

```

=====
def2-SV(P)
=====
*
h def2-SV(P)
# h      (4s) / [2s]      {31}
*
  3 s
  13.010701000      0.19682158000E-01
  1.9622572000     0.13796524000
  0.44453796000     0.47831935000
  1 s
  0.12194962000     1.00000000000
*
*
he def2-SV(P)
# he     (4s1p) / [2s1p]   {31/1}
*
  3 s
  38.354936737      0.23814288905E-01
  5.7689081479      0.15490906777
  1.2399407035      0.46998096633
  1 s
  0.29757815953     1.00000000000
  1 p
  1.00000000000     1.00000000000
*
*
li def2-SV(P)
# li     (7s3p) / [3s2p]   {511/21}
*
  5 s
  266.27785516      0.64920150325E-02
  40.069783447      0.47747863215E-01
  9.0559944389      0.20268796111
  2.4503009051      0.48606574817
  0.72209571855     0.43626977955
  1 s
  0.52810884721E-01  1.00000000000
  1 s
  0.20960948798E-01  1.00000000000
  2 p
  1.45000000000      0.25860000000
  0.30000000000      1.00000000000
  1 p
  0.82000000000E-01  1.00000000000
*
*
be def2-SV(P)
# be     (7s4p) / [3s2p]   {511/31}
*
  5 s
  515.18616125      0.55615307983E-02
  77.511037595      0.41190068062E-01
  17.552481693      0.17913378108
  4.8028940596      0.44736716455
  1.4516214316      0.42009581920
  1 s
  0.13281633620     1.00000000000
  1 s

```

```

0.45837372213E-01  1.0000000000
  3 p
  3.6316917145      -0.29033998305E-01
0.71695694366      -0.16877854032
0.19541932860      -0.51403419628
  1 p
0.60515465890E-01  1.0000000000
*
*
b def2-SV(P)
# b      (7s4p1d) / [3s2p1d]      {511/31/1}
*
  5 s
  839.31830086      -0.55929201074E-02
  126.26464843      -0.41565520771E-01
  28.620600763      -0.18299816983
  7.8793722710      -0.46540391866
  2.4088857172      -0.44173884791
  1 s
0.25105109036      1.0000000000
  1 s
0.83648866069E-01  1.0000000000
  3 p
  6.0332223619      -0.35603672456E-01
  1.2499157866      -0.19895775769
  0.33871676350      -0.50850202618
  1 p
0.96415632351E-01  1.0000000000
  1 d
0.50000000000      1.0000000000
*
*
c def2-SV(P)
# c      (7s4p1d) / [3s2p1d]      {511/31/1}
*
  5 s
  1238.4016938      0.54568832082E-02
  186.29004992      0.40638409211E-01
  42.251176346      0.18025593888
  11.676557932      0.46315121755
  3.5930506482      0.44087173314
  1 s
0.40245147363      1.0000000000
  1 s
0.13090182668      1.0000000000
  3 p
  9.4680970621      0.38387871728E-01
  2.0103545142      0.21117025112
  0.54771004707      0.51328172114
  1 p
0.15268613795      1.0000000000
  1 d
0.80000000000      1.0000000000
*
*
n def2-SV(P)
# n      (7s4p1d) / [3s2p1d]      {511/31/1}
*
  5 s
  1712.8415853      -0.53934125305E-02

```

257.64812677	-0.40221581118E-01
58.458245853	-0.17931144990
16.198367905	-0.46376317823
5.0052600809	-0.44171422662
1 s	
0.58731856571	1.0000000000
1 s	
0.18764592253	1.0000000000
3 p	
13.571470233	-0.40072398852E-01
2.9257372874	-0.21807045028
0.79927750754	-0.51294466049
1 p	
0.21954348034	1.0000000000
1 d	
1.0000000000	1.0000000000
*	
*	
o def2-SV(P)	
# o (7s4p1d) / [3s2p1d] {511/31/1}	
*	
5 s	
2266.1767785	-0.53431809926E-02
340.87010191	-0.39890039230E-01
77.363135167	-0.17853911985
21.479644940	-0.46427684959
6.6589433124	-0.44309745172
1 s	
0.80975975668	1.0000000000
1 s	
0.25530772234	1.0000000000
3 p	
17.721504317	0.43394573193E-01
3.8635505440	0.23094120765
1.0480920883	0.51375311064
1 p	
0.27641544411	1.0000000000
1 d	
1.2000000000	1.0000000000
*	
*	
f def2-SV(P)	
# f (7s4p1d) / [3s2p1d] {511/31/1}	
*	
5 s	
2894.8325990	-0.53408255515E-02
435.41939120	-0.39904258866E-01
98.843328866	-0.17912768038
27.485198001	-0.46758090825
8.5405498171	-0.44653131020
1 s	
1.0654578038	1.0000000000
1 s	
0.33247346748	1.0000000000
3 p	
22.696633924	-0.45212874436E-01
4.9872339257	-0.23754317067
1.3491613954	-0.51287353587
1 p	
0.34829881977	1.0000000000

```

1 d
1.4000000000      1.0000000000
*
*
ne def2-SV(P)
# ne      (7s4p1d) / [3s2p1d]      {511/31/1}
*
5 s
3598.9736625     -0.53259297003E-02
541.32073112     -0.39817417969E-01
122.90450062     -0.17914358188
34.216617022     -0.46893582977
10.650584124     -0.44782537577
1 s
1.3545953960      1.0000000000
1 s
0.41919362639     1.0000000000
3 p
28.424053785     -0.46031944795E-01
6.2822510953     -0.23993183041
1.6978715079     -0.50871724964
1 p
0.43300700172     1.0000000000
1 d
1.8880000000      1.0000000000
*
*
na def2-SV(P)
# na      (10s6p1d) / [4s2p1d]      {5311/51/1}
*
5 s
4098.2003908     -0.58535911879E-02
616.49374031     -0.43647161872E-01
139.96644001     -0.19431465884
39.073441051     -0.48685065731
11.929847205     -0.41881705137
3 s
20.659966030      0.85949689854E-01
1.9838860978     -0.56359144041
0.64836323942     -0.51954009048
1 s
0.52443967404E-01  1.0000000000
1 s
0.28048160742E-01  1.0000000000
5 p
75.401862017      0.15435362532E-01
17.274818978      0.99738293184E-01
5.1842347425      0.31209593966
1.6601211973      0.49295674807
0.51232528958      0.32420398318
1 p
0.52000000000E-01  1.0000000000
1 d
0.13100000000      0.0000000000
*
*
mg def2-SV(P)
# mg      (10s7p1d) / [4s3p1d]      {5311/511/1}
*
5 s

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4953.8339196      -0.57778967498E-02
745.18044154     -0.43124761082E-01
169.21604972     -0.19268216987
47.300672019     -0.48641439116
14.461336973     -0.42550894077
 3 s
24.768174789     0.87956969984E-01
2.4940945349     -0.55165058128
0.87807584533    -0.53443294833
 1 s
0.87212782497E-01 1.0000000000
 1 s
0.33599293780E-01 1.0000000000
 5 p
98.053010494     -0.14480564601E-01
22.586932277     -0.95495750787E-01
6.8391509842     -0.30787672651
2.2332843818     -0.49936292886
0.71606599387    -0.31503476213
 1 p
0.18914796195     1.0000000000
 1 p
0.53768755187E-01 1.0000000000
 1 d
0.10100000000     1.0000000000
*
*
al def2-SV(P)
# al      (10s7p1d) / [4s3p1d]      {5311/511/1}
*
 5 s
5887.5727030     0.13483347987E-02
885.61225996     0.10071576809E-01
201.13604899     0.45132454056E-01
56.284974674     0.11461268043
17.229551243     0.10159608943
 3 s
29.340249922     0.69347454208E-01
3.0439630420     -0.42528117679
1.1285539518     -0.41449832210
 1 s
0.14234175160     1.0000000000
 1 s
0.54400192313E-01 1.0000000000
 5 p
145.11918809     0.63963373134E-02
33.717894833     0.44189359965E-01
10.369863083     0.15581575993
3.5135616036     0.28635286951
1.1980050273     0.22921423248
 1 p
0.26583005913     1.0000000000
 1 p
0.71003361994E-01 1.0000000000
 1 d
0.30000000000     1.0000000000
*
*
si def2-SV(P)
# si      (10s7p1d) / [4s3p1d]      {5311/511/1}

```

*

5 s
6903.7118686 0.13373962995E-02
1038.4346419 0.99966546241E-02
235.87581480 0.44910165101E-01
66.069385169 0.11463638540
20.247945761 0.10280063858

3 s
34.353481730 0.70837285010E-01
3.6370788192 -0.43028836252
1.4002048599 -0.41382774969

1 s
0.20484414805 1.0000000000

1 s
0.77994095468E-01 1.0000000000

5 p
179.83907373 0.61916656462E-02
41.907258846 0.43399431982E-01
12.955294367 0.15632019351
4.4383267393 0.29419996982
1.5462247904 0.23536823814

1 p
0.35607612302 1.0000000000

1 p
0.10008513762 1.0000000000

1 d
0.35000000000 1.0000000000

*

*

p def2-SV(P)

p (10s7p1d) / [4s3p1d] {5311/511/1}

*

5 s
8002.4795106 0.57503489302E-02
1203.6813590 0.43007628959E-01
273.44227031 0.19363986252
76.655541517 0.49651693399
23.516927435 0.44983262479

3 s
39.791683439 0.95188129789E-01
4.2770343323 -0.57649840368
1.6940256888 -0.54239583865

1 s
0.27567674644 1.0000000000

1 s
0.10495590099 1.0000000000

5 p
219.50755823 0.92100565257E-02
51.274155030 0.65409765745E-01
15.921595892 0.24033730279
5.5069913481 0.46318321788
1.9537719426 0.37392563382

1 p
0.47803397932 1.0000000000

1 p
0.13657952621 1.0000000000

1 d
0.45000000000 1.0000000000

*

*

```

s def2-SV(P)
# s      (10s7p1d) / [4s3p1d]      {5311/511/1}
*
  5 s
  9184.9303010      -0.22294387756E-02
  1381.5105503      -0.16683029937E-01
  313.87147580      -0.75262436116E-01
  88.053870623      -0.19376827038
  27.039914905      -0.17718020803
  3 s
  45.648731303      -0.10736062573
  4.9664522326      0.65066293018
  2.0116242047      0.59712155354
  1 s
  0.35661077013      1.0000000000
  1 s
  0.13507221477      1.0000000000
  5 p
  261.98233439      -0.92729929822E-02
  61.306894736      -0.66547669241E-01
  19.103729887      -0.24828595903
  6.6567720378      -0.48703847402
  2.3959635161      -0.39337850312
  1 p
  0.61776161679      1.0000000000
  1 p
  0.16993376871      1.0000000000
  1 d
  0.55000000000      1.0000000000
*
*
c1 def2-SV(P)
# c1      (10s7p1d) / [4s3p1d]      {5311/511/1}
*
  5 s
  10449.827566      0.19708362484E-02
  1571.7365221      0.14754727977E-01
  357.12065523      0.66679112875E-01
  100.25185935      0.17228924084
  30.812727554      0.15883786100
  3 s
  51.923789434      -0.10009298909
  5.7045760975      0.60841752753
  2.3508376809      0.54352153355
  1 s
  0.44605124672      1.0000000000
  1 s
  0.16848856190      1.0000000000
  5 p
  307.66790569      -0.87801484118E-02
  72.102015515      -0.63563355471E-01
  22.532680262      -0.24016428276
  7.8991765444      -0.47798866557
  2.8767268321      -0.38515850005
  1 p
  0.77459363955      1.0000000000
  1 p
  0.21037699698      1.0000000000
  1 d
  0.65000000000      1.0000000000

```

```

*
*
ar def2-SV(P)
# ar      (10s7p1d) / [4s3p1d]      {5311/511/1}
*
  5 s
11797.119765      0.20214479973E-02
1774.3522753     0.15139852688E-01
403.18875733     0.68525400873E-01
113.24933999     0.17762929207
34.835298193     0.16496495001
  3 s
58.614775042     -0.10343394000
6.4922045078     0.63133365899
2.7117014403     0.54887572301
  1 s
0.54412974538    1.00000000000
  1 s
0.20517411136    1.00000000000
  5 p
356.28707256     -0.87321783271E-02
83.593132866     -0.63680317444E-01
26.186704029     -0.24311906886
9.2257275925     -0.48956069653
3.3922754954     -0.39229190040
  1 p
0.94740534010    1.00000000000
  1 p
0.25659135062    1.00000000000
  1 d
0.69600000000    1.00000000000
*
*
k def2-SV(P)
# k      (14s9p2d) / [5s3p2d]      {63311/531/11}
*
  6 s
31478.746764     0.39838653994E-02
4726.8876066     0.30501759762E-01
1075.4345353     0.15073752622
303.39811023     0.51912939801
98.327112831     1.0366957005
33.636222177     0.76398963199
  3 s
65.639209962     -0.28242617106
7.3162592218     1.6914935860
2.8902580135     1.2965331953
  3 s
4.5459748965     -0.76343555273E-02
0.70404124062     0.25635718960E-01
0.28266888959     0.16606859208E-01
  1 s
0.29058164020E-01 1.00000000000
  1 s
0.12111638157E-01 1.00000000000
  5 p
361.22492154     0.20906479823E-01
84.670222166     0.15043641740
26.469088236     0.55440061077
9.2658077615     1.0409009991

```


3.3423388293	0.67825341194
3 p	
1.5100876104	0.75248191146
0.56568375163	1.3708585031
0.20817008495	0.66047633079
1 p	
0.41737000000E-01	1.0000000000
1 d	
0.35300000000	1.0000000000
1 d	
0.98000000000E-01	1.0000000000
*	
*	
ca def2-SV(P)	
# ca (14s9p4d) / [5s3p2d] {63311/531/31}	
*	
6 s	
35138.713929	0.39482520740E-02
5276.4111348	0.30234243552E-01
1200.4692589	0.14952019681
338.71810542	0.51597345713
109.85385922	1.0339510296
37.608880299	0.76937933526
3 s	
73.107977555	-0.28268525011
8.2407705688	1.6796092142
3.2959812993	1.2803766016
3 s	
5.2341800914	-0.76868604561E-02
0.84187220515	0.25382375978E-01
0.36510294029	0.16512171511E-01
1 s	
0.51222402884E-01	1.0000000000
1 s	
0.19825111408E-01	1.0000000000
5 p	
413.11313893	0.20327135354E-01
96.935786224	0.14730276362
30.372154659	0.54887167322
10.684776830	1.0440659818
3.8821258350	0.68653490684
3 p	
1.7993016295	0.75410246871
0.69189056530	1.3409296599
0.26364024096	0.56391989435
1 p	
0.74979000000E-01	1.0000000000
3 d	
5.4979093879	0.73770011433E-01
1.3177128032	0.26052853169
0.32188682649	0.45233836380
1 d	
0.70528614919E-01	1.0000000000
*	
*	
sc def2-SV(P)	
# sc (14s9p5d) / [5s3p2d] {63311/531/41}	
*	
6 s	
38956.081804	0.39293205858E-02

5849.5733637	0.30093221229E-01
1330.8813154	0.14890370950
375.55534165	0.51464282906
121.87261370	1.0337708070
41.760243729	0.77436851627
3 s	
81.060633953	-0.28318552316
9.2059823972	1.6770806984
3.7063215732	1.2594733678
3 s	
5.9888909988	-0.77821367493E-02
0.97363432378	0.25499692745E-01
0.42041019223	0.16191560820E-01
1 s	
0.59440551913E-01	1.0000000000
1 s	
0.22897806303E-01	1.0000000000
5 p	
466.31481262	0.19984300385E-01
109.51217097	0.14561043072
34.375921827	0.54687466223
12.142096955	1.0479006012
4.4336767669	0.68894890327
3 p	
2.0971291866	0.75619214724
0.80977606956	1.3178212235
0.30834046588	0.54312268173
1 p	
0.89748000000E-01	1.0000000000
4 d	
19.240334928	0.27039082144E-01
5.1178995899	0.13803684743
1.6554278827	0.34869086403
0.54016355610	0.48594185717
1 d	
0.16211214518	0.343744449689
*	
*	
ti def2-SV(P)	
# ti (14s9p5d) / [5s3p2d] {63311/531/41}	
*	
6 s	
42961.512185	0.39127635355E-02
6450.9759169	0.29969820489E-01
1467.7210915	0.14836352707
414.20997355	0.51347285324
134.48715840	1.0335365483
46.122209796	0.77854233930
3 s	
89.447762543	-0.28385401259
10.223346060	1.6772785333
4.1353774271	1.2411928456
3 s	
6.7896181452	-0.78399994518E-02
1.1106730691	0.25495493019E-01
0.47565975578	0.16061172892E-01
1 s	
0.65986956934E-01	1.0000000000
1 s	
0.25210342250E-01	1.0000000000

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5 p
522.03684782      0.19754179642E-01
122.68649489      0.14460677619
38.572903611      0.54669004165
13.672169319      1.0531647540
5.0118529359      0.69111213363
3 p
2.4131928282      0.75803437136
0.93252270050      1.3036241399
0.35429058390      0.53638653300
1 p
0.10156100000      1.00000000000
4 d
23.465125957      0.26536380115E-01
6.3332593832      0.13796453963
2.0766489946      0.35312644228
0.69027361954      0.48647124166
1 d
0.21088738554      0.33026314258
*
*
v def2-SV(P)
# v      (14s9p5d) / [5s3p2d]      {63311/531/41}
*
6 s
47160.376060      0.14498688908E-02
7081.4110871      0.11106435251E-01
1611.1621223      0.55005423585E-01
454.72940551      0.19060252591
147.71321208      0.38435022957
50.699538950      0.29095546792
3 s
98.262492669      -0.10942337856
11.294293099      0.64539490399
4.5853360105      0.47117880777
3 s
7.6359689588      -0.22454949054
1.2539836689      0.72594852764
0.53271935387      0.45560582748
1 s
0.72246239566E-01      1.00000000000
1 s
0.27358087448E-01      1.00000000000
5 p
580.55044988      0.97315110917E-02
136.52341127      0.71531241137E-01
42.983958820      0.27197688414
15.282798763      0.52618988893
5.6202495154      0.34452533498
3 p
2.7485386415      0.34040396496
1.0618550073      0.57983996120
0.40235518645      0.23911643083
1 p
0.11124800000      1.00000000000
4 d
27.358434017      0.26641927050E-01
7.4540604253      0.13995311726
2.4633917847      0.35751066639
0.82480925277      0.48488354148

```

```

1 d
0.25257904742      0.32332844995
*
*
cr def2-SV(P)
# cr      (14s9p5d) / [5s3p2d]      {63311/531/41}
*
6 s
51528.086349      0.14405823106E-02
7737.2103487      0.11036202287E-01
1760.3748470      0.54676651806E-01
496.87706544      0.18965038103
161.46520598      0.38295412850
55.466352268      0.29090050668
3 s
107.54732999      -0.10932281100
12.408671897      0.64472599471
5.0423628826      0.46262712560
3 s
8.5461640165      -0.22711013286
1.3900441221      0.73301527591
0.56066602876      0.44225565433
1 s
0.71483705972E-01  1.00000000000
1 s
0.28250687604E-01  1.00000000000
5 p
640.48536096      0.96126715203E-02
150.69711194      0.70889834655E-01
47.503755296      0.27065258990
16.934120165      0.52437343414
6.2409680590      0.34107994714
3 p
3.0885463206      0.33973986903
1.1791047769      0.57272062927
0.43369774432      0.24582728206
1 p
0.12067500000      1.00000000000
4 d
27.559479426      0.30612488044E-01
7.4687020327      0.15593270944
2.4345903574      0.36984421276
0.78244754808      0.47071118077
1 d
0.21995774311      0.33941649889
*
*
mn def2-SV(P)
# mn      (14s9p5d) / [5s3p2d]      {63311/531/41}
*
6 s
56137.009037      0.14321304702E-02
8429.2063943      0.10972509162E-01
1917.8277233      0.54382468712E-01
541.36230198      0.18884335129
176.00069142      0.38198025054
60.500477010      0.29156772596
3 s
117.17282882      -0.10933661328
13.596973368      0.64305039431

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5.5483996341	0.45848970584
3 s	
9.4662853530	-0.22538977259
1.5595006070	0.72307758657
0.65230205868	0.45300721536
1 s	
0.84003734475E-01	1.0000000000
1 s	
0.31256098581E-01	1.0000000000
5 p	
706.00497535	0.95055518167E-02
166.19728820	0.70356271142E-01
52.452061906	0.27005556982
18.746932862	0.52574344602
6.9282991622	0.34254033223
3 p	
3.4772204938	0.33994073736
1.3406906449	0.57203836254
0.50498803038	0.23847605831
1 p	
0.12765000000	1.0000000000
4 d	
35.423264935	0.26985304111E-01
9.7814221451	0.14383458648
3.2673488767	0.36418958377
1.1026472189	0.48152670661
1 d	
0.33743205934	0.31458754360
*	
*	
fe def2-SV(P)	
# fe (14s9p5d) / [5s3p2d] {63311/531/41}	
*	
6 s	
60923.640643	0.14302254466E-02
9147.8893982	0.10958790038E-01
2081.3505927	0.54332554248E-01
587.55977067	0.18884995009
191.09043990	0.38253069946
65.732730112	0.29308335984
3 s	
127.25891928	-0.10964564925
14.830913010	0.64387631332
6.0653307408	0.45472347323
3 s	
10.449943710	-0.22539639952
1.7245228003	0.72164398156
0.71772177325	0.44985492922
1 s	
0.91449828308E-01	1.0000000000
1 s	
0.33706691021E-01	1.0000000000
5 p	
773.43750995	0.94325735144E-02
182.15149714	0.70029620575E-01
57.547272758	0.26993651996
20.614988935	0.52700011047
7.6348557890	0.34284148028
3 p	
3.8719327990	0.33974402988

1.4924724132	0.56842594005
0.56061284958	0.23649365839
1 p	
0.13491500000	1.00000000000
4 d	
38.968133419	0.27879664382E-01
10.800067078	0.14858319982
3.6136457999	0.36905479496
1.2129967888	0.47745100883
1 d	
0.36524393170	0.31418142304
*	
*	
co def2-SV(P)	
# co (14s9p5d) / [5s3p2d] {63311/531/41}	
*	
6 s	
65902.208257	0.14284614936E-02
9895.3896027	0.10946072783E-01
2251.4305789	0.54285953890E-01
635.61097084	0.18885179079
206.78820681	0.38301634994
71.179242971	0.29443551266
3 s	
137.77268040	-0.10990221736
16.118079243	0.64455537395
6.6030327710	0.45116787924
3 s	
11.479915788	-0.22593846910
1.8956426324	0.72231409008
0.78466232067	0.44903812296
1 s	
0.98425774432E-01	1.00000000000
1 s	
0.35945741932E-01	1.00000000000
5 p	
843.64358575	0.93866097254E-02
198.76386994	0.69880208716E-01
62.854963098	0.27037070345
22.562842280	0.52904786880
8.3713209127	0.34357029579
3 p	
4.2858719800	0.34027999036
1.6508041817	0.56693392384
0.61834231096	0.23617979783
1 p	
0.14130800000	1.00000000000
4 d	
42.927867612	0.28487788365E-01
11.942533053	0.15206951283
4.0046495664	0.37310913999
1.3413193804	0.47549837676
1 d	
0.40015009743	0.31346831424
*	
*	
ni def2-SV(P)	
# ni (14s9p5d) / [5s3p2d] {63311/531/41}	
*	
6 s	

71074.803211	0.14260386729E-02
10672.020941	0.10928236994E-01
2428.1389007	0.54212626938E-01
685.53595148	0.18874768902
223.10072863	0.38324616985
76.842014042	0.29550637144
3 s	
148.71122016	-0.11014443059
17.459154987	0.64521426988
7.1625280665	0.44797838103
3 s	
12.556137125	-0.22645403224
2.0735740488	0.72320959286
0.85382640602	0.44868026476
1 s	
0.10536766271	1.0000000000
1 s	
0.38134087688E-01	1.0000000000
5 p	
916.73608662	0.93439635610E-02
216.06139913	0.69737374902E-01
68.383914817	0.27073495012
24.593843952	0.53078301549
9.1392960204	0.34410229438
3 p	
4.7193371746	0.34076082016
1.8161849234	0.56580169611
0.67840750720	0.23616717361
1 p	
0.14658800000	1.0000000000
4 d	
47.093832108	0.28982316948E-01
13.146463975	0.15494995950
4.4170548925	0.37633115111
1.4771565078	0.47365096014
1 d	
0.43735921792	0.31247837833
*	
*	
cu def2-SV(P)	
# cu (14s9p5d) / [5s3p2d] {63311/531/41}	
*	
6 s	
76381.348056	0.14336079896E-02
11468.777499	0.10986749865E-01
2609.4246495	0.54513652465E-01
736.75033098	0.18990128258
239.82419958	0.38581959211
82.656829252	0.29790607498
3 s	
160.13544196	-0.11146778567
18.834177695	0.65349301031
7.7176595741	0.44770534421
3 s	
13.710846717	-0.22870911122
2.2349895670	0.73464423031
0.87818360069	0.43273070874
1 s	
0.87187458064E-01	1.0000000000
1 s	

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0.32969114665E-01  1.0000000000
  5 p
991.24075782      0.93878498798E-02
233.69376116      0.70208282458E-01
74.020930927      0.27323522220
26.664967447      0.53580792728
9.9192087478      0.34575794906
  3 p
5.1519553926      0.34229108083
1.9638205828      0.56456592484
0.71560097037     0.24078584318
  1 p
0.15506500000     1.00000000000
  4 d
47.335049590      0.32375547758E-01
13.161666077      0.16810218684
4.3693777244      0.38477707982
1.4132925109      0.46147880178
  1 d
0.38878001452     0.32388873258
*
*
zn def2-SV(P)
# zn      (14s9p5d) / [5s3p2d]      {63311/531/41}
*
  6 s
82000.711629      0.14210764000E-02
12312.471777      0.10891499487E-01
2801.3944193      0.54057188059E-01
790.99424302      0.18847463904
257.56551079      0.38346549346
88.814933400      0.29723794197
  3 s
171.86353716      -0.11051849523
20.302534785      0.64607716984
8.3464123068      0.44220117322
  3 s
14.847536940      -0.22705309278
2.4495029507      0.72433217935
0.99845821824     0.44836495592
  1 s
0.11891307937     1.00000000000
  1 s
0.42297428760E-01  1.00000000000
  5 p
1071.5185372      0.92767797235E-02
252.69712152      0.69541149434E-01
80.100829126      0.27156772564
28.903393172      0.53401355573
10.768899879      0.34501323446
  3 p
5.6446212530      0.34129600164
2.1678291347      0.56390521973
0.80540898341     0.23676109735
  1 p
0.16245500000     1.00000000000
  4 d
56.088939191      0.29588869140E-01
15.751908917      0.15872571404
5.3115812367      0.37976229159

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1.7737904917      0.46898959172
 1 d
0.51975583665      0.30907149078
*
*
ga def2-SV(P)
# ga      (14s10p6d) / [5s4p3d]      {63311/5311/411}
*
 6 s
87842.126296      0.14271588798E-02
13189.496402      0.10938894097E-01
3000.9482141      0.54308200127E-01
847.38425966      0.18951055983
276.00980642      0.38615185918
95.216672071      0.30051082719
 3 s
184.00703968      -0.111244461963
21.827051433      0.64831322918
9.0026963761      0.44358383594
 3 s
16.033176938      -0.23014299555
2.6707724878      0.72946861516
1.1252834170      0.46214976951
 1 s
0.15967608829      1.00000000000
 1 s
0.57643044753E-01  1.00000000000
 5 p
1167.2665844      0.90974021307E-02
275.38062789      0.68456273343E-01
87.375073070      0.26922293888
31.597254670      0.53507897882
11.824122798      0.35279062760
 3 p
6.2881845133      0.33938244530
2.5199853240      0.56871947608
1.0169726306      0.27717694939
 1 p
0.24748373604      1.00000000000
 1 p
0.66685294163E-01  1.00000000000
 4 d
65.354237674      0.27370146382E-01
18.504656747      0.15099463976
6.3179620632      0.37485328545
2.1641389426      0.47510606851
 1 d
0.66693092754      0.29843287401
 1 d
0.20700000000      1.00000000000
*
*
ge def2-SV(P)
# ge      (14s10p6d) / [5s4p3d]      {63311/5311/411}
*
 6 s
93889.836642      0.14233976060E-02
14097.497528      0.10910795654E-01
3207.5477309      0.54183705943E-01
905.76727269      0.18922820349

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295.11014693	0.38612847001
101.84713141	0.30164050736
3 s	
196.56719662	-0.11118770940
23.405292522	0.64616007369
9.6839116702	0.44188904568
3 s	
17.269736544	-0.23027421375
2.8964622160	0.73017169398
1.2553621412	0.46197222255
1 s	
0.20213081492	1.0000000000
1 s	
0.73867910982E-01	1.0000000000
5 p	
1259.2085995	0.90115464252E-02
297.15626382	0.67986841689E-01
94.353387522	0.26853856488
34.176329677	0.53659649219
12.816139615	0.35633514961
3 p	
6.8471029784	0.33900693119
2.7717363939	0.56809365264
1.1458418175	0.27246539884
1 p	
0.30679631536	1.0000000000
1 p	
0.89283644115E-01	1.0000000000
4 d	
74.782168177	0.25755860205E-01
21.310849759	0.14536816132
7.3464792363	0.37134209859
2.5656271395	0.48002998436
1 d	
0.81981773070	0.28978790744
1 d	
0.24600000000	1.0000000000
*	
*	
as def2-SV(P)	
# as (14s10p6d) / [5s4p3d] {63311/5311/411}	
*	
6 s	
100146.52554	0.14258349617E-02
15036.861711	0.10930176963E-01
3421.2902833	0.54294174610E-01
966.16965717	0.18976078153
314.87394026	0.38775195453
108.70823790	0.30402812040
3 s	
209.54238950	-0.11162094204
25.038221139	0.64697607762
10.390964343	0.44223608673
3 s	
18.555090093	-0.22994190569
3.1281217449	0.73319107613
1.3884885073	0.45533653943
1 s	
0.24714362141	1.0000000000
1 s	

```

0.91429428670E-01  1.0000000000
  5 p
1355.6443507      0.89182507898E-02
319.99929270     0.67454750717E-01
101.67734092     0.26759772110
36.886323845     0.53776844520
13.861115909     0.35992570244
  3 p
  7.4260666912   0.34036849637
  3.0316247187   0.57030149334
  1.2783078340   0.26606170238
  1 p
0.37568503356    1.0000000000
  1 p
0.11394805454    1.0000000000
  4 d
  84.445514539   0.24518402724E-01
  24.190416102   0.14107454677
  8.4045015119   0.36875228915
  2.9808970748   0.48409561362
  1 d
0.97909243359   0.28250268781
  1 d
0.29300000000   1.0000000000
*
*
se def2-SV(P)
# se      (14s10p6d) / [5s4p3d]      {63311/5311/411}
*
  6 s
106612.20027     0.14274889113E-02
16007.604701     0.10943525114E-01
3642.1699707     0.54374171596E-01
1028.5912993     0.19018092947
335.30298888     0.38913021696
115.80129154     0.30620207088
  3 s
222.93325020    -0.11198808009
26.726257934    0.64752124207
11.124501923    0.44241976651
  3 s
19.888520061    -0.22857227762
3.3668473803    0.73591359951
1.5249277839    0.44330199577
  1 s
0.29630037912   1.0000000000
  1 s
0.11009288974   1.0000000000
  5 p
1455.9068120     0.88203597043E-02
343.75101831     0.66875851967E-01
109.29554964     0.26640578080
39.707711022     0.53834928422
14.950185232     0.36303281993
  3 p
  8.0208962094   0.34153807025
  3.2934649756   0.57257906583
  1.4058602438   0.25549813222
  1 p
0.45076123226   1.0000000000

```

```

1 p
0.13353413325      1.0000000000
4 d
94.494024044      0.23490101098E-01
27.188185260      0.13747735767
9.5091567352      0.36649929124
3.4170516853      0.48750989884
1 d
1.1479590083      0.27657943383
1 d
0.33800000000     1.0000000000
*
*
br def2-SV(P)
# br      (14s10p6d) / [5s4p3d]      {63311/5311/411}
*
6 s
113286.38776      0.14283037779E-02
17009.626303      0.10950417496E-01
3870.1842567      0.54421006604E-01
1093.0357227      0.19047907695
356.39721797      0.39024642737
123.12539643      0.30814432514
3 s
236.74084007      -0.11228065671
28.468661070      0.64775962312
11.883443722      0.44235575986
3 s
21.269633312      -0.22642576323
3.6129226841      0.73823712008
1.6626648969      0.42683868694
1 s
0.34823793232      1.0000000000
1 s
0.13019031394      1.0000000000
5 p
1560.2801881      0.87166669072E-02
368.47859205      0.66243637420E-01
117.22978849      0.26495610385
42.648909248      0.53839160587
16.087225096      0.36579387888
3 p
8.6352810058      0.34248787366
3.5613665502      0.57500678213
1.5292626609      0.24330394172
1 p
0.53064294848      1.0000000000
1 p
0.15702758965      1.0000000000
4 d
104.85518642      0.22650147581E-01
30.281143688      0.13455483230
10.651394267      0.36474454537
3.8699456233      0.49044587056
1 d
1.3240876762      0.27137289040
1 d
0.38900000000     1.0000000000
*
*

```

kr def2-SV(P)
kr (14s10p6d) / [5s4p3d] {63311/5311/411}
*

6 s
120165.64875 0.14294234496E-02
18042.500169 0.10959597020E-01
4105.1800388 0.54479647470E-01
1159.4447248 0.19081239122
378.13810346 0.39140445949
130.67610045 0.31007346689
3 s
250.96373353 -0.11258604011
30.265930380 0.64816322524
12.668110757 0.44240238994
3 s
22.697940101 -0.22391964908
3.8673017398 0.74060953026
1.8013706671 0.40803658445
1 s
0.40308639136 1.0000000000
1 s
0.15170527749 1.0000000000
5 p
1668.5736623 0.86215009803E-02
394.13862798 0.65665506884E-01
125.46644854 0.26366576697
45.704992729 0.53867658574
17.270133229 0.36865167502
3 p
9.2699487770 0.34346189015
3.8364617719 0.57784776196
1.6467163312 0.23075615197
1 p
0.61479686489 1.0000000000
1 p
0.18319467414 1.0000000000
4 d
115.55868603 0.21945485333E-01
33.477985864 0.13211212879
11.834450207 0.36333306964
4.3408254894 0.49300484446
1 d
1.5079273157 0.26676858913
1 d
0.44300000000 1.0000000000

*
*
rb def2-SV(P)
rb (7s6p2d) / [5s3p2d] {31111/411/11}
*

3 s
4.6687885071 0.29008526793
2.9442428420 -0.67740090428
0.58171262989 0.45712389487
1 s
0.45147933555 1.0000000000
1 s
0.21604923532 1.0000000000
1 s
0.32088816526E-01 1.0000000000

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1 s
0.13833878175E-01 1.0000000000
4 p
5.5234179480 0.51234729472E-01
3.4120149646 -0.17337025646
0.76899021792 0.43339683188
0.33088071786 0.55354332721
1 p
0.13423268441 1.0000000000
1 p
0.20642679613E-01 1.0000000000
1 d
0.22600000000 1.0000000000
1 d
0.27432280711E-01 1.0000000000
*
rb def2-ecp
*
ncore = 28 lmax = 3
# coefficient r^n exponent
f -12.3169000 2 3.8431140
s-f 89.5001980 2 5.0365510
0.4937610 2 1.9708490
12.3169000 2 3.8431140
p-f 58.5689740 2 4.2583410
0.4317910 2 1.4707090
12.3169000 2 3.8431140
d-f 26.2248980 2 3.0231270
0.9628390 2 0.6503830
12.3169000 2 3.8431140
*
*
sr def2-SV(P)
# sr (6s6p5d) / [4s3p2d] {3111/411/41}
*
3 s
5.9276428767 0.19698765364
3.0691274814 -0.64852205985
0.70675488028 0.62064729022
1 s
0.33824024280 1.0000000000
1 s
0.61768869200E-01 1.0000000000
1 s
0.25767593093E-01 1.0000000000
4 p
2.4324720000 -0.37145059848
1.6642340000 0.37856824234
0.59455471858 0.59874487803
0.26152621998 0.35314019512
1 p
0.10258814042 1.0000000000
1 p
0.33223404030E-01 1.0000000000
4 d
3.6180810000 -0.75010000000E-02

```

```

0.99665600000    0.10809800000
0.39073500000    0.27854000000
0.12277000000    0.47731800000
  1 d
0.36655000000E-01 0.44818300000
*
sr def2-ecp
*
  ncore =    28      lmax =    3
#   coefficient   r^n      exponent
f
  -15.8059920     2        4.6339750
s-f
  135.4794300     2        7.4000740
  17.5344630     2        3.6063790
  15.8059920     2        4.6339750
p-f
  88.3597090     2        6.4848680
  15.3943720     2        3.2880530
  15.8059920     2        4.6339750
d-f
  29.8889870     2        4.6228410
  6.6594140     2        2.2469040
  15.8059920     2        4.6339750
*
*
y def2-SV(P)
# y   (7s6p5d) / [5s3p2d]   {31111/411/41}
*
  3 s
  5.1329580000    -1.3864845457
  4.2401920000    1.9459581166
  1.2982800000    0.44182603154
  1 s
  0.82904954347    1.0000000000
  1 s
  0.34752758911    1.0000000000
  1 s
  0.68418878574E-01 1.0000000000
  1 s
  0.27323992904E-01 1.0000000000
  4 p
  2.7279200000    -0.37249884912
  1.9790500000    0.32572065996
  0.79980886805    0.50094655502
  0.38409397354    0.44385929493
  1 p
  0.16173582264    1.0000000000
  1 p
  0.30000000000E-01 1.0000000000
  4 d
  3.9030833060    -0.98209792625E-02
  1.1363234302    0.19183629664
  0.45617043877    0.40597788539
  0.17470950748    0.43861485518
  1 d
  0.61978796638E-01 1.0000000000
*
y def2-ecp
*
```

```

ncore = 28          lmax = 3
#      coefficient  r^n      exponent
f      -19.1221981  2        6.5842120
      -2.4363754  2        3.2921060
s-f    135.1538441  2        7.4880494
      15.5524413  2        3.7440247
      19.1221981  2        6.5842120
      2.4363754  2        3.2921060
p-f    87.7849917  2        6.4453772
      11.5640660  2        3.2226886
      19.1221981  2        6.5842120
      2.4363754  2        3.2921060
d-f    29.7010007  2        4.6584472
      5.5399685  2        2.3292236
      19.1221981  2        6.5842120
      2.4363754  2        3.2921060

```

*
*

```

zr def2-SV(P)
# zr (7s6p5d) / [5s3p2d] {31111/411/41}

```

*

```

3 s
5.8737890000      0.54255558714
4.2872700000     -0.95241333244
1.4641370000     -0.13703926411
1 s
0.83727682345    0.88521584390
1 s
0.36849806511    1.00000000000
1 s
0.77806859124E-01 1.00000000000
1 s
0.30273088330E-01 1.00000000000
4 p
2.8742240000     -0.46624086918
2.1199010000     0.45883133891
0.78845821105    0.58853912475
0.36332579847    0.35822232244
1 p
0.14951762021    1.00000000000
1 p
0.30000000000E-01 1.00000000000
4 d
4.2898623878     -0.12212868080E-01
1.3615557498     0.19692423520
0.56937550689    0.42057831659
0.22674948677    0.42757027999
1 d
0.83011031631E-01 1.00000000000

```

*

```

zr def2-ecp
#      coefficient  r^n      exponent
f      -21.0937760  2        7.5400000

```


	-3.0806943	2	3.7700000
s-f	150.2675911	2	8.2000000
	18.9762165	2	4.0897278
	21.0937760	2	7.5400000
	3.0806943	2	3.7700000
p-f	99.6221237	2	7.1100000
	14.1687333	2	3.5967980
	21.0937760	2	7.5400000
	3.0806943	2	3.7700000
d-f	35.0451235	2	5.3500000
	6.1112595	2	2.4918215
	21.0937760	2	7.5400000
	3.0806943	2	3.7700000

*

*

nb def2-SV(P)

nb (7s6p5d) / [5s3p2d] {31111/411/41}

*

3 s		
6.5663010000	-0.94917907866	
4.5864380000	1.5736372883	
3.7537700000	0.36380422981	
1 s		
0.84187717437	1.0000000000	
1 s		
0.38160666177	1.0000000000	
1 s		
0.85819911368E-01	1.0000000000	
1 s		
0.32702330370E-01	1.0000000000	
4 p		
3.0700630000	-0.51025115881	
2.2379640000	0.53570598017	
0.80801969671	0.63102216351	
0.35783343432	0.30205908942	
1 p		
0.13820085283	1.0000000000	
1 p		
0.36000000000E-01	1.0000000000	
4 d		
4.6170975867	-0.13574476955E-01	
1.5663438480	0.20374310496	
0.66952425826	0.42997453105	
0.27140946867	0.41799754848	
1 d		
0.10054426592	1.0000000000	

*

nb def2-ecp

*

#	ncore =	coefficient	r^n	lmax =	exponent
	28			3	
f		-22.9295500	2		8.4900000
		-3.6663099	2		4.2500000
s-f		165.1791435	2		8.9000000
		21.9929744	2		4.4300000

	22.9295500	2	8.4900000
	3.6663099	2	4.2500000
p-f	111.7944145	2	7.7700000
	16.6334833	2	3.9600000
	22.9295500	2	8.4900000
	3.6663099	2	4.2500000
d-f	38.1122488	2	6.0500000
	8.0391673	2	2.8400000
	22.9295500	2	8.4900000
	3.6663099	2	4.2500000

*

*

mo def2-SV(P)

mo (7s6p5d) / [5s3p2d] {31111/411/41}

*

3 s		
7.2033800000	-0.89310617237	
5.0522950000	1.6074095756	
2.9135330000	0.27804186088	
1 s		
0.97858218681	1.0000000000	
1 s		
0.44369153753	1.0000000000	
1 s		
0.92150090705E-01	1.0000000000	
1 s		
0.34802246935E-01	1.0000000000	
4 p		
3.1518660000	-0.71873040872	
2.4534820000	0.76442887870	
0.85030192180	0.64808585640	
0.36918237179	0.26792115234	
1 p		
0.13490627460	1.0000000000	
1 p		
0.38200000000E-01	1.0000000000	
4 d		
5.0044445497	-0.21587364862E-01	
1.7736823324	0.20958680086	
0.76950591696	0.43730880599	
0.31530878939	0.41123927009	
1 d		
0.11754374390	1.0000000000	

*

mo def2-ecp

*

ncore =	28	lmax =	3
#	coefficient	r^n	exponent
f	-24.8051771	2	9.4500000
	-4.1537815	2	4.7200000
s-f	180.1031085	2	9.7145938
	24.9972279	2	4.6805004
	24.8051771	2	9.4500000
	4.1537815	2	4.7200000
p-f	123.7727523	2	8.1421366

```

19.5302280    2    4.6259863
24.8051771    2    9.4500000
4.1537815     2    4.7200000
d-f
48.3750223    2    6.6184148
8.8920527     2    3.2487516
24.8051771    2    9.4500000
4.1537815     2    4.7200000
*
*
tc def2-SV(P)
# tc      (7s6p5d) / [5s3p2d]      {31111/411/41}
*
3 s
7.4344020000    -1.1436289973
5.5513270000    1.8752000559
3.0230860000    0.23952854431
1 s
1.0647443990    1.0000000000
1 s
0.48127808497    1.0000000000
1 s
0.98299016952E-01    1.0000000000
1 s
0.36659977936E-01    1.0000000000
4 p
3.4490050000    -0.72277510434
2.6927370000    0.76458962802
0.94427370692    0.64533225171
0.41348148619    0.27195668811
1 p
0.15488152305    1.0000000000
1 p
0.40300000000E-01    1.0000000000
4 d
5.0906268699    -0.32176405405E-01
2.0156178510    0.21280802536
0.88113887240    0.44403309175
0.36427094833    0.40796933085
1 d
0.13678402297    1.0000000000
*
tc def2-ecp
*
ncore =      28          lmax =      3
# coefficient    r^n          exponent
f
-26.5624475     2          10.4000000
-4.5856805      2          5.2000000
s-f
195.1591659     2          10.4223462
28.0926033      2          5.0365160
26.5624475      2          10.4000000
4.5856805        2          5.2000000
p-f
135.2845662     2          8.9504494
21.8065043      2          4.8544394
26.5624475      2          10.4000000
4.5856805        2          5.2000000
d-f

```

	54.3297294	2	6.9456968
	11.1550679	2	3.9705849
	26.5624475	2	10.4000000
	4.5856805	2	5.2000000

*
*

```

ru def2-SV(P)
# ru      (7s6p5d) / [5s3p2d]      {31111/411/41}
*
  3 s
  7.9365700000      -1.1772083350
  5.9842450000      1.6197059592
  4.8822200000      0.51065807556
  1 s
  1.1031002163      1.0000000000
  1 s
  0.49818875261     1.0000000000
  1 s
  0.10678711393     1.0000000000
  1 s
  0.39191775872E-01 1.0000000000
  4 p
  3.7546090000     -0.70777873563
  2.9165710000     0.74954391484
  1.0322209568     0.64660609645
  0.45249553774    0.27029086816
  1 p
  0.16987042198    1.0000000000
  1 p
  0.430000000000E-01 1.0000000000
  4 d
  5.7341846619     -0.35266111560E-01
  2.2483686294     0.21802502222
  0.98376978359    0.44709565013
  0.40379445583    0.40371732508
  1 d
  0.14978618173    1.0000000000
*
ru def2-ecp
*
  ncore =      28          lmax =      3
#      coefficient      r^n          exponent
f
  -28.3406163      2          11.3600000
  -4.9446292       2          5.6800000
s-f
  209.8229712      2          11.1052693
  30.6547264       2          5.4147454
  28.3406163       2          11.3600000
  4.9446292        2          5.6800000
p-f
  146.3361823      2          9.7712707
  24.1278772       2          5.0739908
  28.3406163       2          11.3600000
  4.9446292        2          5.6800000
d-f
  67.5158967       2          7.6714231
  9.8701041        2          4.1365647
  28.3406163       2          11.3600000
  4.9446292        2          5.6800000

```

```

*
*
rh def2-SV(P)
# rh      (7s6p5d) / [5s3p2d]      {31111/411/41}
*
  3 s
  7.9177440000      1.4014042010
  6.8412070000      -1.7975072656
  2.9598400000      -0.16225754497
  1 s
  1.3166643441      0.87495110714
  1 s
  0.56907152172      1.0000000000
  1 s
  0.10059695193      1.0000000000
  1 s
  0.37071460798E-01  1.0000000000
  4 p
  4.1360790000      -0.55183328018
  2.9462810000      0.61370533515
  1.0792431924      0.64005434538
  0.46611217769      0.25958050755
  1 p
  0.17453169991      1.0000000000
  1 p
  0.41000000000E-01  1.0000000000
  4 d
  6.8847131641      -0.15962387985E-01
  2.3837304391      0.23047555829
  1.0184384022      0.44075804028
  0.39957494644      0.39567661996
  1 d
  0.13951120264      1.0000000000
*
rh def2-ecp
*
  ncore =    28      lmax =    3
#      coefficient  r^n      exponent
f
      -30.0934557    2      12.3100000
      -5.2184819    2      6.1600000
s-f
      225.3477535    2      11.7200000
      32.8231890     2      5.8200000
      30.0934557     2      12.3100000
      5.2184819      2      6.1600000
p-f
      158.7094116    2      10.4200000
      26.4441005     2      5.4500000
      30.0934557     2      12.3100000
      5.2184819      2      6.1600000
d-f
      62.7586257     2      8.8200000
      10.9787195     2      3.8700000
      30.0934557     2      12.3100000
      5.2184819      2      6.1600000
*
*
pd def2-SV(P)
# pd      (7s6p5d) / [5s3p2d]      {31111/411/41}

```

```

*
  3 s
  8.4756400000      1.2392391076
  7.1657170000     -1.6563109970
  3.1821100000     -0.13178619060
  1 s
  1.3973644196      1.0000000000
  1 s
  0.60532955868     1.0000000000
  1 s
  0.10229514209     1.0000000000
  1 s
  0.37338972881E-01  1.0000000000
  4 p
  4.2460970000     -0.82324104973
  3.3925940000      0.87084659933
  1.1975891264      0.63512225791
  0.52673750585     0.27225338752
  1 p
  0.20607094098     1.0000000000
  1 p
  0.37000000000E-01  1.0000000000
  4 d
  7.3613290985     -0.17199885828E-01
  2.6291037258      0.23313745275
  1.1292744634      0.44536385867
  0.44471659896     0.39293650406
  1 d
  0.15544893836     1.0000000000
*
pd def2-ecp
*
ncore =      28      lmax =      3
#      coefficient  r^n      exponent
f      -31.9295543   2      13.2700000
      -5.3982169    2      6.6300000
s-f    240.2290403    2      12.4300000
      35.1719435    2      6.1707594
      31.9295543    2      13.2700000
      5.3982169    2      6.6300000
p-f    170.4172760    2      11.0800000
      28.4721329    2      5.8295541
      31.9295543    2      13.2700000
      5.3982169    2      6.6300000
d-f    69.0138449     2      9.5100000
      11.7508616    2      4.1397811
      31.9295543    2      13.2700000
      5.3982169    2      6.6300000
*
*
ag def2-SV(P)
# ag      (7s6p5d) / [5s3p2d]      {31111/411/41}
*
  3 s
  9.0884420000     -1.9808918797
  7.5407310000     2.7554513347

```

```

2.7940050000      0.22715408381
 1 s
1.4918135849      1.00000000000
 1 s
0.63579159445     1.00000000000
 1 s
0.10368414161     1.00000000000
 1 s
0.37460004363E-01 1.00000000000
 4 p
4.4512400000     -0.99352103771
3.6752630000      1.0500525237
1.2610620905      0.64747532537
0.54212477498     0.25621550723
 1 p
0.20221617026     1.00000000000
 1 p
0.41200000000E-01 1.00000000000
 4 d
7.7956672292     -0.17042912377E-01
2.8926510238      0.23446154803
1.2474273203      0.44765877533
0.49313817671     0.39064954560
 1 d
0.17285032603     1.00000000000
*
ag def2-ecp
*
  ncore =    28      lmax =    3
#      coefficient  r^n      exponent
f
      -33.6899201    2      14.2200000
      -5.5311202    2      7.1100000
s-f
      255.1393645    2      13.1300000
      36.8661215     2      6.5100000
      33.6899201     2      14.2200000
      5.5311202      2      7.1100000
p-f
      182.1818687    2      11.7400000
      30.3577515     2      6.2000000
      33.6899201     2      14.2200000
      5.5311202      2      7.1100000
d-f
      73.7192609     2      10.2100000
      12.5021171     2      4.3800000
      33.6899201     2      14.2200000
      5.5311202      2      7.1100000
*
*
cd def2-SV(P)
# cd      (7s6p5d) / [5s3p2d]      {31111/411/41}
*
  3 s
9.7270110000     -1.7930075316
7.8375230000      2.6110318971
5.0891940000      0.10748428949
 1 s
1.4981738327      1.00000000000
 1 s

```

```

0.67281383129      1.0000000000
 1 s
0.13297424875      1.0000000000
 1 s
0.46915090488E-01  1.0000000000
 4 p
 4.7427160000      -1.0411923051
 3.9366550000      1.1003682332
 1.3569243142      0.65366639411
0.58791569541      0.24632369113
 1 p
0.21371239619      1.0000000000
 1 p
0.51600000000E-01  1.0000000000
 4 d
 7.8631040859      -0.21376239365E-01
 3.2935059133      0.22596399568
 1.4503676025      0.45294402972
0.59373316766      0.39218971958
 1 d
0.21760141520      1.0000000000
*
cd def2-ecp
*
  ncore =      28          lmax =      3
#   coefficient   r^n      exponent
f
  -35.4766256     2          15.1847957
  -5.6176768     2          7.5923978
s-f
  270.0094832    2          13.8358689
  38.7673080     2          6.8572704
  35.4766256     2          15.1847957
  5.6176768     2          7.5923978
p-f
  193.8296294    2          12.4049710
  31.8965252     2          6.5677995
  35.4766256     2          15.1847957
  5.6176768     2          7.5923978
d-f
  79.1936470     2          10.8969253
  13.2308267     2          4.6411649
  35.4766256     2          15.1847957
  5.6176768     2          7.5923978
*
*
in def2-SV(P)
# in      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
  6 s
  283.52297445    0.70132141424E-03
  23.324282101    -0.90887432418E-01
  16.868026844    0.28096825177
  6.7866498137    -0.70697832452
  1.6782596016    0.98671644913
0.78396870439    0.62568576302
  2 s
  1.8276654775    -0.34151640249
0.83753492534    -0.59696724334
  1 s

```



```

0.16643068973      1.0000000000
 1 s
0.61143742809E-01  1.0000000000
 4 p
14.699191826      0.92248042349E-01
 8.8709038051     -0.32437029300
 1.1342905889     0.61162217018
0.52667652433     0.17609640386
 1 p
 2.3284433667     1.0000000000
 1 p
0.16859144934     1.0000000000
 1 p
0.50070381081E-01 1.0000000000
 5 d
31.378655926      0.54007004722E-02
18.290046326     -0.11208558948E-01
 3.2551894590     0.30384519161
 1.3874842584     0.54078109979
0.54248962672     0.38232680038
 1 d
0.18000000000     1.0000000000
*
in def2-ecp
*
  ncore =    28          lmax =    3
#   coefficient   r^n      exponent
f
    -13.7280780    2         12.5390560
    -18.2068660    2         12.5525610
s-f
    281.1223500    2         15.3928220
    61.9014700    2          8.0558640
    13.7280780    2         12.5390560
    18.2068660    2         12.5525610
p-f
    67.4621540    2         13.9286720
   134.9492500    2         13.3472340
    14.7461400    2          7.6141320
    29.6392620    2          7.3183650
    13.7280780    2         12.5390560
    18.2068660    2         12.5525610
d-f
    35.4932540    2         14.0347150
    53.1787730    2         14.5116160
     9.1772810    2          5.5505500
    12.3924100    2          5.0594150
    13.7280780    2         12.5390560
    18.2068660    2         12.5525610
*
*
sn def2-SV(P)
# sn      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
  6 s
375.95156177      0.15224884228E-02
23.661818008     -0.16776065030
19.946281315     0.33989090393
 6.8240270454    -0.84441791529
 1.8771488722     0.92646952846

```

```

0.82033199226      0.53091094490
  2 s
10.341549887      -0.90331119154E-02
1.3672524155      0.22980877714
  1 s
0.18314843823      1.00000000000
  1 s
0.69547226146E-01  1.00000000000
  4 p
21.293597748      0.37103218279E-01
8.8171842499      -0.32351709661
1.2347028371      0.83846760898
0.57869142617      0.23294977050
  1 p
2.5084050284      1.00000000000
  1 p
0.21298577719      1.00000000000
  1 p
0.67364584657E-01  1.00000000000
  5 d
39.693023177      0.39185734275E-02
20.852179275      -0.68210073667E-02
3.6907832774      0.27938420495
1.5849404530      0.52607409874
0.62772693365      0.36149465348
  1 d
0.20500000000      1.00000000000
*
sn def2-ecp
*
  ncore =    28      lmax =    3
#      coefficient  r^n      exponent
f
      -12.5763330   2      12.2823480
      -16.5959440   2      12.2721500
s-f
      279.9886820   2      17.4204140
      62.3778100   2      7.6311550
      12.5763330   2      12.2823480
      16.5959440   2      12.2721500
p-f
      66.1625230   2      16.1310240
      132.1743960   2      15.6280770
      16.3394170   2      7.3256080
      32.4889590   2      6.9425190
      12.5763330   2      12.2823480
      16.5959440   2      12.2721500
d-f
      36.3874410   2      15.5149760
      54.5078410   2      15.1881600
      8.6968230    2      5.4560240
      12.8402080   2      5.3631050
      12.5763330   2      12.2823480
      16.5959440   2      12.2721500
*
*
sb def2-SV(P)
# sb      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
  6 s

```

372.76139166	0.15878057239E-02
22.689478596	-0.15027605583
18.391547037	0.35915813039
7.6406271414	-0.74805091065
1.9052000235	0.92017581656
0.93007107773	0.46754079597
2 s	
10.584496987	-0.14845336778E-01
1.4680242769	0.35289492025
1 s	
0.21621190032	1.0000000000
1 s	
0.83546307041E-01	1.0000000000
4 p	
15.926550950	0.13206950012
10.052739237	-0.41511149340
1.2682183726	0.74197972626
0.57196620929	0.15580772750
1 p	
2.6190751238	1.0000000000
1 p	
0.25183282652	1.0000000000
1 p	
0.83389127684E-01	1.0000000000
5 d	
45.485063360	0.32556415807E-02
18.504059617	-0.54952972010E-02
3.9156032308	0.27988806353
1.7142196009	0.51273377761
0.69675478242	0.33288802736
1 d	
0.23060000000	1.0000000000

*

sb def2-ecp

*

#	ncore = 28	lmax = 3	coefficient	r^n	exponent
f			-15.3668010	2	14.4449780
			-20.2961380	2	14.4492950
s-f			281.0715810	2	16.3308650
			61.7166040	2	8.5565420
			15.3668010	2	14.4449780
			20.2961380	2	14.4492950
p-f			67.4573800	2	14.4703370
			134.9335030	2	13.8161940
			14.7163440	2	8.4249240
			29.5185120	2	8.0927280
			15.3668010	2	14.4449780
			20.2961380	2	14.4492950
d-f			35.4478150	2	14.8863310
			53.1434660	2	15.1463190
			9.1792230	2	5.9082670
			13.2402530	2	5.5943220
			15.3668010	2	14.4449780
			20.2961380	2	14.4492950

*

```

*
te def2-SV(P)
# te      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
  6 s
396.47954659      0.26307731203E-02
21.919773309     -0.13203517066
18.061271390     0.36203197834
8.1403463241     -0.75591120276
2.0705998798     0.79192928400
0.97715185085    0.40558342540
  2 s
11.263563841     -0.15212984183E-01
1.6122696062     0.35202140517
  1 s
0.25095401705    1.00000000000
  1 s
0.97478452576E-01 1.00000000000
  4 p
17.479502221     0.11517799182
10.433943171     -0.41205302672
1.3623024763     0.78760578076
0.59239616258    0.15283299018
  1 p
2.7961737670     1.00000000000
  1 p
0.29766401026    1.00000000000
  1 p
0.96151090240E-01 1.00000000000
  5 d
50.821835991     0.33763474774E-02
18.884095378     -0.35221408938E-02
4.2527304630     0.28254216065
1.8757557092     0.52039372916
0.77069282849    0.32213541689
  1 d
0.25000000000    1.00000000000
*
te def2-ecp
*
  ncore =      28      lmax =      3
#      coefficient      r^n      exponent
f
      -15.7454500      2      15.2061680
      -20.7424480      2      15.2017020
s-f
      281.0458430      2      16.8144730
      61.6206560      2      8.7935260
      15.7454500      2      15.2061680
      20.7424480      2      15.2017020
p-f
      67.4494640      2      14.8778010
      134.9043040      2      14.2697310
      14.6895470      2      8.7244350
      29.4150630      2      8.2915150
      15.7454500      2      15.2061680
      20.7424480      2      15.2017020
d-f
      35.4320570      2      15.2050080
      53.1356870      2      15.2258480

```

```

          9.0698020    2          6.0717690
          13.1223040    2          5.8047600
          15.7454500    2          15.2061680
          20.7424480    2          15.2017020
*
*
i def2-SV(P)
# i      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
  6 s
445.90489176      0.20037290389E-02
23.336842412     -0.14989397324
19.583446104      0.36436474913
8.5112089186     -0.75538138199
2.1996161861      0.82816359356
1.0668970454      0.42161048110
  2 s
11.720547572     -0.16160234511E-01
1.7625986449      0.35271525193
  1 s
0.28697476318      1.00000000000
  1 s
0.11227609607      1.00000000000
  4 p
20.499027254      0.77159335656E-01
10.558754576     -0.38370372780
1.5015895485      0.83554174719
0.64597173095      0.16787259488
  1 p
3.0288656771      1.00000000000
  1 p
0.34506591841      1.00000000000
  1 p
0.11134513813      1.00000000000
  5 d
51.235354920      0.40345130346E-02
15.616239482     -0.50768108881E-02
4.5266002139      0.29151065356
2.0529808766      0.51145783605
0.87640281623      0.31232025297
  1 d
0.30900000000      1.00000000000
*
i def2-ecp
*
  ncore =    28          lmax =    3
#      coefficient      r^n          exponent
f
      -21.8420400      2          19.4586090
      -28.4681910      2          19.3492600
      -0.2437130      2          4.8237670
      -0.3208040      2          4.8843150
s-f
      49.9942930      2          40.0158350
      281.0253170      2          17.4297470
      61.5733260      2          9.0054840
      21.8420400      2          19.4586090
      28.4681910      2          19.3492600
      0.2437130      2          4.8237670
      0.3208040      2          4.8843150

```

```

p-f
    67.4428410    2    15.3554660
    134.8811370   2    14.9718330
    14.6750510    2    8.9601640
    29.3756660    2    8.2590960
    21.8420400    2    19.4586090
    28.4681910    2    19.3492600
    0.2437130     2    4.8237670
    0.3208040     2    4.8843150

d-f
    35.4395290    2    15.0689080
    53.1760570    2    14.5553220
    9.0671950     2    6.7186470
    13.2069370    2    6.4563930
    0.0893350     2    1.1917790
    0.0523800     2    1.2911570
    21.8420400    2    19.4586090
    28.4681910    2    19.3492600
    0.2437130     2    4.8237670
    0.3208040     2    4.8843150

```

*

*

```

xe def2-SV(P)
# xe (11s10p8d2f) / [6s5p3d2f] {521111/34111/611/11}

```

*

```

5 s
6420.2481656    0.25092173886E-03
983.54530664    0.16251948178E-02
219.43881364    0.46037106451E-02
23.012587807    -0.14698707182
18.048324490    0.57524870348
2 s
11.752550163    0.66038420156
6.2390917199    0.38470524721
1 s
2.6257211320    1.0000000000
1 s
1.2905042943    1.0000000000
1 s
0.36204185060    1.0000000000
1 s
0.14069888091    1.0000000000
3 p
193.81432545    0.95394802497E-03
21.725228086    0.57393353332E-01
9.8891605641    -0.27974266640
4 p
13.960683826    -0.50950157807E-01
4.0928947097    0.36669211800
2.2546815460    0.72619456861
1.1546596184    0.35555871740
1 p
0.52321923128    1.0000000000
1 p
0.21945569800    1.0000000000
1 p
0.86158996836E-01 1.0000000000
6 d
135.60300038    0.81873543290E-03
38.727062692    0.60897654151E-02

```

```

15.377328089      -0.92782985596E-02
5.2602537686      0.22890785589
2.6590627424      0.44434407051
1.2938205124      0.36029482992
 1 d
0.58050830139      1.0000000000
 1 d
0.18000000000      1.0000000000
 1 f
0.49652793000      1.0000000000
 1 f
2.50000000000      1.0000000000
*
xe def2-ecp
*
  ncore =    28          lmax =    3
#   coefficient   r^n      exponent
f
  -23.0892950     2         20.8815570
  -30.0744750     2         20.7834430
   -0.2882270     2          5.2533890
   -0.3869240     2          5.3611880
s-f
   49.9979620     2         40.0051840
  281.0133030     2         17.8122140
   61.5382550     2          9.3041500
   23.0892950     2         20.8815570
   30.0744750     2         20.7834430
    0.2882270     2          5.2533890
    0.3869240     2          5.3611880
p-f
   67.4391420     2         15.7017720
  134.8747110     2         15.2586080
   14.6633000     2          9.2921840
   29.3547300     2          8.5590030
   23.0892950     2         20.8815570
   30.0744750     2         20.7834430
    0.2882270     2          5.2533890
    0.3869240     2          5.3611880
d-f
   35.4369080     2         15.1856000
   53.1957720     2         14.2845000
    9.0462320     2          7.1218890
   13.2236810     2          6.9919630
    0.0848530     2          0.6239460
    0.0441550     2          0.6472840
   23.0892950     2         20.8815570
   30.0744750     2         20.7834430
    0.2882270     2          5.2533890
    0.3869240     2          5.3611880
*
*
cs def2-SV(P)
# cs      (7s6p2d) / [5s3p2d]      {31111/411/11}
*
  3 s
5.8778113443      0.12859994983
4.3631538286      -0.34632569725
1.8048475155      0.69930637051
 1 s

```

```

0.37485237136      1.0000000000
 1 s
0.16384858778      1.0000000000
 1 s
0.27230462048E-01  1.0000000000
 1 s
0.11991533212E-01  1.0000000000
 4 p
 4.2751856154      0.45723074174E-01
 1.9656663360      -0.25019961976
0.47689195212      0.55660850066
0.21529749588      0.58218553406
 1 p
0.91450850296E-01  1.0000000000
 1 p
0.17592078473E-01  1.0000000000
 1 d
0.13300000000      1.0000000000
 1 d
0.33216214821E-01  1.0000000000
*
cs def2-ecp
*
ncore =    46          lmax =    3
# coefficient  r^n      exponent
f          -28.8843090    2          3.1232690
s-f          84.5477300    2          4.0797500
           16.6541730    2          2.4174060
           28.8843090    2          3.1232690
p-f          157.0490590    2          5.5140800
           26.4233070    2          2.1603160
           28.8843090    2          3.1232690
d-f          13.1727530    2          1.8074100
           3.3428330    2          0.8581820
           28.8843090    2          3.1232690
*
*
ba def2-SV(P)
# ba      (6s6p5d) / [4s3p2d]      {3111/411/41}
*
 3 s
 2.3961900000      -5.9554766710
 2.2433050000      6.6805648241
0.71740200000      -0.57055347037
 1 s
0.27420073547      1.0000000000
 1 s
0.40933264188E-01  1.0000000000
 1 s
0.18060156423E-01  1.0000000000
 4 p
 2.9267420000      0.79815276764
 2.5207180000      -1.0707548832
0.67578180854      0.34940781448
0.31985844531      0.65041110673
 1 p

```



```

0.13221792446      1.0000000000
  1 p
0.33039565349E-01  1.0000000000
  4 d
0.96631500000     -0.90893800000
0.89382800000     0.94724000000
0.27319500000     0.32205700000
0.10389100000     0.47326000000
  1 d
0.35578000000E-01  0.36597700000
*
ba def2-ecp
*
  ncore =      46      lmax =      3
#      coefficient  r^n      exponent
f      -33.4731740    2      3.5894650
s-f      427.8458160    2      9.5269860
      204.4175300    2      4.4875100
      33.4731740    2      3.5894650
p-f      293.6058640    2      8.3159300
      294.1933160    2      4.2922170
      33.4731740    2      3.5894650
d-f      112.5504020    2      5.9161080
      181.7826210    2      2.8748420
      33.4731740    2      3.5894650
*
*
la def2-SV(P)
# la      (7s6p5d) / [6s3p2d]      {211111/411/41}
*
  2 s
  5.0873990000     -0.44173707857
  4.2709780000     0.85812489720
  1 s
  2.1823803999     1.00000000000
  1 s
0.48954926461     1.00000000000
  1 s
0.23292032550     1.00000000000
  1 s
0.55595529876E-01  1.00000000000
  1 s
0.22795184937E-01  1.00000000000
  4 p
  3.0251610000     -0.28580266655
  2.3820950000     0.51718364644
0.67246658081     -0.44823115995
0.32519427171     -0.58864843930
  1 p
0.13635489374     1.00000000000
  1 p
0.25100000000E-01  1.00000000000
  4 d
  1.2667182018     -0.17445579381
0.89049882672     0.25137236211
0.32947291040     0.44604068240

```

```

0.13398788830      0.44878277154
  1 d
0.51275503081E-01  1.0000000000
*
la def2-ecp
*
  ncore =    46      lmax =    3
#   coefficient   r^n      exponent
f
  -36.0100160     2        4.0286000
s-f
  91.9321770     2        3.3099000
  -3.7887640     2        1.6550000
  36.0100160     2        4.0286000
p-f
  63.7594860     2        2.8368000
  -0.6479580     2        1.4184000
  36.0100160     2        4.0286000
d-f
  36.1161730     2        2.0213000
  0.2191140     2        1.0107000
  36.0100160     2        4.0286000
*
*
hf def2-SV(P)
# hf      (7s6p5d) / [6s3p2d]      {211111/411/41}
*
  2 s
  14.592485000    -0.80196298812
  11.547491000    1.5261602829
  1 s
  4.9112973928    1.0000000000
  1 s
  0.79665469409    1.0000000000
  1 s
  0.34234072894    1.0000000000
  1 s
  0.98109197714E-01  1.0000000000
  1 s
  0.36190984443E-01  1.0000000000
  4 p
  6.7265310000    0.65076205466
  5.9599790000    -0.83713508620
  1.0921117054    0.50570506286
  0.49702823217    0.51965388691
  1 p
  0.20258973792    1.0000000000
  1 p
  0.33600000000E-01  1.0000000000
  4 d
  3.9820623229    -0.42446023944E-01
  1.3077987772    0.18409232564
  0.53272310298    0.41484423516
  0.20564954488    0.44224303497
  1 d
  0.73099858787E-01  1.0000000000
*
hf def2-ecp
*
  ncore =    60      lmax =    3

```

```

#      coefficient  r^n      exponent
f      10.0467225   2        1.7857698
s-f    1499.2847107  2        14.7699590
      40.2821014    2        7.3849794
      -10.0467225  2        1.7857698
p-f    397.7330053   2        9.8494895
      19.3164059   2        4.9247445
      -10.0467225  2        1.7857698
d-f    101.3298053   2        6.0967564
      5.8734382    2        3.0483782
      -10.0467225  2        1.7857698
*
*
ta def2-SV(P)
# ta      (7s6p5d) / [6s3p2d]      {211111/411/41}
*
  2 s
  14.400000000  0.99343296745
  12.000000000 -1.6510077975
  1 s
  5.0701477302  1.0000000000
  1 s
  0.86033356487 1.0000000000
  1 s
  0.37158938894 1.0000000000
  1 s
  0.10745336254 1.0000000000
  1 s
  0.39142776556E-01 1.0000000000
  4 p
  7.4188720000  0.26979695152
  5.6984100000 -0.46968874449
  1.1777211960  0.50905100155
  0.54478533555  0.52298161137
  1 p
  0.22309270117  1.0000000000
  1 p
  0.43100000000E-01 1.0000000000
  4 d
  3.9738796278 -0.52799310714E-01
  1.4528884813  0.18558319471
  0.61042908544  0.42959071631
  0.24216276510  0.43497228232
  1 d
  0.87909318337E-01 1.0000000000
*
*
ta def2-ecp
*
  ncore = 60      lmax = 3
#      coefficient  r^n      exponent
f      12.0179609   2        2.0178811
s-f    1345.8806470  2        14.5464077
      36.7668062    2        7.2732038
      -12.0179609   2        2.0178811

```

```

p-f      378.4253015   2      9.9355653
         22.2930909   2      4.9677824
        -12.0179609   2      2.0178811
d-f      104.8839557   2      6.3473769
         8.7558481    2      3.1736885
        -12.0179609   2      2.0178811
*
*
w def2-SV(P)
# w      (7s6p5d) / [6s3p2d]      {211111/411/41}
*
  2 s
 15.000000000      -0.53315505392
 12.000000000      1.0014141748
  1 s
 5.2610967725     1.0000000000
  1 s
0.92785370307     1.0000000000
  1 s
0.40334458241     1.0000000000
  1 s
0.11585976646     1.0000000000
  1 s
0.41800474073E-01 1.0000000000
  4 p
 7.2496570000     0.45857265530
 6.0848760000     -0.66720686321
 1.2523777812     0.52090351989
0.58569208922     0.51885687511
  1 p
0.24106964301     1.0000000000
  1 p
0.40300000000E-01 1.0000000000
  4 d
 4.0131231332     -0.63416491808E-01
 1.6237452450     0.18452733732
0.69187452392     0.44121676843
0.27865835325     0.43158409241
  1 d
0.10225296446     1.0000000000
*
w def2-ecp
*
  ncore =    60      lmax =    3
#      coefficient  r^n      exponent
f
      14.1525795    2      2.2588885
s-f
1192.3958823      2      14.3228564
 32.5229332       2      7.1614281
-14.1525795       2      2.2588885
p-f
 359.0319671      2      10.0216411
 24.0303802       2      5.0108204
-14.1525795       2      2.2588885
d-f
 108.3013490      2      6.5979974
 10.9825283       2      3.2989987

```

```

-14.1525795      2      2.2588885
*
*
re def2-SV(P)
# re      (7s6p5d) / [6s3p2d]      {211111/411/41}
*
  2 s
 14.781862000      -1.1395193885
 12.324075000      1.9371421121
  1 s
  5.5098597284      1.0000000000
  1 s
 0.98874104687      1.0000000000
  1 s
 0.42833312030      1.0000000000
  1 s
 0.12296804533      1.0000000000
  1 s
 0.43949851581E-01  1.0000000000
  4 p
  7.4040050000      0.54510937865
  6.3502060000      -0.76096056536
  1.3311713455      0.53252276765
 0.62659600547      0.51483045040
  1 p
 0.25922718696      1.0000000000
  1 p
 0.483000000000E-01  1.0000000000
  4 d
  4.0616274916      -0.76667295205E-01
  1.8487943286      0.18067495215
 0.78702048429      0.45160766937
 0.32069843172      0.43261236266
  1 d
 0.11892742980      1.0000000000
*
re def2-ecp
*
  ncore =      60      lmax =      3
#      coefficient      r^n      exponent
f
      16.4498523      2      2.5086506
s-f
      1038.9515723      2      14.0993051
      29.5617383      2      7.0496525
      -16.4498523      2      2.5086506
p-f
      339.5435096      2      10.1077169
      24.9136965      2      5.0538583
      -16.4498523      2      2.5086506
d-f
      111.6996527      2      6.8486179
      12.6243293      2      3.4243090
      -16.4498523      2      2.5086506
*
*
os def2-SV(P)
# os      (7s6p5d) / [6s3p2d]      {211111/411/41}
*
  2 s

```

```

15.286736000      -1.0647114485
12.700638000      1.8433193269
 1 s
5.7094832504      1.0000000000
 1 s
1.0689228744      1.0000000000
 1 s
0.46783543749     1.0000000000
 1 s
0.13253456992     1.0000000000
 1 s
0.47101982911E-01 1.0000000000
 4 p
7.9362790000      0.33899369659
6.3036410000      -0.56379438345
1.4351579676      0.52360040577
0.68442749722     0.52445339821
 1 p
0.28347394974     1.0000000000
 1 p
0.58100000000E-01 1.0000000000
 4 d
3.5808150000      -0.42773932262
3.1961650000      0.44501403992
1.0550226354      0.43689459722
0.41588406618     0.48220605799
 1 d
0.14653507868     1.0000000000
*
os def2-ecp
*
  ncore =      60          lmax =      3
#      coefficient      r^n          exponent
f
      18.9094570      2          2.7670751
s-f
      885.4057191      2          13.8757539
      25.9670401      2          6.9378769
      -18.9094570      2          2.7670751
p-f
      320.0839019      2          10.1937926
      26.1487649      2          5.0968962
      -18.9094570      2          2.7670751
d-f
      115.0448431      2          7.0992385
      13.6225746      2          3.5496192
      -18.9094570      2          2.7670751
*
*
ir def2-SV(P)
# ir      (7s6p5d) / [6s3p2d]      {2111111/411/41}
*
  2 s
15.293709000      -1.6731899791
13.573682000      2.3934378976
 1 s
5.8213436542      1.0000000000
 1 s
1.1520364268      1.0000000000
 1 s

```

```

0.51104895338      1.0000000000
 1 s
0.14084043578      1.0000000000
 1 s
0.49828673085E-01  1.0000000000
 4 p
 8.6697960000      0.21469187346
 6.2456140000      -0.44863071815
 1.5657036153      0.50653393257
0.75577412863      0.54052273352
 1 p
0.31306011113      1.0000000000
 1 p
0.54800000000E-01  1.0000000000
 4 d
 3.6994850000      -0.54840155965
 3.3617430000      0.56835425804
 1.1177053710      0.44304381513
0.44322534858      0.47078394930
 1 d
0.15641305125      1.0000000000
*
ir def2-ecp
*
  ncore =    60          lmax =    3
#   coefficient  r^n      exponent
f
      21.5310311      2          3.0340719
s-f
      732.2691998      2          13.6522026
      26.4847209      2          6.8261013
      -21.5310311      2          3.0340719
p-f
      299.4894736      2          10.2798684
      26.4662335      2          5.1399341
      -21.5310311      2          3.0340719
d-f
      124.4575945      2          7.3498590
      14.0359952      2          3.6749295
      -21.5310311      2          3.0340719
*
*
pt def2-SV(P)
# pt      (7s6p5d) / [6s3p2d]      {211111/411/41}
*
  2 s
 16.559563000      -0.53808800717
 13.892440000      0.91402161377
 1 s
 5.8531044732      1.0000000000
 1 s
 1.2498640609      1.0000000000
 1 s
0.55606439459      1.0000000000
 1 s
0.13793093812      1.0000000000
 1 s
0.48989034059E-01  1.0000000000
 4 p
 8.1000000000      0.72955608128

```

```

7.20000000000 -0.95441807252
1.5588402917 0.57140490320
0.73230402180 0.49508234268
1 p
0.30270484669 1.00000000000
1 p
0.50000000000E-01 1.00000000000
4 d
4.6299536825 -0.87774450596E-01
2.1980241252 0.21158360681
0.93629991261 0.46533857641
0.37160028160 0.41129165525
1 d
0.13155928617 1.00000000000
*
pt def2-ecp
*
ncore = 60 lmax = 3
# coefficient r^n exponent
f
24.3143757 2 3.3095686
s-f
579.2238609 2 13.4286513
29.6694906 2 6.7143256
-24.3143757 2 3.3095686
p-f
280.8607742 2 10.3659442
26.7453820 2 5.1829721
-24.3143757 2 3.3095686
d-f
120.3964443 2 7.6004795
15.8109206 2 3.8002397
-24.3143757 2 3.3095686
*
*
au def2-SV(P)
# au (7s6p5d) / [6s3p2d] {211111/411/41}
*
2 s
20.115299000 -0.15910719389
12.193477000 0.79105526778
1 s
6.0735294368 1.00000000000
1 s
1.3174451569 1.00000000000
1 s
0.58596768244 1.00000000000
1 s
0.13875427354 1.00000000000
1 s
0.48876985527E-01 1.00000000000
4 p
8.6096650000 0.50053018599
7.3353260000 -0.72681584494
1.6575296365 0.57315511417
0.78159310216 0.49579068859
1 p
0.32384840661 1.00000000000
1 p
0.54000000000E-01 1.00000000000

```



```

4 d
4.1439490000 -0.37099566643
3.5682570000 0.40197233762
1.2345757130 0.46001988624
0.48190232338 0.46152130958
1 d
0.16490636769 1.00000000000
*
au def2-ecp
*
ncore = 60 lmax = 3
# coefficient r^n exponent
f
30.4900889 2 4.7898200
5.1710738 2 2.3949100
s-f
426.8466792 2 13.2051000
37.0070829 2 6.6025500
-30.4900889 2 4.7898200
-5.1710738 2 2.3949100
p-f
261.1995804 2 10.4520200
26.9624960 2 5.2260100
-30.4900889 2 4.7898200
-5.1710738 2 2.3949100
d-f
124.7906656 2 7.8511000
16.3007257 2 3.9255500
-30.4900889 2 4.7898200
-5.1710738 2 2.3949100
*
*
hg def2-SV(P)
# hg (7s6p5d) / [6s3p2d] {211111/411/41}
*
2 s
26.842049000 -0.26845096483E-01
10.320909000 0.81771278143
1 s
6.3656242291 1.00000000000
1 s
1.3898932095 1.00000000000
1 s
0.63706742699 1.00000000000
1 s
0.16047725098 1.00000000000
1 s
0.56410423453E-01 1.00000000000
4 p
9.7729900000 0.21210940502
7.1690950000 -0.44026342153
1.7559567931 0.58406314464
0.83145670425 0.49359746203
1 p
0.34494917659 1.00000000000
1 p
0.70000000000E-01 1.00000000000
4 d
4.2800000000 -0.32033414305
3.4800000000 0.37748470203

```

```

1.2535869926      0.48342275878
0.50841366863    0.43493523158
  l  d
0.18501599388    1.00000000000
*
hg def2-ecp
*
  ncore =      60      lmax =      3
#      coefficient  r^n      exponent
f
      30.3649964      2      3.8857911
s-f
      275.7372117      2      12.9815487
      49.0892125      2      6.4907744
      -30.3649964      2      3.8857911
p-f
      241.5400740      2      10.5380958
      27.3965908      2      5.2690479
      -30.3649964      2      3.8857911
d-f
      127.8670076      2      8.1017205
      16.6083115      2      4.0508603
      -30.3649964      2      3.8857911
*
*
t1 def2-SV(P)
# t1      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
  6  s
45.356924655      0.50938157397E-02
20.278843336      -0.14805704314
14.420612394      0.36768453564
6.2161909754      -0.66820394623
1.5002511178      0.96232806743
0.76330879305      0.33175999361
  2  s
7.8193195283      -0.18828631537E-01
1.3176904042      0.32093431467
  1  s
0.17643545481      1.00000000000
  1  s
0.65296835238E-01  1.00000000000
  4  p
9.0323058024      0.22738839085
7.5356419671      -0.35117975889
1.0521421998      0.25690085604
0.50303932656      0.84549942764E-01
  1  p
2.0067660913      1.00000000000
  1  p
0.16675605056      1.00000000000
  1  p
0.48596401464E-01  1.00000000000
  5  d
9.4421940760      0.58250776986E-01
7.4410003381      -0.11789199301
1.9831617772      0.34232057636
0.91671748567      0.47557282350
0.39647207885      0.30528029435
  1  d

```

```

0.15500000000      1.0000000000
*
t1 def2-ecp
*
ncore =      60      lmax =      3
# coefficient  r^n      exponent
f
      15.8254880      2      5.6263990
      21.1040210      2      5.5489520
      2.9151270      2      2.8749460
      3.8969030      2      2.8214510
s-f
      281.2846630      2      12.1678050
      62.4342510      2      8.2949090
      -15.8254880      2      5.6263990
      -21.1040210      2      5.5489520
      -2.9151270      2      2.8749460
      -3.8969030      2      2.8214510
p-f
      4.6334080      2      7.1514920
      9.3417560      2      5.1728650
      72.2992530      2      9.8910720
      144.5580370      2      9.0033910
      -15.8254880      2      5.6263990
      -21.1040210      2      5.5489520
      -2.9151270      2      2.8749460
      -3.8969030      2      2.8214510
d-f
      35.9430390      2      7.1302180
      53.9095930      2      6.9269060
      10.3819390      2      5.4175700
      15.5838220      2      5.1386810
      -15.8254880      2      5.6263990
      -21.1040210      2      5.5489520
      -2.9151270      2      2.8749460
      -3.8969030      2      2.8214510
*
*
pb def2-SV(P)
# pb      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
      6 s
      55.727520333      0.29681153058E-02
      20.302912827      -0.14352634362
      14.558628750      0.37554188507
      6.5370530973      -0.67253099800
      1.5933900686      0.95887533909
      0.83051419711      0.32593632538
      2 s
      8.0719473648      -0.20412061217E-01
      1.4165737490      0.32865829049
      1 s
      0.20418933370      1.0000000000
      1 s
      0.77159007761E-01      1.0000000000
      4 p
      9.5531412199      0.20542943990
      7.5327685129      -0.36407590058
      1.1185539567      0.32217481686
      0.53739855255      0.96677743015E-01

```

```

1 p
2.1359869828      1.0000000000
1 p
0.20027494801    1.0000000000
1 p
0.63408011513E-01  1.0000000000
5 d
13.494505735     0.11571042371E-01
7.0609770411    -0.66746645076E-01
2.1581835375     0.33978760942
1.0148541418     0.48523039273
0.44632672920    0.29682924018
1 d
0.17500000000    1.0000000000
*
pb def2-ecp
*
ncore = 60      lmax = 3
# coefficient r^n exponent
f
12.2098920     2      3.8875120
16.1902910     2      3.8119630
s-f
281.2854990    2      12.2963030
62.5202170     2      8.6326340
-12.2098920    2      3.8875120
-16.1902910    2      3.8119630
p-f
72.2768970     2      10.2417900
144.5910830    2      8.9241760
4.7586930      2      6.5813420
9.9406210      2      6.2554030
-12.2098920    2      3.8875120
-16.1902910    2      3.8119630
d-f
35.8485070     2      7.7543360
53.7243420     2      7.7202810
10.1152560     2      4.9702640
14.8337310     2      4.5637890
-12.2098920    2      3.8875120
-16.1902910    2      3.8119630
*
*
bi def2-SV(P)
# bi (10s7p6d) / [4s4p2d] {6211/4111/51}
*
6 s
175.19632102    0.80278879028E-03
19.820147783    -0.14624461250
14.960110102    0.37435719885
6.7065785571    -0.68476017748
1.7391967524    0.90967322081
0.94504730591    0.38695797807
2 s
8.4636832909    -0.20037183144E-01
1.5317838545    0.31054408682
1 s
0.23405391503    1.0000000000
1 s
0.90268814613E-01  1.0000000000

```

```

4 p
10.672046293      0.14391258793
7.1992185915     -0.37994608603
1.5359697528     0.53268032065
0.72201275727    0.23037698678
1 p
2.8508661858     1.00000000000
1 p
0.23769418731    1.00000000000
1 p
0.78768140453E-01 1.00000000000
5 d
15.834273510     0.85062993231E-02
7.0956896087    -0.65954380016E-01
2.3363137007     0.33707163406
1.1208861366     0.49128719933
0.50309487376    0.29095930644
1 d
0.20000000000    1.00000000000
*
bi def2-ecp
*
ncore =      60          lmax =      3
#      coefficient      r^n          exponent
f
      13.7133830      2          4.2145460
      18.1943080      2          4.1334000
s-f
      283.2642270      2          13.0430900
      62.4719590      2          8.2216820
      -13.7133830      2          4.2145460
      -18.1943080      2          4.1334000
p-f
      72.0014990      2          10.4677770
      144.0022770      2          9.1189010
      5.0079450      2          6.7547910
      9.9915500      2          6.2525920
      -13.7133830      2          4.2145460
      -18.1943080      2          4.1334000
d-f
      36.3962590      2          8.0814740
      54.5976640      2          7.8905950
      9.9842940      2          4.9555560
      14.9814850      2          4.7045590
      -13.7133830      2          4.2145460
      -18.1943080      2          4.1334000
*
*
po def2-SV(P)
# po      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
6 s
278.13783916     0.91690497839E-03
19.659291105     -0.14713009283
15.016229647     0.38790413631
7.1149978720     -0.67059966298
1.7879214122     0.91212928327
0.94021655206    0.29153755200
2 s
8.7584161749     -0.21561417525E-01

```

```

1.6503945866      0.31638990001
 1 s
0.26329582133      1.00000000000
 1 s
0.10190654304      1.00000000000
 4 p
10.445945973       0.23631841405
 8.0293101888      -0.45017818996
 1.3588798023       0.44160334658
0.66829182929       0.14575285544
 1 p
 2.4460635387       1.00000000000
 1 p
0.27242942777       1.00000000000
 1 p
0.88796031338E-01   1.00000000000
 5 d
18.292670150        0.72030963652E-02
 7.1695578539       -0.66160544754E-01
 2.5029225180        0.34363449378
 1.2115945443        0.50529101033
0.54713334240       0.28301155453
 1 d
0.21500000000       1.00000000000

```

*

po def2-ecp

*

```

ncore = 60          lmax = 3
#      coefficient   r^n      exponent
f
      17.4282950      2          5.0132700
      23.3803530      2          4.9846400
      0.1633920       2          1.3267600
      0.3245660       2          1.5287580
s-f
      283.2447060      2          13.2772270
      62.3964610       2          8.3995180
      -17.4282950      2          5.0132700
      -23.3803530      2          4.9846400
      -0.1633920       2          1.3267600
      -0.3245660       2          1.5287580
p-f
      71.9917160       2          10.6656820
      143.9718710      2          9.2837530
      4.9496150        2          6.8727490
      9.7404990         2          6.3261500
      -17.4282950      2          5.0132700
      -23.3803530      2          4.9846400
      -0.1633920       2          1.3267600
      -0.3245660       2          1.5287580
d-f
      36.3783830       2          8.2148660
      54.5627150       2          8.0086960
      9.8894990         2          5.0552270
      14.6938770       2          4.7825530
      -17.4282950      2          5.0132700
      -23.3803530      2          4.9846400
      -0.1633920       2          1.3267600
      -0.3245660       2          1.5287580

```

*

```

*
at def2-SV(P)
# at      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
  6 s
303.23376176      0.63504969788E-03
20.289449240     -0.13823165350
15.383783126      0.38333193283
7.4702184232     -0.66837560338
1.8731608346      0.91545877992
0.97426847543     0.25559567998
  2 s
8.9610112498     -0.23092977605E-01
1.7804284294      0.31690635939
  1 s
0.29269461143      1.0000000000
  1 s
0.11395353119      1.0000000000
  4 p
10.722023134      0.26194870008
8.4823338656     -0.46607228264
1.3474291294      0.42119853309
0.62824011467     0.10643224457
  1 p
2.4814896839      1.0000000000
  1 p
0.31036518470      1.0000000000
  1 p
0.10144862043      1.0000000000
  5 d
20.799819604      0.65227965381E-02
7.1664616770     -0.67780885217E-01
2.6934397048      0.33954991335
1.3175112423      0.50899559178
0.59997066293     0.27526771759
  1 d
0.23500000000      1.0000000000
*
at def2-ecp
*
  ncore =      60      lmax =      3
#      coefficient      r^n      exponent
f
      19.8701980      2      5.8121630
      26.4164520      2      5.7537150
      0.9949700      2      2.5134720
      1.4907010      2      2.5362610
s-f
      49.9571580      2      30.2008320
      283.2103710      2      13.6123060
      62.2810520      2      8.5293400
      -19.8701980      2      5.8121630
      -26.4164520      2      5.7537150
      -0.9949700      2      2.5134720
      -1.4907010      2      2.5362610
p-f
      71.9823710      2      10.8540650
      143.9035320      2      9.4682290
      4.8717590      2      7.0311140
      8.9830590      2      6.1438580

```

	-19.8701980	2	5.8121630
	-26.4164520	2	5.7537150
	-0.9949700	2	2.5134720
	-1.4907010	2	2.5362610
d-f			
	36.3632370	2	8.3135150
	54.5489700	2	7.9989650
	9.7762850	2	5.1799660
	14.2647550	2	4.9422260
	-19.8701980	2	5.8121630
	-26.4164520	2	5.7537150
	-0.9949700	2	2.5134720
	-1.4907010	2	2.5362610
*			
*			
rn def2-SV(P)			
# rn	(11s10p8d2f) / [6s5p3d2f]		{521111/34111/611/11}
*			
	5 s		
	5187.7442468	0.16097034848E-03	
	768.14491207	0.10508214789E-02	
	159.35182065	0.27375438093E-02	
	21.863432724	-0.55045904905	
	18.388689978	0.78321373922	
	2 s		
	24.816226448	-0.82636797204E-01	
	7.2923301677	1.0926256000	
	1 s		
	2.0850437166	1.0000000000	
	1 s		
	1.0915245945	1.0000000000	
	1 s		
	0.34915708428	1.0000000000	
	1 s		
	0.13648422952	1.0000000000	
	3 p		
	194.68918723	0.26265814046E-03	
	11.210013525	0.19952302621	
	7.5298316489	-0.45994479561	
	4 p		
	9.0845000304	-0.23093917426	
	6.2631489717	0.39747614192	
	2.2545193734	0.83026693838	
	1.1180666918	0.51467013112	
	1 p		
	0.47444492594	1.0000000000	
	1 p		
	0.20172354616	1.0000000000	
	1 p		
	0.79503144392E-01	1.0000000000	
	6 d		
	75.302723665	0.73590238429E-03	
	17.965913830	0.89490827389E-02	
	7.3741298033	-0.76641663693E-01	
	3.2296258578	0.22975404602	
	1.7937840508	0.43991495311	
	0.94633319732	0.35259395198	
	1 d		
	0.46860482223	1.0000000000	
	1 d		


```

0.200000000000      1.000000000000
  1 f
0.418060000000      1.000000000000
  1 f
2.100000000000      1.000000000000
*
rn def2-ecp
*
  ncore =    60      lmax =    3
#      coefficient  r^n      exponent
f
      21.7972900    2        6.3485710
      28.9468050    2        6.2959490
      1.4473650    2        2.8821180
      2.1779640    2        2.9080480
s-f
      49.9655510    2        30.1512420
      283.0700000    2        14.5212410
      62.0028700    2        8.0520380
      -21.7972900   2        6.3485710
      -28.9468050   2        6.2959490
      -1.4473650    2        2.8821180
      -2.1779640    2        2.9080480
p-f
      71.9691190    2        11.0099420
      143.8605590    2        9.6176250
      4.7147610     2        7.3360080
      9.0130650     2        6.4062530
      -21.7972900   2        6.3485710
      -28.9468050   2        6.2959490
      -1.4473650    2        2.8821180
      -2.1779640    2        2.9080480
d-f
      36.3683650    2        8.3692200
      54.5517610    2        8.1169750
      9.6344870     2        5.3536560
      14.3879020    2        5.0972120
      -21.7972900   2        6.3485710
      -28.9468050   2        6.2959490
      -1.4473650    2        2.8821180
      -2.1779640    2        2.9080480
*
=====
def2-SVP
=====
*
h def2-SVP
# h      (4s1p) / [2s1p]      {31/1}
*
  3 s
  13.010701000      0.19682158000E-01
  1.9622572000      0.13796524000
  0.44453796000      0.47831935000
  1 s
  0.12194962000      1.00000000000
  1 p
  0.80000000000      1.00000000000
*
*
he def2-SVP

```

```

# he      (4s1p) / [2s1p]      {31/1}
*
  3 s
 38.354936737      0.23814288905E-01
 5.7689081479      0.15490906777
 1.2399407035      0.46998096633
  1 s
0.29757815953      1.00000000000
  1 p
 1.00000000000      1.00000000000
*
*
li def2-SVP
# li      (7s3p) / [3s2p]      {511/21}
*
  5 s
 266.27785516      0.64920150325E-02
 40.069783447      0.47747863215E-01
 9.0559944389      0.20268796111
 2.4503009051      0.48606574817
 0.72209571855      0.43626977955
  1 s
0.52810884721E-01  1.00000000000
  1 s
0.20960948798E-01  1.00000000000
  2 p
 1.45000000000      0.25860000000
 0.30000000000      1.00000000000
  1 p
0.82000000000E-01  1.00000000000
*
*
be def2-SVP
# be      (7s4p) / [3s2p]      {511/31}
*
  5 s
 515.18616125      0.55615307983E-02
 77.511037595      0.41190068062E-01
 17.552481693      0.17913378108
 4.8028940596      0.44736716455
 1.4516214316      0.42009581920
  1 s
0.13281633620      1.00000000000
  1 s
0.45837372213E-01  1.00000000000
  3 p
 3.6316917145      -0.29033998305E-01
 0.71695694366      -0.16877854032
 0.19541932860      -0.51403419628
  1 p
0.60515465890E-01  1.00000000000
*
*
b def2-SVP
# b      (7s4p1d) / [3s2p1d]    {511/31/1}
*
  5 s
 839.31830086      -0.55929201074E-02
 126.26464843      -0.41565520771E-01
 28.620600763      -0.18299816983

```

```

7.8793722710      -0.46540391866
2.4088857172      -0.44173884791
 1 s
0.25105109036      1.00000000000
 1 s
0.83648866069E-01  1.00000000000
 3 p
 6.0332223619      -0.35603672456E-01
 1.2499157866      -0.19895775769
0.33871676350      -0.50850202618
 1 p
0.96415632351E-01  1.00000000000
 1 d
0.50000000000      1.00000000000
*
*
c def2-SVP
# c      (7s4p1d) / [3s2p1d]      {511/31/1}
*
 5 s
1238.4016938      0.54568832082E-02
186.29004992      0.40638409211E-01
42.251176346      0.18025593888
11.676557932      0.46315121755
 3.5930506482      0.44087173314
 1 s
0.40245147363      1.00000000000
 1 s
0.13090182668      1.00000000000
 3 p
 9.4680970621      0.38387871728E-01
 2.0103545142      0.21117025112
0.54771004707      0.51328172114
 1 p
0.15268613795      1.00000000000
 1 d
0.80000000000      1.00000000000
*
*
n def2-SVP
# n      (7s4p1d) / [3s2p1d]      {511/31/1}
*
 5 s
1712.8415853      -0.53934125305E-02
257.64812677      -0.40221581118E-01
58.458245853      -0.17931144990
16.198367905      -0.46376317823
 5.0052600809      -0.44171422662
 1 s
0.58731856571      1.00000000000
 1 s
0.18764592253      1.00000000000
 3 p
13.571470233      -0.40072398852E-01
 2.9257372874      -0.21807045028
0.79927750754      -0.51294466049
 1 p
0.21954348034      1.00000000000
 1 d
1.00000000000      1.00000000000

```

```

*
*
o def2-SVP
# o      (7s4p1d) / [3s2p1d]      {511/31/1}
*
  5 s
  2266.1767785      -0.53431809926E-02
  340.87010191     -0.39890039230E-01
  77.363135167     -0.17853911985
  21.479644940     -0.46427684959
  6.6589433124     -0.44309745172
  1 s
  0.80975975668     1.0000000000
  1 s
  0.25530772234     1.0000000000
  3 p
  17.721504317      0.43394573193E-01
  3.8635505440      0.23094120765
  1.0480920883      0.51375311064
  1 p
  0.27641544411     1.0000000000
  1 d
  1.2000000000      1.0000000000
*
*
f def2-SVP
# f      (7s4p1d) / [3s2p1d]      {511/31/1}
*
  5 s
  2894.8325990      -0.53408255515E-02
  435.41939120      -0.39904258866E-01
  98.843328866      -0.17912768038
  27.485198001      -0.46758090825
  8.5405498171      -0.44653131020
  1 s
  1.0654578038      1.0000000000
  1 s
  0.33247346748     1.0000000000
  3 p
  22.696633924      -0.45212874436E-01
  4.9872339257      -0.23754317067
  1.3491613954      -0.51287353587
  1 p
  0.34829881977     1.0000000000
  1 d
  1.4000000000      1.0000000000
*
*
ne def2-SVP
# ne     (7s4p1d) / [3s2p1d]      {511/31/1}
*
  5 s
  3598.9736625      -0.53259297003E-02
  541.32073112      -0.39817417969E-01
  122.90450062      -0.17914358188
  34.216617022      -0.46893582977
  10.650584124      -0.44782537577
  1 s
  1.3545953960      1.0000000000
  1 s

```

```

0.41919362639      1.0000000000
  3 p
28.424053785      -0.46031944795E-01
6.2822510953      -0.23993183041
1.6978715079      -0.50871724964
  1 p
0.43300700172      1.0000000000
  1 d
1.88800000000      1.0000000000
*
*
na def2-SVP
# na      (10s6p1d) / [4s2p1d]      {5311/51/1}
*
  5 s
4098.2003908      -0.58535911879E-02
616.49374031      -0.43647161872E-01
139.96644001      -0.19431465884
39.073441051      -0.48685065731
11.929847205      -0.41881705137
  3 s
20.659966030      0.85949689854E-01
1.9838860978      -0.56359144041
0.64836323942      -0.51954009048
  1 s
0.52443967404E-01  1.0000000000
  1 s
0.28048160742E-01  1.0000000000
  5 p
75.401862017      0.15435362532E-01
17.274818978      0.99738293184E-01
5.1842347425      0.31209593966
1.6601211973      0.49295674807
0.51232528958      0.32420398318
  1 p
0.52000000000E-01  1.0000000000
  1 d
0.13100000000      0.0000000000
*
*
mg def2-SVP
# mg      (10s7p1d) / [4s3p1d]      {5311/511/1}
*
  5 s
4953.8339196      -0.57778967498E-02
745.18044154      -0.43124761082E-01
169.21604972      -0.19268216987
47.300672019      -0.48641439116
14.461336973      -0.42550894077
  3 s
24.768174789      0.87956969984E-01
2.4940945349      -0.55165058128
0.87807584533      -0.53443294833
  1 s
0.87212782497E-01  1.0000000000
  1 s
0.33599293780E-01  1.0000000000
  5 p
98.053010494      -0.14480564601E-01
22.586932277      -0.95495750787E-01

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```

6.8391509842      -0.30787672651
2.2332843818      -0.49936292886
0.71606599387     -0.31503476213
 1 p
0.18914796195     1.00000000000
 1 p
0.53768755187E-01 1.00000000000
 1 d
0.10100000000     1.00000000000
*
*
al def2-SVP
# al      (10s7p1d) / [4s3p1d]      {5311/511/1}
*
 5 s
5887.5727030      0.13483347987E-02
885.61225996      0.10071576809E-01
201.13604899      0.45132454056E-01
56.284974674      0.11461268043
17.229551243      0.10159608943
 3 s
29.340249922      0.69347454208E-01
3.0439630420     -0.42528117679
1.1285539518     -0.41449832210
 1 s
0.14234175160     1.00000000000
 1 s
0.54400192313E-01 1.00000000000
 5 p
145.11918809      0.63963373134E-02
33.717894833      0.44189359965E-01
10.369863083      0.15581575993
3.5135616036      0.28635286951
1.1980050273      0.22921423248
 1 p
0.26583005913     1.00000000000
 1 p
0.71003361994E-01 1.00000000000
 1 d
0.30000000000     1.00000000000
*
*
si def2-SVP
# si      (10s7p1d) / [4s3p1d]      {5311/511/1}
*
 5 s
6903.7118686      0.13373962995E-02
1038.4346419      0.99966546241E-02
235.87581480      0.44910165101E-01
66.069385169      0.11463638540
20.247945761      0.10280063858
 3 s
34.353481730      0.70837285010E-01
3.6370788192     -0.43028836252
1.4002048599     -0.41382774969
 1 s
0.20484414805     1.00000000000
 1 s
0.77994095468E-01 1.00000000000
 5 p

```

179.83907373	0.61916656462E-02
41.907258846	0.43399431982E-01
12.955294367	0.15632019351
4.4383267393	0.29419996982
1.5462247904	0.23536823814
1 p	
0.35607612302	1.0000000000
1 p	
0.10008513762	1.0000000000
1 d	
0.35000000000	1.0000000000
*	
*	
p def2-SVP	
# p (10s7p1d) / [4s3p1d] {5311/511/1}	
*	
5 s	
8002.4795106	0.57503489302E-02
1203.6813590	0.43007628959E-01
273.44227031	0.19363986252
76.655541517	0.49651693399
23.516927435	0.44983262479
3 s	
39.791683439	0.95188129789E-01
4.2770343323	-0.57649840368
1.6940256888	-0.54239583865
1 s	
0.27567674644	1.0000000000
1 s	
0.10495590099	1.0000000000
5 p	
219.50755823	0.92100565257E-02
51.274155030	0.65409765745E-01
15.921595892	0.24033730279
5.5069913481	0.46318321788
1.9537719426	0.37392563382
1 p	
0.47803397932	1.0000000000
1 p	
0.13657952621	1.0000000000
1 d	
0.45000000000	1.0000000000
*	
*	
s def2-SVP	
# s (10s7p1d) / [4s3p1d] {5311/511/1}	
*	
5 s	
9184.9303010	-0.22294387756E-02
1381.5105503	-0.16683029937E-01
313.87147580	-0.75262436116E-01
88.053870623	-0.19376827038
27.039914905	-0.17718020803
3 s	
45.648731303	-0.10736062573
4.9664522326	0.65066293018
2.0116242047	0.59712155354
1 s	
0.35661077013	1.0000000000
1 s	

```

0.13507221477      1.0000000000
  5 p
261.98233439      -0.92729929822E-02
61.306894736      -0.66547669241E-01
19.103729887      -0.24828595903
6.6567720378      -0.48703847402
2.3959635161      -0.39337850312
  1 p
0.61776161679      1.0000000000
  1 p
0.16993376871      1.0000000000
  1 d
0.55000000000      1.0000000000
*
*
cl def2-SVP
# cl      (10s7p1d) / [4s3p1d]      {5311/511/1}
*
  5 s
10449.827566      0.19708362484E-02
1571.7365221      0.14754727977E-01
357.12065523      0.66679112875E-01
100.25185935      0.17228924084
30.812727554      0.15883786100
  3 s
51.923789434      -0.10009298909
5.7045760975      0.60841752753
2.3508376809      0.54352153355
  1 s
0.44605124672      1.0000000000
  1 s
0.16848856190      1.0000000000
  5 p
307.66790569      -0.87801484118E-02
72.102015515      -0.63563355471E-01
22.532680262      -0.24016428276
7.8991765444      -0.47798866557
2.8767268321      -0.38515850005
  1 p
0.77459363955      1.0000000000
  1 p
0.21037699698      1.0000000000
  1 d
0.65000000000      1.0000000000
*
*
ar def2-SVP
# ar      (10s7p1d) / [4s3p1d]      {5311/511/1}
*
  5 s
11797.119765      0.20214479973E-02
1774.3522753      0.15139852688E-01
403.18875733      0.68525400873E-01
113.24933999      0.17762929207
34.835298193      0.16496495001
  3 s
58.614775042      -0.10343394000
6.4922045078      0.63133365899
2.7117014403      0.54887572301
  1 s

```



```

0.54412974538      1.0000000000
  1 s
0.20517411136      1.0000000000
  5 p
356.28707256      -0.87321783271E-02
83.593132866      -0.63680317444E-01
26.186704029      -0.24311906886
9.2257275925      -0.48956069653
3.3922754954      -0.39229190040
  1 p
0.94740534010      1.0000000000
  1 p
0.25659135062      1.0000000000
  1 d
0.69600000000      1.0000000000
*
*
k def2-SVP
# k      (14s9p2d) / [5s3p2d]      {63311/531/11}
*
  6 s
31478.746764      0.39838653994E-02
4726.8876066      0.30501759762E-01
1075.4345353      0.15073752622
303.39811023      0.51912939801
98.327112831      1.0366957005
33.636222177      0.76398963199
  3 s
65.639209962      -0.28242617106
7.3162592218      1.6914935860
2.8902580135      1.2965331953
  3 s
4.5459748965      -0.76343555273E-02
0.70404124062      0.25635718960E-01
0.28266888959      0.16606859208E-01
  1 s
0.29058164020E-01  1.0000000000
  1 s
0.12111638157E-01  1.0000000000
  5 p
361.22492154      0.20906479823E-01
84.670222166      0.15043641740
26.469088236      0.55440061077
9.2658077615      1.0409009991
3.3423388293      0.67825341194
  3 p
1.5100876104      0.75248191146
0.56568375163      1.3708585031
0.20817008495      0.66047633079
  1 p
0.41737000000E-01  1.0000000000
  1 d
0.35300000000      1.0000000000
  1 d
0.98000000000E-01  1.0000000000
*
*
ca def2-SVP
# ca      (14s9p4d) / [5s3p2d]      {63311/531/31}
*

```

```

6 s
35138.713929      0.39482520740E-02
5276.4111348     0.30234243552E-01
1200.4692589     0.14952019681
338.71810542    0.51597345713
109.85385922    1.0339510296
37.608880299    0.76937933526
3 s
73.107977555    -0.28268525011
8.2407705688    1.6796092142
3.2959812993    1.2803766016
3 s
5.2341800914    -0.76868604561E-02
0.84187220515    0.25382375978E-01
0.36510294029    0.16512171511E-01
1 s
0.51222402884E-01  1.0000000000
1 s
0.19825111408E-01  1.0000000000
5 p
413.11313893    0.20327135354E-01
96.935786224    0.14730276362
30.372154659    0.54887167322
10.684776830    1.0440659818
3.8821258350    0.68653490684
3 p
1.7993016295    0.75410246871
0.69189056530    1.3409296599
0.26364024096    0.56391989435
1 p
0.74979000000E-01  1.0000000000
3 d
5.4979093879    0.73770011433E-01
1.3177128032    0.26052853169
0.32188682649    0.45233836380
1 d
0.70528614919E-01  1.0000000000
*
*
sc def2-SVP
# sc      (14s9p5d1f) / [5s3p2d1f]      {63311/531/41/1}
*
6 s
38956.081804    0.39293205858E-02
5849.5733637    0.30093221229E-01
1330.8813154    0.14890370950
375.55534165    0.51464282906
121.87261370    1.0337708070
41.760243729    0.77436851627
3 s
81.060633953    -0.28318552316
9.2059823972    1.6770806984
3.7063215732    1.2594733678
3 s
5.9888909988    -0.77821367493E-02
0.97363432378    0.25499692745E-01
0.42041019223    0.16191560820E-01
1 s
0.59440551913E-01  1.0000000000
1 s

```

```

0.22897806303E-01  1.0000000000
  5 p
466.31481262      0.19984300385E-01
109.51217097      0.14561043072
34.375921827      0.54687466223
12.142096955      1.0479006012
4.4336767669      0.68894890327
  3 p
2.0971291866      0.75619214724
0.80977606956      1.3178212235
0.30834046588      0.54312268173
  1 p
0.89748000000E-01  1.0000000000
  4 d
19.240334928      0.27039082144E-01
5.1178995899      0.13803684743
1.6554278827      0.34869086403
0.54016355610      0.48594185717
  1 d
0.16211214518      0.34374449689
  1 f
0.34500000000      1.0000000000
*
*
ti def2-SVP
# ti      (14s9p5d1f) / [5s3p2d1f]      {63311/531/41/1}
*
  6 s
42961.512185      0.39127635355E-02
6450.9759169      0.29969820489E-01
1467.7210915      0.14836352707
414.20997355      0.51347285324
134.48715840      1.0335365483
46.122209796      0.77854233930
  3 s
89.447762543      -0.28385401259
10.223346060      1.6772785333
4.1353774271      1.2411928456
  3 s
6.7896181452      -0.78399994518E-02
1.1106730691      0.25495493019E-01
0.47565975578      0.16061172892E-01
  1 s
0.65986956934E-01  1.0000000000
  1 s
0.25210342250E-01  1.0000000000
  5 p
522.03684782      0.19754179642E-01
122.68649489      0.14460677619
38.572903611      0.54669004165
13.672169319      1.0531647540
5.0118529359      0.69111213363
  3 p
2.4131928282      0.75803437136
0.93252270050      1.3036241399
0.35429058390      0.53638653300
  1 p
0.10156100000      1.0000000000
  4 d
23.465125957      0.26536380115E-01

```

```

6.3332593832      0.13796453963
2.0766489946      0.35312644228
0.69027361954     0.48647124166
  1 d
0.21088738554     0.33026314258
  1 f
0.56200000000     1.00000000000
*
*
v def2-SVP
# v      (14s9p5d1f) / [5s3p2d1f]      {63311/531/41/1}
*
  6 s
47160.376060      0.14498688908E-02
7081.4110871      0.11106435251E-01
1611.1621223      0.55005423585E-01
454.72940551      0.19060252591
147.71321208      0.38435022957
50.699538950      0.29095546792
  3 s
98.262492669      -0.10942337856
11.294293099      0.64539490399
4.5853360105      0.47117880777
  3 s
7.6359689588      -0.22454949054
1.2539836689      0.72594852764
0.53271935387     0.45560582748
  1 s
0.72246239566E-01  1.00000000000
  1 s
0.27358087448E-01  1.00000000000
  5 p
580.55044988      0.97315110917E-02
136.52341127      0.71531241137E-01
42.983958820      0.27197688414
15.282798763      0.52618988893
5.6202495154      0.34452533498
  3 p
2.7485386415      0.34040396496
1.0618550073      0.57983996120
0.40235518645     0.23911643083
  1 p
0.11124800000     1.00000000000
  4 d
27.358434017      0.26641927050E-01
7.4540604253      0.13995311726
2.4633917847      0.35751066639
0.82480925277     0.48488354148
  1 d
0.25257904742     0.32332844995
  1 f
0.83100000000     1.00000000000
*
*
cr def2-SVP
# cr      (14s9p5d1f) / [5s3p2d1f]      {63311/531/41/1}
*
  6 s
51528.086349      0.14405823106E-02
7737.2103487      0.11036202287E-01

```

1760.3748470	0.54676651806E-01
496.87706544	0.18965038103
161.46520598	0.38295412850
55.466352268	0.29090050668
3 s	
107.54732999	-0.10932281100
12.408671897	0.64472599471
5.0423628826	0.46262712560
3 s	
8.5461640165	-0.22711013286
1.3900441221	0.73301527591
0.56066602876	0.44225565433
1 s	
0.71483705972E-01	1.0000000000
1 s	
0.28250687604E-01	1.0000000000
5 p	
640.48536096	0.96126715203E-02
150.69711194	0.70889834655E-01
47.503755296	0.27065258990
16.934120165	0.52437343414
6.2409680590	0.34107994714
3 p	
3.0885463206	0.33973986903
1.1791047769	0.57272062927
0.43369774432	0.24582728206
1 p	
0.12067500000	1.0000000000
4 d	
27.559479426	0.30612488044E-01
7.4687020327	0.15593270944
2.4345903574	0.36984421276
0.78244754808	0.47071118077
1 d	
0.21995774311	0.33941649889
1 f	
1.1470000000	1.0000000000
*	
*	
mn def2-SVP	
# mn (14s9p5d1f) / [5s3p2d1f] {63311/531/41/1}	
*	
6 s	
56137.009037	0.14321304702E-02
8429.2063943	0.10972509162E-01
1917.8277233	0.54382468712E-01
541.36230198	0.18884335129
176.00069142	0.38198025054
60.500477010	0.29156772596
3 s	
117.17282882	-0.10933661328
13.596973368	0.64305039431
5.5483996341	0.45848970584
3 s	
9.4662853530	-0.22538977259
1.5595006070	0.72307758657
0.65230205868	0.45300721536
1 s	
0.84003734475E-01	1.0000000000
1 s	

```

0.31256098581E-01  1.0000000000
  5 p
706.00497535      0.95055518167E-02
166.19728820      0.70356271142E-01
52.452061906      0.27005556982
18.746932862      0.52574344602
6.9282991622      0.34254033223
  3 p
3.4772204938      0.33994073736
1.3406906449      0.57203836254
0.50498803038     0.23847605831
  1 p
0.12765000000     1.0000000000
  4 d
35.423264935      0.26985304111E-01
9.7814221451      0.14383458648
3.2673488767      0.36418958377
1.1026472189      0.48152670661
  1 d
0.33743205934     0.31458754360
  1 f
1.3260000000      1.0000000000
*
*
fe def2-SVP
# fe      (14s9p5d1f) / [5s3p2d1f]      {63311/531/41/1}
*
  6 s
60923.640643      0.14302254466E-02
9147.8893982      0.10958790038E-01
2081.3505927      0.54332554248E-01
587.55977067      0.18884995009
191.09043990      0.38253069946
65.732730112      0.29308335984
  3 s
127.25891928      -0.10964564925
14.830913010      0.64387631332
6.0653307408      0.45472347323
  3 s
10.449943710      -0.22539639952
1.7245228003      0.72164398156
0.71772177325     0.44985492922
  1 s
0.91449828308E-01  1.0000000000
  1 s
0.33706691021E-01  1.0000000000
  5 p
773.43750995      0.94325735144E-02
182.15149714      0.70029620575E-01
57.547272758      0.26993651996
20.614988935      0.52700011047
7.6348557890      0.34284148028
  3 p
3.8719327990      0.33974402988
1.4924724132      0.56842594005
0.56061284958     0.23649365839
  1 p
0.13491500000     1.0000000000
  4 d
38.968133419      0.27879664382E-01

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10.800067078      0.14858319982
3.6136457999     0.36905479496
1.2129967888     0.47745100883
1 d
0.36524393170    0.31418142304
1 f
1.5980000000     1.0000000000
*
*
co def2-SVP
# co      (14s9p5d1f) / [5s3p2d1f]      {63311/531/41/1}
*
6 s
65902.208257     0.14284614936E-02
9895.3896027     0.10946072783E-01
2251.4305789     0.54285953890E-01
635.61097084     0.18885179079
206.78820681     0.38301634994
71.179242971     0.29443551266
3 s
137.77268040     -0.10990221736
16.118079243     0.64455537395
6.6030327710     0.45116787924
3 s
11.479915788     -0.22593846910
1.8956426324     0.72231409008
0.78466232067    0.44903812296
1 s
0.98425774432E-01  1.0000000000
1 s
0.35945741932E-01  1.0000000000
5 p
843.64358575     0.93866097254E-02
198.76386994     0.69880208716E-01
62.854963098     0.27037070345
22.562842280     0.52904786880
8.3713209127     0.34357029579
3 p
4.2858719800     0.34027999036
1.6508041817     0.56693392384
0.61834231096    0.23617979783
1 p
0.14130800000    1.0000000000
4 d
42.927867612     0.28487788365E-01
11.942533053     0.15206951283
4.0046495664     0.37310913999
1.3413193804     0.47549837676
1 d
0.40015009743    0.31346831424
1 f
1.9030000000     1.0000000000
*
*
ni def2-SVP
# ni      (14s9p5d1f) / [5s3p2d1f]      {63311/531/41/1}
*
6 s
71074.803211     0.14260386729E-02
10672.020941     0.10928236994E-01

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2428.1389007	0.54212626938E-01
685.53595148	0.18874768902
223.10072863	0.38324616985
76.842014042	0.29550637144
3 s	
148.71122016	-0.11014443059
17.459154987	0.64521426988
7.1625280665	0.44797838103
3 s	
12.556137125	-0.22645403224
2.0735740488	0.72320959286
0.85382640602	0.44868026476
1 s	
0.10536766271	1.0000000000
1 s	
0.38134087688E-01	1.0000000000
5 p	
916.73608662	0.93439635610E-02
216.06139913	0.69737374902E-01
68.383914817	0.27073495012
24.593843952	0.53078301549
9.1392960204	0.34410229438
3 p	
4.7193371746	0.34076082016
1.8161849234	0.56580169611
0.67840750720	0.23616717361
1 p	
0.14658800000	1.0000000000
4 d	
47.093832108	0.28982316948E-01
13.146463975	0.15494995950
4.4170548925	0.37633115111
1.4771565078	0.47365096014
1 d	
0.43735921792	0.31247837833
1 f	
2.1740000000	1.0000000000
*	
*	
cu def2-SVP	
# cu (14s9p5d1f) / [5s3p2d1f] {63311/531/41/1}	
*	
6 s	
76381.348056	0.14336079896E-02
11468.777499	0.10986749865E-01
2609.4246495	0.54513652465E-01
736.75033098	0.18990128258
239.82419958	0.38581959211
82.656829252	0.29790607498
3 s	
160.13544196	-0.11146778567
18.834177695	0.65349301031
7.7176595741	0.44770534421
3 s	
13.710846717	-0.22870911122
2.2349895670	0.73464423031
0.87818360069	0.43273070874
1 s	
0.87187458064E-01	1.0000000000
1 s	


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0.32969114665E-01  1.0000000000
  5 p
991.24075782      0.93878498798E-02
233.69376116      0.70208282458E-01
74.020930927      0.27323522220
26.664967447      0.53580792728
9.9192087478      0.34575794906
  3 p
5.1519553926      0.34229108083
1.9638205828      0.56456592484
0.71560097037      0.24078584318
  1 p
0.15506500000      1.00000000000
  4 d
47.335049590      0.32375547758E-01
13.161666077      0.16810218684
4.3693777244      0.38477707982
1.4132925109      0.46147880178
  1 d
0.38878001452      0.32388873258
  1 f
2.23300000000      1.00000000000
*
*
zn def2-SVP
# zn      (14s9p5d1f) / [5s3p2d1f]      {63311/531/41/1}
*
  6 s
82000.711629      0.14210764000E-02
12312.471777      0.10891499487E-01
2801.3944193      0.54057188059E-01
790.99424302      0.18847463904
257.56551079      0.38346549346
88.814933400      0.29723794197
  3 s
171.86353716      -0.11051849523
20.302534785      0.64607716984
8.3464123068      0.44220117322
  3 s
14.847536940      -0.22705309278
2.4495029507      0.72433217935
0.99845821824      0.44836495592
  1 s
0.11891307937      1.00000000000
  1 s
0.42297428760E-01  1.00000000000
  5 p
1071.5185372      0.92767797235E-02
252.69712152      0.69541149434E-01
80.100829126      0.27156772564
28.903393172      0.53401355573
10.768899879      0.34501323446
  3 p
5.6446212530      0.34129600164
2.1678291347      0.56390521973
0.80540898341      0.23676109735
  1 p
0.16245500000      1.00000000000
  4 d
56.088939191      0.29588869140E-01

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15.751908917      0.15872571404
5.3115812367      0.37976229159
1.7737904917      0.46898959172
 1 d
0.51975583665     0.30907149078
 1 f
2.6140000000      1.0000000000
*
*
ga def2-SVP
# ga      (14s10p6d) / [5s4p3d]      {63311/5311/411}
*
 6 s
87842.126296      0.14271588798E-02
13189.496402      0.10938894097E-01
3000.9482141      0.54308200127E-01
847.38425966      0.18951055983
276.00980642      0.38615185918
95.216672071      0.30051082719
 3 s
184.00703968      -0.11124461963
21.827051433      0.64831322918
9.0026963761      0.44358383594
 3 s
16.033176938      -0.23014299555
2.6707724878      0.72946861516
1.1252834170      0.46214976951
 1 s
0.15967608829     1.0000000000
 1 s
0.57643044753E-01 1.0000000000
 5 p
1167.2665844      0.90974021307E-02
275.38062789      0.68456273343E-01
87.375073070      0.26922293888
31.597254670      0.53507897882
11.824122798      0.35279062760
 3 p
6.2881845133      0.33938244530
2.5199853240      0.56871947608
1.0169726306      0.27717694939
 1 p
0.24748373604     1.0000000000
 1 p
0.66685294163E-01 1.0000000000
 4 d
65.354237674      0.27370146382E-01
18.504656747      0.15099463976
6.3179620632      0.37485328545
2.1641389426      0.47510606851
 1 d
0.66693092754     0.29843287401
 1 d
0.20700000000     1.0000000000
*
*
ge def2-SVP
# ge      (14s10p6d) / [5s4p3d]      {63311/5311/411}
*
 6 s

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93889.836642	0.14233976060E-02
14097.497528	0.10910795654E-01
3207.5477309	0.54183705943E-01
905.76727269	0.18922820349
295.11014693	0.38612847001
101.84713141	0.30164050736
3 s	
196.56719662	-0.11118770940
23.405292522	0.64616007369
9.6839116702	0.44188904568
3 s	
17.269736544	-0.23027421375
2.8964622160	0.73017169398
1.2553621412	0.46197222255
1 s	
0.20213081492	1.0000000000
1 s	
0.73867910982E-01	1.0000000000
5 p	
1259.2085995	0.90115464252E-02
297.15626382	0.67986841689E-01
94.353387522	0.26853856488
34.176329677	0.53659649219
12.816139615	0.35633514961
3 p	
6.8471029784	0.33900693119
2.7717363939	0.56809365264
1.1458418175	0.27246539884
1 p	
0.30679631536	1.0000000000
1 p	
0.89283644115E-01	1.0000000000
4 d	
74.782168177	0.25755860205E-01
21.310849759	0.14536816132
7.3464792363	0.37134209859
2.5656271395	0.48002998436
1 d	
0.81981773070	0.28978790744
1 d	
0.24600000000	1.0000000000
*	
*	
as def2-SVP	
# as (14s10p6d) / [5s4p3d] {63311/5311/411}	
*	
6 s	
100146.52554	0.14258349617E-02
15036.861711	0.10930176963E-01
3421.2902833	0.54294174610E-01
966.16965717	0.18976078153
314.87394026	0.38775195453
108.70823790	0.30402812040
3 s	
209.54238950	-0.11162094204
25.038221139	0.64697607762
10.390964343	0.44223608673
3 s	
18.555090093	-0.22994190569
3.1281217449	0.73319107613

1.3884885073	0.45533653943
1 s	
0.24714362141	1.0000000000
1 s	
0.91429428670E-01	1.0000000000
5 p	
1355.6443507	0.89182507898E-02
319.99929270	0.67454750717E-01
101.67734092	0.26759772110
36.886323845	0.53776844520
13.861115909	0.35992570244
3 p	
7.4260666912	0.34036849637
3.0316247187	0.57030149334
1.2783078340	0.26606170238
1 p	
0.37568503356	1.0000000000
1 p	
0.11394805454	1.0000000000
4 d	
84.445514539	0.24518402724E-01
24.190416102	0.14107454677
8.4045015119	0.36875228915
2.9808970748	0.48409561362
1 d	
0.97909243359	0.28250268781
1 d	
0.29300000000	1.0000000000
*	
*	
se def2-SVP	
# se (14s10p6d) / [5s4p3d] {63311/5311/411}	
*	
6 s	
106612.20027	0.14274889113E-02
16007.604701	0.10943525114E-01
3642.1699707	0.54374171596E-01
1028.5912993	0.19018092947
335.30298888	0.38913021696
115.80129154	0.30620207088
3 s	
222.93325020	-0.11198808009
26.726257934	0.64752124207
11.124501923	0.44241976651
3 s	
19.888520061	-0.22857227762
3.3668473803	0.73591359951
1.5249277839	0.44330199577
1 s	
0.29630037912	1.0000000000
1 s	
0.11009288974	1.0000000000
5 p	
1455.9068120	0.88203597043E-02
343.75101831	0.66875851967E-01
109.29554964	0.26640578080
39.707711022	0.53834928422
14.950185232	0.36303281993
3 p	
8.0208962094	0.34153807025

3.2934649756	0.57257906583
1.4058602438	0.25549813222
1 p	
0.45076123226	1.0000000000
1 p	
0.13353413325	1.0000000000
4 d	
94.494024044	0.23490101098E-01
27.188185260	0.13747735767
9.5091567352	0.36649929124
3.4170516853	0.48750989884
1 d	
1.1479590083	0.27657943383
1 d	
0.33800000000	1.0000000000
*	
*	
br def2-SVP	
# br (14s10p6d) / [5s4p3d] {63311/5311/411}	
*	
6 s	
113286.38776	0.14283037779E-02
17009.626303	0.10950417496E-01
3870.1842567	0.54421006604E-01
1093.0357227	0.19047907695
356.39721797	0.39024642737
123.12539643	0.30814432514
3 s	
236.74084007	-0.11228065671
28.468661070	0.64775962312
11.883443722	0.44235575986
3 s	
21.269633312	-0.22642576323
3.6129226841	0.73823712008
1.6626648969	0.42683868694
1 s	
0.34823793232	1.0000000000
1 s	
0.13019031394	1.0000000000
5 p	
1560.2801881	0.87166669072E-02
368.47859205	0.66243637420E-01
117.22978849	0.26495610385
42.648909248	0.53839160587
16.087225096	0.36579387888
3 p	
8.6352810058	0.34248787366
3.5613665502	0.57500678213
1.5292626609	0.24330394172
1 p	
0.53064294848	1.0000000000
1 p	
0.15702758965	1.0000000000
4 d	
104.85518642	0.22650147581E-01
30.281143688	0.13455483230
10.651394267	0.36474454537
3.8699456233	0.49044587056
1 d	
1.3240876762	0.27137289040

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1 d
0.389000000000      1.000000000000
*
*
kr def2-SVP
# kr      (14s10p6d) / [5s4p3d]      {63311/5311/411}
*
6 s
120165.64875      0.14294234496E-02
18042.500169      0.10959597020E-01
4105.1800388      0.54479647470E-01
1159.4447248      0.19081239122
378.13810346      0.391404445949
130.67610045      0.31007346689
3 s
250.96373353      -0.11258604011
30.265930380      0.64816322524
12.668110757      0.44240238994
3 s
22.697940101      -0.22391964908
3.8673017398      0.74060953026
1.8013706671      0.40803658445
1 s
0.40308639136      1.000000000000
1 s
0.15170527749      1.000000000000
5 p
1668.5736623      0.86215009803E-02
394.13862798      0.65665506884E-01
125.46644854      0.26366576697
45.704992729      0.53867658574
17.270133229      0.36865167502
3 p
9.2699487770      0.34346189015
3.8364617719      0.57784776196
1.6467163312      0.23075615197
1 p
0.61479686489      1.000000000000
1 p
0.18319467414      1.000000000000
4 d
115.55868603      0.21945485333E-01
33.477985864      0.13211212879
11.834450207      0.36333306964
4.3408254894      0.49300484446
1 d
1.5079273157      0.26676858913
1 d
0.443000000000      1.000000000000
*
*
rb def2-SVP
# rb      (7s6p2d) / [5s3p2d]      {31111/411/11}
*
3 s
4.6687885071      0.29008526793
2.9442428420      -0.67740090428
0.58171262989      0.45712389487
1 s
0.45147933555      1.000000000000

```

```

1 s
0.21604923532      1.0000000000
1 s
0.32088816526E-01  1.0000000000
1 s
0.13833878175E-01  1.0000000000
4 p
5.5234179480      0.51234729472E-01
3.4120149646      -0.17337025646
0.76899021792     0.43339683188
0.33088071786     0.55354332721
1 p
0.13423268441     1.0000000000
1 p
0.20642679613E-01  1.0000000000
1 d
0.22600000000     1.0000000000
1 d
0.27432280711E-01  1.0000000000
*
rb def2-ecp
*
ncore =      28      lmax =      3
# coefficient  r^n      exponent
f
-12.3169000    2      3.8431140
s-f
89.5001980    2      5.0365510
0.4937610     2      1.9708490
12.3169000    2      3.8431140
p-f
58.5689740    2      4.2583410
0.4317910     2      1.4707090
12.3169000    2      3.8431140
d-f
26.2248980    2      3.0231270
0.9628390     2      0.6503830
12.3169000    2      3.8431140
*
*
sr def2-SVP
# sr (6s6p5d) / [4s3p2d] {3111/411/41}
*
3 s
5.9276428767     0.19698765364
3.0691274814     -0.64852205985
0.70675488028    0.62064729022
1 s
0.33824024280    1.0000000000
1 s
0.61768869200E-01  1.0000000000
1 s
0.25767593093E-01  1.0000000000
4 p
2.4324720000     -0.37145059848
1.6642340000     0.37856824234
0.59455471858    0.59874487803
0.26152621998    0.35314019512
1 p
0.10258814042    1.0000000000

```

```

1 p
0.33223404030E-01 1.0000000000
4 d
3.6180810000 -0.75010000000E-02
0.99665600000 0.10809800000
0.39073500000 0.27854000000
0.12277000000 0.47731800000
1 d
0.36655000000E-01 0.44818300000
*
sr def2-ecp
*
ncore = 28 lmax = 3
# coefficient r^n exponent
f -15.8059920 2 4.6339750
s-f 135.4794300 2 7.4000740
17.5344630 2 3.6063790
15.8059920 2 4.6339750
p-f 88.3597090 2 6.4848680
15.3943720 2 3.2880530
15.8059920 2 4.6339750
d-f 29.8889870 2 4.6228410
6.6594140 2 2.2469040
15.8059920 2 4.6339750
*
*
y def2-SVP
# y (7s6p5d1f) / [5s3p2d1f] {31111/411/41/1}
*
3 s
5.1329580000 -1.3864845457
4.2401920000 1.9459581166
1.2982800000 0.44182603154
1 s
0.82904954347 1.0000000000
1 s
0.34752758911 1.0000000000
1 s
0.68418878574E-01 1.0000000000
1 s
0.27323992904E-01 1.0000000000
4 p
2.7279200000 -0.37249884912
1.9790500000 0.32572065996
0.79980886805 0.50094655502
0.38409397354 0.44385929493
1 p
0.16173582264 1.0000000000
1 p
0.30000000000E-01 1.0000000000
4 d
3.9030833060 -0.98209792625E-02
1.1363234302 0.19183629664
0.45617043877 0.40597788539
0.17470950748 0.43861485518
1 d

```



```

0.61978796638E-01  1.0000000000
 1 f
0.26515000000  1.0000000000
*
y def2-ecp
*
  ncore = 28          lmax = 3
# coefficient  r^n      exponent
f
  -19.1221981  2          6.5842120
  -2.4363754  2          3.2921060
s-f
  135.1538441  2          7.4880494
  15.5524413  2          3.7440247
  19.1221981  2          6.5842120
  2.4363754  2          3.2921060
p-f
  87.7849917  2          6.4453772
  11.5640660  2          3.2226886
  19.1221981  2          6.5842120
  2.4363754  2          3.2921060
d-f
  29.7010007  2          4.6584472
  5.5399685  2          2.3292236
  19.1221981  2          6.5842120
  2.4363754  2          3.2921060
*
*
zr def2-SVP
# zr (7s6p5d1f) / [5s3p2d1f] {31111/411/41/1}
*
  3 s
  5.8737890000  0.54255558714
  4.2872700000  -0.95241333244
  1.4641370000  -0.13703926411
  1 s
  0.83727682345  0.88521584390
  1 s
  0.36849806511  1.00000000000
  1 s
  0.77806859124E-01  1.00000000000
  1 s
  0.30273088330E-01  1.00000000000
  4 p
  2.8742240000  -0.46624086918
  2.1199010000  0.45883133891
  0.78845821105  0.58853912475
  0.36332579847  0.35822232244
  1 p
  0.14951762021  1.00000000000
  1 p
  0.30000000000E-01  1.00000000000
  4 d
  4.2898623878  -0.12212868080E-01
  1.3615557498  0.19692423520
  0.56937550689  0.42057831659
  0.22674948677  0.42757027999
  1 d
  0.83011031631E-01  1.00000000000
  1 f

```

```

0.39261000000      1.0000000000
*
zr def2-ecp
*
ncore =      28      lmax =      3
# coefficient  r^n      exponent
f      -21.0937760    2      7.5400000
      -3.0806943    2      3.7700000
s-f      150.2675911    2      8.2000000
      18.9762165    2      4.0897278
      21.0937760    2      7.5400000
      3.0806943    2      3.7700000
p-f      99.6221237    2      7.1100000
      14.1687333    2      3.5967980
      21.0937760    2      7.5400000
      3.0806943    2      3.7700000
d-f      35.0451235    2      5.3500000
      6.1112595    2      2.4918215
      21.0937760    2      7.5400000
      3.0806943    2      3.7700000
*
*
nb def2-SVP
# nb      (7s6p5d1f) / [5s3p2d1f]      {31111/411/41/1}
*
3 s
6.5663010000      -0.94917907866
4.5864380000      1.5736372883
3.7537700000      0.36380422981
1 s
0.84187717437      1.0000000000
1 s
0.38160666177      1.0000000000
1 s
0.85819911368E-01  1.0000000000
1 s
0.32702330370E-01  1.0000000000
4 p
3.0700630000      -0.51025115881
2.2379640000      0.53570598017
0.80801969671      0.63102216351
0.35783343432      0.30205908942
1 p
0.13820085283      1.0000000000
1 p
0.36000000000E-01  1.0000000000
4 d
4.6170975867      -0.13574476955E-01
1.5663438480      0.20374310496
0.66952425826      0.42997453105
0.27140946867      0.41799754848
1 d
0.10054426592      1.0000000000
1 f
0.52270000000      1.0000000000
*

```

```

nb def2-ecp
*
  ncore =    28          lmax =    3
#   coefficient      r^n      exponent
f
  -22.9295500      2      8.4900000
  -3.6663099      2      4.2500000
s-f
  165.1791435      2      8.9000000
  21.9929744      2      4.4300000
  22.9295500      2      8.4900000
  3.6663099      2      4.2500000
p-f
  111.7944145      2      7.7700000
  16.6334833      2      3.9600000
  22.9295500      2      8.4900000
  3.6663099      2      4.2500000
d-f
  38.1122488      2      6.0500000
  8.0391673      2      2.8400000
  22.9295500      2      8.4900000
  3.6663099      2      4.2500000
*
*
mo def2-SVP
# mo      (7s6p5d1f) / [5s3p2d1f]      {31111/411/41/1}
*
  3 s
  7.2033800000      -0.89310617237
  5.0522950000      1.6074095756
  2.9135330000      0.27804186088
  1 s
  0.97858218681      1.0000000000
  1 s
  0.44369153753      1.0000000000
  1 s
  0.92150090705E-01      1.0000000000
  1 s
  0.34802246935E-01      1.0000000000
  4 p
  3.1518660000      -0.71873040872
  2.4534820000      0.76442887870
  0.85030192180      0.64808585640
  0.36918237179      0.26792115234
  1 p
  0.13490627460      1.0000000000
  1 p
  0.38200000000E-01      1.0000000000
  4 d
  5.0044445497      -0.21587364862E-01
  1.7736823324      0.20958680086
  0.76950591696      0.43730880599
  0.31530878939      0.41123927009
  1 d
  0.11754374390      1.0000000000
  1 f
  0.65545000000      1.0000000000
*
mo def2-ecp
*

```

```

ncore = 28          lmax = 3
#      coefficient  r^n      exponent
f      -24.8051771  2        9.4500000
      -4.1537815   2        4.7200000
s-f    180.1031085  2        9.7145938
      24.9972279   2        4.6805004
      24.8051771   2        9.4500000
      4.1537815    2        4.7200000
p-f    123.7727523  2        8.1421366
      19.5302280   2        4.6259863
      24.8051771   2        9.4500000
      4.1537815    2        4.7200000
d-f    48.3750223   2        6.6184148
      8.8920527    2        3.2487516
      24.8051771   2        9.4500000
      4.1537815    2        4.7200000
*
*
tc def2-SVP
# tc      (7s6p5d1f) / [5s3p2d1f]      {31111/411/41/1}
*
  3 s
  7.4344020000      -1.1436289973
  5.5513270000       1.8752000559
  3.0230860000       0.23952854431
  1 s
  1.0647443990       1.0000000000
  1 s
  0.48127808497      1.0000000000
  1 s
  0.98299016952E-01  1.0000000000
  1 s
  0.36659977936E-01  1.0000000000
  4 p
  3.4490050000      -0.72277510434
  2.6927370000       0.76458962802
  0.94427370692      0.64533225171
  0.41348148619      0.27195668811
  1 p
  0.15488152305      1.0000000000
  1 p
  0.40300000000E-01  1.0000000000
  4 d
  5.0906268699      -0.32176405405E-01
  2.0156178510       0.21280802536
  0.88113887240      0.44403309175
  0.36427094833      0.40796933085
  1 d
  0.13678402297      1.0000000000
  1 f
  0.79085000000      1.0000000000
*
tc def2-ecp
*
ncore = 28          lmax = 3
#      coefficient  r^n      exponent

```

```

f
      -26.5624475    2    10.4000000
      -4.5856805    2    5.2000000
s-f
      195.1591659    2    10.4223462
      28.0926033    2    5.0365160
      26.5624475    2    10.4000000
      4.5856805    2    5.2000000
p-f
      135.2845662    2    8.9504494
      21.8065043    2    4.8544394
      26.5624475    2    10.4000000
      4.5856805    2    5.2000000
d-f
      54.3297294    2    6.9456968
      11.1550679    2    3.9705849
      26.5624475    2    10.4000000
      4.5856805    2    5.2000000
*
*
ru def2-SVP
# ru      (7s6p5d1f) / [5s3p2d1f]      {31111/411/41/1}
*
  3 s
  7.9365700000    -1.1772083350
  5.9842450000    1.6197059592
  4.8822200000    0.51065807556
  1 s
  1.1031002163    1.0000000000
  1 s
  0.49818875261    1.0000000000
  1 s
  0.10678711393    1.0000000000
  1 s
  0.39191775872E-01  1.0000000000
  4 p
  3.7546090000    -0.70777873563
  2.9165710000    0.74954391484
  1.0322209568    0.64660609645
  0.45249553774    0.27029086816
  1 p
  0.16987042198    1.0000000000
  1 p
  0.430000000000E-01  1.0000000000
  4 d
  5.7341846619    -0.35266111560E-01
  2.2483686294    0.21802502222
  0.98376978359    0.44709565013
  0.40379445583    0.40371732508
  1 d
  0.14978618173    1.0000000000
  1 f
  0.94314000000    1.0000000000
*
ru def2-ecp
*
  ncore =    28      lmax =    3
#      coefficient  r^n      exponent
f
      -28.3406163    2    11.3600000

```

```

-4.9446292      2      5.6800000
s-f
209.8229712    2      11.1052693
30.6547264     2      5.4147454
28.3406163     2      11.3600000
4.9446292      2      5.6800000
p-f
146.3361823    2      9.7712707
24.1278772     2      5.0739908
28.3406163     2      11.3600000
4.9446292      2      5.6800000
d-f
67.5158967     2      7.6714231
9.8701041      2      4.1365647
28.3406163     2      11.3600000
4.9446292      2      5.6800000
*
*
rh def2-SVP
# rh      (7s6p5d1f) / [5s3p2d1f]      {31111/411/41/1}
*
  3 s
  7.9177440000      1.4014042010
  6.8412070000      -1.7975072656
  2.9598400000      -0.16225754497
  1 s
  1.3166643441      0.87495110714
  1 s
  0.56907152172     1.00000000000
  1 s
  0.10059695193     1.00000000000
  1 s
  0.37071460798E-01 1.00000000000
  4 p
  4.1360790000      -0.55183328018
  2.9462810000      0.61370533515
  1.0792431924      0.64005434538
  0.46611217769     0.25958050755
  1 p
  0.17453169991     1.00000000000
  1 p
  0.41000000000E-01 1.00000000000
  4 d
  6.8847131641      -0.15962387985E-01
  2.3837304391      0.23047555829
  1.0184384022      0.44075804028
  0.39957494644     0.39567661996
  1 d
  0.13951120264     1.00000000000
  1 f
  1.0949900000      1.00000000000
*
rh def2-ecp
*
ncore =      28      lmax =      3
# coefficient  r^n      exponent
f
-30.0934557    2      12.3100000
-5.2184819     2      6.1600000
s-f

```

	225.3477535	2	11.7200000
	32.8231890	2	5.8200000
	30.0934557	2	12.3100000
	5.2184819	2	6.1600000
p-f			
	158.7094116	2	10.4200000
	26.4441005	2	5.4500000
	30.0934557	2	12.3100000
	5.2184819	2	6.1600000
d-f			
	62.7586257	2	8.8200000
	10.9787195	2	3.8700000
	30.0934557	2	12.3100000
	5.2184819	2	6.1600000
*			
*			
pd def2-SVP			
# pd	(7s6p5d1f) / [5s3p2d1f]		{31111/411/41/1}
*			
3 s			
	8.4756400000	1.2392391076	
	7.1657170000	-1.6563109970	
	3.1821100000	-0.13178619060	
1 s			
	1.3973644196	1.0000000000	
1 s			
	0.60532955868	1.0000000000	
1 s			
	0.10229514209	1.0000000000	
1 s			
	0.37338972881E-01	1.0000000000	
4 p			
	4.2460970000	-0.82324104973	
	3.3925940000	0.87084659933	
	1.1975891264	0.63512225791	
	0.52673750585	0.27225338752	
1 p			
	0.20607094098	1.0000000000	
1 p			
	0.37000000000E-01	1.0000000000	
4 d			
	7.3613290985	-0.17199885828E-01	
	2.6291037258	0.23313745275	
	1.1292744634	0.44536385867	
	0.44471659896	0.39293650406	
1 d			
	0.15544893836	1.0000000000	
1 f			
	1.2462900000	1.0000000000	
*			
pd def2-ecp			
*			
ncore =	28	lmax =	3
#	coefficient	r^n	exponent
f			
	-31.9295543	2	13.2700000
	-5.3982169	2	6.6300000
s-f			
	240.2290403	2	12.4300000
	35.1719435	2	6.1707594

	31.9295543	2	13.2700000
	5.3982169	2	6.6300000
p-f	170.4172760	2	11.0800000
	28.4721329	2	5.8295541
	31.9295543	2	13.2700000
	5.3982169	2	6.6300000
d-f	69.0138449	2	9.5100000
	11.7508616	2	4.1397811
	31.9295543	2	13.2700000
	5.3982169	2	6.6300000
*			
*			
ag def2-SVP			
# ag	(7s6p5d1f) / [5s3p2d1f]		{31111/411/41/1}
*			
	3 s		
	9.0884420000	-1.9808918797	
	7.5407310000	2.7554513347	
	2.7940050000	0.22715408381	
	1 s		
	1.4918135849	1.0000000000	
	1 s		
	0.63579159445	1.0000000000	
	1 s		
	0.10368414161	1.0000000000	
	1 s		
	0.37460004363E-01	1.0000000000	
	4 p		
	4.4512400000	-0.99352103771	
	3.6752630000	1.0500525237	
	1.2610620905	0.64747532537	
	0.54212477498	0.25621550723	
	1 p		
	0.20221617026	1.0000000000	
	1 p		
	0.41200000000E-01	1.0000000000	
	4 d		
	7.7956672292	-0.17042912377E-01	
	2.8926510238	0.23446154803	
	1.2474273203	0.44765877533	
	0.49313817671	0.39064954560	
	1 d		
	0.17285032603	1.0000000000	
	1 f		
	1.3971100000	1.0000000000	
*			
ag def2-ecp			
*			
	ncore = 28	lmax = 3	
#	coefficient	r^n	exponent
f			
	-33.6899201	2	14.2200000
	-5.5311202	2	7.1100000
s-f	255.1393645	2	13.1300000
	36.8661215	2	6.5100000
	33.6899201	2	14.2200000
	5.5311202	2	7.1100000


```

p-f
    182.1818687    2    11.7400000
    30.3577515    2    6.2000000
    33.6899201    2    14.2200000
    5.5311202     2    7.1100000
d-f
    73.7192609    2    10.2100000
    12.5021171    2    4.3800000
    33.6899201    2    14.2200000
    5.5311202     2    7.1100000
*
*
cd def2-SVP
# cd      (7s6p5d1f) / [5s3p2d1f]      {31111/411/41/1}
*
  3 s
  9.7270110000    -1.7930075316
  7.8375230000     2.6110318971
  5.0891940000     0.10748428949
  1 s
  1.4981738327     1.0000000000
  1 s
  0.67281383129     1.0000000000
  1 s
  0.13297424875     1.0000000000
  1 s
  0.46915090488E-01  1.0000000000
  4 p
  4.7427160000    -1.0411923051
  3.9366550000     1.1003682332
  1.3569243142     0.65366639411
  0.58791569541     0.24632369113
  1 p
  0.21371239619     1.0000000000
  1 p
  0.51600000000E-01  1.0000000000
  4 d
  7.8631040859    -0.21376239365E-01
  3.2935059133     0.22596399568
  1.4503676025     0.45294402972
  0.59373316766     0.39218971958
  1 d
  0.21760141520     1.0000000000
  1 f
  1.5981300000     1.0000000000
*
cd def2-ecp
*
  ncore =    28      lmax =    3
#      coefficient      r^n      exponent
f
    -35.4766256     2      15.1847957
    -5.6176768     2      7.5923978
s-f
    270.0094832     2      13.8358689
    38.7673080     2      6.8572704
    35.4766256     2      15.1847957
    5.6176768     2      7.5923978
p-f
    193.8296294     2      12.4049710

```

```

31.8965252      2      6.5677995
35.4766256      2      15.1847957
5.6176768       2      7.5923978
d-f
79.1936470      2      10.8969253
13.2308267      2      4.6411649
35.4766256      2      15.1847957
5.6176768       2      7.5923978
*
*
in def2-SVP
# in      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
  6 s
283.52297445    0.70132141424E-03
23.324282101   -0.90887432418E-01
16.868026844    0.28096825177
6.7866498137   -0.70697832452
1.6782596016    0.98671644913
0.78396870439   0.62568576302
  2 s
1.8276654775   -0.34151640249
0.83753492534   -0.59696724334
  1 s
0.16643068973    1.0000000000
  1 s
0.61143742809E-01  1.0000000000
  4 p
14.699191826    0.92248042349E-01
8.8709038051   -0.32437029300
1.1342905889    0.61162217018
0.52667652433   0.17609640386
  1 p
2.3284433667    1.0000000000
  1 p
0.16859144934    1.0000000000
  1 p
0.50070381081E-01  1.0000000000
  5 d
31.378655926    0.54007004722E-02
18.290046326   -0.11208558948E-01
3.2551894590    0.30384519161
1.3874842584    0.54078109979
0.54248962672   0.38232680038
  1 d
0.18000000000    1.0000000000
*
in def2-ecp
*
  ncore =      28      lmax =      3
#      coefficient      r^n      exponent
f
      -13.7280780      2      12.5390560
      -18.2068660      2      12.5525610
s-f
      281.1223500      2      15.3928220
      61.9014700      2      8.0558640
      13.7280780      2      12.5390560
      18.2068660      2      12.5525610
p-f

```

	67.4621540	2	13.9286720
	134.9492500	2	13.3472340
	14.7461400	2	7.6141320
	29.6392620	2	7.3183650
	13.7280780	2	12.5390560
	18.2068660	2	12.5525610
d-f			
	35.4932540	2	14.0347150
	53.1787730	2	14.5116160
	9.1772810	2	5.5505500
	12.3924100	2	5.0594150
	13.7280780	2	12.5390560
	18.2068660	2	12.5525610
*			
*			
sn def2-SVP			
# sn	(10s7p6d) / [4s4p2d]		{6211/4111/51}
*			
	6 s		
	375.95156177	0.15224884228E-02	
	23.661818008	-0.16776065030	
	19.946281315	0.33989090393	
	6.8240270454	-0.84441791529	
	1.8771488722	0.92646952846	
	0.82033199226	0.53091094490	
	2 s		
	10.341549887	-0.90331119154E-02	
	1.3672524155	0.22980877714	
	1 s		
	0.18314843823	1.0000000000	
	1 s		
	0.69547226146E-01	1.0000000000	
	4 p		
	21.293597748	0.37103218279E-01	
	8.8171842499	-0.32351709661	
	1.2347028371	0.83846760898	
	0.57869142617	0.23294977050	
	1 p		
	2.5084050284	1.0000000000	
	1 p		
	0.21298577719	1.0000000000	
	1 p		
	0.67364584657E-01	1.0000000000	
	5 d		
	39.693023177	0.39185734275E-02	
	20.852179275	-0.68210073667E-02	
	3.6907832774	0.27938420495	
	1.5849404530	0.52607409874	
	0.62772693365	0.36149465348	
	1 d		
	0.20500000000	1.0000000000	
*			
sn def2-ecp			
*			
	ncore = 28	lmax = 3	
#	coefficient	r^n	exponent
f			
	-12.5763330	2	12.2823480
	-16.5959440	2	12.2721500
s-f			

	279.9886820	2	17.4204140
	62.3778100	2	7.6311550
	12.5763330	2	12.2823480
	16.5959440	2	12.2721500
p-f			
	66.1625230	2	16.1310240
	132.1743960	2	15.6280770
	16.3394170	2	7.3256080
	32.4889590	2	6.9425190
	12.5763330	2	12.2823480
	16.5959440	2	12.2721500
d-f			
	36.3874410	2	15.5149760
	54.5078410	2	15.1881600
	8.6968230	2	5.4560240
	12.8402080	2	5.3631050
	12.5763330	2	12.2823480
	16.5959440	2	12.2721500

*
*

sb def2-SVP

sb (10s7p6d) / [4s4p2d] {6211/4111/51}

*

6	s		
372.76139166		0.15878057239E-02	
22.689478596		-0.15027605583	
18.391547037		0.35915813039	
7.6406271414		-0.74805091065	
1.9052000235		0.92017581656	
0.93007107773		0.46754079597	
2	s		
10.584496987		-0.14845336778E-01	
1.4680242769		0.35289492025	
1	s		
0.21621190032		1.0000000000	
1	s		
0.83546307041E-01		1.0000000000	
4	p		
15.926550950		0.13206950012	
10.052739237		-0.41511149340	
1.2682183726		0.74197972626	
0.57196620929		0.15580772750	
1	p		
2.6190751238		1.0000000000	
1	p		
0.25183282652		1.0000000000	
1	p		
0.83389127684E-01		1.0000000000	
5	d		
45.485063360		0.32556415807E-02	
18.504059617		-0.54952972010E-02	
3.9156032308		0.27988806353	
1.7142196009		0.51273377761	
0.69675478242		0.33288802736	
1	d		
0.23060000000		1.0000000000	

*

sb def2-ecp

*

ncore = 28 lmax = 3

#	coefficient	r^n	exponent
f	-15.3668010	2	14.4449780
	-20.2961380	2	14.4492950
s-f	281.0715810	2	16.3308650
	61.7166040	2	8.5565420
	15.3668010	2	14.4449780
	20.2961380	2	14.4492950
p-f	67.4573800	2	14.4703370
	134.9335030	2	13.8161940
	14.7163440	2	8.4249240
	29.5185120	2	8.0927280
	15.3668010	2	14.4449780
	20.2961380	2	14.4492950
d-f	35.4478150	2	14.8863310
	53.1434660	2	15.1463190
	9.1792230	2	5.9082670
	13.2402530	2	5.5943220
	15.3668010	2	14.4449780
	20.2961380	2	14.4492950
*			
*			
te	def2-SVP		
#	te	(10s7p6d) / [4s4p2d]	{6211/4111/51}
*			
	6 s		
	396.47954659	0.26307731203E-02	
	21.919773309	-0.13203517066	
	18.061271390	0.36203197834	
	8.1403463241	-0.75591120276	
	2.0705998798	0.79192928400	
	0.97715185085	0.40558342540	
	2 s		
	11.263563841	-0.15212984183E-01	
	1.6122696062	0.35202140517	
	1 s		
	0.25095401705	1.0000000000	
	1 s		
	0.97478452576E-01	1.0000000000	
	4 p		
	17.479502221	0.11517799182	
	10.433943171	-0.41205302672	
	1.3623024763	0.78760578076	
	0.59239616258	0.15283299018	
	1 p		
	2.7961737670	1.0000000000	
	1 p		
	0.29766401026	1.0000000000	
	1 p		
	0.96151090240E-01	1.0000000000	
	5 d		
	50.821835991	0.33763474774E-02	
	18.884095378	-0.35221408938E-02	
	4.2527304630	0.28254216065	
	1.8757557092	0.52039372916	
	0.77069282849	0.32213541689	
	1 d		

```

0.250000000000      1.000000000000
*
te def2-ecp
*
ncore =      28          lmax =      3
# coefficient      r^n          exponent
f
      -15.7454500      2          15.2061680
      -20.7424480      2          15.2017020
s-f
      281.0458430      2          16.8144730
      61.6206560      2           8.7935260
      15.7454500      2          15.2061680
      20.7424480      2          15.2017020
p-f
      67.4494640      2          14.8778010
      134.9043040      2          14.2697310
      14.6895470      2           8.7244350
      29.4150630      2           8.2915150
      15.7454500      2          15.2061680
      20.7424480      2          15.2017020
d-f
      35.4320570      2          15.2050080
      53.1356870      2          15.2258480
      9.0698020      2           6.0717690
      13.1223040      2           5.8047600
      15.7454500      2          15.2061680
      20.7424480      2          15.2017020
*
*
i def2-SVP
# i      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
  6 s
445.90489176      0.20037290389E-02
23.336842412      -0.14989397324
19.583446104      0.36436474913
8.5112089186      -0.75538138199
2.1996161861      0.82816359356
1.0668970454      0.42161048110
  2 s
11.720547572      -0.16160234511E-01
1.7625986449      0.35271525193
  1 s
0.28697476318      1.00000000000
  1 s
0.11227609607      1.00000000000
  4 p
20.499027254      0.77159335656E-01
10.558754576      -0.38370372780
1.5015895485      0.83554174719
0.64597173095      0.16787259488
  1 p
3.0288656771      1.00000000000
  1 p
0.34506591841      1.00000000000
  1 p
0.11134513813      1.00000000000
  5 d
51.235354920      0.40345130346E-02

```

```

15.616239482      -0.50768108881E-02
4.5266002139      0.29151065356
2.0529808766      0.51145783605
0.87640281623     0.31232025297
  1 d
0.30900000000     1.00000000000
*
i def2-ecp
*
  ncore =    28      lmax =    3
#   coefficient   r^n      exponent
f
  -21.8420400     2        19.4586090
  -28.4681910     2        19.3492600
   -0.2437130     2         4.8237670
   -0.3208040     2         4.8843150
s-f
  49.9942930     2        40.0158350
 281.0253170     2        17.4297470
  61.5733260     2         9.0054840
  21.8420400     2        19.4586090
  28.4681910     2        19.3492600
   0.2437130     2         4.8237670
   0.3208040     2         4.8843150
p-f
  67.4428410     2        15.3554660
134.8811370     2        14.9718330
  14.6750510     2         8.9601640
  29.3756660     2         8.2590960
  21.8420400     2        19.4586090
  28.4681910     2        19.3492600
   0.2437130     2         4.8237670
   0.3208040     2         4.8843150
d-f
  35.4395290     2        15.0689080
  53.1760570     2        14.5553220
   9.0671950     2         6.7186470
  13.2069370     2         6.4563930
   0.0893350     2         1.1917790
   0.0523800     2         1.2911570
  21.8420400     2        19.4586090
  28.4681910     2        19.3492600
   0.2437130     2         4.8237670
   0.3208040     2         4.8843150
*
*
xe def2-SVP
# xe   (11s10p8d2f) / [6s5p3d2f]   {521111/34111/611/11}
*
  5 s
6420.2481656     0.25092173886E-03
983.54530664     0.16251948178E-02
219.43881364     0.46037106451E-02
23.012587807     -0.14698707182
18.048324490     0.57524870348
  2 s
11.752550163     0.66038420156
6.2390917199     0.38470524721
  1 s
2.6257211320     1.00000000000

```

```

1 s
1.2905042943      1.0000000000
1 s
0.36204185060    1.0000000000
1 s
0.14069888091    1.0000000000
3 p
193.81432545     0.95394802497E-03
21.725228086     0.57393353332E-01
9.8891605641     -0.27974266640
4 p
13.960683826     -0.50950157807E-01
4.0928947097     0.36669211800
2.2546815460     0.72619456861
1.1546596184     0.35555871740
1 p
0.52321923128    1.0000000000
1 p
0.21945569800    1.0000000000
1 p
0.86158996836E-01 1.0000000000
6 d
135.60300038     0.81873543290E-03
38.727062692     0.60897654151E-02
15.377328089     -0.92782985596E-02
5.2602537686     0.22890785589
2.6590627424     0.44434407051
1.2938205124     0.36029482992
1 d
0.58050830139    1.0000000000
1 d
0.18000000000    1.0000000000
1 f
0.49652793000    1.0000000000
1 f
2.50000000000    1.0000000000
*
xe def2-ecp
*
ncore = 28      lmax = 3
#      coefficient  r^n      exponent
f
      -23.0892950    2        20.8815570
      -30.0744750    2        20.7834430
      -0.2882270    2         5.2533890
      -0.3869240    2         5.3611880
s-f
      49.9979620    2         40.0051840
      281.0133030   2         17.8122140
      61.5382550    2          9.3041500
      23.0892950    2        20.8815570
      30.0744750    2        20.7834430
      0.2882270    2         5.2533890
      0.3869240    2         5.3611880
p-f
      67.4391420    2        15.7017720
      134.8747110   2        15.2586080
      14.6633000    2          9.2921840
      29.3547300    2         8.5590030
      23.0892950    2        20.8815570

```


	30.0744750	2	20.7834430
	0.2882270	2	5.2533890
	0.3869240	2	5.3611880
d-f			
	35.4369080	2	15.1856000
	53.1957720	2	14.2845000
	9.0462320	2	7.1218890
	13.2236810	2	6.9919630
	0.0848530	2	0.6239460
	0.0441550	2	0.6472840
	23.0892950	2	20.8815570
	30.0744750	2	20.7834430
	0.2882270	2	5.2533890
	0.3869240	2	5.3611880

*

*

cs def2-SVP

cs (7s6p2d) / [5s3p2d] {31111/411/11}

*

3	s		
5.8778113443		0.12859994983	
4.3631538286		-0.34632569725	
1.8048475155		0.69930637051	
1	s		
0.37485237136		1.0000000000	
1	s		
0.16384858778		1.0000000000	
1	s		
0.27230462048E-01		1.0000000000	
1	s		
0.11991533212E-01		1.0000000000	
4	p		
4.2751856154		0.45723074174E-01	
1.9656663360		-0.25019961976	
0.47689195212		0.55660850066	
0.21529749588		0.58218553406	
1	p		
0.91450850296E-01		1.0000000000	
1	p		
0.17592078473E-01		1.0000000000	
1	d		
0.13300000000		1.0000000000	
1	d		
0.33216214821E-01		1.0000000000	

*

cs def2-ecp

*

ncore =	46	lmax =	3
#	coefficient	r^n	exponent
f	-28.8843090	2	3.1232690
s-f			
	84.5477300	2	4.0797500
	16.6541730	2	2.4174060
	28.8843090	2	3.1232690
p-f			
	157.0490590	2	5.5140800
	26.4233070	2	2.1603160
	28.8843090	2	3.1232690
d-f			

```

13.1727530    2    1.8074100
3.3428330    2    0.8581820
28.8843090   2    3.1232690
*
*
ba def2-SVP
# ba      (6s6p5d) / [4s3p2d]      {3111/411/41}
*
  3 s
  2.3961900000    -5.9554766710
  2.2433050000     6.6805648241
  0.717402000000  -0.57055347037
  1 s
  0.27420073547    1.0000000000
  1 s
  0.40933264188E-01  1.0000000000
  1 s
  0.18060156423E-01  1.0000000000
  4 p
  2.9267420000     0.79815276764
  2.5207180000    -1.0707548832
  0.67578180854    0.34940781448
  0.31985844531    0.65041110673
  1 p
  0.13221792446    1.0000000000
  1 p
  0.33039565349E-01  1.0000000000
  4 d
  0.966315000000   -0.90893800000
  0.893828000000    0.94724000000
  0.273195000000    0.32205700000
  0.103891000000    0.47326000000
  1 d
  0.35578000000E-01  0.36597700000
*
ba def2-ecp
*
  ncore =    46      lmax =    3
#      coefficient  r^n      exponent
f
  -33.4731740      2      3.5894650
s-f
  427.8458160      2      9.5269860
  204.4175300      2      4.4875100
  33.4731740      2      3.5894650
p-f
  293.6058640      2      8.3159300
  294.1933160      2      4.2922170
  33.4731740      2      3.5894650
d-f
  112.5504020      2      5.9161080
  181.7826210      2      2.8748420
  33.4731740      2      3.5894650
*
*
la def2-SVP
# la      (7s6p5d1f) / [6s3p2d1f]  {211111/411/41/1}
*
  2 s
  5.0873990000    -0.44173707857

```

```

4.2709780000      0.85812489720
 1 s
2.1823803999      1.00000000000
 1 s
0.48954926461     1.00000000000
 1 s
0.23292032550     1.00000000000
 1 s
0.55595529876E-01 1.00000000000
 1 s
0.22795184937E-01 1.00000000000
 4 p
3.0251610000     -0.28580266655
2.3820950000      0.51718364644
0.67246658081    -0.44823115995
0.32519427171    -0.58864843930
 1 p
0.13635489374     1.00000000000
 1 p
0.25100000000E-01 1.00000000000
 4 d
1.2667182018     -0.17445579381
0.89049882672     0.25137236211
0.32947291040     0.44604068240
0.13398788830     0.44878277154
 1 d
0.51275503081E-01 1.00000000000
 1 f
0.25683000000     1.00000000000
*
la def2-ecp
*
  ncore =      46          lmax =      3
#      coefficient      r^n      exponent
f
s-f      -36.0100160      2      4.0286000
          91.9321770      2      3.3099000
          -3.7887640      2      1.6550000
          36.0100160      2      4.0286000
p-f
          63.7594860      2      2.8368000
          -0.6479580      2      1.4184000
          36.0100160      2      4.0286000
d-f
          36.1161730      2      2.0213000
          0.2191140      2      1.0107000
          36.0100160      2      4.0286000
*
*
hf def2-SVP
# hf      (7s6p5d1f) / [6s3p2d1f]      {211111/411/41/1}
*
  2 s
14.592485000     -0.80196298812
11.547491000     1.5261602829
 1 s
4.9112973928     1.00000000000
 1 s
0.79665469409     1.00000000000

```

```

1 s
0.34234072894      1.0000000000
1 s
0.98109197714E-01  1.0000000000
1 s
0.36190984443E-01  1.0000000000
4 p
6.7265310000      0.65076205466
5.9599790000     -0.83713508620
1.0921117054      0.50570506286
0.49702823217     0.51965388691
1 p
0.20258973792     1.0000000000
1 p
0.336000000000E-01  1.0000000000
4 d
3.9820623229     -0.42446023944E-01
1.3077987772      0.18409232564
0.53272310298     0.41484423516
0.20564954488     0.44224303497
1 d
0.73099858787E-01  1.0000000000
1 f
0.31547000000     1.0000000000
*
hf def2-ecp
*
ncore =      60      lmax =      3
#      coefficient  r^n      exponent
f
      10.0467225    2        1.7857698
s-f
      1499.2847107  2        14.7699590
      40.2821014   2        7.3849794
      -10.0467225  2        1.7857698
p-f
      397.7330053   2        9.8494895
      19.3164059   2        4.9247445
      -10.0467225  2        1.7857698
d-f
      101.3298053   2        6.0967564
      5.8734382    2        3.0483782
      -10.0467225  2        1.7857698
*
*
ta def2-SVP
# ta      (7s6p5d1f) / [6s3p2d1f]      {211111/411/41/1}
*
2 s
14.400000000      0.99343296745
12.000000000     -1.6510077975
1 s
5.0701477302      1.0000000000
1 s
0.86033356487     1.0000000000
1 s
0.37158938894     1.0000000000
1 s
0.10745336254     1.0000000000
1 s

```

```

0.39142776556E-01  1.0000000000
  4 p
  7.4188720000      0.26979695152
  5.6984100000     -0.46968874449
  1.1777211960     0.50905100155
  0.54478533555    0.52298161137
  1 p
  0.22309270117    1.00000000000
  1 p
  0.43100000000E-01 1.00000000000
  4 d
  3.9738796278    -0.52799310714E-01
  1.4528884813    0.18558319471
  0.61042908544    0.42959071631
  0.24216276510    0.43497228232
  1 d
  0.87909318337E-01 1.00000000000
  1 f
  0.37386000000    1.00000000000
*
ta def2-ecp
*
  ncore =      60          lmax =      3
#      coefficient  r^n      exponent
f
      12.0179609      2          2.0178811
s-f
      1345.8806470      2          14.5464077
      36.7668062      2          7.2732038
      -12.0179609      2          2.0178811
p-f
      378.4253015      2          9.9355653
      22.2930909      2          4.9677824
      -12.0179609      2          2.0178811
d-f
      104.8839557      2          6.3473769
      8.7558481      2          3.1736885
      -12.0179609      2          2.0178811
*
*
w def2-SVP
# w      (7s6p5d1f) / [6s3p2d1f]      {211111/411/41/1}
*
  2 s
  15.000000000      -0.53315505392
  12.000000000      1.0014141748
  1 s
  5.2610967725      1.00000000000
  1 s
  0.92785370307      1.00000000000
  1 s
  0.40334458241      1.00000000000
  1 s
  0.11585976646      1.00000000000
  1 s
  0.41800474073E-01 1.00000000000
  4 p
  7.2496570000      0.45857265530
  6.0848760000     -0.66720686321
  1.2523777812      0.52090351989

```

```

0.58569208922      0.51885687511
 1 p
0.24106964301      1.00000000000
 1 p
0.403000000000E-01  1.00000000000
 4 d
 4.0131231332      -0.63416491808E-01
 1.6237452450      0.18452733732
0.69187452392      0.44121676843
0.27865835325      0.43158409241
 1 d
0.10225296446      1.00000000000
 1 f
0.43199000000      1.00000000000
*
w def2-ecp
*
  ncore =      60      lmax =      3
#      coefficient      r^n      exponent
f
      14.1525795      2      2.2588885
s-f
1192.3958823      2      14.3228564
 32.5229332      2      7.1614281
 -14.1525795      2      2.2588885
p-f
 359.0319671      2      10.0216411
 24.0303802      2      5.0108204
 -14.1525795      2      2.2588885
d-f
 108.3013490      2      6.5979974
 10.9825283      2      3.2989987
 -14.1525795      2      2.2588885
*
*
re def2-SVP
# re      (7s6p5d1f) / [6s3p2d1f]      {211111/411/41/1}
*
 2 s
14.781862000      -1.1395193885
12.324075000      1.9371421121
 1 s
 5.5098597284      1.00000000000
 1 s
0.98874104687      1.00000000000
 1 s
0.42833312030      1.00000000000
 1 s
0.12296804533      1.00000000000
 1 s
0.43949851581E-01  1.00000000000
 4 p
 7.4040050000      0.54510937865
 6.3502060000      -0.76096056536
 1.3311713455      0.53252276765
0.62659600547      0.51483045040
 1 p
0.25922718696      1.00000000000
 1 p
0.483000000000E-01  1.00000000000

```

```

4 d
4.0616274916      -0.76667295205E-01
1.8487943286      0.18067495215
0.78702048429     0.45160766937
0.32069843172     0.43261236266
1 d
0.11892742980     1.00000000000
1 f
0.48989000000     1.00000000000
*
re def2-ecp
*
ncore =      60      lmax =      3
#      coefficient  r^n      exponent
f
      16.4498523    2      2.5086506
s-f
      1038.9515723  2      14.0993051
      29.5617383   2      7.0496525
      -16.4498523  2      2.5086506
p-f
      339.5435096   2      10.1077169
      24.9136965   2      5.0538583
      -16.4498523  2      2.5086506
d-f
      111.6996527   2      6.8486179
      12.6243293   2      3.4243090
      -16.4498523  2      2.5086506
*
*
os def2-SVP
# os      (7s6p5d1f) / [6s3p2d1f]      {211111/411/41/1}
*
2 s
15.286736000      -1.0647114485
12.700638000      1.8433193269
1 s
5.7094832504      1.00000000000
1 s
1.0689228744      1.00000000000
1 s
0.46783543749     1.00000000000
1 s
0.13253456992     1.00000000000
1 s
0.47101982911E-01 1.00000000000
4 p
7.9362790000      0.33899369659
6.3036410000      -0.56379438345
1.4351579676      0.52360040577
0.68442749722     0.52445339821
1 p
0.28347394974     1.00000000000
1 p
0.58100000000E-01 1.00000000000
4 d
3.5808150000      -0.42773932262
3.1961650000      0.44501403992
1.0550226354      0.43689459722
0.41588406618     0.48220605799

```

```

1 d
0.14653507868      1.0000000000
1 f
0.55065000000     1.0000000000
*
os def2-ecp
*
ncore =      60      lmax =      3
# coefficient  r^n      exponent
f
      18.9094570      2      2.7670751
s-f
      885.4057191      2      13.8757539
      25.9670401      2      6.9378769
      -18.9094570      2      2.7670751
p-f
      320.0839019      2      10.1937926
      26.1487649      2      5.0968962
      -18.9094570      2      2.7670751
d-f
      115.0448431      2      7.0992385
      13.6225746      2      3.5496192
      -18.9094570      2      2.7670751
*
*
ir def2-SVP
# ir      (7s6p5d1f) / [6s3p2d1f]      {211111/411/41/1}
*
2 s
15.293709000      -1.6731899791
13.573682000      2.3934378976
1 s
5.8213436542      1.0000000000
1 s
1.1520364268      1.0000000000
1 s
0.51104895338      1.0000000000
1 s
0.14084043578      1.0000000000
1 s
0.49828673085E-01  1.0000000000
4 p
8.6697960000      0.21469187346
6.2456140000      -0.44863071815
1.5657036153      0.50653393257
0.75577412863      0.54052273352
1 p
0.31306011113      1.0000000000
1 p
0.54800000000E-01  1.0000000000
4 d
3.6994850000      -0.54840155965
3.3617430000      0.56835425804
1.1177053710      0.44304381513
0.44322534858      0.47078394930
1 d
0.15641305125      1.0000000000
1 f
0.61008000000      1.0000000000
*

```



```

ir def2-ecp
*
  ncore =    60          lmax =    3
#   coefficient      r^n      exponent
f
      21.5310311      2          3.0340719
s-f
      732.2691998      2          13.6522026
      26.4847209      2          6.8261013
      -21.5310311      2          3.0340719
p-f
      299.4894736      2          10.2798684
      26.4662335      2          5.1399341
      -21.5310311      2          3.0340719
d-f
      124.4575945      2          7.3498590
      14.0359952      2          3.6749295
      -21.5310311      2          3.0340719
*
*
pt def2-SVP
# pt      (7s6p5d1f) / [6s3p2d1f]      {211111/411/41/1}
*
  2 s
  16.559563000      -0.53808800717
  13.892440000      0.91402161377
  1 s
  5.8531044732      1.00000000000
  1 s
  1.2498640609      1.00000000000
  1 s
  0.55606439459      1.00000000000
  1 s
  0.13793093812      1.00000000000
  1 s
  0.48989034059E-01  1.00000000000
  4 p
  8.1000000000      0.72955608128
  7.2000000000      -0.95441807252
  1.5588402917      0.57140490320
  0.73230402180      0.49508234268
  1 p
  0.30270484669      1.00000000000
  1 p
  0.50000000000E-01  1.00000000000
  4 d
  4.6299536825      -0.87774450596E-01
  2.1980241252      0.21158360681
  0.93629991261      0.46533857641
  0.37160028160      0.41129165525
  1 d
  0.13155928617      1.00000000000
  1 f
  0.66813000000      1.00000000000
*
pt def2-ecp
*
  ncore =    60          lmax =    3
#   coefficient      r^n      exponent
f

```

	24.3143757	2	3.3095686
s-f	579.2238609	2	13.4286513
	29.6694906	2	6.7143256
	-24.3143757	2	3.3095686
p-f	280.8607742	2	10.3659442
	26.7453820	2	5.1829721
	-24.3143757	2	3.3095686
d-f	120.3964443	2	7.6004795
	15.8109206	2	3.8002397
	-24.3143757	2	3.3095686
*			
*			
au	def2-SVP		
#	au	(7s6p5d1f) / [6s3p2d1f]	{211111/411/41/1}
*			
	2 s		
	20.115299000	-0.15910719389	
	12.193477000	0.79105526778	
	1 s		
	6.0735294368	1.0000000000	
	1 s		
	1.3174451569	1.0000000000	
	1 s		
	0.58596768244	1.0000000000	
	1 s		
	0.13875427354	1.0000000000	
	1 s		
	0.48876985527E-01	1.0000000000	
	4 p		
	8.6096650000	0.50053018599	
	7.3353260000	-0.72681584494	
	1.6575296365	0.57315511417	
	0.78159310216	0.49579068859	
	1 p		
	0.32384840661	1.0000000000	
	1 p		
	0.54000000000E-01	1.0000000000	
	4 d		
	4.1439490000	-0.37099566643	
	3.5682570000	0.40197233762	
	1.2345757130	0.46001988624	
	0.48190232338	0.46152130958	
	1 d		
	0.16490636769	1.0000000000	
	1 f		
	0.72482000000	1.0000000000	
*			
au	def2-ecp		
*			
	ncore =	60	lmax = 3
#	coefficient	r^n	exponent
f			
	30.4900889	2	4.7898200
	5.1710738	2	2.3949100
s-f	426.8466792	2	13.2051000
	37.0070829	2	6.6025500

```

-30.4900889    2    4.7898200
-5.1710738    2    2.3949100
p-f
261.1995804    2    10.4520200
26.9624960    2    5.2260100
-30.4900889    2    4.7898200
-5.1710738    2    2.3949100
d-f
124.7906656    2    7.8511000
16.3007257    2    3.9255500
-30.4900889    2    4.7898200
-5.1710738    2    2.3949100
*
*
hg def2-SVP
# hg      (7s6p5d1f) / [6s3p2d1f]      {211111/411/41/1}
*
  2 s
26.842049000   -0.26845096483E-01
10.320909000   0.81771278143
  1 s
6.3656242291   1.0000000000
  1 s
1.3898932095   1.0000000000
  1 s
0.63706742699   1.0000000000
  1 s
0.16047725098   1.0000000000
  1 s
0.56410423453E-01 1.0000000000
  4 p
9.7729900000    0.21210940502
7.1690950000   -0.44026342153
1.7559567931    0.58406314464
0.83145670425    0.49359746203
  1 p
0.34494917659   1.0000000000
  1 p
0.70000000000E-01 1.0000000000
  4 d
4.2800000000   -0.32033414305
3.4800000000    0.37748470203
1.2535869926    0.48342275878
0.50841366863    0.43493523158
  1 d
0.18501599388   1.0000000000
  1 f
0.79569000000   1.0000000000
*
hg def2-ecp
*
ncore =      60      lmax =      3
#      coefficient  r^n      exponent
f
30.3649964    2      3.8857911
s-f
275.7372117   2      12.9815487
49.0892125    2      6.4907744
-30.3649964   2      3.8857911
p-f

```

```

                241.5400740    2           10.5380958
                27.3965908    2           5.2690479
                -30.3649964    2           3.8857911
d-f
                127.8670076    2           8.1017205
                16.6083115    2           4.0508603
                -30.3649964    2           3.8857911
*
*
t1 def2-SVP
# t1      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
    6 s
    45.356924655      0.50938157397E-02
    20.278843336      -0.14805704314
    14.420612394      0.36768453564
    6.2161909754      -0.66820394623
    1.5002511178      0.96232806743
    0.76330879305      0.33175999361
    2 s
    7.8193195283      -0.18828631537E-01
    1.3176904042      0.32093431467
    1 s
    0.17643545481      1.0000000000
    1 s
    0.65296835238E-01  1.0000000000
    4 p
    9.0323058024      0.22738839085
    7.5356419671      -0.35117975889
    1.0521421998      0.25690085604
    0.50303932656      0.84549942764E-01
    1 p
    2.0067660913      1.0000000000
    1 p
    0.16675605056      1.0000000000
    1 p
    0.48596401464E-01  1.0000000000
    5 d
    9.4421940760      0.58250776986E-01
    7.4410003381      -0.11789199301
    1.9831617772      0.34232057636
    0.91671748567      0.47557282350
    0.39647207885      0.30528029435
    1 d
    0.15500000000      1.0000000000
*
t1 def2-ecp
*
    ncore =    60          lmax =    3
#      coefficient      r^n          exponent
f
    15.8254880      2          5.6263990
    21.1040210      2          5.5489520
    2.9151270      2          2.8749460
    3.8969030      2          2.8214510
s-f
    281.2846630      2          12.1678050
    62.4342510      2          8.2949090
    -15.8254880      2          5.6263990
    -21.1040210      2          5.5489520

```

	-2.9151270	2	2.8749460
	-3.8969030	2	2.8214510
p-f			
	4.6334080	2	7.1514920
	9.3417560	2	5.1728650
	72.2992530	2	9.8910720
	144.5580370	2	9.0033910
	-15.8254880	2	5.6263990
	-21.1040210	2	5.5489520
	-2.9151270	2	2.8749460
	-3.8969030	2	2.8214510
d-f			
	35.9430390	2	7.1302180
	53.9095930	2	6.9269060
	10.3819390	2	5.4175700
	15.5838220	2	5.1386810
	-15.8254880	2	5.6263990
	-21.1040210	2	5.5489520
	-2.9151270	2	2.8749460
	-3.8969030	2	2.8214510

*

*

pb def2-SVP

pb (10s7p6d) / [4s4p2d] {6211/4111/51}

*

6 s		
55.727520333	0.29681153058E-02	
20.302912827	-0.14352634362	
14.558628750	0.37554188507	
6.5370530973	-0.67253099800	
1.5933900686	0.95887533909	
0.83051419711	0.32593632538	
2 s		
8.0719473648	-0.20412061217E-01	
1.4165737490	0.32865829049	
1 s		
0.20418933370	1.0000000000	
1 s		
0.77159007761E-01	1.0000000000	
4 p		
9.5531412199	0.20542943990	
7.5327685129	-0.36407590058	
1.1185539567	0.32217481686	
0.53739855255	0.96677743015E-01	
1 p		
2.1359869828	1.0000000000	
1 p		
0.20027494801	1.0000000000	
1 p		
0.63408011513E-01	1.0000000000	
5 d		
13.494505735	0.11571042371E-01	
7.0609770411	-0.66746645076E-01	
2.1581835375	0.33978760942	
1.0148541418	0.48523039273	
0.44632672920	0.29682924018	
1 d		
0.17500000000	1.0000000000	

*

pb def2-ecp

```

*
ncore = 60          lmax = 3
# coefficient      r^n      exponent
f
    12.2098920     2        3.8875120
    16.1902910     2        3.8119630
s-f
    281.2854990    2        12.2963030
    62.5202170     2        8.6326340
    -12.2098920    2        3.8875120
    -16.1902910    2        3.8119630
p-f
    72.2768970     2        10.2417900
    144.5910830    2        8.9241760
    4.7586930      2        6.5813420
    9.9406210      2        6.2554030
    -12.2098920    2        3.8875120
    -16.1902910    2        3.8119630
d-f
    35.8485070     2        7.7543360
    53.7243420     2        7.7202810
    10.1152560     2        4.9702640
    14.8337310     2        4.5637890
    -12.2098920    2        3.8875120
    -16.1902910    2        3.8119630
*
*
bi def2-SVP
# bi      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
  6 s
  175.19632102      0.80278879028E-03
  19.820147783      -0.14624461250
  14.960110102      0.37435719885
  6.7065785571      -0.68476017748
  1.7391967524      0.90967322081
  0.94504730591     0.38695797807
  2 s
  8.4636832909      -0.20037183144E-01
  1.5317838545      0.31054408682
  1 s
  0.23405391503     1.0000000000
  1 s
  0.90268814613E-01 1.0000000000
  4 p
  10.672046293      0.14391258793
  7.1992185915      -0.37994608603
  1.5359697528      0.53268032065
  0.72201275727     0.23037698678
  1 p
  2.8508661858      1.0000000000
  1 p
  0.23769418731     1.0000000000
  1 p
  0.78768140453E-01 1.0000000000
  5 d
  15.834273510      0.85062993231E-02
  7.0956896087      -0.65954380016E-01
  2.3363137007      0.33707163406
  1.1208861366      0.49128719933

```

```

0.50309487376      0.29095930644
  1 d
0.20000000000      1.00000000000
*
bi def2-ecp
*
  ncore =      60          lmax =      3
#   coefficient      r^n          exponent
f
      13.7133830      2          4.2145460
      18.1943080      2          4.1334000
s-f
      283.2642270      2          13.0430900
      62.4719590      2          8.2216820
      -13.7133830      2          4.2145460
      -18.1943080      2          4.1334000
p-f
      72.0014990      2          10.4677770
      144.0022770      2          9.1189010
      5.0079450      2          6.7547910
      9.9915500      2          6.2525920
      -13.7133830      2          4.2145460
      -18.1943080      2          4.1334000
d-f
      36.3962590      2          8.0814740
      54.5976640      2          7.8905950
      9.9842940      2          4.9555560
      14.9814850      2          4.7045590
      -13.7133830      2          4.2145460
      -18.1943080      2          4.1334000
*
*
po def2-SVP
# po      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
  6 s
278.13783916      0.91690497839E-03
19.659291105      -0.14713009283
15.016229647      0.38790413631
7.1149978720      -0.67059966298
1.7879214122      0.91212928327
0.94021655206      0.29153755200
  2 s
8.7584161749      -0.21561417525E-01
1.6503945866      0.31638990001
  1 s
0.26329582133      1.00000000000
  1 s
0.10190654304      1.00000000000
  4 p
10.445945973      0.23631841405
8.0293101888      -0.45017818996
1.3588798023      0.44160334658
0.66829182929      0.14575285544
  1 p
2.4460635387      1.00000000000
  1 p
0.27242942777      1.00000000000
  1 p
0.88796031338E-01  1.00000000000

```

```

5 d
18.292670150      0.72030963652E-02
7.1695578539     -0.66160544754E-01
2.5029225180     0.343634449378
1.2115945443     0.50529101033
0.54713334240    0.28301155453
1 d
0.21500000000    1.00000000000
*
po def2-ecp
*
ncore = 60          lmax = 3
#      coefficient  r^n      exponent
f
      17.4282950    2         5.0132700
      23.3803530    2         4.9846400
      0.1633920     2         1.3267600
      0.3245660     2         1.5287580
s-f
      283.2447060    2         13.2772270
      62.3964610    2         8.3995180
      -17.4282950   2         5.0132700
      -23.3803530   2         4.9846400
      -0.1633920    2         1.3267600
      -0.3245660    2         1.5287580
p-f
      71.9917160     2         10.6656820
      143.9718710    2         9.2837530
      4.9496150      2         6.8727490
      9.7404990      2         6.3261500
      -17.4282950   2         5.0132700
      -23.3803530   2         4.9846400
      -0.1633920    2         1.3267600
      -0.3245660    2         1.5287580
d-f
      36.3783830     2         8.2148660
      54.5627150     2         8.0086960
      9.8894990      2         5.0552270
      14.6938770     2         4.7825530
      -17.4282950   2         5.0132700
      -23.3803530   2         4.9846400
      -0.1633920    2         1.3267600
      -0.3245660    2         1.5287580
*
*
at def2-SVP
# at      (10s7p6d) / [4s4p2d]      {6211/4111/51}
*
6 s
303.23376176     0.63504969788E-03
20.289449240     -0.13823165350
15.383783126     0.38333193283
7.4702184232     -0.66837560338
1.8731608346     0.91545877992
0.97426847543    0.25559567998
2 s
8.9610112498     -0.23092977605E-01
1.7804284294     0.31690635939
1 s
0.29269461143    1.00000000000

```



```

1 s
0.11395353119      1.0000000000
4 p
10.722023134      0.26194870008
8.4823338656     -0.46607228264
1.3474291294      0.42119853309
0.62824011467     0.10643224457
1 p
2.4814896839      1.0000000000
1 p
0.31036518470      1.0000000000
1 p
0.10144862043      1.0000000000
5 d
20.799819604      0.65227965381E-02
7.1664616770     -0.67780885217E-01
2.6934397048      0.33954991335
1.3175112423      0.50899559178
0.59997066293     0.27526771759
1 d
0.23500000000     1.0000000000
*
at def2-ecp
*
ncore =      60      lmax =      3
# coefficient  r^n      exponent
f
      19.8701980      2      5.8121630
      26.4164520      2      5.7537150
      0.9949700      2      2.5134720
      1.4907010      2      2.5362610
s-f
      49.9571580      2      30.2008320
      283.2103710      2      13.6123060
      62.2810520      2      8.5293400
      -19.8701980      2      5.8121630
      -26.4164520      2      5.7537150
      -0.9949700      2      2.5134720
      -1.4907010      2      2.5362610
p-f
      71.9823710      2      10.8540650
      143.9035320      2      9.4682290
      4.8717590      2      7.0311140
      8.9830590      2      6.1438580
      -19.8701980      2      5.8121630
      -26.4164520      2      5.7537150
      -0.9949700      2      2.5134720
      -1.4907010      2      2.5362610
d-f
      36.3632370      2      8.3135150
      54.5489700      2      7.9989650
      9.7762850      2      5.1799660
      14.2647550      2      4.9422260
      -19.8701980      2      5.8121630
      -26.4164520      2      5.7537150
      -0.9949700      2      2.5134720
      -1.4907010      2      2.5362610
*
*
rn def2-SVP

```

rn (11s10p8d2f) / [6s5p3d2f] {521111/34111/611/11}

*
5 s
5187.7442468 0.16097034848E-03
768.14491207 0.10508214789E-02
159.35182065 0.27375438093E-02
21.863432724 -0.55045904905
18.388689978 0.78321373922
2 s
24.816226448 -0.82636797204E-01
7.2923301677 1.0926256000
1 s
2.0850437166 1.0000000000
1 s
1.0915245945 1.0000000000
1 s
0.34915708428 1.0000000000
1 s
0.13648422952 1.0000000000
3 p
194.68918723 0.26265814046E-03
11.210013525 0.19952302621
7.5298316489 -0.45994479561
4 p
9.0845000304 -0.23093917426
6.2631489717 0.39747614192
2.2545193734 0.83026693838
1.1180666918 0.51467013112
1 p
0.47444492594 1.0000000000
1 p
0.20172354616 1.0000000000
1 p
0.79503144392E-01 1.0000000000
6 d
75.302723665 0.73590238429E-03
17.965913830 0.89490827389E-02
7.3741298033 -0.76641663693E-01
3.2296258578 0.22975404602
1.7937840508 0.43991495311
0.94633319732 0.35259395198
1 d
0.46860482223 1.0000000000
1 d
0.20000000000 1.0000000000
1 f
0.41806000000 1.0000000000
1 f
2.1000000000 1.0000000000

*
rn def2-ecp
*

#	ncore = 60	lmax = 3	
f	coefficient	r^n	exponent
	21.7972900	2	6.3485710
	28.9468050	2	6.2959490
	1.4473650	2	2.8821180
	2.1779640	2	2.9080480

s-f

	49.9655510	2	30.1512420
	283.0700000	2	14.5212410
	62.0028700	2	8.0520380
	-21.7972900	2	6.3485710
	-28.9468050	2	6.2959490
	-1.4473650	2	2.8821180
	-2.1779640	2	2.9080480
p-f			
	71.9691190	2	11.0099420
	143.8605590	2	9.6176250
	4.7147610	2	7.3360080
	9.0130650	2	6.4062530
	-21.7972900	2	6.3485710
	-28.9468050	2	6.2959490
	-1.4473650	2	2.8821180
	-2.1779640	2	2.9080480
d-f			
	36.3683650	2	8.3692200
	54.5517610	2	8.1169750
	9.6344870	2	5.3536560
	14.3879020	2	5.0972120
	-21.7972900	2	6.3485710
	-28.9468050	2	6.2959490
	-1.4473650	2	2.8821180
	-2.1779640	2	2.9080480

*

=====
def2-TZVP
=====

*

h def2-TZVP

h (5s1p) / [3s1p] {311/1}

*

3	s		
34.061341000		0.60251978000E-02	
5.1235746000		0.45021094000E-01	
1.1646626000		0.20189726000	
1	s		
0.32723041000		1.00000000000	
1	s		
0.10307241000		1.00000000000	
1	p		
0.80000000000		1.00000000000	

*

*

he def2-TZVP

he (5s1p) / [3s1p] {311/1}

*

3	s		
98.078321616		0.75803064967E-02	
14.764404247		0.54848620937E-01	
3.3185831473		0.22074382186	
1	s		
0.87413869551		1.00000000000	
1	s		
0.24459897208		1.00000000000	
1	p		
1.00000000000		1.00000000000	

*

*

```

li def2-TZVP
# li      (11s3p) / [5s3p]      {62111/111}
*
  6 s
6269.2628010      0.20540968826E-03
940.31612431     0.15916554089E-02
214.22107528     0.82869829707E-02
60.759840184     0.33856374249E-01
19.915152032     0.11103225876
7.3171509797     0.27449383329
  2 s
2.9724674216     0.23792456411
1.2639852314     0.30765411924
  1 s
0.51427489953    1.00000000000
  1 s
0.77030885901E-01 1.00000000000
  1 s
0.28938896433E-01 1.00000000000
  1 p
0.40000000000    1.00000000000
  1 p
0.60000000000E-01 1.00000000000
  1 p
3.32700000000    1.00000000000
*
*
be def2-TZVP
# be      (11s4p1d) / [5s3p1d]  {62111/121/1}
*
  6 s
4700.2365626     0.23584389316E-03
704.82845622     0.18243791019E-02
160.43110478     0.93966148224E-02
45.425347336     0.36908924159E-01
14.798334125     0.10897561281
5.3512452537     0.21694284551
  2 s
2.1542044819     0.44695408857
0.93363744400    0.20866985771
  1 s
0.18791432989    1.00000000000
  1 s
0.74648267947E-01 1.00000000000
  1 s
0.32650484598E-01 1.00000000000
  1 p
3.6316917145     -0.29033998305E-01
  2 p
0.71695694366    -0.16877854032
0.19541932860    -0.51403419628
  1 p
0.60515465890E-01 1.00000000000
  1 d
0.18000000000    0.00000000000
*
*
b def2-TZVP
# b      (11s6p2d1f) / [5s3p2d1f]  {62111/411/11/1}
*

```

```

6 s
8564.8660687      0.22837198155E-03
1284.1516263     0.17682576447E-02
292.27871604     0.91407080516E-02
82.775469176     0.36342638989E-01
27.017939269     0.11063458441
9.8149619660     0.23367344321
2 s
3.9318559059     0.41818777978
1.6595599712     0.22325473798
1 s
0.35762965239    1.00000000000
1 s
0.14246277496    1.00000000000
1 s
0.60560594768E-01 1.00000000000
4 p
22.453875803     0.50265575179E-02
5.1045058330     0.32801738965E-01
1.4986081344     0.13151230768
0.50927831315    0.33197167769
1 p
0.18147077798    0.47314319570
1 p
0.64621893904E-01 0.25802783943
1 d
0.66100000000    1.00000000000
1 d
0.19900000000    1.00000000000
1 f
0.49000000000    1.00000000000
*
*
c def2-TZVP
# c      (11s6p2d1f) / [5s3p2d1f]      {62111/411/11/1}
*
6 s
13575.349682     0.22245814352E-03
2035.2333680     0.17232738252E-02
463.22562359     0.89255715314E-02
131.20019598     0.35727984502E-01
42.853015891     0.11076259931
15.584185766     0.24295627626
2 s
6.2067138508     0.41440263448
2.5764896527     0.23744968655
1 s
0.57696339419    1.00000000000
1 s
0.22972831358    1.00000000000
1 s
0.95164440028E-01 1.00000000000
4 p
34.697232244     0.53333657805E-02
7.9582622826     0.35864109092E-01
2.3780826883     0.14215873329
0.81433208183    0.34270471845
1 p
0.28887547253    0.46445822433
1 p

```

```

0.10056823671      0.24955789874
  1 d
1.0970000000      1.0000000000
  1 d
0.3180000000      1.0000000000
  1 f
0.7610000000      1.0000000000
*
*
n def2-TZVP
# n      (11s6p2d1f) / [5s3p2d1f]      {62111/411/11/1}
*
  6 s
19730.800647      0.21887984991E-03
2957.8958745      0.16960708803E-02
673.22133595      0.87954603538E-02
190.68249494      0.35359382605E-01
62.295441898      0.11095789217
22.654161182      0.24982972552
  2 s
  8.9791477428      0.40623896148
  3.6863002370      0.24338217176
  1 s
0.84660076805      1.0000000000
  1 s
0.33647133771      1.0000000000
  1 s
0.13647653675      1.0000000000
  4 p
  49.200380510      0.55552416751E-02
  11.346790537      0.38052379723E-01
  3.4273972411      0.14953671029
  1.1785525134      0.34949305230
  1 p
0.41642204972      0.45843153697
  1 p
0.14260826011      0.24428771672
  1 d
  1.6540000000      1.0000000000
  1 d
0.46900000000      1.0000000000
  1 f
  1.0930000000      1.0000000000
*
*
o def2-TZVP
# o      (11s6p2d1f) / [5s3p2d1f]      {62111/411/11/1}
*
  6 s
27032.382631      0.21726302465E-03
4052.3871392      0.16838662199E-02
922.32722710      0.87395616265E-02
261.24070989      0.35239968808E-01
85.354641351      0.11153519115
31.035035245      0.25588953961
  2 s
  12.260860728      0.39768730901
  4.9987076005      0.24627849430
  1 s
  1.1703108158      1.0000000000

```

```

1 s
0.46474740994      1.0000000000
1 s
0.18504536357      1.0000000000
4 p
63.274954801       0.60685103418E-02
14.627049379       0.41912575824E-01
4.4501223456       0.16153841088
1.5275799647       0.35706951311
1 p
0.52935117943      0.44794207502
1 p
0.17478421270      0.24446069663
1 d
2.3140000000       1.0000000000
1 d
0.64500000000     1.0000000000
1 f
1.4280000000       1.0000000000
*
*
f def2-TZVP
# f      (11s6p2d1f) / [5s3p2d1f]      {62111/411/11/1}
*
6 s
35479.100441       0.21545014888E-03
5318.4728983       0.16700686527E-02
1210.4810975       0.86733211476E-02
342.85518140       0.35049933175E-01
112.01943181       0.11165320133
40.714740248       0.25988506647
2 s
16.039678111       0.39422966880
6.5038186740       0.24998238551
1 s
1.5440477509       1.0000000000
1 s
0.61223452862      1.0000000000
1 s
0.24027979698      1.0000000000
4 p
80.233900483       0.63685999134E-02
18.594010743       0.44303143530E-01
5.6867902653       0.16867248708
1.9511006294       0.36166346255
1 p
0.66970211298      0.44202901491
1 p
0.21651300410      0.24319875730
1 d
3.1070000000       1.0000000000
1 d
0.85500000000     1.0000000000
1 f
1.9170000000       1.0000000000
*
*
ne def2-TZVP
# ne     (11s6p2d1f) / [5s3p2d1f]     {62111/411/11/1}
*

```

```

6 s
45069.464022      0.21687155182E-03
6755.9768656     0.16812736757E-02
1537.6502864     0.87356062782E-02
435.51697667    0.35361266922E-01
142.28655638    0.11321521454
51.692153804    0.26654653104
 2 s
20.315870490    0.39631959951
8.2021942646    0.25582811251
 1 s
1.9681276278    1.0000000000
 1 s
0.77904756001   1.0000000000
 1 s
0.30229502043   1.0000000000
 4 p
99.782996032    0.65569234163E-02
23.176124101    0.45888009138E-01
7.1163945872    0.17331287812
2.4418711435    0.36475267512
 1 p
0.83389605766   0.43831075171
 1 p
0.26607311301   0.24160029835
 1 d
4.0140000000    1.0000000000
 1 d
1.0960000000    1.0000000000
 1 f
2.5440000000    1.0000000000
*
*
na def2-TZVP
# na      (14s8p3d) / [5s4p3d]      {73211/5111/111}
*
 7 s
26041.109927    0.61806342811E-03
3906.1268548    0.47748604414E-02
888.97454993    0.24471684829E-01
251.45497961    0.94755394977E-01
81.650143512    0.26867496920
28.904158401    0.47925475440
10.625782932    0.33248591469
 3 s
53.769410179    0.19527731872E-01
16.308243025    0.92648010794E-01
2.3730384125    -0.39938670172
 2 s
0.95730772603    1.6428595391
0.40806460959    0.55692596966
 1 s
0.49967582329E-01  1.0000000000
 1 s
0.19268616250E-01  1.0000000000
 5 p
138.07979989    0.57951891929E-02
32.232700393    0.41620846251E-01
9.9816075360    0.16281916885
3.4822033928    0.36011784647

```


1.2299134620	0.44858979889
1 p	
0.41743959423	0.23040759559
1 p	
0.30000000000E-01	1.0000000000
1 p	
0.91000000000E-01	1.0000000000
1 d	
2.6090000000	1.0000000000
1 d	
0.4300000000	0.0000000000
1 d	
0.1000000000	0.0000000000

*
*
mg def2-TZVP
mg (14s8p3d) / [5s4p3d] {73211/5111/111}
*

7 s	
31438.349555	0.60912311326E-03
4715.5153354	0.47066196465E-02
1073.1629247	0.24135820657E-01
303.57238768	0.93628959834E-01
98.626251042	0.26646742093
34.943808417	0.47890929917
12.859785199	0.33698490286
3 s	
64.876913004	0.19180889307E-01
19.725520777	0.90913704392E-01
2.8951804339	-0.39563756125
2 s	
1.1960454710	1.6827603373
0.54329451156	0.52141091954
1 s	
0.10099104092	1.0000000000
1 s	
0.36865728085E-01	1.0000000000
5 p	
179.87189612	0.53799549018E-02
42.120069376	0.39318014098E-01
13.120503032	0.15740129476
4.6257503609	0.35919094128
1.6695211016	0.45533379310
1 p	
0.58551012105	0.21986432910
1 p	
0.18914796195	1.0000000000
1 p	
0.53768755187E-01	1.0000000000
1 d	
3.4440000000	1.0000000000
1 d	
0.2900000000	1.0000000000
1 d	
0.70000000000E-01	1.0000000000

*
*
al def2-TZVP
al (14s9p3d1f) / [5s5p2d1f] {73211/51111/21/1}
*

```

7 s
37792.550772      0.57047888709E-03
5668.0682165     0.44093016538E-02
1289.8582841     0.22630967411E-01
364.86596028     0.88025644295E-01
118.57631515     0.25223701612
42.024867605     0.45960547169
15.499501629     0.33277886014
3 s
75.208026598     0.19250560190E-01
23.031408972     0.87906743952E-01
3.6348797649     -0.34246704535
2 s
1.6065049957     1.5106266058
0.76103394581    0.58071016470
1 s
0.16556708849    1.0000000000
1 s
0.60041577113E-01 1.0000000000
5 p
452.52303192     0.23110812466E-02
107.08195049     0.18568641823E-01
34.131021255     0.87216237035E-01
12.587037428     0.26902101523
4.9811919704     0.52128324272
1 p
2.0070350900     0.60271687494
1 p
0.80083714374    1.0000000000
1 p
0.20178927472    1.0000000000
1 p
0.57895550392E-01 1.0000000000
2 d
1.5700000000     0.20000000000
0.3330000000     1.0000000000
1 d
0.1110000000     1.0000000000
1 f
0.2440000000     1.0000000000
*
*
si def2-TZVP
# si      (14s9p3d1f) / [5s5p2d1f]      {73211/51111/21/1}
*
7 s
44773.358078     0.55914765868E-03
6717.1992104     0.43206040189E-02
1528.8960325     0.22187096460E-01
432.54746585     0.86489249116E-01
140.61505226     0.24939889716
49.857636724     0.46017197366
18.434974885     0.34250236575
3 s
86.533886111     0.21300063007E-01
26.624606846     0.94676139318E-01
4.4953057159     -0.32616264859
2 s
2.1035045710     1.3980803850
1.0106094922     0.63865786699

```

1 s	
0.23701751489	1.0000000000
1 s	
0.85703405362E-01	1.0000000000
5 p	
394.47503628	0.26285693959E-02
93.137683104	0.20556257749E-01
29.519608742	0.92070262801E-01
10.781663791	0.25565889739
4.1626574778	0.42111707185
1 p	
1.6247972989	0.34401746318
1 p	
0.54306660493	1.0000000000
1 p	
0.20582073956	1.0000000000
1 p	
0.70053487306E-01	1.0000000000
2 d	
2.3030000000	0.2000000000
0.4760000000	1.0000000000
1 d	
0.1600000000	1.0000000000
1 f	
0.3360000000	1.0000000000
*	
*	
p def2-TZVP	
# p (14s9p3d1f) / [5s5p2d1f] {73211/51111/21/1}	
*	
7 s	
52426.999233	0.55207164100E-03
7863.2660552	0.42678595308E-02
1789.5227333	0.21931529186E-01
506.27300165	0.85667168373E-01
164.60698546	0.24840686605
58.391918722	0.46336753971
21.643663201	0.35350558156
3 s	
99.013837620	0.21895679958E-01
30.550439817	0.95650470295E-01
5.4537087661	-0.29454270186
2 s	
2.6503362563	1.3294381200
1.2726688867	0.66109396473
1 s	
0.31645005203	1.0000000000
1 s	
0.11417466938	1.0000000000
5 p	
472.27219248	0.25710623052E-02
111.58882756	0.20250297999E-01
35.445936418	0.91580716787E-01
12.990776875	0.25749454014
5.0486221658	0.42862899758
1 p	
1.9934049566	0.34359817849
1 p	
0.66527284430	1.0000000000
1 p	

```

0.25516832128      1.0000000000
  1 p
0.90357762251E-01  1.0000000000
  2 d
  3.1200000000      0.2000000000
0.648000000000     1.0000000000
  1 d
0.218000000000     1.0000000000
  1 f
0.452000000000     1.0000000000
*
*
s def2-TZVP
# s      (14s9p3d1f) / [5s5p2d1f]      {73211/51111/21/1}
*
  7 s
  60700.928104      0.54695944225E-03
  9102.6106854      0.42297224557E-02
  2071.4166009      0.21747824159E-01
  586.02476821      0.85100053589E-01
  190.55395021      0.24799128459
  67.630384260      0.46703640406
  25.127306905      0.36434587550
  3 s
  112.57463010      0.21670040240E-01
  34.795554217      0.93602301760E-01
  6.5115556215      -0.26068001422
  2 s
  3.2399032261      1.2842089435
  1.5477160881      0.66036416584
  1 s
0.40541030112      1.0000000000
  1 s
0.14550651059      1.0000000000
  5 p
  564.36716027      0.24796796317E-02
  133.42624379      0.19677930250E-01
  42.468271189      0.89980008258E-01
  15.616527580      0.25705880575
  6.1093988469      0.43515167292
  1 p
  2.4404160198      0.34883240595
  1 p
0.83882201296      1.0000000000
  1 p
0.31288746900      1.0000000000
  1 p
0.10770109004      1.0000000000
  2 d
  3.7560000000      0.2000000000
0.812000000000     1.0000000000
  1 d
0.273000000000     1.0000000000
  1 f
0.557000000000     1.0000000000
*
*
cl def2-TZVP
# cl      (14s9p3d1f) / [5s5p2d1f]      {73211/51111/21/1}
*

```

```

7 s
69507.990945      0.54314897497E-03
10426.156880     0.41990463961E-02
2373.2334061     0.21592141679E-01
671.56420071     0.84598850094E-01
218.41999790     0.24757249724
77.572249714     0.47016930228
28.888815277     0.37436370716
3 s
127.10527185     0.25182166603E-01
39.339582961     0.10786112456
7.6740679989    -0.27408821574
2 s
3.8745627630     1.3213875014
1.8385832573     0.68636955368
1 s
0.50229057542     1.0000000000
1 s
0.17962723420     1.0000000000
5 p
666.50423284     0.23632663836E-02
157.64241690     0.18879300374E-01
50.262520978     0.87206341273E-01
18.536078105     0.25285612970
7.2940532777     0.43507154820
1 p
2.9433248995     0.35026513165
1 p
1.0404970818     1.0000000000
1 p
0.38456415080     1.0000000000
1 p
0.13069642732     1.0000000000
2 d
4.6100000000     0.20000000000
1.0110000000     1.0000000000
1 d
0.33900000000     1.0000000000
1 f
0.70600000000     1.0000000000
*
*
ar def2-TZVP
# ar      (14s9p3d1f) / [5s5p2d1f]      {73211/51111/21/1}
*
7 s
79111.422998     0.51029325002E-03
11864.746009     0.39463036981E-02
2700.1642973     0.20307073910E-01
763.95943485     0.79691825214E-01
248.45150561     0.23420623836
88.283581000     0.44833849481
32.948607069     0.36408167400
3 s
142.55358000     0.26387407001E-01
44.163688009     0.11226433999
8.9524995000    -0.26178922001
2 s
4.5546920941     1.3002484998
2.1444079001     0.67197237009

```

1 s	
0.60708777004	1.0000000000
1 s	
0.21651431999	1.0000000000
5 p	
776.77541998	0.22028005003E-02
183.80107018	0.17694180008E-01
58.694003175	0.82431293717E-01
21.701591695	0.24207278863
8.5821489635	0.42263558251
1 p	
3.4922679161	0.34151806086
1 p	
1.2637426998	1.0000000000
1 p	
0.46607870005	1.0000000000
1 p	
0.15766003000	1.0000000000
2 d	
5.5510000000	0.20000000000
1.2350000000	1.0000000000
1 d	
0.41200000000	1.0000000000
1 f	
0.89000000000	1.0000000000
*	
*	
k def2-TZVP	
# k (17s11p3d) / [6s4p3d] {842111/6311/111}	
*	
8 s	
153976.18325	0.23662636107E-03
23082.497672	0.18342929137E-02
5253.2344745	0.95310527769E-02
1486.9550133	0.38638406980E-01
484.06333726	0.12480768502
173.56653980	0.29278861009
67.116381464	0.40633425860
26.339502054	0.20077215860
4 s	
172.87693567	-0.24200960936E-01
53.058649063	-0.11553095040
7.9212753964	0.57455545175
3.2108880472	0.57023185107
2 s	
4.5662070895	-0.22615763466
0.70209907282	0.75528392045
1 s	
0.28258942635	1.0000000000
1 s	
0.35805824617E-01	1.0000000000
1 s	
0.15819213245E-01	1.0000000000
6 p	
728.18449873	0.26150689792E-02
172.13265061	0.20673630835E-01
54.829847075	0.93205603870E-01
20.166266494	0.25436518210
7.8610728806	0.39131132810
3.1105213132	0.22481345943

```

3 p
11.757337492 -0.25777289217E-01
1.5139617411 0.57359428604
0.58328591795 1.0798320002
1 p
0.21570478076 1.0000000000
1 p
0.41737000000E-01 1.0000000000
1 d
0.93000000000 1.0000000000
1 d
0.18000000000 1.0000000000
1 d
0.54000000000E-01 1.0000000000
*
*
ca def2-TZVP
# ca (17s12p4d) / [6s5p3d] {842111/63111/211}
*
8 s
172517.32685 0.23317502546E-03
25861.519275 0.18076521980E-02
5885.6618668 0.93943844255E-02
1665.9730031 0.38108409009E-01
542.36718148 0.12331203853
194.57803492 0.29004470954
75.303597636 0.40587151157
29.574062589 0.20398410743
4 s
191.20074660 -0.24419759759E-01
58.840299883 -0.11547027448
8.9642540845 0.56356636717
3.6856960541 0.56709682704
2 s
5.2464289726 -0.22825334325
0.84862621528 0.72625219172
1 s
0.36743300538 1.0000000000
1 s
0.66821582613E-01 1.0000000000
1 s
0.26759730445E-01 1.0000000000
6 p
836.97262058 0.25258346092E-02
197.93040142 0.20076506686E-01
63.135558054 0.91302987366E-01
23.282687170 0.25247029915
9.1176444932 0.39426326344
3.6336120139 0.23011559492
3 p
13.494163120 -0.26495021951E-01
1.8139259790 0.55088108210
0.71981826006 1.0280616620
1 p
0.27629576992 1.0000000000
1 p
0.74979000000E-01 1.0000000000
1 p
0.26927000000E-01 1.0000000000
2 d

```

```

5.4979093879      0.73770011433E-01
1.3177128032      0.26052853169
  1 d
0.32188682649     0.45233836380
  1 d
0.70528614919E-01  1.00000000000
*
*
sc def2-TZVP
# sc      (17s11p7d1f) / [6s4p4d1f]      {842111/6311/4111/1}
*
  8 s
191612.91874      0.23076475942E-03
28723.850363      0.17890329946E-02
6537.0116490      0.92990401140E-02
1850.3097171      0.37739438011E-01
602.38855156      0.12227148359
216.17324766      0.28814821470
83.712517880      0.40517543099
32.908707189      0.20566019623
  4 s
211.34393234      -0.24527991462E-01
65.128920139      -0.11570158142
10.034311535      0.55995283317
4.1596884597      0.56087765073
  2 s
6.0009041613      -0.22840494325
0.98255784150      0.71948970378
  1 s
0.42483192773      1.00000000000
  1 s
0.77185462096E-01  1.00000000000
  1 s
0.30147219702E-01  1.00000000000
  6 p
947.34122823      0.24737208744E-02
224.09699732      0.19742967060E-01
71.560334882      0.90357147549E-01
26.444824490      0.25201602503
10.393798285      0.39675535929
4.1606304559      0.23208624517
  3 p
15.565737135      -0.27129423974E-01
2.1121544865      0.55109256629
0.84184709021      1.0090635806
  1 p
0.32297542652      1.00000000000
  1 p
0.89748000000E-01  1.00000000000
  4 d
30.989390993      0.11902837431E-01
8.6905465069      0.67655856850E-01
2.9520256337      0.21332539722
1.0761910745      0.38391075578
  1 d
0.38338915095      0.43354716259
  1 d
0.12534686113      0.24509263822
  1 d
0.41000000000E-01  0.00000000000

```



```

1 f
0.34500000000 1.0000000000
*
*
ti def2-TZVP
# ti (17s11p7d1f) / [6s4p4d1f] {842111/6311/4111/1}
*
8 s
211575.69025 0.23318151011E-03
31714.945058 0.18079690851E-02
7217.5476543 0.93984311352E-02
2042.9394247 0.38156853618E-01
665.12896208 0.12374757197
238.74942264 0.29208551143
92.508691001 0.41226800855
36.403919209 0.21090534061
4 s
232.72624607 -0.24920140738E-01
71.791209711 -0.11746490087
11.158534615 0.56503342318
4.6548135416 0.56211101812
2 s
6.8034629174 -0.23011425503
1.1201076403 0.72103186735
1 s
0.48080118839 1.0000000000
1 s
0.85157274977E-01 1.0000000000
1 s
0.32657477046E-01 1.0000000000
6 p
1063.1474732 0.24690839320E-02
251.56507061 0.19773345523E-01
80.408554854 0.90987976672E-01
29.768193269 0.25559900413
11.736830556 0.40489386764
4.7142375230 0.23693402558
3 p
17.796803704 -0.27878639615E-01
2.4272698680 0.55672914668
0.96823445537 1.0055447350
1 p
0.37056694165 1.0000000000
1 p
0.10156100000 1.0000000000
4 d
37.713384723 0.11513835092E-01
10.692931184 0.67246343996E-01
3.6728446990 0.21484207775
1.3588590303 0.38890892779
1 d
0.49213295253 0.43040835243
1 d
0.16330520653 0.23253305465
1 d
0.54000000000E-01 0.0000000000
1 f
0.56200000000 1.0000000000
*
*

```

```
v def2-TZVP
# v      (17s11p7d1f) / [6s4p4d1f]      {842111/6311/4111/1}
*
```

```
  8 s
232340.65058      0.23072410092E-03
34828.841170     0.17888178962E-02
7926.5448691    0.92992490131E-02
2243.7733046    0.37761463347E-01
730.59322944    0.12255909662
262.32219631    0.28963508811
101.70403805    0.41004702955
40.064784617    0.21113610858
  4 s
255.24014968    -0.24458116338E-01
78.804646961    -0.11527205366
12.340598946    0.55174749453
5.1742019219    0.54504528489
  2 s
7.6513894469    -0.22967638286
1.2639759898    0.71683769077
  1 s
0.53861761721    1.0000000000
  1 s
0.92719296124E-01  1.0000000000
  1 s
0.34998055176E-01  1.0000000000
  6 p
1184.2369151    0.24449826729E-02
280.23075192    0.19643454466E-01
89.643627137    0.90796949190E-01
33.242411253    0.25650768222
13.144514452    0.40815393750
5.2948534140    0.23860378268
  3 p
20.175586851    -0.28241489023E-01
2.7605865197    0.55574635619
1.1008900902    0.99319919270
  1 p
0.42013310739    1.0000000000
  1 p
0.11124800000    1.0000000000
  4 d
43.861134864    0.11487174238E-01
12.516021891    0.68247153977E-01
4.3313854957    0.21837784195
1.6138855773    0.39245212296
  1 d
0.58749573961    0.42634466786
  1 d
0.19515723011    0.22646562601
  1 d
0.65000000000E-01  0.0000000000
  1 f
0.83100000000    1.0000000000
```

```
*
```

```
cr def2-TZVP
# cr      (17s11p7d1f) / [6s4p4d1f]      {842111/6311/4111/1}
*
```

```
  8 s
```

254477.80704	0.23386945693E-03
38131.797054	0.18142601800E-02
8675.2930607	0.94363925721E-02
2455.0099848	0.38343639367E-01
799.16217787	0.12459194837
286.90021489	0.29489696029
111.25413232	0.41846149607
43.864152636	0.21633763420
4 s	
279.32669173	-0.23450908111E-01
86.274732376	-0.11080370027
13.555756113	0.53028965842
5.6978112751	0.51603516947
2 s	
8.5636582615	-0.38109545675
1.3988296768	1.1991591436
1 s	
0.57288171116	1.0000000000
1 s	
0.90096171317E-01	1.0000000000
1 s	
0.34125885135E-01	1.0000000000
6 p	
1306.4398864	0.24277326185E-02
309.25311441	0.19544041017E-01
98.996273963	0.90651794553E-01
36.756916451	0.25699279154
14.566657077	0.40935504891
5.8739937432	0.23729388849
3 p	
22.890999695	-0.28166026613E-01
3.0855001822	0.56034120148
1.2132329118	0.98119019650
1 p	
0.44931680699	1.0000000000
1 p	
0.12067500000	1.0000000000
4 d	
43.720074476	0.13622964026E-01
12.391242652	0.78935180133E-01
4.2639442006	0.23833840000
1.5525221790	0.39526851122
1 d	
0.53761929485	0.41061717056
1 d	
0.16493173074	0.24440410795
1 d	
0.51000000000E-01	0.0000000000
1 f	
1.1470000000	1.0000000000
*	
*	
mn def2-TZVP	
# mn (17s11p7d1f) / [6s4p4d1f]	{842111/6311/4111/1}
*	
8 s	
277185.00153	0.22838385133E-03
41550.769890	0.17707650375E-02
9455.9700152	0.92077209994E-02
2676.5206482	0.37415971825E-01

871.46687530	0.12164861426
312.98306420	0.28824392499
121.44454051	0.41041600847
47.922598829	0.21372375145
4 s	
303.66723163	-0.24589926140E-01
93.881403187	-0.11602608038
14.879421214	0.55112059677
6.2865200745	0.53707560756
2 s	
9.4858591337	-0.22889262695
1.5698706158	0.71196169587
1 s	
0.65903213608	1.0000000000
1 s	
0.10686292371	1.0000000000
1 s	
0.39267435433E-01	1.0000000000
6 p	
1444.7978182	0.23994136455E-02
342.06551197	0.19369286864E-01
109.58400891	0.90236108988E-01
40.747988173	0.25745467851
16.188626566	0.41272351958
6.5484505964	0.24087700007
3 p	
25.357086437	-0.28707174058E-01
3.4830168782	0.55208100712
1.3858800906	0.97226901379
1 p	
0.52555094893	1.0000000000
1 p	
0.12765000000	1.0000000000
4 d	
56.563189119	0.11543245295E-01
16.278734711	0.70299845987E-01
5.6964273914	0.22450770821
2.1411147942	0.39703065434
1 d	
0.78291801938	0.41941039165
1 d	
0.25952311214	0.21887261673
1 d	
0.86000000000E-01	0.0000000000
1 f	
1.3260000000	1.0000000000
*	
*	
fe def2-TZVP	
# fe (17s11p7d1f) / [6s4p4d1f]	{842111/6311/4111/1}
*	
8 s	
300784.84637	0.22806273096E-03
45088.970557	0.17681788761E-02
10262.516317	0.91927083490E-02
2905.2897293	0.37355495807E-01
946.11487137	0.12151108426
339.87832894	0.28818881468
131.94425588	0.41126612677
52.111494077	0.21518583573

```

4 s
329.48839267      -0.24745216477E-01
101.92332739      -0.11683089050
16.240462745      0.55293621136
6.8840675801      0.53601640182
2 s
10.470693782      -0.22912708577
1.7360039648      0.71159319984
1 s
0.72577288979      1.00000000000
1 s
0.11595528203      1.00000000000
1 s
0.41968227746E-01  1.00000000000
6 p
1585.3959970      0.23793960179E-02
375.38006499      0.19253154755E-01
120.31816501      0.90021836536E-01
44.788749031      0.25798172356
17.829278584      0.41492649744
7.2247153786      0.24207474784
3 p
28.143219756      -0.29041755152E-01
3.8743241412      0.55312260343
1.5410752281      0.96771136842
1 p
0.58285615250      1.00000000000
1 p
0.13491500000      1.00000000000
4 d
61.996675034      0.11971972255E-01
17.873732552      0.73210135410E-01
6.2744782934      0.23103094314
2.3552337175      0.39910706494
1 d
0.85432239901      0.41391589765
1 d
0.27869254413      0.21909269782
1 d
0.91000000000E-01  0.00000000000
1 f
1.59800000000      1.00000000000
*
*
co def2-TZVP
# co      (17s11p7d1f) / [6s4p4d1f]      {842111/6311/4111/1}
*
8 s
325817.01553      0.22568462484E-03
48839.636453      0.17499397533E-02
11114.937307      0.91003134097E-02
3146.1603642      0.36996256837E-01
1024.4378465      0.12044269621
368.02508816      0.28598731649
142.91229205      0.40908312004
56.482649209      0.21500145739
4 s
356.40298318      -0.24767059678E-01
110.31165215      -0.11702139134
17.659634834      0.55215522200

```

7.5059030479	0.53246877060
2 s	
11.501807176	-0.22942470077
1.9081994606	0.71180933514
1 s	
0.79396696891	1.00000000000
1 s	
0.12444448829	1.00000000000
1 s	
0.44444645379E-01	1.00000000000
6 p	
1731.1369144	0.23905767685E-02
409.91750438	0.19382999967E-01
131.45648578	0.90905448509E-01
48.987439714	0.26146681577
19.537078992	0.42157264570
7.9287281634	0.24571813557
3 p	
31.076017584	-0.29438069973E-01
4.2835180697	0.55615568168
1.7022921563	0.96772195064
1 p	
0.64202908602	1.00000000000
1 p	
0.14130800000	1.00000000000
4 d	
68.140745239	0.11983845360E-01
19.685241019	0.73688540475E-01
6.9322128825	0.23085496779
2.6025125694	0.39281059225
1 d	
0.94016837302	0.40203412228
1 d	
0.30381457794	0.21415606743
1 d	
0.98000000000E-01	0.00000000000
1 f	
1.90300000000	1.00000000000
*	
*	
ni def2-TZVP	
# ni (17s11p7d1f) / [6s4p4d1f]	{842111/6311/4111/1}
*	
8 s	
351535.72935	0.22529386884E-03
52695.809283	0.17468616223E-02
11992.468293	0.90849992136E-02
3394.5776689	0.36940748447E-01
1105.3594585	0.12032819950
397.14677769	0.28596715057
154.27542974	0.40983020196
61.018723780	0.21620642851
4 s	
384.45559739	-0.24651279268E-01
119.04879199	-0.11658505277
19.137012223	0.54864126676
8.1526718562	0.52640051122
2 s	
12.579408642	-0.22797884293
2.0870866081	0.70703738215

1 s		
0.86432568555	1.0000000000	
1 s		
0.13283169217	1.0000000000	
1 s		
0.46845327726E-01	1.0000000000	
6 p		
1883.0907486	0.23748258443E-02	
445.95155320	0.19289457172E-01	
143.08430815	0.90718211507E-01	
53.372920722	0.26181414117	
21.321919357	0.42309149832	
8.6643561994	0.24641686015	
3 p		
34.144255211	-0.29677129163E-01	
4.7122455921	0.55616824096	
1.8709231845	0.96357766460	
1 p		
0.70370016267	1.0000000000	
1 p		
0.14658800000	1.0000000000	
4 d		
74.591603465	0.12077454672E-01	
21.590632752	0.74637262154E-01	
7.6246142580	0.23236775502	
2.8632206762	0.39042651680	
1 d		
1.0311063388	0.39509498921	
1 d		
0.33060760691	0.21138769167	
1 d		
0.10600000000	0.0000000000	
1 f		
2.1740000000	1.0000000000	
*		
*		
cu def2-TZVP		
# cu (17s11p7d1f) / [6s4p4d1f]	{842111/6311/4111/1}	
*		
8 s		
377518.79923	0.22811766128E-03	
56589.984311	0.17688035931E-02	
12878.711706	0.91993460227E-02	
3645.3752143	0.37411016434E-01	
1187.0072945	0.12189873737	
426.46421902	0.28983900714	
165.70660164	0.41531872174	
65.598942707	0.21905799287	
4 s		
414.41265811	-0.24682525053E-01	
128.32056039	-0.11716827406	
20.622089750	0.55301315941	
8.7821226045	0.52242718609	
2 s		
13.741372006	-0.22736061821	
2.2431246833	0.71761210873	
1 s		
0.89370549079	1.0000000000	
1 s		
0.10836699534	1.0000000000	

```

1 s
0.38806178058E-01 1.0000000000
6 p
2034.7596692 0.23524822298E-02
481.90468106 0.19134070751E-01
154.67482963 0.90171105278E-01
57.740576969 0.26063284735
23.099052811 0.42093485770
9.3882478591 0.24344615121
3 p
37.596171210 -0.28991094530E-01
5.1240690810 0.54919083831
2.0119996085 0.93793330488
1 p
0.73860686002 1.0000000000
1 p
0.15506500000 1.0000000000
4 d
74.129460637 0.14363216676E-01
21.359842587 0.86628177096E-01
7.4995240537 0.25631430541
2.7601394169 0.40374062368
1 d
0.95362061236 0.39427042447
1 d
0.28420862520 0.23091146816
1 d
0.85000000000E-01 0.0000000000
1 f
2.23300000000 1.0000000000
*
*
zn def2-TZVP
# zn (17s12p7d1f) / [6s5p4d1f] {842111/63111/4111/1}
*
8 s
405924.31028 0.22442017483E-03
60846.955735 0.17402086626E-02
13847.343092 0.90513339565E-02
3919.6158551 0.36817341445E-01
1276.3594167 0.12004850256
458.67254435 0.28576057621
178.28725246 0.41087462062
70.612192837 0.21816962456
4 s
443.88077950 -0.24934274984E-01
137.55875267 -0.11817955766
22.268083479 0.55367318468
9.5217310606 0.52628934936
2 s
14.874114065 -0.22929955254
2.4647517612 0.71135484742
1 s
1.0113272238 1.0000000000
1 s
0.14919852089 1.0000000000
1 s
0.51441872981E-01 1.0000000000
6 p
2205.3508534 0.23356240448E-02

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522.35300699	0.19031022634E-01
167.73055542	0.89955758675E-01
62.670045373	0.26113248631
25.109749456	0.42348448173
10.225142681	0.24618926885
3 p	
40.713442521	-0.30029667592E-01
5.6247090696	0.55575254864
2.2279949116	0.95581013442
1 p	
0.83354741691	1.0000000000
1 p	
0.16245500000	1.0000000000
1 p	
0.47769000000E-01	1.0000000000
4 d	
88.554315311	0.12728170015E-01
25.721525557	0.79394499843E-01
9.1278367624	0.24491506805
3.4312364064	0.40390526479
1 d	
1.2308920645	0.40158491145
1 d	
0.39031845112	0.21579805034
1 d	
0.12400000000	0.0000000000
1 f	
2.6140000000	1.0000000000
*	
*	
ga def2-TZVP	
# ga (17s12p8d1f) / [6s5p4d1f] {842111/63111/5111/1}	
*	
8 s	
435548.66254	0.23646329650E-03
65289.589031	0.18335271776E-02
14858.784256	0.95371863081E-02
4205.9734729	0.38803412468E-01
1369.6416431	0.12661604848
492.30348905	0.30175310292
191.41923233	0.43543934218
75.840558665	0.23282363780
4 s	
474.30810613	-0.26743707958E-01
147.10297560	-0.12654657542
23.982599435	0.58840346839
10.298230094	0.56324271589
2 s	
16.050381430	-0.24516439508
2.6988468784	0.74578049593
1 s	
1.1428588736	1.0000000000
1 s	
0.20217652251	1.0000000000
1 s	
0.71980152032E-01	1.0000000000
6 p	
2432.0171070	0.22434065928E-02
576.12049582	0.18342265336E-01
185.11584354	0.87279697167E-01

69.246572556	0.25684868351
27.818107777	0.42398378107
11.420229938	0.25701340043
3 p	
42.819661530	-0.19326519119E-01
6.3885901000	0.31571386917
2.6698993326	0.57617792822
1 p	
1.0781783834	1.0000000000
1 p	
0.22796559371	1.0000000000
1 p	
0.62836234833E-01	1.0000000000
5 d	
103.92331829	0.11464613652E-01
30.371094389	0.73625747383E-01
10.872078097	0.23505107382
4.1549137954	0.40318563513
1.5345659145	0.40824748152
1 d	
0.51114263830	0.20502439263
1 d	
0.30622000000	1.0000000000
1 d	
0.11391309000	1.0000000000
1 f	
0.30996095000	1.0000000000
*	
*	
ge def2-TZVP	
# ge (17s12p8d1f) / [6s5p4d1f]	{842111/63111/5111/1}
*	
8 s	
466115.00592	0.22487264660E-03
69875.420762	0.17435426729E-02
15903.276716	0.90691482206E-02
4501.8233453	0.36906174685E-01
1466.0570924	0.12050167907
527.07841728	0.28748641703
205.00395074	0.41622321885
81.251596065	0.22397845695
4 s	
505.74661282	-0.25184609291E-01
156.96593744	-0.11898929721
25.761448176	0.54930135870
11.106654687	0.52939309129
2 s	
17.272059104	-0.22854595728
2.9438289048	0.68377930317
1 s	
1.2839164916	1.0000000000
1 s	
0.25873337445	1.0000000000
1 s	
0.93524913177E-01	1.0000000000
6 p	
2633.9346241	0.22143925310E-02
624.00161628	0.18140899141E-01
200.58528404	0.86632184922E-01
75.097081525	0.25649020592

30.214388474	0.42658611262
12.440087567	0.26200527313
3 p	
45.981316002	-0.20321767678E-01
6.9945654416	0.32013744527
2.9686001327	0.59051014555
1 p	
1.2320988495	1.0000000000
1 p	
0.28981614974	1.0000000000
1 p	
0.85564606447E-01	1.0000000000
5 d	
119.44887581	0.10586544521E-01
35.062915293	0.69601280945E-01
12.636924529	0.22807035287
4.8888672922	0.40301067220
1.8453195392	0.41304847015
1 d	
0.63571158892	0.19639209740
1 d	
0.35492132000	1.0000000000
1 d	
0.13155709000	1.0000000000
1 f	
0.36210645000	1.0000000000
*	
*	
as def2-TZVP	
# as (17s13p8d1f) / [6s5p4d1f]	{842111/64111/5111/1}
*	
8 s	
498032.42158	0.22740196900E-03
74656.868743	0.17632816413E-02
16990.960004	0.91728040381E-02
4809.6200321	0.37337829344E-01
1566.2887055	0.12199536117
563.21360499	0.29137475324
219.11179978	0.42326351479
86.866061030	0.22921464278
4 s	
538.19512479	-0.25254197297E-01
167.14850224	-0.11915461115
27.605517159	0.54628495980
11.947858521	0.53001520976
2 s	
18.538023133	-0.23479188136
3.2018985739	0.69167053428
1 s	
1.4356522077	1.0000000000
1 s	
0.31837805200	1.0000000000
1 s	
0.11622632186	1.0000000000
6 p	
2678.9421546	0.23318955287E-02
634.61765840	0.19042149977E-01
203.93967606	0.90229744913E-01
76.323890369	0.26169037693
30.664124943	0.41857168155

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12.505056732      0.23447830190
 4 p
49.256229549     -0.21235539870E-01
7.7274891466     0.30470206668
3.5410493476     0.52888373107
1.6985585501     0.37272250955
 1 p
0.76848071044    1.00000000000
 1 p
0.30050823260    1.00000000000
 1 p
0.98190639437E-01 1.00000000000
 5 d
135.33289305     0.99291144106E-02
39.860212744     0.66568843496E-01
14.446428359     0.22275768307
5.6432900356     0.40309224382
2.1668188623     0.41671667946
 1 d
0.76514970569    0.18935502288
 1 d
0.42434653000    1.00000000000
 1 d
0.16331527000    1.00000000000
 1 f
0.43271941000    1.00000000000
*
*
se def2-TZVP
# se      (17s13p8d1f) / [6s5p4d1f]      {842111/64111/5111/1}
*
 8 s
531071.66696     0.24108973168E-03
79603.044117     0.18696431441E-02
18115.844240     0.97271616536E-02
5127.8923194     0.39604793031E-01
1669.9130839     0.12948855136
600.57534527     0.30959437289
233.70021247     0.45115769216
92.672443932     0.24579189033
 4 s
571.57513675     -0.26895707881E-01
177.63686375     -0.12670989353
29.517767052     0.57699001719
12.824399795     0.56369075408
 2 s
19.848235841     -0.25132415534
3.4744018486     0.72905416980
 1 s
1.5988910849     1.00000000000
 1 s
0.38333469387     1.00000000000
 1 s
0.14049742459     1.00000000000
 6 p
2815.3500566     0.25569026854E-02
666.92558298     0.20874026901E-01
214.34213188     0.98772096250E-01
80.246687942     0.28471821221
32.251081288     0.45003584934

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13.106432562	0.24416091055	
4 p		
53.366108516	-0.21558456273E-01	
8.1827777195	0.32662310638	
3.6239945672	0.57740499319	
1.6341591401	0.34301320826	
1 p		
0.58418320228	1.0000000000	
1 p		
0.23966269279	1.0000000000	
1 p		
0.88785134803E-01	1.0000000000	
5 d		
151.82910279	0.93970276988E-02	
44.839992523	0.64086503991E-01	
16.328999510	0.21834238004	
6.4305057612	0.40314789649	
2.5048025169	0.41966491490	
1 d		
0.90271148434	0.18366663432	
1 d		
0.47683613000	1.0000000000	
1 d		
0.18535160000	1.0000000000	
1 f		
0.48866905000	1.0000000000	
*		
*		
br def2-TZVP		
# br (17s13p8d1f) / [6s5p4d1f]	{842111/64111/5111/1}	
*		
8 s		
565073.25256	0.23660314690E-03	
84701.723179	0.18348332508E-02	
19276.271900	0.95465849860E-02	
5456.4284576	0.38877142153E-01	
1776.9503500	0.12718314231	
639.19398276	0.30437662191	
248.78823961	0.44490940497	
98.678305494	0.24381643058	
4 s		
606.07824568	-0.26527158709E-01	
188.45598484	-0.12484584809	
31.497144506	0.56468683559	
13.736008320	0.55555268564	
2 s		
21.203212766	-0.24940920493	
3.7616420178	0.71213119743	
1 s		
1.7735933962	1.0000000000	
1 s		
0.45197413664	1.0000000000	
1 s		
0.16613377099	1.0000000000	
6 p		
3019.6955723	0.24971049798E-02	
715.35481126	0.20419267596E-01	
229.98328751	0.96897148309E-01	
86.167844615	0.28053901252	
34.667870802	0.44606390473	

14.113870307	0.24410073923	
4 p		
57.085653082	-0.21855950710E-01	
8.8193845840	0.32707075320	
3.9340302872	0.57855229520	
1.7998830384	0.33570987698	
1 p		
0.66899410512	1.0000000000	
1 p		
0.27136238231	1.0000000000	
1 p		
0.10083790243	1.0000000000	
5 d		
168.85370257	0.89663981988E-02	
49.977949919	0.62062059316E-01	
18.274913338	0.21474732384	
7.2455694631	0.40335336746	
2.8562315025	0.42208813080	
1 d		
1.0459621144	0.17874813267	
1 d		
0.56865655000	1.0000000000	
1 d		
0.22031490000	1.0000000000	
1 f		
0.57083312000	1.0000000000	
*		
*		
kr def2-TZVP		
# kr (17s13p8d1f) / [6s5p4d1f]	{842111/64111/5111/1}	
*		
8 s		
600250.97575	0.23740610399E-03	
89976.650781	0.18410240539E-02	
20476.814225	0.95795580699E-02	
5796.1554078	0.39020650488E-01	
1887.5913196	0.12772645628	
679.11458519	0.30596521300	
264.38244511	0.44857474437	
104.88368574	0.24722957327	
4 s		
641.47370764	-0.26745279805E-01	
199.57524820	-0.12571122567	
33.545462954	0.56483736390	
14.683955144	0.55972765539	
2 s		
22.603101860	-0.25298771800	
4.0650682991	0.70992159965	
1 s		
1.9611027060	1.0000000000	
1 s		
0.52465147979	1.0000000000	
1 s		
0.19332399511	1.0000000000	
6 p		
3232.9589614	0.24885607974E-02	
765.96442694	0.20379007428E-01	
246.33940810	0.96977188584E-01	
92.365283041	0.28199960954	
37.199509551	0.45116254358	

15.172166534	0.24917131496
4 p	
60.931321698	-0.22173603519E-01
9.4792600646	0.32838462778
4.2564686326	0.58124997120
1.9729313762	0.32863541783
1 p	
0.76337108716	1.0000000000
1 p	
0.30943625526	1.0000000000
1 p	
0.11569704458	1.0000000000
5 d	
186.41760904	0.86120284601E-02
55.274124345	0.60394406304E-01
20.283219120	0.21181331869
8.0884536976	0.40366293413
3.2214033853	0.42402860686
1 d	
1.1952170102	0.17441742274
1 d	
0.64800000000	1.0000000000
1 d	
0.25100000000	1.0000000000
1 f	
0.62800000000	1.0000000000
*	
*	
rb def2-TZVP	
# rb (7s7p3d) / [6s4p3d] {211111/4111/111}	
*	
2 s	
7.4744618040	0.26997866363
6.7296180594	-0.42629251814
1 s	
2.7816640004	1.0000000000
1 s	
0.53452175148	1.0000000000
1 s	
0.22368793034	1.0000000000
1 s	
0.32410407052E-01	1.0000000000
1 s	
0.14171047424E-01	1.0000000000
4 p	
5.6720643194	0.48114224135E-01
3.3320183956	-0.18485131426
0.80150054910	0.42811864954
0.36302220227	0.58673165411
1 p	
0.15733924392	1.0000000000
1 p	
0.40000000000E-01	1.0000000000
1 p	
0.16000000000E-01	1.0000000000
1 d	
0.25907866956	0.76806746340E-01
1 d	
0.42507438045E-01	0.37846160487
1 d	

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0.11909276840E-01  1.0000000000
*
rb def2-ecp
*
  ncore =    28          lmax =    3
#   coefficient  r^n      exponent
f      -12.3169000    2        3.8431140
s-f      89.5001980    2        5.0365510
         0.4937610    2        1.9708490
         12.3169000    2        3.8431140
p-f      58.5689740    2        4.2583410
         0.4317910    2        1.4707090
         12.3169000    2        3.8431140
d-f      26.2248980    2        3.0231270
         0.9628390    2        0.6503830
         12.3169000    2        3.8431140
*
*
sr def2-TZVP
# sr      (7s7p5d) / [6s4p3d]      {211111/4111/311}
*
  2  s
  10.000000000    -0.18530550262
  8.5000000000    0.33970355376
  1  s
  3.0057048856    1.0000000000
  1  s
  0.61161287650    1.0000000000
  1  s
  0.27393841217    1.0000000000
  1  s
  0.57435564563E-01  1.0000000000
  1  s
  0.23338198665E-01  1.0000000000
  4  p
  7.5883077869    0.33731690287E-01
  3.6731307392    -0.20523185005
  0.90496618455    0.49209972665
  0.43310256408    0.62105296512
  1  p
  0.20222168964    1.0000000000
  1  p
  0.72000000000E-01  1.0000000000
  1  p
  0.25000000000E-01  1.0000000000
  3  d
  3.6180810000    -0.75010000000E-02
  0.99665600000    0.10809800000
  0.39073500000    0.27854000000
  1  d
  0.12277000000    1.0000000000
  1  d
  0.36655000000E-01  1.0000000000
*
sr def2-ecp
*

```



```

ncore = 28          lmax = 3
# coefficient      r^n      exponent
f
-15.8059920      2          4.6339750
s-f
135.4794300     2          7.4000740
17.5344630      2          3.6063790
15.8059920      2          4.6339750
p-f
88.3597090      2          6.4848680
15.3943720      2          3.2880530
15.8059920      2          4.6339750
d-f
29.8889870      2          4.6228410
6.6594140       2          2.2469040
15.8059920      2          4.6339750
*
*
y def2-TZVP
# y      (7s7p5d1f) / [6s4p3d1f]      {211111/4111/311/1}
*
2 s
10.000000000    -0.17487686796
8.500000000     0.34152345084
1 s
3.3653905454    1.00000000000
1 s
0.68860679385    1.00000000000
1 s
0.31191502936    1.00000000000
1 s
0.70326042567E-01  1.00000000000
1 s
0.27733859327E-01  1.00000000000
4 p
8.0554093616     0.36410978939E-01
4.0163458751    -0.20872572547
1.0232915404     0.48956929335
0.49843561636    0.60611943833
1 p
0.23307661842    1.00000000000
1 p
0.80000000000E-01  1.00000000000
1 p
0.27000000000E-01  1.00000000000
3 d
3.9030833060    -0.98209792625E-02
1.1363234302     0.19183629664
0.45617043877    0.40597788539
1 d
0.17470950748    1.00000000000
1 d
0.61978796638E-01  1.00000000000
1 f
0.26515000000    1.00000000000
*
y def2-ecp
*
ncore = 28          lmax = 3
# coefficient      r^n      exponent

```

```

f
    -19.1221981    2    6.5842120
    -2.4363754    2    3.2921060
s-f
    135.1538441    2    7.4880494
    15.5524413    2    3.7440247
    19.1221981    2    6.5842120
    2.4363754    2    3.2921060
p-f
    87.7849917    2    6.4453772
    11.5640660    2    3.2226886
    19.1221981    2    6.5842120
    2.4363754    2    3.2921060
d-f
    29.7010007    2    4.6584472
    5.5399685    2    2.3292236
    19.1221981    2    6.5842120
    2.4363754    2    3.2921060
*
*
zr def2-TZVP
# zr      (7s7p5d1f) / [6s4p3d1f]      {211111/4111/311/1}
*
    2 s
    11.0000000000    -0.19075595257
    9.5000000000    0.33895588754
    1 s
    3.6383667759    1.0000000000
    1 s
    0.76822026698    1.0000000000
    1 s
    0.34036824036    1.0000000000
    1 s
    0.75261298085E-01    1.0000000000
    1 s
    0.30131404705E-01    1.0000000000
    4 p
    8.6066305543    0.40404260236E-01
    4.4400979958    -0.21187745201
    1.1281026946    0.49164266891
    0.54346076310    0.57303370658
    1 p
    0.25022406048    1.0000000000
    1 p
    0.85000000000E-01    1.0000000000
    1 p
    0.29000000000E-01    1.0000000000
    3 d
    4.5567957795    -0.96190569023E-02
    1.2904939797    0.20569990155
    0.51646987222    0.41831381851
    1 d
    0.19349797794    1.0000000000
    1 d
    0.67309809967E-01    1.0000000000
    1 f
    0.39261000000    1.0000000000
*
zr def2-ecp
*

```

```

ncore = 28          lmax = 3
# coefficient      r^n      exponent
f
  -21.0937760      2          7.5400000
  -3.0806943      2          3.7700000
s-f
  150.2675911     2          8.2000000
  18.9762165     2          4.0897278
  21.0937760     2          7.5400000
  3.0806943      2          3.7700000
p-f
  99.6221237     2          7.1100000
  14.1687333     2          3.5967980
  21.0937760     2          7.5400000
  3.0806943      2          3.7700000
d-f
  35.0451235     2          5.3500000
  6.1112595     2          2.4918215
  21.0937760     2          7.5400000
  3.0806943      2          3.7700000
*
*
nb def2-TZVP
# nb      (7s7p5d1f) / [6s4p3d1f]      {211111/4111/311/1}
*
  2 s
  12.000000000    -0.20219507530
  10.500000000    0.33640105939
  1 s
  3.9276062854    1.00000000000
  1 s
  0.85976543258    1.00000000000
  1 s
  0.39074087505    1.00000000000
  1 s
  0.86387259879E-01  1.00000000000
  1 s
  0.32906200326E-01  1.00000000000
  4 p
  9.2056285646     0.43347689874E-01
  4.8679632125    -0.21302479233
  1.2442155792     0.48102127136
  0.60390590312    0.53917858960
  1 p
  0.27967675553    1.00000000000
  1 p
  0.90000000000E-01  1.00000000000
  1 p
  0.30000000000E-01  1.00000000000
  3 d
  4.6170975867    -0.13574476955E-01
  1.5663438480     0.20374310496
  0.66952425826    0.42997453105
  1 d
  0.27140946867    1.00000000000
  1 d
  0.10054426592    1.00000000000
  1 f
  0.52270000000    1.00000000000
*

```

nb def2-ecp

```
*
# ncore = 28          lmax = 3
# coefficient r^n      exponent
f      -22.9295500    2          8.4900000
      -3.6663099     2          4.2500000
s-f    165.1791435    2          8.9000000
      21.9929744     2          4.4300000
      22.9295500     2          8.4900000
      3.6663099      2          4.2500000
p-f    111.7944145    2          7.7700000
      16.6334833     2          3.9600000
      22.9295500     2          8.4900000
      3.6663099      2          4.2500000
d-f    38.1122488     2          6.0500000
      8.0391673      2          2.8400000
      22.9295500     2          8.4900000
      3.6663099      2          4.2500000
*
*
```

mo def2-TZVP

```
# mo      (7s7p5d1f) / [6s4p3d1f]      {211111/4111/311/1}
```

```
*
*
2 s
14.000000000    -0.22490043406
12.500000000    0.33151248555
1 s
4.0921501803    1.00000000000
1 s
0.97053602586    1.00000000000
1 s
0.44217620170    1.00000000000
1 s
0.92915024334E-01  1.00000000000
1 s
0.35016314389E-01  1.00000000000
4 p
8.8931117915    0.69994449475E-01
5.4689112270    -0.23547141883
1.3548473007    0.46315460007
0.65494867461    0.48820184710
1 p
0.30428197472    1.00000000000
1 p
0.10000000000    1.00000000000
1 p
0.33000000000E-01  1.00000000000
3 d
5.0044445497    -0.21587364862E-01
1.7736823324    0.20958680086
0.76950591696    0.43730880599
1 d
0.31530878939    1.00000000000
1 d
0.11754374390    1.00000000000
1 f
```

```

0.65545000000      1.0000000000
*
mo def2-ecp
*
  ncore =      28          lmax =      3
#   coefficient   r^n      exponent
f      -24.8051771      2      9.4500000
      -4.1537815      2      4.7200000
s-f      180.1031085      2      9.7145938
      24.9972279      2      4.6805004
      24.8051771      2      9.4500000
      4.1537815      2      4.7200000
p-f      123.7727523      2      8.1421366
      19.5302280      2      4.6259863
      24.8051771      2      9.4500000
      4.1537815      2      4.7200000
d-f      48.3750223      2      6.6184148
      8.8920527      2      3.2487516
      24.8051771      2      9.4500000
      4.1537815      2      4.7200000
*
*
tc def2-TZVP
# tc      (7s7p5d1f) / [6s4p3d1f]      {211111/4111/311/1}
*
  2 s
  15.000000000      -0.19945408941
  12.910581694      0.33689922245
  1 s
  4.4493321158      1.0000000000
  1 s
  1.0548409451      1.0000000000
  1 s
  0.47909677246      1.0000000000
  1 s
  0.99124162989E-01      1.0000000000
  1 s
  0.36882799789E-01      1.0000000000
  4 p
  10.027138011      0.61481602710E-01
  5.8463419741      -0.23600729385
  1.4968345491      0.47746483995
  0.72934632066      0.50731543496
  1 p
  0.33913558879      1.0000000000
  1 p
  0.11000000000      1.0000000000
  1 p
  0.35000000000E-01      1.0000000000
  3 d
  5.0906268699      -0.32176405405E-01
  2.0156178510      0.21280802536
  0.88113887240      0.44403309175
  1 d
  0.36427094833      1.0000000000
  1 d

```

```

0.13678402297      1.0000000000
 1 f
0.79085000000     1.0000000000
*
tc def2-ecp
*
  ncore =      28          lmax =      3
#   coefficient   r^n      exponent
f
    -26.5624475    2        10.4000000
    -4.5856805    2         5.2000000
s-f
    195.1591659    2        10.4223462
    28.0926033    2         5.0365160
    26.5624475    2        10.4000000
    4.5856805     2         5.2000000
p-f
    135.2845662    2         8.9504494
    21.8065043    2         4.8544394
    26.5624475    2        10.4000000
    4.5856805     2         5.2000000
d-f
    54.3297294    2         6.9456968
    11.1550679    2         3.9705849
    26.5624475    2        10.4000000
    4.5856805     2         5.2000000
*
*
ru def2-TZVP
# ru   (7s7p5d1f) / [6s4p3d1f]   {211111/4111/311/1}
*
  2 s
16.000000000     -0.20634002919
13.910581694     0.33550437725
  1 s
4.7967971407     1.00000000000
  1 s
1.1555425594     1.00000000000
  1 s
0.52455741182     1.00000000000
  1 s
0.10734572646     1.00000000000
  1 s
0.39432760192E-01 1.00000000000
  4 p
11.187208671     0.53225073263E-01
 6.2477688734    -0.22731662050
 1.6279472859     0.47869486056
0.79326493538     0.50213311567
  1 p
0.36707276865     1.00000000000
  1 p
0.11500000000     1.00000000000
  1 p
0.37000000000E-01 1.00000000000
  3 d
 5.7341846619    -0.35266111560E-01
 2.2483686294     0.21802502222
0.98376978359     0.44709565013
  1 d

```

```

0.40379445583      1.0000000000
  1 d
0.14978618173      1.0000000000
  1 f
0.94314000000      1.0000000000
*
ru def2-ecp
*
  ncore =    28      lmax =    3
#      coefficient  r^n      exponent
f
      -28.3406163    2      11.3600000
      -4.9446292    2      5.6800000
s-f
      209.8229712    2      11.1052693
      30.6547264    2      5.4147454
      28.3406163    2      11.3600000
      4.9446292    2      5.6800000
p-f
      146.3361823    2      9.7712707
      24.1278772    2      5.0739908
      28.3406163    2      11.3600000
      4.9446292    2      5.6800000
d-f
      67.5158967    2      7.6714231
      9.8701041    2      4.1365647
      28.3406163    2      11.3600000
      4.9446292    2      5.6800000
*
*
rh def2-TZVP
# rh      (7s7p6d1f) / [6s4p3d1f]      {211111/4111/411/1}
*
  2 s
  17.000000000      -0.16690803139
  13.910581694      0.34235001652
  1 s
  5.2481265288      1.0000000000
  1 s
  1.2262575928      1.0000000000
  1 s
  0.53930216349      1.0000000000
  1 s
  0.10130730377      1.0000000000
  1 s
  0.37124139005E-01  1.0000000000
  4 p
  11.767103631      0.59494859388E-01
  6.7485133083      -0.23735853477
  1.7502679834      0.49019334303
  0.84321166133      0.50623933751
  1 p
  0.38295544759      1.0000000000
  1 p
  0.11500000000      1.0000000000
  1 p
  0.37000000000E-01  1.0000000000
  4 d
  19.857830136      0.66960778187E-02
  10.061378139      -0.21981738213E-01

```

```

2.2619546477      0.37918706236
0.97098845035      0.67289976592
  1 d
0.38391195297      1.0000000000
  1 d
0.13537026904      1.0000000000
  1 f
1.0949900000      1.0000000000
*
rh def2-ecp
*
  ncore =      28      lmax =      3
#      coefficient      r^n      exponent
f
      -30.0934557      2      12.3100000
      -5.2184819      2      6.1600000
s-f
      225.3477535      2      11.7200000
      32.8231890      2      5.8200000
      30.0934557      2      12.3100000
      5.2184819      2      6.1600000
p-f
      158.7094116      2      10.4200000
      26.4441005      2      5.4500000
      30.0934557      2      12.3100000
      5.2184819      2      6.1600000
d-f
      62.7586257      2      8.8200000
      10.9787195      2      3.8700000
      30.0934557      2      12.3100000
      5.2184819      2      6.1600000
*
*
pd def2-TZVP
# pd      (7s7p6d1f) / [6s4p3d1f]      {211111/4111/411/1}
*
  2 s
18.000000000      -0.16605388598
14.662134308      0.34899955055
  1 s
5.6388709265      1.0000000000
  1 s
1.3198953252      1.0000000000
  1 s
0.57817908509      1.0000000000
  1 s
0.10352166239      1.0000000000
  1 s
0.37548442674E-01      1.0000000000
  4 p
12.552899300      0.61728998206E-01
7.2444496380      -0.24178626753
1.8905941078      0.49453200915
0.90737168760      0.50454362626
  1 p
0.40877210813      1.0000000000
  1 p
0.11500000000      1.0000000000
  1 p
0.37000000000E-01      1.0000000000

```



```

4 d
22.357457575      0.39559479546E-02
10.682526382     -0.14039011601E-01
2.4858232550      0.24219476776
1.0735333903      0.42580283281
1 d
0.42613842853     1.00000000000
1 d
0.15046355385     1.00000000000
1 f
1.2462900000      1.00000000000
*
pd def2-ecp
*
ncore = 28          lmax = 3
# coefficient      r^n      exponent
f
-31.9295543       2        13.2700000
-5.3982169        2        6.6300000
s-f
240.2290403       2        12.4300000
35.1719435        2        6.1707594
31.9295543       2        13.2700000
5.3982169         2        6.6300000
p-f
170.4172760       2        11.0800000
28.4721329        2        5.8295541
31.9295543       2        13.2700000
5.3982169         2        6.6300000
d-f
69.0138449        2        9.5100000
11.7508616        2        4.1397811
31.9295543       2        13.2700000
5.3982169         2        6.6300000
*
*
ag def2-TZVP
# ag (7s7p6d1f) / [6s4p3d1f] {211111/4111/411/1}
*
2 s
19.000000000      -0.16600104141
15.428199933      0.35665095918
1 s
6.0553507268      1.00000000000
1 s
1.4162368935      1.00000000000
1 s
0.61758635858     1.00000000000
1 s
0.10474197431     1.00000000000
1 s
0.37685106264E-01 1.00000000000
4 p
13.188180180      0.66928737147E-01
7.7952789138      -0.24735235409
2.0351571912      0.49154280216
0.98093914842     0.49741609006
1 p
0.44451179958     1.00000000000
1 p

```

```

0.130000000000      1.0000000000
  1 p
0.412000000000E-01  1.0000000000
  4 d
 25.784397351      0.35645063082E-02
 11.396636755      -0.12984262784E-01
  2.7345581361      0.24108826548
  1.1873583605      0.42412330744
  1 d
0.47316910566      1.0000000000
  1 d
0.16746017986      1.0000000000
  1 f
  1.3971100000      1.0000000000
*
ag def2-ecp
*
  ncore =    28      lmax =    3
#      coefficient  r^n      exponent
f
      -33.6899201    2      14.2200000
      -5.5311202    2      7.1100000
s-f
      255.1393645    2      13.1300000
      36.8661215    2      6.5100000
      33.6899201    2      14.2200000
      5.5311202     2      7.1100000
p-f
      182.1818687    2      11.7400000
      30.3577515    2      6.2000000
      33.6899201    2      14.2200000
      5.5311202     2      7.1100000
d-f
      73.7192609     2      10.2100000
      12.5021171     2      4.3800000
      33.6899201     2      14.2200000
      5.5311202     2      7.1100000
*
*
cd def2-TZVP
# cd      (7s7p6d1f) / [6s4p3d1f]      {211111/4111/411/1}
*
  2 s
 20.0000000000      -0.17401196927
 16.309051661      0.37137277194
  1 s
  6.4512709901      1.0000000000
  1 s
  1.5350047390      1.0000000000
  1 s
0.68983631523      1.0000000000
  1 s
0.13475720977      1.0000000000
  1 s
0.47416874527E-01  1.0000000000
  4 p
 14.000681404      0.69333062793E-01
  8.3094019872      -0.25420103681
  2.2020058122      0.49200980368
  1.0779246137      0.49702118131

```

```

1 p
0.50111879846      1.0000000000
1 p
0.160000000000    1.0000000000
1 p
0.516000000000E-01  1.0000000000
4 d
30.380789793      0.32545123835E-02
11.474551578      -0.14212074843E-01
3.0507394903      0.24961756436
1.3622028524      0.44905635176
1 d
0.56399409888     1.0000000000
1 d
0.20916686535     1.0000000000
1 f
1.5981300000      1.0000000000
*
cd def2-ecp
*
ncore = 28          lmax = 3
# coefficient      r^n          exponent
f
-35.4766256       2            15.1847957
-5.6176768        2            7.5923978
s-f
270.0094832       2            13.8358689
38.7673080        2            6.8572704
35.4766256        2            15.1847957
5.6176768         2            7.5923978
p-f
193.8296294       2            12.4049710
31.8965252        2            6.5677995
35.4766256        2            15.1847957
5.6176768         2            7.5923978
d-f
79.1936470        2            10.8969253
13.2308267        2            4.6411649
35.4766256        2            15.1847957
5.6176768         2            7.5923978
*
*
in def2-TZVP
# in (10s9p8d2f) / [6s5p3d2f] {421111/33111/611/11}
*
4 s
847.79276774      0.12432052471E-03
72.041054824      0.23600367607E-02
41.061316522      -0.85588299453E-02
12.407609713      0.62952032489
2 s
11.640316941      1.5543429200
6.3695642727      0.67492488361
1 s
1.7063236353      1.0000000000
1 s
0.78666967936     1.0000000000
1 s
0.16965196873     1.0000000000
1 s

```

```

0.62074858667E-01  1.0000000000
  3 p
268.28136685      0.11542193636E-03
14.781553782     0.77779830292E-01
8.8041476194     -0.28332389472
  3 p
2.3717277227     0.47896111744
1.1927065422     0.48293819961
0.58352812041    0.16843883728
  1 p
0.23280968310    1.0000000000
  1 p
0.88674065208E-01 1.0000000000
  1 p
0.33598828267E-01 1.0000000000
  6 d
94.282575063     0.43652729696E-03
19.716431102     0.63918753088
19.600106824     -0.64663115577
3.5643186737     0.21187579614
1.7017801400     0.42129321741
0.76456615531    0.38418127707
  1 d
0.31826765584    1.0000000000
  1 d
0.10000000000    1.0000000000
  1 f
0.26415991000    1.0000000000
  1 f
0.90000000000    1.0000000000
*
in def2-ecp
*
  ncore =    28          lmax =    3
#   coefficient  r^n      exponent
f
   -13.7280780    2        12.5390560
   -18.2068660    2        12.5525610
s-f
   281.1223500    2        15.3928220
   61.9014700    2         8.0558640
   13.7280780    2        12.5390560
   18.2068660    2        12.5525610
p-f
   67.4621540    2        13.9286720
  134.9492500    2        13.3472340
   14.7461400    2         7.6141320
   29.6392620    2         7.3183650
   13.7280780    2        12.5390560
   18.2068660    2        12.5525610
d-f
   35.4932540    2        14.0347150
   53.1787730    2        14.5116160
    9.1772810    2         5.5505500
   12.3924100    2         5.0594150
   13.7280780    2        12.5390560
   18.2068660    2        12.5525610
*
*
sn def2-TZVP

```

sn (10s9p8d2f) / [6s5p3d2f] {421111/331111/611/11}

```

*
  4 s
1577.0715931      0.17042767713E-03
235.26601078     0.81467057272E-03
38.206330645     -0.39057904293E-02
13.097031765     0.53245922343
  2 s
11.681492759     1.5435287275
5.9647604361     0.76421510041
  1 s
1.8891070740     1.0000000000
  1 s
0.88514080630     1.0000000000
  1 s
0.20500105152     1.0000000000
  1 s
0.76748551032E-01 1.0000000000
  3 p
221.55767496     0.31125177983E-03
21.084021433     0.31108097016E-01
8.7600138521     -0.27571560918
  3 p
2.5912909722     0.45912328666
1.3426801157     0.49682867217
0.67732735829     0.18962377821
  1 p
0.29418756752     1.0000000000
  1 p
0.11863762052     1.0000000000
  1 p
0.46215750632E-01 1.0000000000
  6 d
108.33210154     0.46561853277E-03
23.703936630     0.54063163067E-01
22.339843906     -0.58928768877E-01
4.0874834028     0.19588500896
1.9737354146     0.42301799185
0.90158257692     0.39252716176
  1 d
0.38237153649     1.0000000000
  1 d
0.12000000000     1.0000000000
  1 f
0.29392848500     1.0000000000
  1 f
1.00000000000     1.0000000000

```

*
sn def2-ecp

```

*
ncore = 28      lmax = 3
#      coefficient  r^n      exponent
f      -12.5763330   2        12.2823480
      -16.5959440   2        12.2721500
s-f    279.9886820   2        17.4204140
      62.3778100   2         7.6311550
      12.5763330   2        12.2823480
      16.5959440   2        12.2721500

```

p-f	66.1625230	2	16.1310240
	132.1743960	2	15.6280770
	16.3394170	2	7.3256080
	32.4889590	2	6.9425190
	12.5763330	2	12.2823480
	16.5959440	2	12.2721500
d-f	36.3874410	2	15.5149760
	54.5078410	2	15.1881600
	8.6968230	2	5.4560240
	12.8402080	2	5.3631050
	12.5763330	2	12.2823480
	16.5959440	2	12.2721500

*

*

sb def2-TZVP

sb (10s9p8d2f) / [6s5p3d2f] {421111/33111/611/11}

*

4 s		
1612.4199933	0.28540380783E-03	
238.84452097	0.13393778746E-02	
23.998118809	-0.49388154574E-01	
15.193124213	0.43392227254	
2 s		
11.736409733	0.92125519965	
6.5259774794	0.79235280226	
1 s		
2.0247451872	1.0000000000	
1 s		
0.97113418587	1.0000000000	
1 s		
0.24254333998	1.0000000000	
1 s		
0.92206608177E-01	1.0000000000	
3 p		
215.68393354	0.26051823221E-03	
16.374479088	0.73728000195E-01	
9.7216283345	-0.27230028128	
3 p		
2.7982643154	0.46472692374	
1.4711045033	0.50364242075	
0.75165385301	0.18706666294	
1 p		
0.33168699849	1.0000000000	
1 p		
0.13931606366	1.0000000000	
1 p		
0.56399307526E-01	1.0000000000	
6 d		
115.90312253	0.53140915051E-03	
30.474233720	0.59411139166E-02	
18.228418239	-0.10563706947E-01	
4.3291456646	0.20348177341	
2.1294818496	0.42748378928	
0.99682636692	0.38539560809	
1 d		
0.43347239863	1.0000000000	
1 d		
0.14000000000	1.0000000000	

```

1 f
0.32369706000      1.0000000000
1 f
1.10000000000      1.00000000000
*
sb def2-ecp
*
ncore =      28      lmax =      3
#      coefficient      r^n      exponent
f
      -15.3668010      2      14.4449780
      -20.2961380      2      14.4492950
s-f
      281.0715810      2      16.3308650
      61.7166040      2      8.5565420
      15.3668010      2      14.4449780
      20.2961380      2      14.4492950
p-f
      67.4573800      2      14.4703370
      134.9335030      2      13.8161940
      14.7163440      2      8.4249240
      29.5185120      2      8.0927280
      15.3668010      2      14.4449780
      20.2961380      2      14.4492950
d-f
      35.4478150      2      14.8863310
      53.1434660      2      15.1463190
      9.1792230      2      5.9082670
      13.2402530      2      5.5943220
      15.3668010      2      14.4449780
      20.2961380      2      14.4492950
*
*
te def2-TZVP
# te      (11s9p8d2f) / [6s5p3d2f]      {521111/33111/611/11}
*
5 s
6213.2001650      0.17392073280E-03
920.89640017      0.11933589842E-02
199.28042708      0.36256556777E-02
24.774233098      -0.59791033012E-01
14.838199169      0.95943203263
2 s
12.278761954      0.75942429936
6.3807845532      0.35331689542
1 s
2.2228405205      1.00000000000
1 s
1.0776043442      1.00000000000
1 s
0.28136649025      1.00000000000
1 s
0.10781573341      1.00000000000
3 p
204.29400852      0.40605406751E-03
18.208759358      0.60255451613E-01
9.9211024302      -0.27491671277
3 p
3.1441528685      0.43154849974
1.7220884031      0.55403079110

```

```

0.89098945714      0.24087311227
 1 p
0.39804719568      1.00000000000
 1 p
0.16538785242      1.00000000000
 1 p
0.65082695586E-01  1.00000000000
 6 d
121.51055249       0.63490629024E-03
32.968794396       0.61811936324E-02
19.249862451       -0.88929825218E-02
4.7198407254       0.20159884764
2.3428061416       0.42976049013
1.1135379412       0.38247126751
 1 d
0.49200061510      1.00000000000
 1 d
0.16000000000      1.00000000000
 1 f
0.38255757000      1.00000000000
 1 f
1.85000000000      1.00000000000
*
te def2-ecp
*
  ncore =    28          lmax =    3
#   coefficient   r^n      exponent
f
  -15.7454500     2         15.2061680
  -20.7424480     2         15.2017020
s-f
  281.0458430     2         16.8144730
   61.6206560     2          8.7935260
   15.7454500     2         15.2061680
   20.7424480     2         15.2017020
p-f
   67.4494640     2         14.8778010
  134.9043040     2         14.2697310
   14.6895470     2          8.7244350
   29.4150630     2          8.2915150
   15.7454500     2         15.2061680
   20.7424480     2         15.2017020
d-f
   35.4320570     2         15.2050080
   53.1356870     2         15.2258480
    9.0698020     2          6.0717690
   13.1223040     2          5.8047600
   15.7454500     2         15.2061680
   20.7424480     2         15.2017020
*
*
i def2-TZVP
# i      (11s10p8d2f) / [6s5p3d2f]      {521111/34111/611/11}
*
  5 s
5899.5791533       0.24188269271E-03
898.54238765       0.15474041742E-02
200.37237912       0.42836684457E-02
31.418053840       -0.39417936275E-01
15.645987838       0.96086691992

```


2	s		
11.815741857		0.75961524091	
6.4614458287		0.42495501835	
1	s		
2.3838067579		1.0000000000	
1	s		
1.1712089662		1.0000000000	
1	s		
0.32115875757		1.0000000000	
1	s		
0.12387919364		1.0000000000	
3	p		
197.30030547		0.73951226905E-03	
20.061411349		0.66168450008E-01	
9.7631460485		-0.28554662348	
4	p		
12.984316904		-0.49096186164E-01	
3.6199503008		0.38914432482	
2.0232273090		0.65610817262	
1.0367490559		0.31803551647	
1	p		
0.45937816000		1.0000000000	
1	p		
0.19116532928		1.0000000000	
1	p		
0.74878813023E-01		1.0000000000	
6	d		
119.12671745		0.82596039573E-03	
33.404240134		0.68377675770E-02	
17.805918203		-0.10308158997E-01	
4.8990510353		0.22670457658	
2.4516753106		0.44180113937	
1.1820693432		0.36775472225	
1	d		
0.52923110068		1.0000000000	
1	d		
0.17000000000		1.0000000000	
1	f		
0.44141808000		1.0000000000	
1	f		
2.18000000000		1.0000000000	
*			
i	def2-ecp		
*			
n	core =	28	lmax = 3
#	coefficient	r^n	exponent
f			
	-21.8420400	2	19.4586090
	-28.4681910	2	19.3492600
	-0.2437130	2	4.8237670
	-0.3208040	2	4.8843150
s-f			
	49.9942930	2	40.0158350
	281.0253170	2	17.4297470
	61.5733260	2	9.0054840
	21.8420400	2	19.4586090
	28.4681910	2	19.3492600
	0.2437130	2	4.8237670
	0.3208040	2	4.8843150
p-f			

	67.4428410	2	15.3554660
	134.8811370	2	14.9718330
	14.6750510	2	8.9601640
	29.3756660	2	8.2590960
	21.8420400	2	19.4586090
	28.4681910	2	19.3492600
	0.2437130	2	4.8237670
	0.3208040	2	4.8843150
d-f			
	35.4395290	2	15.0689080
	53.1760570	2	14.5553220
	9.0671950	2	6.7186470
	13.2069370	2	6.4563930
	0.0893350	2	1.1917790
	0.0523800	2	1.2911570
	21.8420400	2	19.4586090
	28.4681910	2	19.3492600
	0.2437130	2	4.8237670
	0.3208040	2	4.8843150
*			
*			
xe def2-TZVP			
# xe	(11s10p8d2f) / [6s5p3d2f]		{5211111/341111/611/11}
*			
5 s			
6420.2481656	0.25092173886E-03		
983.54530664	0.16251948178E-02		
219.43881364	0.46037106451E-02		
23.012587807	-0.14698707182		
18.048324490	0.57524870348		
2 s			
11.752550163	0.66038420156		
6.2390917199	0.38470524721		
1 s			
2.6257211320	1.0000000000		
1 s			
1.2905042943	1.0000000000		
1 s			
0.36204185060	1.0000000000		
1 s			
0.14069888091	1.0000000000		
3 p			
193.81432545	0.95394802497E-03		
21.725228086	0.57393353332E-01		
9.8891605641	-0.27974266640		
4 p			
13.960683826	-0.50950157807E-01		
4.0928947097	0.36669211800		
2.2546815460	0.72619456861		
1.1546596184	0.35555871740		
1 p			
0.52321923128	1.0000000000		
1 p			
0.21945569800	1.0000000000		
1 p			
0.86158996836E-01	1.0000000000		
6 d			
135.60300038	0.81873543290E-03		
38.727062692	0.60897654151E-02		
15.377328089	-0.92782985596E-02		

```

5.2602537686      0.22890785589
2.6590627424      0.44434407051
1.2938205124      0.36029482992
  1 d
0.58050830139     1.00000000000
  1 d
0.18000000000     1.00000000000
  1 f
0.49652793000     1.00000000000
  1 f
2.50000000000     1.00000000000
*
xe def2-ecp
*
  ncore =    28          lmax =    3
#   coefficient   r^n      exponent
f
  -23.0892950     2         20.8815570
  -30.0744750     2         20.7834430
   -0.2882270     2          5.2533890
   -0.3869240     2          5.3611880
s-f
  49.9979620     2         40.0051840
 281.0133030     2         17.8122140
  61.5382550     2          9.3041500
  23.0892950     2         20.8815570
  30.0744750     2         20.7834430
   0.2882270     2          5.2533890
   0.3869240     2          5.3611880
p-f
  67.4391420     2         15.7017720
 134.8747110     2         15.2586080
  14.6633000     2          9.2921840
  29.3547300     2          8.5590030
  23.0892950     2         20.8815570
  30.0744750     2         20.7834430
   0.2882270     2          5.2533890
   0.3869240     2          5.3611880
d-f
  35.4369080     2         15.1856000
  53.1957720     2         14.2845000
   9.0462320     2          7.1218890
  13.2236810     2          6.9919630
   0.0848530     2          0.6239460
   0.0441550     2          0.6472840
  23.0892950     2         20.8815570
  30.0744750     2         20.7834430
   0.2882270     2          5.2533890
   0.3869240     2          5.3611880
*
*
cs def2-TZVP
# cs      (7s6p3d) / [5s3p3d]      {31111/411/111}
*
  3 s
  5.8778113443     0.12859994983
  4.3631538286    -0.34632569725
  1.8048475155     0.69930637051
  1 s
0.37485237136     1.00000000000

```

```

1 s
0.16384858778      1.0000000000
1 s
0.27230462048E-01  1.0000000000
1 s
0.11991533212E-01  1.0000000000
4 p
4.2751856154      0.45723074174E-01
1.9656663360     -0.25019961976
0.47689195212     0.55660850066
0.21529749588     0.58218553406
1 p
0.91450850296E-01  1.0000000000
1 p
0.17592078473E-01  1.0000000000
1 d
0.27941471548     0.15040680034
1 d
0.62419809739E-01  0.36150912942
1 d
0.15987870156E-01  1.0000000000
*
cs def2-ecp
*
ncore =      46          lmax =      3
# coefficient  r^n      exponent
f
s-f
-28.8843090    2          3.1232690
84.5477300    2          4.0797500
16.6541730    2          2.4174060
28.8843090    2          3.1232690
p-f
157.0490590   2          5.5140800
26.4233070    2          2.1603160
28.8843090    2          3.1232690
d-f
13.1727530    2          1.8074100
3.3428330     2          0.8581820
28.8843090    2          3.1232690
*
*
ba def2-TZVP
# ba (7s7p5d1f) / [6s4p3d1f] {211111/4111/311/1}
*
2 s
6.0000000000    -0.56587174838
4.9822082226    0.97514768535
1 s
2.1451943914    1.0000000000
1 s
0.41486174100   1.0000000000
1 s
0.19214757016   1.0000000000
1 s
0.48465890337E-01  1.0000000000
1 s
0.20138298948E-01  1.0000000000
4 p
5.5000000000    -0.44586312998

```

```

4.9017938336      0.67755479813
2.6142685062     -0.46010554954
0.47903394983    0.68749608021
  1 p
0.19415138747    1.00000000000
  1 p
0.34917622027E-01  1.00000000000
  1 p
0.16320065666E-01  1.00000000000
  3 d
0.96631500000    -0.90893800000
0.89382800000    0.94724000000
0.27319500000    0.32205700000
  1 d
0.10389100000    1.00000000000
  1 d
0.35578000000E-01  1.00000000000
  1 f
0.65760000000    0.00000000000
*
ba def2-ecp
*
  ncore =      46          lmax =      3
#      coefficient      r^n      exponent
f
      -33.4731740      2          3.5894650
s-f
      427.8458160      2          9.5269860
      204.4175300      2          4.4875100
      33.4731740      2          3.5894650
p-f
      293.6058640      2          8.3159300
      294.1933160      2          4.2922170
      33.4731740      2          3.5894650
d-f
      112.5504020      2          5.9161080
      181.7826210      2          2.8748420
      33.4731740      2          3.5894650
*
*
la def2-TZVP
# la      (7s7p5d1f) / [6s4p3d1f]      {211111/4111/311/1}
*
  2 s
5.0873990000     -0.44174952534
4.2709780000     0.85812466843
  1 s
2.1823656045     1.00000000000
  1 s
0.48966533785     1.00000000000
  1 s
0.23301675348     1.00000000000
  1 s
0.55719523051E-01  1.00000000000
  1 s
0.22854708808E-01  1.00000000000
  4 p
6.0000000000     -0.11397960924E-01
3.6808191615     0.14675038550
2.3265462081     -0.35581819167

```

```

0.64342629633      0.45834955229
  1 p
0.33584281962      1.00000000000
  1 p
0.16519051916      1.00000000000
  1 p
0.35400000000E-01  1.00000000000
  3 d
  1.2675288018     -0.17569274035
0.89395340284      0.25139922933
0.33095767339      0.44603267053
  1 d
0.13461377501      1.00000000000
  1 d
0.51441629839E-01  1.00000000000
  1 f
0.25683000000      1.00000000000
*
la def2-ecp
*
  ncore =    46      lmax =    3
#      coefficient  r^n      exponent
f
s-f      -36.0100160    2      4.0286000
          91.9321770    2      3.3099000
          -3.7887640    2      1.6550000
          36.0100160    2      4.0286000
p-f
          63.7594860    2      2.8368000
          -0.6479580    2      1.4184000
          36.0100160    2      4.0286000
d-f
          36.1161730    2      2.0213000
          0.2191140    2      1.0107000
          36.0100160    2      4.0286000
*
*
hf def2-TZVP
# hf      (9s7p5d1f) / [6s4p3d1f]      {411111/4111/311/1}
*
  4 s
24.000000000      0.19369448644
16.000000000      -3.5064630782
14.400000000      4.3082581000
10.304504667      -0.91045809742
  1 s
  3.8426510824      1.00000000000
  1 s
0.93296029049      1.00000000000
  1 s
0.42615320942      1.00000000000
  1 s
0.93366560195E-01  1.00000000000
  1 s
0.35532895141E-01  1.00000000000
  4 p
17.000000000      -0.30316491880E-01
11.738072097      0.10139279686
  4.9203967161      -0.28227924657

```

```

1.1251726138      0.52032008501
 1 p
0.54220114055      1.00000000000
 1 p
0.25659447877      1.00000000000
 1 p
0.650000000000E-01  1.00000000000
 3 d
 3.9820623229      -0.42446023944E-01
 1.3077987772      0.18409232564
0.53272310298      0.41484423516
 1 d
0.20564954488      1.00000000000
 1 d
0.73099858787E-01  1.00000000000
 1 f
0.31547000000      1.00000000000
*
hf def2-ecp
*
  ncore =    60      lmax =    3
#      coefficient  r^n      exponent
f
      10.0467225    2      1.7857698
s-f
      1499.2847107  2      14.7699590
      40.2821014    2      7.3849794
      -10.0467225   2      1.7857698
p-f
      397.7330053    2      9.8494895
      19.3164059    2      4.9247445
      -10.0467225   2      1.7857698
d-f
      101.3298053    2      6.0967564
      5.8734382     2      3.0483782
      -10.0467225   2      1.7857698
*
*
ta def2-TZVP
# ta      (9s7p5d1f) / [6s4p3d1f]      {411111/4111/311/1}
*
 4 s
24.473650944      0.20590322488
18.721372549      -0.74670795514
11.500000000      3.4071363897
10.350000000      -2.8175487609
 1 s
 3.8436180089      1.00000000000
 1 s
 1.0202266016      1.00000000000
 1 s
0.46774781869      1.00000000000
 1 s
0.10323186670      1.00000000000
 1 s
0.38674461203E-01  1.00000000000
 4 p
17.000000000      -0.32577305616E-01
12.008186536      0.10336287365
 5.0278760583      -0.28526521696

```

```

1.1937124184      0.51790141155
 1 p
0.57889707053      1.00000000000
 1 p
0.27225198801      1.00000000000
 1 p
0.650000000000E-01  1.00000000000
 3 d
 3.9738796278      -0.52799310714E-01
 1.4528884813      0.18558319471
0.61042908544      0.42959071631
 1 d
0.24216276510      1.00000000000
 1 d
0.87909318337E-01  1.00000000000
 1 f
0.37386000000      1.00000000000
*
ta def2-ecp
*
  ncore =    60          lmax =    3
#      coefficient      r^n      exponent
f
      12.0179609      2          2.0178811
s-f
      1345.8806470      2          14.5464077
      36.7668062      2          7.2732038
      -12.0179609      2          2.0178811
p-f
      378.4253015      2          9.9355653
      22.2930909      2          4.9677824
      -12.0179609      2          2.0178811
d-f
      104.8839557      2          6.3473769
      8.7558481      2          3.1736885
      -12.0179609      2          2.0178811
*
*
w def2-TZVP
# w      (8s7p6d1f) / [6s4p3d1f]      {311111/4111/411/1}
*
 3 s
30.000000000      0.32246483410
27.000000000      -0.46692257214
13.078045684      0.42699563776
 1 s
 4.8100449717      1.00000000000
 1 s
0.98497804263      1.00000000000
 1 s
0.44910485344      1.00000000000
 1 s
0.11448352920      1.00000000000
 1 s
0.41720421956E-01  1.00000000000
 4 p
17.000000000      -0.37817768433E-01
12.431973432      0.10905673845
 5.1586217658      -0.29399955020
 1.2801454812      0.51560726697

```



```

1 p
0.62856790898      1.0000000000
1 p
0.29380423553      1.0000000000
1 p
0.650000000000E-01  1.0000000000
4 d
7.4064737315      0.86993963018E-01
5.9026268603      -0.17667540011
1.2984756750      0.55145697030
0.57153508541     0.95313596535
1 d
0.23845526606     1.0000000000
1 d
0.91144267331E-01  1.0000000000
1 f
0.43199000000     1.0000000000
*
w def2-ecp
*
ncore = 60          lmax = 3
# coefficient      r^n          exponent
f
14.1525795        2            2.2588885
s-f
1192.3958823      2            14.3228564
32.5229332        2            7.1614281
-14.1525795       2            2.2588885
p-f
359.0319671       2            10.0216411
24.0303802        2            5.0108204
-14.1525795       2            2.2588885
d-f
108.3013490       2            6.5979974
10.9825283        2            3.2989987
-14.1525795       2            2.2588885
*
*
re def2-TZVP
# re (8s7p6d1f) / [6s4p3d1f] {311111/4111/411/1}
*
3 s
30.000000000      0.31780717811
27.000000000      -0.46492321332
13.078045684      0.45723641305
1 s
5.0352712861     1.0000000000
1 s
1.0482706438     1.0000000000
1 s
0.47708773413    1.0000000000
1 s
0.12225857255    1.0000000000
1 s
0.44007400609E-01 1.0000000000
4 p
18.000000000     -0.26890962397E-01
12.318606250     0.99711498502E-01
5.3719234505     -0.29289398145
1.3506646748     0.51466301434

```

```

1 p
0.66212816808      1.0000000000
1 p
0.31071385193      1.0000000000
1 p
0.700000000000E-01  1.0000000000
4 d
7.7352877672      0.83901798556E-01
6.0949443610      -0.17722258734
1.3871105497      0.55238259692
0.62324027854      0.91980111239
1 d
0.26517328547      1.0000000000
1 d
0.10321096849      1.0000000000
1 f
0.48989000000      1.0000000000
*
re def2-ecp
*
ncore =      60      lmax =      3
#      coefficient      r^n      exponent
f
      16.4498523      2      2.5086506
s-f
      1038.9515723      2      14.0993051
      29.5617383      2      7.0496525
      -16.4498523      2      2.5086506
p-f
      339.5435096      2      10.1077169
      24.9136965      2      5.0538583
      -16.4498523      2      2.5086506
d-f
      111.6996527      2      6.8486179
      12.6243293      2      3.4243090
      -16.4498523      2      2.5086506
*
*
os def2-TZVP
# os      (8s7p6d1f) / [6s4p3d1f]      {311111/4111/411/1}
*
3 s
30.000000000      0.32213004804
27.000000000      -0.47922918137
13.524730005      0.47465946837
1 s
5.2402883472      1.0000000000
1 s
1.1306661245      1.0000000000
1 s
0.51689966917      1.0000000000
1 s
0.13222953545      1.0000000000
1 s
0.47220318801E-01  1.0000000000
4 p
15.500000000      0.16016463376
14.000000000      -0.23201520402
5.5458290420      0.29772587274
1.4139502215      -0.54253238176

```

```

1 p
0.68136686765      1.0000000000
1 p
0.30911452647      1.0000000000
1 p
0.520000000000E-01  1.0000000000
4 d
8.2945059487      0.69648222110E-01
6.3060397430      -0.16444229630
1.4890109110      0.55154541033
0.67315390607      0.88461370291
1 d
0.28590805222      1.0000000000
1 d
0.11058012051      1.0000000000
1 f
0.55065000000      1.0000000000
*
os def2-ecp
*
ncore = 60          lmax = 3
# coefficient      r^n      exponent
f
      18.9094570      2          2.7670751
s-f
      885.4057191      2          13.8757539
      25.9670401      2          6.9378769
      -18.9094570      2          2.7670751
p-f
      320.0839019      2          10.1937926
      26.1487649      2          5.0968962
      -18.9094570      2          2.7670751
d-f
      115.0448431      2          7.0992385
      13.6225746      2          3.5496192
      -18.9094570      2          2.7670751
*
*
ir def2-TZVP
# ir      (8s7p6d1f) / [6s4p3d1f]      {311111/4111/411/1}
*
3 s
30.000000000      0.30797903228
27.000000000      -0.46726361781
13.961973911      0.47161003146
1 s
5.3956977802      1.0000000000
1 s
1.2149128721      1.0000000000
1 s
0.55885743756      1.0000000000
1 s
0.14097974313      1.0000000000
1 s
0.50021924989E-01  1.0000000000
4 p
15.902664143      -0.16290720099
14.415830698      0.23483212987
5.7597608991      -0.30305337176
1.5008913108      0.55512982069

```

```

1 p
0.72348035957      1.0000000000
1 p
0.32785980328      1.0000000000
1 p
0.560000000000E-01  1.0000000000
4 d
8.6321692504      0.75000099949E-01
6.5898192302     -0.17326965173
1.5808379663      0.55065196913
0.71827834905      0.85273641436
1 d
0.30571851998      1.0000000000
1 d
0.11827071879      1.0000000000
1 f
0.61008000000      1.0000000000
*
ir def2-ecp
*
ncore =      60      lmax =      3
#      coefficient      r^n      exponent
f
      21.5310311      2      3.0340719
s-f
      732.2691998      2      13.6522026
      26.4847209      2      6.8261013
      -21.5310311      2      3.0340719
p-f
      299.4894736      2      10.2798684
      26.4662335      2      5.1399341
      -21.5310311      2      3.0340719
d-f
      124.4575945      2      7.3498590
      14.0359952      2      3.6749295
      -21.5310311      2      3.0340719
*
*
pt def2-TZVP
# pt      (8s7p6d1f) / [6s4p3d1f]      {311111/4111/411/1}
*
3 s
30.000000000      0.27148263900
27.000000000      -0.42226758774
14.408318564      0.44361581995
1 s
5.5335788010      1.0000000000
1 s
1.2986438223      1.0000000000
1 s
0.58759393108      1.0000000000
1 s
0.13845587261      1.0000000000
1 s
0.49204459888E-01  1.0000000000
4 p
15.500000000      -0.15672718629
14.000000000      0.23853412989
6.1161212339      -0.31041379733
1.5715586385      0.56473525089

```

```

1 p
0.75132510781      1.0000000000
1 p
0.33306466812      1.0000000000
1 p
0.570000000000E-01  1.0000000000
4 d
8.3207937611      0.62945798646E-01
7.4207226520      -0.90271847072E-01
1.6570410639      0.16812526416
0.73943569960      0.25045416970
1 d
0.30510856008      1.0000000000
1 d
0.11350405268      1.0000000000
1 f
0.66813000000      1.0000000000
*
pt def2-ecp
*
ncore = 60          lmax = 3
# coefficient      r^n          exponent
f
      24.3143757      2          3.3095686
s-f
      579.2238609      2          13.4286513
      29.6694906      2          6.7143256
      -24.3143757      2          3.3095686
p-f
      280.8607742      2          10.3659442
      26.7453820      2          5.1829721
      -24.3143757      2          3.3095686
d-f
      120.3964443      2          7.6004795
      15.8109206      2          3.8002397
      -24.3143757      2          3.3095686
*
*
au def2-TZVP
# au      (8s7p6d1f) / [6s4p3d1f]      {311111/4111/411/1}
*
3 s
30.000000000      0.20749231108
27.000000000      -0.33267893394
14.746824331      0.38302817958
1 s
5.6017248938      1.0000000000
1 s
1.3874162443      1.0000000000
1 s
0.62923031957      1.0000000000
1 s
0.14027517613      1.0000000000
1 s
0.49379413761E-01  1.0000000000
4 p
15.500000000      0.15001711880
14.000000000      -0.23609813183
6.4227368205      0.31458896948
1.6595601681      -0.57279670446

```

```

1 p
0.79402913993      1.0000000000
1 p
0.35125155397      1.0000000000
1 p
0.450000000000E-01  1.0000000000
4 d
9.5524098656      0.40145559502E-01
7.2698886937      -0.93690906606E-01
1.7746496789      0.31746282317
0.79960541055      0.46795192483
1 d
0.33252279372      1.0000000000
1 d
0.12445133105      1.0000000000
1 f
0.72482000000      1.0000000000
*
au def2-ecp
*
ncore = 60          lmax = 3
# coefficient      r^n          exponent
f
30.4900889        2            4.7898200
5.1710738         2            2.3949100
s-f
426.8466792       2            13.2051000
37.0070829        2            6.6025500
-30.4900889       2            4.7898200
-5.1710738        2            2.3949100
p-f
261.1995804       2            10.4520200
26.9624960        2            5.2260100
-30.4900889       2            4.7898200
-5.1710738        2            2.3949100
d-f
124.7906656       2            7.8511000
16.3007257        2            3.9255500
-30.4900889       2            4.7898200
-5.1710738        2            2.3949100
*
*
hg def2-TZVP
# hg (8s8p6d1f) / [6s5p3d1f] {311111/41111/411/1}
*
3 s
48.013786990      0.58008164912E-02
21.239875095      -0.17328165235
15.876100879      0.36416685034
1 s
5.5180531820      1.0000000000
1 s
1.5099145479      1.0000000000
1 s
0.70683482159     1.0000000000
1 s
0.16266265576     1.0000000000
1 s
0.56960589112E-01 1.0000000000
4 p

```

```

17.500000000    -0.86457187331E-01
15.252594855    0.15327318234
6.4404715169    -0.30274955249
1.8180159920    0.54361285026
 1 p
0.90067981801    1.0000000000
 1 p
0.41304540122    1.0000000000
 1 p
0.11845702655    1.0000000000
 1 p
0.36087619349E-01  1.0000000000
 4 d
10.028197701    0.39922353165E-01
7.5920661493    -0.94774230522E-01
1.9144256118    0.31164157463
0.88641552102    0.45567078406
 1 d
0.38154235320    1.0000000000
 1 d
0.14880740086    1.0000000000
 1 f
0.79569000000    1.0000000000
*
hg def2-ecp
*
  ncore =    60          lmax =    3
#      coefficient      r^n      exponent
f
      30.3649964        2          3.8857911
s-f
      275.7372117        2          12.9815487
      49.0892125         2           6.4907744
      -30.3649964        2          3.8857911
p-f
      241.5400740        2          10.5380958
      27.3965908         2           5.2690479
      -30.3649964        2          3.8857911
d-f
      127.8670076        2           8.1017205
      16.6083115         2           4.0508603
      -30.3649964        2          3.8857911
*
*
t1 def2-TZVP
# t1      (10s9p8d2f) / [6s5p3d2f]      {421111/33111/611/11}
*
 4 s
729.65038145    0.13672829828E-03
46.665548707    0.60443439951E-02
20.970448726    -0.20022066697
14.149588677    0.40801678488
 2 s
20.730134285    -0.71861135918E-01
6.1527631309    0.98057508445
 1 s
1.5757324480    1.0000000000
 1 s
0.74980169458    1.0000000000
 1 s

```

0.19536816194	1.0000000000
1 s	
0.70878767298E-01	1.0000000000
3 p	
15.383852616	0.61717949180
14.814929544	-0.72859235151
6.7261253658	0.40438195364
3 p	
1.9626182149	0.43157661160
1.0331857851	0.39230403853
0.53837445996	0.14007406820
1 p	
0.24446611676	1.0000000000
1 p	
0.90785377260E-01	1.0000000000
1 p	
0.33401321498E-01	1.0000000000
6 d	
57.606819928	0.16054811114E-03
9.7368866667	0.24456562496E-01
6.9256201679	-0.69914775031E-01
2.1396230731	0.19496269490
1.0836187110	0.29731629705
0.52356298209	0.23728708102
1 d	
0.23842309375	1.0000000000
1 d	
0.95000000000E-01	1.0000000000
1 f	
0.28435000000	1.0000000000
1 f	
0.95000000000	1.0000000000

*

tl def2-ecp

*

#	ncore = 60	coefficient	lmax = 3	r^n	exponent
f		15.8254880	2		5.6263990
		21.1040210	2		5.5489520
		2.9151270	2		2.8749460
		3.8969030	2		2.8214510
s-f		281.2846630	2		12.1678050
		62.4342510	2		8.2949090
		-15.8254880	2		5.6263990
		-21.1040210	2		5.5489520
		-2.9151270	2		2.8749460
		-3.8969030	2		2.8214510
p-f		4.6334080	2		7.1514920
		9.3417560	2		5.1728650
		72.2992530	2		9.8910720
		144.5580370	2		9.0033910
		-15.8254880	2		5.6263990
		-21.1040210	2		5.5489520
		-2.9151270	2		2.8749460
		-3.8969030	2		2.8214510
d-f		35.9430390	2		7.1302180

53.9095930	2	6.9269060
10.3819390	2	5.4175700
15.5838220	2	5.1386810
-15.8254880	2	5.6263990
-21.1040210	2	5.5489520
-2.9151270	2	2.8749460
-3.8969030	2	2.8214510

*
*

pb def2-TZVP

pb (10s9p8d2f) / [6s5p3d2f] {421111/331111/611/11}

*

4 s		
591.61124370	0.22126521076E-03	
46.757232559	0.56961959130E-02	
20.746462696	-0.21374063831	
14.610796419	0.40502620616	
2 s		
20.222637612	-0.83541883299E-01	
6.4767324865	0.97910892388	
1 s		
1.6600600927	1.0000000000	
1 s		
0.80431655001	1.0000000000	
1 s		
0.22627039020	1.0000000000	
1 s		
0.84014530665E-01	1.0000000000	
3 p		
15.189102118	0.61952303583	
14.693144415	-0.72498497086	
6.8705890048	0.37680007984	
3 p		
2.2021426123	0.40196284806	
1.2209125119	0.46058131862	
0.63367559815	0.19367655397	
1 p		
0.28202837058	1.0000000000	
1 p		
0.11333375666	1.0000000000	
1 p		
0.43948707430E-01	1.0000000000	
6 d		
61.315369628	0.33870800787E-03	
12.372195840	0.13788683942E-01	
6.9254944983	-0.75979608103E-01	
2.3319539939	0.28113784298	
1.2108730003	0.44474512269	
0.60090478506	0.35326874351	
1 d		
0.28135869813	1.0000000000	
1 d		
0.11500000000	1.0000000000	
1 f		
0.28962000000	1.0000000000	
1 f		
1.0000000000	1.0000000000	

*

pb def2-ecp

*

```

ncore = 60          lmax = 3
#      coefficient  r^n    exponent
f
      12.2098920    2      3.8875120
      16.1902910    2      3.8119630
s-f
      281.2854990   2      12.2963030
      62.5202170   2      8.6326340
      -12.2098920   2      3.8875120
      -16.1902910   2      3.8119630
p-f
      72.2768970    2      10.2417900
      144.5910830   2      8.9241760
      4.7586930     2      6.5813420
      9.9406210     2      6.2554030
      -12.2098920   2      3.8875120
      -16.1902910   2      3.8119630
d-f
      35.8485070    2      7.7543360
      53.7243420    2      7.7202810
      10.1152560    2      4.9702640
      14.8337310    2      4.5637890
      -12.2098920   2      3.8875120
      -16.1902910   2      3.8119630
*
*
bi def2-TZVP
# bi      (10s9p8d2f) / [6s5p3d2f]      {4211111/331111/611/11}
*
  4 s
  716.41435310      0.31254307133E-03
  83.806059047      0.17624768946E-02
  21.116962853      -0.21910983437
  15.491448187      0.40411224931
  2 s
  23.239855029      -0.68255758685E-01
  6.6474255000      0.97888046471
  1 s
  1.7617744005      1.0000000000
  1 s
  0.87252866000     1.0000000000
  1 s
  0.25618895997     1.0000000000
  1 s
  0.97073913006E-01 1.0000000000
  3 p
  15.249644669      0.74560356000
  14.846176053      -0.85578637338
  7.0636826784      0.40149159592
  3 p
  2.5881255616      0.35542729633
  1.5020208499      0.63976991890
  0.76732724388     0.32332773839
  1 p
  0.32797648982     1.0000000000
  1 p
  0.13820335991     1.0000000000
  1 p
  0.55137330969E-01 1.0000000000
  6 d

```

```

66.404481948      0.38102878348E-03
13.858426961      0.10746152442E-01
7.0654519000     -0.71947646845E-01
2.5252144035      0.26195974989
1.3419585000      0.42594750000
0.68340941000     0.33680325627
  1 d
0.32934755420     1.00000000000
  1 d
0.14000000000     1.00000000000
  1 f
0.31271000000     1.00000000000
  1 f
1.05000000000     1.00000000000
*
bi def2-ecp
*
  ncore =      60      lmax =      3
#      coefficient      r^n      exponent
f
      13.7133830      2      4.2145460
      18.1943080      2      4.1334000
s-f
      283.2642270      2      13.0430900
      62.4719590      2      8.2216820
      -13.7133830      2      4.2145460
      -18.1943080      2      4.1334000
p-f
      72.0014990      2      10.4677770
      144.0022770      2      9.1189010
      5.0079450      2      6.7547910
      9.9915500      2      6.2525920
      -13.7133830      2      4.2145460
      -18.1943080      2      4.1334000
d-f
      36.3962590      2      8.0814740
      54.5976640      2      7.8905950
      9.9842940      2      4.9555560
      14.9814850      2      4.7045590
      -13.7133830      2      4.2145460
      -18.1943080      2      4.1334000
*
*
po def2-TZVP
# po      (11s10p8d2f) / [6s5p3d2f]      {521111/34111/611/11}
*
  5 s
6744.8211765      0.76891556363E-04
744.41892532      0.71284827354E-03
131.04029309      0.22057583958E-02
19.662021030     -0.64364713744
16.623025609      0.91997150546
  2 s
23.094002965     -0.70404410177E-01
6.9707398381      0.97886540086
  1 s
1.8497377593      1.00000000000
  1 s
0.93082999263      1.00000000000
  1 s

```

0.28673026462	1.0000000000
1 s	
0.10979212169	1.0000000000
3 p	
253.99024497	0.83876362116E-04
9.8712718748	0.24572710458
7.4489893496	-0.44297763661
4 p	
8.9027395407	-0.13798250445
5.7414667465	0.26304005326
1.9896329823	0.66225846161
0.94703210822	0.39547051892
1 p	
0.37071136280	1.0000000000
1 p	
0.15554706086	1.0000000000
1 p	
0.61173720818E-01	1.0000000000
6 d	
67.943077046	0.48919125336E-03
14.914219894	0.10157120776E-01
7.2973948305	-0.69943263066E-01
2.6826784400	0.26244730680
1.4374143009	0.42702361494
0.73903797417	0.32502435477
1 d	
0.35838153281	1.0000000000
1 d	
0.15000000000	1.0000000000
1 f	
0.33275000000	1.0000000000
1 f	
1.40000000000	1.0000000000

*

po def2-ecp

*

#	ncore = 60	lmax = 3	coefficient	r^n	exponent
f			17.4282950	2	5.0132700
			23.3803530	2	4.9846400
			0.1633920	2	1.3267600
			0.3245660	2	1.5287580
s-f			283.2447060	2	13.2772270
			62.3964610	2	8.3995180
			-17.4282950	2	5.0132700
			-23.3803530	2	4.9846400
			-0.1633920	2	1.3267600
			-0.3245660	2	1.5287580
p-f			71.9917160	2	10.6656820
			143.9718710	2	9.2837530
			4.9496150	2	6.8727490
			9.7404990	2	6.3261500
			-17.4282950	2	5.0132700
			-23.3803530	2	4.9846400
			-0.1633920	2	1.3267600
			-0.3245660	2	1.5287580
d-f					

36.3783830	2	8.2148660
54.5627150	2	8.0086960
9.8894990	2	5.0552270
14.6938770	2	4.7825530
-17.4282950	2	5.0132700
-23.3803530	2	4.9846400
-0.1633920	2	1.3267600
-0.3245660	2	1.5287580

*

*

at def2-TZVP

at (11s10p8d2f) / [6s5p3d2f] {521111/34111/611/11}

*

5 s	
3635.9809356	0.12571463494E-03
537.64129823	0.75950883820E-03
91.600030756	0.25790982348E-02
20.200005804	-0.54772187699
16.893873824	0.78417507786
2 s	
18.177216938	-0.13023627002
7.2317852082	0.96473566747
1 s	
1.9496199739	1.0000000000
1 s	
0.99226695236	1.0000000000
1 s	
0.31957178881	1.0000000000
1 s	
0.12342539809	1.0000000000
3 p	
216.81518928	0.16975297090E-03
10.592298115	0.22683755793
7.4596585430	-0.47336848377
4 p	
8.9484156471	-0.15012953475
5.9694592464	0.27048141788
2.1099088209	0.63671217722
1.0236370373	0.38057472615
1 p	
0.42186356565	1.0000000000
1 p	
0.17757132268	1.0000000000
1 p	
0.69670886939E-01	1.0000000000
6 d	
70.619633393	0.59974022914E-03
16.212096478	0.93445952839E-02
7.3607401479	-0.70748413897E-01
2.9309052592	0.24037366077
1.6085414823	0.41841372624
0.84194162715	0.32832651044
1 d	
0.41335677957	1.0000000000
1 d	
0.17400000000	1.0000000000
1 f	
0.37408000000	1.0000000000
1 f	
1.80000000000	1.0000000000

```

*
at def2-ecp
*
ncore = 60          lmax = 3
# coefficient      r^n      exponent
f
    19.8701980     2         5.8121630
    26.4164520     2         5.7537150
    0.9949700      2         2.5134720
    1.4907010      2         2.5362610
s-f
    49.9571580     2         30.2008320
    283.2103710    2         13.6123060
    62.2810520     2         8.5293400
    -19.8701980    2         5.8121630
    -26.4164520    2         5.7537150
    -0.9949700     2         2.5134720
    -1.4907010     2         2.5362610
p-f
    71.9823710     2         10.8540650
    143.9035320    2         9.4682290
    4.8717590      2         7.0311140
    8.9830590      2         6.1438580
    -19.8701980    2         5.8121630
    -26.4164520    2         5.7537150
    -0.9949700     2         2.5134720
    -1.4907010     2         2.5362610
d-f
    36.3632370     2         8.3135150
    54.5489700     2         7.9989650
    9.7762850      2         5.1799660
    14.2647550     2         4.9422260
    -19.8701980    2         5.8121630
    -26.4164520    2         5.7537150
    -0.9949700     2         2.5134720
    -1.4907010     2         2.5362610
*
*
rn def2-TZVP
# rn      (11s10p8d2f) / [6s5p3d2f]      {521111/34111/611/11}
*
  5 s
5187.7442468      0.16097034848E-03
768.14491207      0.10508214789E-02
159.35182065      0.27375438093E-02
21.863432724      -0.55045904905
18.388689978      0.78321373922
  2 s
24.816226448      -0.82636797204E-01
7.2923301677      1.0926256000
  1 s
2.0850437166      1.0000000000
  1 s
1.0915245945      1.0000000000
  1 s
0.34915708428      1.0000000000
  1 s
0.13648422952      1.0000000000
  3 p
194.68918723      0.26265814046E-03

```

11.210013525	0.19952302621	
7.5298316489	-0.45994479561	
4 p		
9.0845000304	-0.23093917426	
6.2631489717	0.39747614192	
2.2545193734	0.83026693838	
1.1180666918	0.51467013112	
1 p		
0.47444492594	1.00000000000	
1 p		
0.20172354616	1.00000000000	
1 p		
0.79503144392E-01	1.00000000000	
6 d		
75.302723665	0.73590238429E-03	
17.965913830	0.89490827389E-02	
7.3741298033	-0.76641663693E-01	
3.2296258578	0.22975404602	
1.7937840508	0.43991495311	
0.94633319732	0.35259395198	
1 d		
0.46860482223	1.00000000000	
1 d		
0.20000000000	1.00000000000	
1 f		
0.41806000000	1.00000000000	
1 f		
2.10000000000	1.00000000000	
*		
rn def2-ecp		
*		
ncore = 60	lmax = 3	
# coefficient r^n exponent		
f		
21.7972900	2	6.3485710
28.9468050	2	6.2959490
1.4473650	2	2.8821180
2.1779640	2	2.9080480
s-f		
49.9655510	2	30.1512420
283.0700000	2	14.5212410
62.0028700	2	8.0520380
-21.7972900	2	6.3485710
-28.9468050	2	6.2959490
-1.4473650	2	2.8821180
-2.1779640	2	2.9080480
p-f		
71.9691190	2	11.0099420
143.8605590	2	9.6176250
4.7147610	2	7.3360080
9.0130650	2	6.4062530
-21.7972900	2	6.3485710
-28.9468050	2	6.2959490
-1.4473650	2	2.8821180
-2.1779640	2	2.9080480
d-f		
36.3683650	2	8.3692200
54.5517610	2	8.1169750
9.6344870	2	5.3536560
14.3879020	2	5.0972120

-21.7972900	2	6.3485710
-28.9468050	2	6.2959490
-1.4473650	2	2.8821180
-2.1779640	2	2.9080480

*

\$end

=====
def2-TZVPP
=====

*

h def2-TZVPP

h (5s2p1d) / [3s2p1d] {311/11/1}

*

3 s		
34.061341000	0.60251978000E-02	
5.1235746000	0.45021094000E-01	
1.1646626000	0.20189726000	
1 s		
0.32723041000	1.00000000000	
1 s		
0.10307241000	1.00000000000	
1 p		
1.40700000000	1.00000000000	
1 p		
0.38800000000	1.00000000000	
1 d		
1.05700000000	1.00000000000	

*

*

he def2-TZVPP

he (5s2p1d) / [3s2p1d] {311/11/1}

*

3 s		
98.078321616	0.75803064967E-02	
14.764404247	0.54848620937E-01	
3.3185831473	0.22074382186	
1 s		
0.87413869551	1.00000000000	
1 s		
0.24459897208	1.00000000000	
1 p		
3.04400000000	1.00000000000	
1 p		
0.75800000000	1.00000000000	
1 d		
1.96500000000	1.00000000000	

*

*

li def2-TZVPP

li (11s3p1d) / [5s3p1d] {62111/111/1}

*

6 s		
6269.2628010	0.20540968826E-03	
940.31612431	0.15916554089E-02	
214.22107528	0.82869829707E-02	
60.759840184	0.33856374249E-01	
19.915152032	0.11103225876	
7.3171509797	0.27449383329	
2 s		
2.9724674216	0.23792456411	


```

1.2639852314      0.30765411924
 1 s
0.51427489953    1.00000000000
 1 s
0.77030885901E-01 1.00000000000
 1 s
0.28938896433E-01 1.00000000000
 1 p
0.40000000000    1.00000000000
 1 p
0.60000000000E-01 1.00000000000
 1 p
 3.3270000000    1.00000000000
 1 d
0.13190000000    1.00000000000
*
*
be def2-TZVPP
# be      (11s4p1d) / [5s3p1d]      {62111/121/1}
*
 6 s
4700.2365626     0.23584389316E-03
704.82845622    0.18243791019E-02
160.43110478    0.93966148224E-02
45.425347336    0.36908924159E-01
14.798334125    0.10897561281
5.3512452537    0.21694284551
 2 s
2.1542044819    0.44695408857
0.93363744400    0.20866985771
 1 s
0.18791432989    1.00000000000
 1 s
0.74648267947E-01 1.00000000000
 1 s
0.32650484598E-01 1.00000000000
 1 p
 3.6316917145    -0.29033998305E-01
 2 p
0.71695694366    -0.16877854032
0.19541932860    -0.51403419628
 1 p
0.60515465890E-01 1.00000000000
 1 d
0.18000000000    0.00000000000
*
*
b def2-TZVPP
# b      (11s6p2d1f) / [5s3p2d1f]    {62111/411/11/1}
*
 6 s
8564.8660687    0.22837198155E-03
1284.1516263    0.17682576447E-02
292.27871604    0.91407080516E-02
82.775469176    0.36342638989E-01
27.017939269    0.11063458441
9.8149619660    0.23367344321
 2 s
3.9318559059    0.41818777978
1.6595599712    0.22325473798

```

```

1 s
0.35762965239      1.0000000000
1 s
0.14246277496      1.0000000000
1 s
0.60560594768E-01  1.0000000000
4 p
22.453875803      0.50265575179E-02
5.1045058330      0.32801738965E-01
1.4986081344      0.13151230768
0.50927831315      0.33197167769
1 p
0.18147077798      0.47314319570
1 p
0.64621893904E-01  0.25802783943
1 d
0.66100000000      1.0000000000
1 d
0.19900000000      1.0000000000
1 f
0.49000000000      1.0000000000
*
*
c def2-TZVPP
# c      (11s6p2d1f) / [5s3p2d1f]      {62111/411/11/1}
*
6 s
13575.349682      0.22245814352E-03
2035.2333680      0.17232738252E-02
463.22562359      0.89255715314E-02
131.20019598      0.35727984502E-01
42.853015891      0.11076259931
15.584185766      0.24295627626
2 s
6.2067138508      0.41440263448
2.5764896527      0.23744968655
1 s
0.57696339419      1.0000000000
1 s
0.22972831358      1.0000000000
1 s
0.95164440028E-01  1.0000000000
4 p
34.697232244      0.53333657805E-02
7.9582622826      0.35864109092E-01
2.3780826883      0.14215873329
0.81433208183      0.34270471845
1 p
0.28887547253      0.46445822433
1 p
0.10056823671      0.24955789874
1 d
1.09700000000      1.0000000000
1 d
0.31800000000      1.0000000000
1 f
0.76100000000      1.0000000000
*
*
n def2-TZVPP

```

n (11s6p2d1f) / [5s3p2d1f] {62111/411/11/1}

*

6 s	
19730.800647	0.21887984991E-03
2957.8958745	0.16960708803E-02
673.22133595	0.87954603538E-02
190.68249494	0.35359382605E-01
62.295441898	0.11095789217
22.654161182	0.24982972552
2 s	
8.9791477428	0.40623896148
3.6863002370	0.24338217176
1 s	
0.84660076805	1.0000000000
1 s	
0.33647133771	1.0000000000
1 s	
0.13647653675	1.0000000000
4 p	
49.200380510	0.55552416751E-02
11.346790537	0.38052379723E-01
3.4273972411	0.14953671029
1.1785525134	0.34949305230
1 p	
0.41642204972	0.45843153697
1 p	
0.14260826011	0.24428771672
1 d	
1.6540000000	1.0000000000
1 d	
0.4690000000	1.0000000000
1 f	
1.0930000000	1.0000000000

*

*

o def2-TZVPP

o (11s6p2d1f) / [5s3p2d1f] {62111/411/11/1}

*

6 s	
27032.382631	0.21726302465E-03
4052.3871392	0.16838662199E-02
922.32722710	0.87395616265E-02
261.24070989	0.35239968808E-01
85.354641351	0.11153519115
31.035035245	0.25588953961
2 s	
12.260860728	0.39768730901
4.9987076005	0.24627849430
1 s	
1.1703108158	1.0000000000
1 s	
0.46474740994	1.0000000000
1 s	
0.18504536357	1.0000000000
4 p	
63.274954801	0.60685103418E-02
14.627049379	0.41912575824E-01
4.4501223456	0.16153841088
1.5275799647	0.35706951311
1 p	

0.52935117943	0.44794207502
1 p	
0.17478421270	0.24446069663
1 d	
2.3140000000	1.0000000000
1 d	
0.6450000000	1.0000000000
1 f	
1.4280000000	1.0000000000
*	
*	
f def2-TZVPP	
# f (11s6p2d1f) / [5s3p2d1f]	{62111/411/11/1}
*	
6 s	
35479.100441	0.21545014888E-03
5318.4728983	0.16700686527E-02
1210.4810975	0.86733211476E-02
342.85518140	0.35049933175E-01
112.01943181	0.11165320133
40.714740248	0.25988506647
2 s	
16.039678111	0.39422966880
6.5038186740	0.24998238551
1 s	
1.5440477509	1.0000000000
1 s	
0.61223452862	1.0000000000
1 s	
0.24027979698	1.0000000000
4 p	
80.233900483	0.63685999134E-02
18.594010743	0.44303143530E-01
5.6867902653	0.16867248708
1.9511006294	0.36166346255
1 p	
0.66970211298	0.44202901491
1 p	
0.21651300410	0.24319875730
1 d	
3.1070000000	1.0000000000
1 d	
0.8550000000	1.0000000000
1 f	
1.9170000000	1.0000000000
*	
*	
ne def2-TZVPP	
# ne (11s6p2d1f) / [5s3p2d1f]	{62111/411/11/1}
*	
6 s	
45069.464022	0.21687155182E-03
6755.9768656	0.16812736757E-02
1537.6502864	0.87356062782E-02
435.51697667	0.35361266922E-01
142.28655638	0.11321521454
51.692153804	0.26654653104
2 s	
20.315870490	0.39631959951
8.2021942646	0.25582811251

```

1 s
1.9681276278      1.0000000000
1 s
0.77904756001    1.0000000000
1 s
0.30229502043    1.0000000000
4 p
99.782996032     0.65569234163E-02
23.176124101     0.45888009138E-01
7.1163945872     0.17331287812
2.4418711435     0.36475267512
1 p
0.83389605766    0.43831075171
1 p
0.26607311301    0.24160029835
1 d
4.0140000000     1.0000000000
1 d
1.0960000000     1.0000000000
1 f
2.5440000000     1.0000000000
*
*
na def2-TZVPP
# na      (14s8p3d) / [5s4p3d]      {73211/5111/111}
*
7 s
26041.109927     0.61806342811E-03
3906.1268548     0.47748604414E-02
888.97454993     0.24471684829E-01
251.45497961     0.94755394977E-01
81.650143512     0.26867496920
28.904158401     0.47925475440
10.625782932     0.33248591469
3 s
53.769410179     0.19527731872E-01
16.308243025     0.92648010794E-01
2.3730384125     -0.39938670172
2 s
0.95730772603    1.6428595391
0.40806460959    0.55692596966
1 s
0.49967582329E-01  1.0000000000
1 s
0.19268616250E-01  1.0000000000
5 p
138.07979989     0.57951891929E-02
32.232700393     0.41620846251E-01
9.9816075360     0.16281916885
3.4822033928     0.36011784647
1.2299134620     0.44858979889
1 p
0.41743959423    0.23040759559
1 p
0.30000000000E-01  1.0000000000
1 p
0.91000000000E-01  1.0000000000
1 d
2.6090000000     1.0000000000
1 d

```

```

0.430000000000      0.0000000000
 1 d
0.100000000000      0.0000000000
*
*
mg def2-TZVPP
# mg      (14s8p3d) / [5s4p3d]      {73211/5111/111}
*
 7 s
31438.349555      0.60912311326E-03
4715.5153354      0.47066196465E-02
1073.1629247      0.24135820657E-01
303.57238768      0.93628959834E-01
98.626251042      0.26646742093
34.943808417      0.47890929917
12.859785199      0.33698490286
 3 s
64.876913004      0.19180889307E-01
19.725520777      0.90913704392E-01
2.8951804339      -0.39563756125
 2 s
1.1960454710      1.6827603373
0.54329451156      0.52141091954
 1 s
0.10099104092      1.0000000000
 1 s
0.36865728085E-01  1.0000000000
 5 p
179.87189612      0.53799549018E-02
42.120069376      0.39318014098E-01
13.120503032      0.15740129476
4.6257503609      0.35919094128
1.6695211016      0.45533379310
 1 p
0.58551012105      0.21986432910
 1 p
0.18914796195      1.0000000000
 1 p
0.53768755187E-01  1.0000000000
 1 d
3.4440000000      1.0000000000
 1 d
0.290000000000      1.0000000000
 1 d
0.70000000000E-01  1.0000000000
*
*
al def2-TZVPP
# al      (14s9p3d1f) / [5s5p3d1f]      {73211/51111/111/1}
*
 7 s
37792.550772      0.57047888709E-03
5668.0682165      0.44093016538E-02
1289.8582841      0.22630967411E-01
364.86596028      0.88025644295E-01
118.57631515      0.25223701612
42.024867605      0.45960547169
15.499501629      0.33277886014
 3 s
75.208026598      0.19250560190E-01

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```

23.031408972      0.87906743952E-01
3.6348797649     -0.34246704535
 2 s
1.6065049957      1.5106266058
0.76103394581     0.58071016470
 1 s
0.16556708849      1.00000000000
 1 s
0.60041577113E-01  1.00000000000
 5 p
452.52303192      0.23110812466E-02
107.08195049      0.18568641823E-01
34.131021255      0.87216237035E-01
12.587037428      0.26902101523
4.9811919704      0.52128324272
 1 p
2.0070350900      0.60271687494
 1 p
0.80083714374      1.00000000000
 1 p
0.20178927472      1.00000000000
 1 p
0.57895550392E-01  1.00000000000
 1 d
1.57000000000      1.00000000000
 1 d
0.33300000000      1.00000000000
 1 d
0.11100000000      1.00000000000
 1 f
0.24400000000      1.00000000000
*
*
si def2-TZVPP
# si      (14s9p3d1f) / [5s5p3d1f]      {73211/51111/111/1}
*
 7 s
44773.358078      0.55914765868E-03
6717.1992104      0.43206040189E-02
1528.8960325      0.22187096460E-01
432.54746585      0.86489249116E-01
140.61505226      0.24939889716
49.857636724      0.46017197366
18.434974885      0.34250236575
 3 s
86.533886111      0.21300063007E-01
26.624606846      0.94676139318E-01
4.4953057159     -0.32616264859
 2 s
2.1035045710      1.3980803850
1.0106094922      0.63865786699
 1 s
0.23701751489      1.00000000000
 1 s
0.85703405362E-01  1.00000000000
 5 p
394.47503628      0.26285693959E-02
93.137683104      0.20556257749E-01
29.519608742      0.92070262801E-01
10.781663791      0.25565889739

```

4.1626574778	0.42111707185
1 p	
1.6247972989	0.34401746318
1 p	
0.54306660493	1.0000000000
1 p	
0.20582073956	1.0000000000
1 p	
0.70053487306E-01	1.0000000000
1 d	
2.3030000000	1.0000000000
1 d	
0.47600000000	1.0000000000
1 d	
0.16000000000	1.0000000000
1 f	
0.33600000000	1.0000000000
*	
*	
p def2-TZVPP	
# p (14s9p3d1f) / [5s5p3d1f] {73211/51111/111/1}	
*	
7 s	
52426.999233	0.55207164100E-03
7863.2660552	0.42678595308E-02
1789.5227333	0.21931529186E-01
506.27300165	0.85667168373E-01
164.60698546	0.24840686605
58.391918722	0.46336753971
21.643663201	0.35350558156
3 s	
99.013837620	0.21895679958E-01
30.550439817	0.95650470295E-01
5.4537087661	-0.29454270186
2 s	
2.6503362563	1.3294381200
1.2726688867	0.66109396473
1 s	
0.31645005203	1.0000000000
1 s	
0.11417466938	1.0000000000
5 p	
472.27219248	0.25710623052E-02
111.58882756	0.20250297999E-01
35.445936418	0.91580716787E-01
12.990776875	0.25749454014
5.0486221658	0.42862899758
1 p	
1.9934049566	0.34359817849
1 p	
0.66527284430	1.0000000000
1 p	
0.25516832128	1.0000000000
1 p	
0.90357762251E-01	1.0000000000
1 d	
3.1200000000	1.0000000000
1 d	
0.64800000000	1.0000000000
1 d	


```

0.21800000000      1.0000000000
  1 f
0.45200000000      1.0000000000
*
*
s def2-TZVPP
# s      (14s9p3d1f) / [5s5p3d1f]      {73211/51111/111/1}
*
  7 s
60700.928104      0.54695944225E-03
9102.6106854      0.42297224557E-02
2071.4166009      0.21747824159E-01
586.02476821      0.85100053589E-01
190.55395021      0.24799128459
67.630384260      0.46703640406
25.127306905      0.36434587550
  3 s
112.57463010      0.21670040240E-01
34.795554217      0.93602301760E-01
6.5115556215      -0.26068001422
  2 s
3.2399032261      1.2842089435
1.5477160881      0.66036416584
  1 s
0.40541030112      1.0000000000
  1 s
0.14550651059      1.0000000000
  5 p
564.36716027      0.24796796317E-02
133.42624379      0.19677930250E-01
42.468271189      0.89980008258E-01
15.616527580      0.25705880575
6.1093988469      0.43515167292
  1 p
2.4404160198      0.34883240595
  1 p
0.83882201296      1.0000000000
  1 p
0.31288746900      1.0000000000
  1 p
0.10770109004      1.0000000000
  1 d
3.75600000000      1.0000000000
  1 d
0.81200000000      1.0000000000
  1 d
0.27300000000      1.0000000000
  1 f
0.55700000000      1.0000000000
*
*
c1 def2-TZVPP
# c1      (14s9p3d1f) / [5s5p3d1f]      {73211/51111/111/1}
*
  7 s
69507.990945      0.54314897497E-03
10426.156880      0.41990463961E-02
2373.2334061      0.21592141679E-01
671.56420071      0.84598850094E-01
218.41999790      0.24757249724

```

77.572249714	0.47016930228
28.888815277	0.37436370716
3 s	
127.10527185	0.25182166603E-01
39.339582961	0.10786112456
7.6740679989	-0.27408821574
2 s	
3.8745627630	1.3213875014
1.8385832573	0.68636955368
1 s	
0.50229057542	1.0000000000
1 s	
0.17962723420	1.0000000000
5 p	
666.50423284	0.23632663836E-02
157.64241690	0.18879300374E-01
50.262520978	0.87206341273E-01
18.536078105	0.25285612970
7.2940532777	0.43507154820
1 p	
2.9433248995	0.35026513165
1 p	
1.0404970818	1.0000000000
1 p	
0.38456415080	1.0000000000
1 p	
0.13069642732	1.0000000000
1 d	
4.6100000000	1.0000000000
1 d	
1.0110000000	1.0000000000
1 d	
0.33900000000	1.0000000000
1 f	
0.70600000000	1.0000000000
*	
*	
ar def2-TZVPP	
# ar (14s9p3d1f) / [5s5p3d1f] {73211/51111/111/1}	
*	
7 s	
79111.422998	0.51029325002E-03
11864.746009	0.39463036981E-02
2700.1642973	0.20307073910E-01
763.95943485	0.79691825214E-01
248.45150561	0.23420623836
88.283581000	0.44833849481
32.948607069	0.36408167400
3 s	
142.55358000	0.26387407001E-01
44.163688009	0.11226433999
8.9524995000	-0.26178922001
2 s	
4.5546920941	1.3002484998
2.1444079001	0.67197237009
1 s	
0.60708777004	1.0000000000
1 s	
0.21651431999	1.0000000000
5 p	

776.77541998	0.22028005003E-02
183.80107018	0.17694180008E-01
58.694003175	0.82431293717E-01
21.701591695	0.24207278863
8.5821489635	0.42263558251
1 p	
3.4922679161	0.34151806086
1 p	
1.2637426998	1.0000000000
1 p	
0.46607870005	1.0000000000
1 p	
0.15766003000	1.0000000000
1 d	
5.55100000000	1.0000000000
1 d	
1.23500000000	1.0000000000
1 d	
0.41200000000	1.0000000000
1 f	
0.89000000000	1.0000000000
*	
*	
k def2-TZVPP	
# k (17s11p3d) / [6s4p3d] {842111/6311/111}	
*	
8 s	
153976.18325	0.23662636107E-03
23082.497672	0.18342929137E-02
5253.2344745	0.95310527769E-02
1486.9550133	0.38638406980E-01
484.06333726	0.12480768502
173.56653980	0.29278861009
67.116381464	0.40633425860
26.339502054	0.20077215860
4 s	
172.87693567	-0.24200960936E-01
53.058649063	-0.11553095040
7.9212753964	0.57455545175
3.2108880472	0.57023185107
2 s	
4.5662070895	-0.22615763466
0.70209907282	0.75528392045
1 s	
0.28258942635	1.0000000000
1 s	
0.35805824617E-01	1.0000000000
1 s	
0.15819213245E-01	1.0000000000
6 p	
728.18449873	0.26150689792E-02
172.13265061	0.20673630835E-01
54.829847075	0.93205603870E-01
20.166266494	0.25436518210
7.8610728806	0.39131132810
3.1105213132	0.22481345943
3 p	
11.757337492	-0.25777289217E-01
1.5139617411	0.57359428604
0.58328591795	1.0798320002

```

1 p
0.21570478076      1.0000000000
1 p
0.41737000000E-01  1.0000000000
1 d
0.93000000000      1.0000000000
1 d
0.18000000000      1.0000000000
1 d
0.54000000000E-01  1.0000000000
*
*
ca def2-TZVPP
# ca      (17s12p4d) / [6s5p3d]      {842111/63111/211}
*
8 s
172517.32685      0.23317502546E-03
25861.519275      0.18076521980E-02
5885.6618668      0.93943844255E-02
1665.9730031      0.38108409009E-01
542.36718148      0.12331203853
194.57803492      0.29004470954
75.303597636      0.40587151157
29.574062589      0.20398410743
4 s
191.20074660      -0.24419759759E-01
58.840299883      -0.11547027448
8.9642540845      0.56356636717
3.6856960541      0.56709682704
2 s
5.2464289726      -0.22825334325
0.84862621528      0.72625219172
1 s
0.36743300538      1.0000000000
1 s
0.66821582613E-01  1.0000000000
1 s
0.26759730445E-01  1.0000000000
6 p
836.97262058      0.25258346092E-02
197.93040142      0.20076506686E-01
63.135558054      0.91302987366E-01
23.282687170      0.25247029915
9.1176444932      0.39426326344
3.6336120139      0.23011559492
3 p
13.494163120      -0.26495021951E-01
1.8139259790      0.55088108210
0.71981826006      1.0280616620
1 p
0.27629576992      1.0000000000
1 p
0.74979000000E-01  1.0000000000
1 p
0.26927000000E-01  1.0000000000
2 d
5.4979093879      0.73770011433E-01
1.3177128032      0.26052853169
1 d
0.32188682649      0.45233836380

```

```

1 d
0.70528614919E-01 1.0000000000
*
*
sc def2-TZVPP
# sc (17s12p7d2f1g) / [6s5p4d2f1g] {842111/63111/4111/11/1}
*
8 s
191612.91874 0.23076475942E-03
28723.850363 0.17890329946E-02
6537.0116490 0.92990401140E-02
1850.3097171 0.37739438011E-01
602.38855156 0.12227148359
216.17324766 0.28814821470
83.712517880 0.40517543099
32.908707189 0.20566019623
4 s
211.34393234 -0.24527991462E-01
65.128920139 -0.11570158142
10.034311535 0.55995283317
4.1596884597 0.56087765073
2 s
6.0009041613 -0.22840494325
0.98255784150 0.71948970378
1 s
0.42483192773 1.0000000000
1 s
0.77185462096E-01 1.0000000000
1 s
0.30147219702E-01 1.0000000000
6 p
947.34122823 0.24737208744E-02
224.09699732 0.19742967060E-01
71.560334882 0.90357147549E-01
26.444824490 0.25201602503
10.393798285 0.39675535929
4.1606304559 0.23208624517
3 p
15.565737135 -0.27129423974E-01
2.1121544865 0.55109256629
0.84184709021 1.0090635806
1 p
0.32297542652 1.0000000000
1 p
0.12390000000 1.0000000000
1 p
0.47530000000E-01 1.0000000000
4 d
30.989390993 0.11902837431E-01
8.6905465069 0.67655856850E-01
2.9520256337 0.21332539722
1.0761910745 0.38391075578
1 d
0.38338915095 0.43354716259
1 d
0.12534686113 0.24509263822
1 d
0.41000000000E-01 0.0000000000
1 f
0.44200000000 1.0000000000

```

```

1 f
0.11000000000 1.0000000000
1 g
0.24700000000 1.0000000000
*
*
ti def2-TZVPP
# ti (17s12p7d2f1g) / [6s5p4d2f1g] {842111/63111/4111/11/1}
*
8 s
211575.69025 0.23318151011E-03
31714.945058 0.18079690851E-02
7217.5476543 0.93984311352E-02
2042.9394247 0.38156853618E-01
665.12896208 0.12374757197
238.74942264 0.29208551143
92.508691001 0.41226800855
36.403919209 0.21090534061
4 s
232.72624607 -0.24920140738E-01
71.791209711 -0.11746490087
11.158534615 0.56503342318
4.6548135416 0.56211101812
2 s
6.8034629174 -0.23011425503
1.1201076403 0.72103186735
1 s
0.48080118839 1.0000000000
1 s
0.85157274977E-01 1.0000000000
1 s
0.32657477046E-01 1.0000000000
6 p
1063.1474732 0.24690839320E-02
251.56507061 0.19773345523E-01
80.408554854 0.90987976672E-01
29.768193269 0.25559900413
11.736830556 0.40489386764
4.7142375230 0.23693402558
3 p
17.796803704 -0.27878639615E-01
2.4272698680 0.55672914668
0.96823445537 1.0055447350
1 p
0.37056694165 1.0000000000
1 p
0.14180000000 1.0000000000
1 p
0.54270000000E-01 1.0000000000
4 d
37.713384723 0.11513835092E-01
10.692931184 0.67246343996E-01
3.6728446990 0.21484207775
1.3588590303 0.38890892779
1 d
0.49213295253 0.43040835243
1 d
0.16330520653 0.23253305465
1 d
0.54000000000E-01 0.0000000000

```

```

1 f
0.25390000000 1.0000000000
1 f
1.0750000000 1.0000000000
1 g
0.63400000000 1.0000000000
*
*
v def2-TZVPP
# v (17s12p7d2f1g) / [6s5p4d2f1g] {842111/63111/4111/11/1}
*
8 s
232340.65058 0.23072410092E-03
34828.841170 0.17888178962E-02
7926.5448691 0.92992490131E-02
2243.7733046 0.37761463347E-01
730.59322944 0.12255909662
262.32219631 0.28963508811
101.70403805 0.41004702955
40.064784617 0.21113610858
4 s
255.24014968 -0.24458116338E-01
78.804646961 -0.11527205366
12.340598946 0.55174749453
5.1742019219 0.54504528489
2 s
7.6513894469 -0.22967638286
1.2639759898 0.71683769077
1 s
0.53861761721 1.0000000000
1 s
0.92719296124E-01 1.0000000000
1 s
0.34998055176E-01 1.0000000000
6 p
1184.2369151 0.24449826729E-02
280.23075192 0.19643454466E-01
89.643627137 0.90796949190E-01
33.242411253 0.25650768222
13.144514452 0.40815393750
5.2948534140 0.23860378268
3 p
20.175586851 -0.28241489023E-01
2.7605865197 0.55574635619
1.1008900902 0.99319919270
1 p
0.42013310739 1.0000000000
1 p
0.16030000000 1.0000000000
1 p
0.61190000000E-01 1.0000000000
4 d
43.861134864 0.11487174238E-01
12.516021891 0.68247153977E-01
4.3313854957 0.21837784195
1.6138855773 0.39245212296
1 d
0.58749573961 0.42634466786
1 d
0.19515723011 0.22646562601

```

```

1 d
0.650000000000E-01  0.0000000000
1 f
1.70800000000  1.0000000000
1 f
0.39800000000  1.0000000000
1 g
1.00900000000  1.0000000000
*
*
cr def2-TZVPP
# cr      (17s12p7d2f1g) / [6s5p4d2f1g]      {842111/63111/4111/11/1}
*
8 s
254477.80704      0.23386945693E-03
38131.797054      0.18142601800E-02
8675.2930607      0.94363925721E-02
2455.0099848      0.38343639367E-01
799.16217787      0.12459194837
286.90021489      0.29489696029
111.25413232      0.41846149607
43.864152636      0.21633763420
4 s
279.32669173      -0.23450908111E-01
86.274732376      -0.11080370027
13.555756113      0.53028965842
5.6978112751      0.51603516947
2 s
8.5636582615      -0.38109545675
1.3988296768      1.1991591436
1 s
0.57288171116      1.0000000000
1 s
0.90096171317E-01  1.0000000000
1 s
0.34125885135E-01  1.0000000000
6 p
1306.4398864      0.24277326185E-02
309.25311441      0.19544041017E-01
98.996273963      0.90651794553E-01
36.756916451      0.25699279154
14.566657077      0.40935504891
5.8739937432      0.23729388849
3 p
22.890999695      -0.28166026613E-01
3.0855001822      0.56034120148
1.2132329118      0.98119019650
1 p
0.44931680699      1.0000000000
1 p
0.16640000000      1.0000000000
1 p
0.61630000000E-01  1.0000000000
4 d
43.720074476      0.13622964026E-01
12.391242652      0.78935180133E-01
4.2639442006      0.23833840000
1.5525221790      0.39526851122
1 d
0.53761929485      0.41061717056

```



```

1 d
0.16493173074      0.24440410795
1 d
0.51000000000E-01  0.00000000000
1 f
2.3410000000      1.00000000000
1 f
0.54200000000     1.00000000000
1 g
1.3820000000      1.00000000000
*
*
mn def2-TZVPP
# mn      (17s12p7d2f1g) / [6s5p4d2f1g]      {842111/63111/4111/11/1}
*
8 s
277185.00153      0.22838385133E-03
41550.769890      0.17707650375E-02
9455.9700152      0.92077209994E-02
2676.5206482      0.37415971825E-01
871.46687530      0.12164861426
312.98306420      0.28824392499
121.44454051      0.41041600847
47.922598829      0.21372375145
4 s
303.66723163      -0.24589926140E-01
93.881403187      -0.11602608038
14.879421214      0.55112059677
6.2865200745      0.53707560756
2 s
9.4858591337      -0.22889262695
1.5698706158      0.71196169587
1 s
0.65903213608      1.00000000000
1 s
0.10686292371      1.00000000000
1 s
0.39267435433E-01  1.00000000000
6 p
1444.7978182      0.23994136455E-02
342.06551197      0.19369286864E-01
109.58400891      0.90236108988E-01
40.747988173      0.25745467851
16.188626566      0.41272351958
6.5484505964      0.24087700007
3 p
25.357086437      -0.28707174058E-01
3.4830168782      0.55208100712
1.3858800906      0.97226901379
1 p
0.52555094893      1.00000000000
1 p
0.19930000000      1.00000000000
1 p
0.75570000000E-01  1.00000000000
4 d
56.563189119      0.11543245295E-01
16.278734711      0.70299845987E-01
5.6964273914      0.22450770821
2.1411147942      0.39703065434

```

```

1 d
0.78291801938      0.41941039165
1 d
0.25952311214      0.21887261673
1 d
0.860000000000E-01  0.00000000000
1 f
2.97500000000      1.00000000000
1 f
0.720000000000      1.00000000000
1 g
1.75500000000      1.00000000000
*
*
fe def2-TZVPP
# fe      (17s12p7d2f1g) / [6s5p4d2f1g]      {842111/63111/4111/11/1}
*
8 s
300784.84637      0.22806273096E-03
45088.970557      0.17681788761E-02
10262.516317      0.91927083490E-02
2905.2897293      0.37355495807E-01
946.11487137      0.12151108426
339.87832894      0.28818881468
131.94425588      0.41126612677
52.111494077      0.21518583573
4 s
329.48839267      -0.24745216477E-01
101.92332739      -0.11683089050
16.240462745      0.55293621136
6.8840675801      0.53601640182
2 s
10.470693782      -0.22912708577
1.7360039648      0.71159319984
1 s
0.72577288979      1.00000000000
1 s
0.11595528203      1.00000000000
1 s
0.41968227746E-01  1.00000000000
6 p
1585.3959970      0.23793960179E-02
375.38006499      0.19253154755E-01
120.31816501      0.90021836536E-01
44.788749031      0.25798172356
17.829278584      0.41492649744
7.2247153786      0.24207474784
3 p
28.143219756      -0.29041755152E-01
3.8743241412      0.55312260343
1.5410752281      0.96771136842
1 p
0.58285615250      1.00000000000
1 p
0.22040000000      1.00000000000
1 p
0.833800000000E-01  1.00000000000
4 d
61.996675034      0.11971972255E-01
17.873732552      0.73210135410E-01

```

6.2744782934	0.23103094314	
2.3552337175	0.39910706494	
1 d		
0.85432239901	0.41391589765	
1 d		
0.27869254413	0.21909269782	
1 d		
0.91000000000E-01	0.00000000000	
1 f		
3.46500000000	1.00000000000	
1 f		
0.84300000000	1.00000000000	
1 g		
2.12800000000	1.00000000000	
*		
*		
co def2-TZVPP		
# co (17s12p7d2f1g) / [6s5p4d2f1g]	{842111/63111/4111/11/1}	
*		
8 s		
325817.01553	0.22568462484E-03	
48839.636453	0.17499397533E-02	
11114.937307	0.91003134097E-02	
3146.1603642	0.36996256837E-01	
1024.4378465	0.12044269621	
368.02508816	0.28598731649	
142.91229205	0.40908312004	
56.482649209	0.21500145739	
4 s		
356.40298318	-0.24767059678E-01	
110.31165215	-0.11702139134	
17.659634834	0.55215522200	
7.5059030479	0.53246877060	
2 s		
11.501807176	-0.22942470077	
1.9081994606	0.71180933514	
1 s		
0.79396696891	1.00000000000	
1 s		
0.124444448829	1.00000000000	
1 s		
0.44444645379E-01	1.00000000000	
6 p		
1731.1369144	0.23905767685E-02	
409.91750438	0.19382999967E-01	
131.45648578	0.90905448509E-01	
48.987439714	0.26146681577	
19.537078992	0.42157264570	
7.9287281634	0.24571813557	
3 p		
31.076017584	-0.29438069973E-01	
4.2835180697	0.55615568168	
1.7022921563	0.96772195064	
1 p		
0.64202908602	1.00000000000	
1 p		
0.24210000000	1.00000000000	
1 p		
0.91320000000E-01	1.00000000000	
4 d		

68.140745239	0.11983845360E-01	
19.685241019	0.73688540475E-01	
6.9322128825	0.23085496779	
2.6025125694	0.39281059225	
1 d		
0.94016837302	0.40203412228	
1 d		
0.30381457794	0.21415606743	
1 d		
0.980000000000E-01	0.00000000000	
1 f		
3.9550000000	1.00000000000	
1 f		
0.965000000000	1.00000000000	
1 g		
2.50000000000	1.00000000000	
*		
*		
ni def2-TZVPP		
# ni (17s12p7d2f1g) / [6s5p4d2f1g]	{842111/63111/4111/11/1}	
*		
8 s		
351535.72935	0.22529386884E-03	
52695.809283	0.17468616223E-02	
11992.468293	0.90849992136E-02	
3394.5776689	0.36940748447E-01	
1105.3594585	0.12032819950	
397.14677769	0.28596715057	
154.27542974	0.40983020196	
61.018723780	0.21620642851	
4 s		
384.45559739	-0.24651279268E-01	
119.04879199	-0.11658505277	
19.137012223	0.54864126676	
8.1526718562	0.52640051122	
2 s		
12.579408642	-0.22797884293	
2.0870866081	0.70703738215	
1 s		
0.86432568555	1.00000000000	
1 s		
0.13283169217	1.00000000000	
1 s		
0.46845327726E-01	1.00000000000	
6 p		
1883.0907486	0.23748258443E-02	
445.95155320	0.19289457172E-01	
143.08430815	0.90718211507E-01	
53.372920722	0.26181414117	
21.321919357	0.42309149832	
8.6643561994	0.24641686015	
3 p		
34.144255211	-0.29677129163E-01	
4.7122455921	0.55616824096	
1.8709231845	0.96357766460	
1 p		
0.70370016267	1.00000000000	
1 p		
0.264600000000	1.00000000000	
1 p		

```

0.995500000000E-01  1.0000000000
  4 d
  74.591603465      0.12077454672E-01
  21.590632752      0.74637262154E-01
  7.6246142580      0.23236775502
  2.8632206762      0.39042651680
  1 d
  1.0311063388      0.39509498921
  1 d
0.33060760691      0.21138769167
  1 d
0.10600000000      0.00000000000
  1 f
  4.44600000000      1.00000000000
  1 f
  1.08700000000      1.00000000000
  1 g
  2.87200000000      1.00000000000
*
*
cu def2-TZVPP
# cu      (17s12p7d2f1g) / [6s5p4d2f1g]      {842111/63111/4111/11/1}
*
  8 s
  377518.79923      0.22811766128E-03
  56589.984311      0.17688035931E-02
  12878.711706      0.91993460227E-02
  3645.3752143      0.37411016434E-01
  1187.0072945      0.12189873737
  426.46421902      0.28983900714
  165.70660164      0.41531872174
  65.598942707      0.21905799287
  4 s
  414.41265811      -0.24682525053E-01
  128.32056039      -0.11716827406
  20.622089750      0.55301315941
  8.7821226045      0.52242718609
  2 s
  13.741372006      -0.22736061821
  2.2431246833      0.71761210873
  1 s
0.89370549079      1.00000000000
  1 s
0.10836699534      1.00000000000
  1 s
0.38806178058E-01  1.00000000000
  6 p
  2034.7596692      0.23524822298E-02
  481.90468106      0.19134070751E-01
  154.67482963      0.90171105278E-01
  57.740576969      0.26063284735
  23.099052811      0.42093485770
  9.3882478591      0.24344615121
  3 p
  37.596171210      -0.28991094530E-01
  5.1240690810      0.54919083831
  2.0119996085      0.93793330488
  1 p
0.73860686002      1.00000000000
  1 p

```

0.27110000000	1.0000000000	
1 p		
0.99540000000E-01	1.0000000000	
4 d		
74.129460637	0.14363216676E-01	
21.359842587	0.86628177096E-01	
7.4995240537	0.25631430541	
2.7601394169	0.40374062368	
1 d		
0.95362061236	0.39427042447	
1 d		
0.28420862520	0.23091146816	
1 d		
0.85000000000E-01	0.0000000000	
1 f		
1.2090000000	1.0000000000	
1 f		
4.9360000000	1.0000000000	
1 g		
3.2450000000	1.0000000000	
*		
*		
zn def2-TZVPP		
# zn (17s12p7d2f1g) / [6s5p4d2f1g]		{842111/63111/4111/11/1}
*		
8 s		
405924.31028	0.22442017483E-03	
60846.955735	0.17402086626E-02	
13847.343092	0.90513339565E-02	
3919.6158551	0.36817341445E-01	
1276.3594167	0.12004850256	
458.67254435	0.28576057621	
178.28725246	0.41087462062	
70.612192837	0.21816962456	
4 s		
443.88077950	-0.24934274984E-01	
137.55875267	-0.11817955766	
22.268083479	0.55367318468	
9.5217310606	0.52628934936	
2 s		
14.874114065	-0.22929955254	
2.4647517612	0.71135484742	
1 s		
1.0113272238	1.0000000000	
1 s		
0.14919852089	1.0000000000	
1 s		
0.51441872981E-01	1.0000000000	
6 p		
2205.3508534	0.23356240448E-02	
522.35300699	0.19031022634E-01	
167.73055542	0.89955758675E-01	
62.670045373	0.26113248631	
25.109749456	0.42348448173	
10.225142681	0.24618926885	
3 p		
40.713442521	-0.30029667592E-01	
5.6247090696	0.55575254864	
2.2279949116	0.95581013442	
1 p		

```

0.83354741691      1.0000000000
  1 p
0.16245500000     1.0000000000
  1 p
0.47769000000E-01 1.0000000000
  4 d
  88.554315311     0.12728170015E-01
  25.721525557     0.79394499843E-01
  9.1278367624     0.24491506805
  3.4312364064     0.40390526479
  1 d
  1.2308920645     0.40158491145
  1 d
0.39031845112     0.21579805034
  1 d
0.12400000000     0.0000000000
  1 f
  1.4330000000     1.0000000000
  1 f
  5.6940000000     1.0000000000
  1 g
  3.6170000000     1.0000000000
*
*
ga def2-TZVPP
# ga      (17s12p8d1f) / [6s5p4d1f]      {842111/63111/5111/1}
*
  8 s
  435548.66254     0.23646329650E-03
  65289.589031     0.18335271776E-02
  14858.784256     0.95371863081E-02
  4205.9734729     0.38803412468E-01
  1369.6416431     0.12661604848
  492.30348905     0.30175310292
  191.41923233     0.43543934218
  75.840558665     0.23282363780
  4 s
  474.30810613     -0.26743707958E-01
  147.10297560     -0.12654657542
  23.982599435     0.58840346839
  10.298230094     0.56324271589
  2 s
  16.050381430     -0.24516439508
  2.6988468784     0.74578049593
  1 s
  1.1428588736     1.0000000000
  1 s
0.20217652251     1.0000000000
  1 s
0.71980152032E-01 1.0000000000
  6 p
  2432.0171070     0.22434065928E-02
  576.12049582     0.18342265336E-01
  185.11584354     0.87279697167E-01
  69.246572556     0.25684868351
  27.818107777     0.42398378107
  11.420229938     0.25701340043
  3 p
  42.819661530     -0.19326519119E-01
  6.3885901000     0.31571386917

```

2.6698993326	0.57617792822
1 p	
1.0781783834	1.0000000000
1 p	
0.22796559371	1.0000000000
1 p	
0.62836234833E-01	1.0000000000
5 d	
103.92331829	0.11464613652E-01
30.371094389	0.73625747383E-01
10.872078097	0.23505107382
4.1549137954	0.40318563513
1.5345659145	0.40824748152
1 d	
0.51114263830	0.20502439263
1 d	
0.30622000000	1.0000000000
1 d	
0.11391309000	1.0000000000
1 f	
0.30996095000	1.0000000000
*	
*	
ge def2-TZVPP	
# ge (17s12p8d1f) / [6s5p4d1f]	{842111/63111/5111/1}
*	
8 s	
466115.00592	0.22487264660E-03
69875.420762	0.17435426729E-02
15903.276716	0.90691482206E-02
4501.8233453	0.36906174685E-01
1466.0570924	0.12050167907
527.07841728	0.28748641703
205.00395074	0.41622321885
81.251596065	0.22397845695
4 s	
505.74661282	-0.25184609291E-01
156.96593744	-0.11898929721
25.761448176	0.54930135870
11.106654687	0.52939309129
2 s	
17.272059104	-0.22854595728
2.9438289048	0.68377930317
1 s	
1.2839164916	1.0000000000
1 s	
0.25873337445	1.0000000000
1 s	
0.93524913177E-01	1.0000000000
6 p	
2633.9346241	0.22143925310E-02
624.00161628	0.18140899141E-01
200.58528404	0.86632184922E-01
75.097081525	0.25649020592
30.214388474	0.42658611262
12.440087567	0.26200527313
3 p	
45.981316002	-0.20321767678E-01
6.9945654416	0.32013744527
2.9686001327	0.59051014555


```

1 p
1.2320988495      1.0000000000
1 p
0.28981614974    1.0000000000
1 p
0.85564606447E-01  1.0000000000
5 d
119.44887581     0.10586544521E-01
35.062915293     0.69601280945E-01
12.636924529     0.22807035287
4.8888672922     0.40301067220
1.8453195392     0.41304847015
1 d
0.63571158892    0.19639209740
1 d
0.35492132000    1.0000000000
1 d
0.13155709000    1.0000000000
1 f
0.36210645000    1.0000000000
*
*
as def2-TZVPP
# as      (17s13p8d1f) / [6s5p4d1f]      {842111/64111/5111/1}
*
8 s
498032.42158     0.22740196900E-03
74656.868743     0.17632816413E-02
16990.960004     0.91728040381E-02
4809.6200321     0.37337829344E-01
1566.2887055     0.12199536117
563.21360499     0.29137475324
219.11179978     0.42326351479
86.866061030     0.22921464278
4 s
538.19512479     -0.25254197297E-01
167.14850224     -0.11915461115
27.605517159     0.54628495980
11.947858521     0.53001520976
2 s
18.538023133     -0.23479188136
3.2018985739     0.69167053428
1 s
1.4356522077     1.0000000000
1 s
0.31837805200    1.0000000000
1 s
0.11622632186    1.0000000000
6 p
2678.9421546     0.23318955287E-02
634.61765840     0.19042149977E-01
203.93967606     0.90229744913E-01
76.323890369     0.26169037693
30.664124943     0.41857168155
12.505056732     0.23447830190
4 p
49.256229549     -0.21235539870E-01
7.7274891466     0.30470206668
3.5410493476     0.52888373107
1.6985585501     0.37272250955

```

```

1 p
0.76848071044      1.0000000000
1 p
0.30050823260      1.0000000000
1 p
0.98190639437E-01  1.0000000000
5 d
135.33289305       0.99291144106E-02
39.860212744       0.66568843496E-01
14.446428359       0.22275768307
5.6432900356       0.40309224382
2.1668188623       0.41671667946
1 d
0.76514970569      0.18935502288
1 d
0.42434653000      1.0000000000
1 d
0.16331527000      1.0000000000
1 f
0.43271941000      1.0000000000
*
*
se def2-TZVPP
# se      (17s13p8d1f) / [6s5p4d1f]      {842111/64111/5111/1}
*
8 s
531071.66696       0.24108973168E-03
79603.044117       0.18696431441E-02
18115.844240       0.97271616536E-02
5127.8923194       0.39604793031E-01
1669.9130839       0.12948855136
600.57534527       0.30959437289
233.70021247       0.45115769216
92.672443932       0.24579189033
4 s
571.57513675       -0.26895707881E-01
177.63686375       -0.12670989353
29.517767052       0.57699001719
12.824399795       0.56369075408
2 s
19.848235841       -0.25132415534
3.4744018486       0.72905416980
1 s
1.5988910849       1.0000000000
1 s
0.38333469387      1.0000000000
1 s
0.14049742459      1.0000000000
6 p
2815.3500566       0.25569026854E-02
666.92558298       0.20874026901E-01
214.34213188       0.98772096250E-01
80.246687942       0.28471821221
32.251081288       0.45003584934
13.106432562       0.24416091055
4 p
53.366108516       -0.21558456273E-01
8.1827777195       0.32662310638
3.6239945672       0.57740499319
1.6341591401       0.34301320826

```

```

1 p
0.58418320228      1.0000000000
1 p
0.23966269279      1.0000000000
1 p
0.88785134803E-01  1.0000000000
5 d
151.82910279       0.93970276988E-02
44.839992523       0.64086503991E-01
16.328999510       0.21834238004
6.4305057612       0.40314789649
2.5048025169       0.41966491490
1 d
0.90271148434      0.18366663432
1 d
0.47683613000      1.0000000000
1 d
0.18535160000      1.0000000000
1 f
0.48866905000      1.0000000000
*
*
br def2-TZVPP
# br      (17s13p8d1f) / [6s5p4d1f]      {842111/64111/5111/1}
*
8 s
565073.25256       0.23660314690E-03
84701.723179       0.18348332508E-02
19276.271900       0.95465849860E-02
5456.4284576       0.38877142153E-01
1776.9503500       0.12718314231
639.19398276       0.30437662191
248.78823961       0.44490940497
98.678305494       0.24381643058
4 s
606.07824568       -0.26527158709E-01
188.45598484       -0.12484584809
31.497144506       0.56468683559
13.736008320       0.55555268564
2 s
21.203212766       -0.24940920493
3.7616420178       0.71213119743
1 s
1.7735933962       1.0000000000
1 s
0.45197413664       1.0000000000
1 s
0.16613377099       1.0000000000
6 p
3019.6955723       0.24971049798E-02
715.35481126       0.20419267596E-01
229.98328751       0.96897148309E-01
86.167844615       0.28053901252
34.667870802       0.44606390473
14.113870307       0.24410073923
4 p
57.085653082       -0.21855950710E-01
8.8193845840       0.32707075320
3.9340302872       0.57855229520
1.7998830384       0.33570987698

```

1 p		
0.66899410512	1.0000000000	
1 p		
0.27136238231	1.0000000000	
1 p		
0.10083790243	1.0000000000	
5 d		
168.85370257	0.89663981988E-02	
49.977949919	0.62062059316E-01	
18.274913338	0.21474732384	
7.2455694631	0.40335336746	
2.8562315025	0.42208813080	
1 d		
1.0459621144	0.17874813267	
1 d		
0.56865655000	1.0000000000	
1 d		
0.22031490000	1.0000000000	
1 f		
0.57083312000	1.0000000000	
*		
*		
kr def2-TZVPP		
# kr (17s13p8d1f) / [6s5p4d1f]	{842111/64111/5111/1}	
*		
8 s		
600250.97575	0.23740610399E-03	
89976.650781	0.18410240539E-02	
20476.814225	0.95795580699E-02	
5796.1554078	0.39020650488E-01	
1887.5913196	0.12772645628	
679.11458519	0.30596521300	
264.38244511	0.44857474437	
104.88368574	0.24722957327	
4 s		
641.47370764	-0.26745279805E-01	
199.57524820	-0.12571122567	
33.545462954	0.56483736390	
14.683955144	0.55972765539	
2 s		
22.603101860	-0.25298771800	
4.0650682991	0.70992159965	
1 s		
1.9611027060	1.0000000000	
1 s		
0.52465147979	1.0000000000	
1 s		
0.19332399511	1.0000000000	
6 p		
3232.9589614	0.24885607974E-02	
765.96442694	0.20379007428E-01	
246.33940810	0.96977188584E-01	
92.365283041	0.28199960954	
37.199509551	0.45116254358	
15.172166534	0.24917131496	
4 p		
60.931321698	-0.22173603519E-01	
9.4792600646	0.32838462778	
4.2564686326	0.58124997120	
1.9729313762	0.32863541783	

```

1 p
0.76337108716      1.0000000000
1 p
0.30943625526      1.0000000000
1 p
0.11569704458      1.0000000000
5 d
186.41760904       0.86120284601E-02
55.274124345       0.60394406304E-01
20.283219120       0.21181331869
8.0884536976       0.40366293413
3.2214033853       0.42402860686
1 d
1.1952170102       0.17441742274
1 d
0.64800000000      1.0000000000
1 d
0.25100000000      1.0000000000
1 f
0.62800000000      1.0000000000
*
*
rb def2-TZVPP
# rb      (7s7p3d1f) / [6s4p3d1f]      {211111/4111/111/1}
*
2 s
7.4744618040       0.26997866363
6.7296180594       -0.42629251814
1 s
2.7816640004       1.0000000000
1 s
0.53452175148      1.0000000000
1 s
0.22368793034      1.0000000000
1 s
0.32410407052E-01  1.0000000000
1 s
0.14171047424E-01  1.0000000000
4 p
5.6720643194       0.48114224135E-01
3.3320183956       -0.18485131426
0.80150054910      0.42811864954
0.36302220227      0.58673165411
1 p
0.15733924392      1.0000000000
1 p
0.40000000000E-01  1.0000000000
1 p
0.16000000000E-01  1.0000000000
1 d
0.25907866956      0.76806746340E-01
1 d
0.42507438045E-01  0.37846160487
1 d
0.11909276840E-01  1.0000000000
1 f
0.85245000000      0.0000000000
*
rb def2-ecp
*

```

```

ncore = 28          lmax = 3
# coefficient      r^n      exponent
f
-12.3169000      2          3.8431140
s-f
 89.5001980      2          5.0365510
 0.4937610       2          1.9708490
12.3169000       2          3.8431140
p-f
 58.5689740      2          4.2583410
 0.4317910       2          1.4707090
12.3169000       2          3.8431140
d-f
 26.2248980      2          3.0231270
 0.9628390       2          0.6503830
12.3169000       2          3.8431140
*
*
sr def2-TZVPP
# sr (7s7p5d1f) / [6s4p3d1f] {211111/4111/311/1}
*
 2 s
10.0000000000    -0.18530550262
 8.5000000000    0.33970355376
 1 s
 3.0057048856    1.00000000000
 1 s
 0.61161287650   1.00000000000
 1 s
 0.27393841217   1.00000000000
 1 s
 0.57435564563E-01 1.00000000000
 1 s
 0.23338198665E-01 1.00000000000
 4 p
 7.5883077869    0.33731690287E-01
 3.6731307392    -0.20523185005
 0.90496618455   0.49209972665
 0.43310256408   0.62105296512
 1 p
 0.20222168964   1.00000000000
 1 p
 0.72000000000E-01 1.00000000000
 1 p
 0.25000000000E-01 1.00000000000
 3 d
 3.6180810000    -0.75010000000E-02
 0.99665600000   0.10809800000
 0.39073500000   0.27854000000
 1 d
 0.12277000000   1.00000000000
 1 d
 0.36655000000E-01 1.00000000000
 1 f
 0.99540000000   0.00000000000
*
sr def2-ecp
*
ncore = 28          lmax = 3
# coefficient      r^n      exponent

```

f	-15.8059920	2	4.6339750
s-f	135.4794300	2	7.4000740
	17.5344630	2	3.6063790
	15.8059920	2	4.6339750
p-f	88.3597090	2	6.4848680
	15.3943720	2	3.2880530
	15.8059920	2	4.6339750
d-f	29.8889870	2	4.6228410
	6.6594140	2	2.2469040
	15.8059920	2	4.6339750

*

*

y def2-TZVPP

y (7s7p5d2f1g) / [6s4p3d2f1g] {211111/4111/311/11/1}

*

2 s		
10.000000000	-0.17487686796	
8.500000000	0.34152345084	
1 s		
3.3653905454	1.0000000000	
1 s		
0.68860679385	1.0000000000	
1 s		
0.31191502936	1.0000000000	
1 s		
0.70326042567E-01	1.0000000000	
1 s		
0.27733859327E-01	1.0000000000	
4 p		
8.0554093616	0.36410978939E-01	
4.0163458751	-0.20872572547	
1.0232915404	0.48956929335	
0.49843561636	0.60611943833	
1 p		
0.23307661842	1.0000000000	
1 p		
0.80000000000E-01	1.0000000000	
1 p		
0.27000000000E-01	1.0000000000	
3 d		
3.9030833060	-0.98209792625E-02	
1.1363234302	0.19183629664	
0.45617043877	0.40597788539	
1 d		
0.17470950748	1.0000000000	
1 d		
0.61978796638E-01	1.0000000000	
1 f		
0.38611000000	1.0000000000	
1 f		
0.10766000000	1.0000000000	
1 g		
0.11149000000	1.0000000000	

*

y def2-ecp

*

```

ncore = 28          lmax = 3
#      coefficient   r^n      exponent
f      -19.1221981   2          6.5842120
      -2.4363754    2          3.2921060
s-f    135.1538441   2          7.4880494
      15.5524413    2          3.7440247
      19.1221981    2          6.5842120
      2.4363754     2          3.2921060
p-f    87.7849917    2          6.4453772
      11.5640660    2          3.2226886
      19.1221981    2          6.5842120
      2.4363754     2          3.2921060
d-f    29.7010007    2          4.6584472
      5.5399685     2          2.3292236
      19.1221981    2          6.5842120
      2.4363754     2          3.2921060
*
*
zr def2-TZVPP
# zr      (7s7p5d2f1g) / [6s4p3d2f1g]      {211111/4111/311/11/1}
*
  2 s
  11.000000000    -0.19075595257
  9.5000000000    0.33895588754
  1 s
  3.6383667759    1.0000000000
  1 s
  0.76822026698    1.0000000000
  1 s
  0.34036824036    1.0000000000
  1 s
  0.75261298085E-01  1.0000000000
  1 s
  0.30131404705E-01  1.0000000000
  4 p
  8.6066305543     0.40404260236E-01
  4.4400979958    -0.21187745201
  1.1281026946     0.49164266891
  0.54346076310    0.57303370658
  1 p
  0.25022406048    1.0000000000
  1 p
  0.85000000000E-01  1.0000000000
  1 p
  0.29000000000E-01  1.0000000000
  3 d
  4.5567957795    -0.96190569023E-02
  1.2904939797     0.20569990155
  0.51646987222    0.41831381851
  1 d
  0.19349797794    1.0000000000
  1 d
  0.67309809967E-01  1.0000000000
  1 f
  0.65322000000    1.0000000000
  1 f

```



```

0.18293000000      1.0000000000
  1 g
0.28989000000      1.0000000000
*
zr def2-ecp
*
  ncore =    28          lmax =    3
#   coefficient   r^n      exponent
f
    -21.0937760     2        7.5400000
    -3.0806943     2        3.7700000
s-f
    150.2675911     2        8.2000000
    18.9762165     2        4.0897278
    21.0937760     2        7.5400000
    3.0806943     2        3.7700000
p-f
    99.6221237     2        7.1100000
    14.1687333     2        3.5967980
    21.0937760     2        7.5400000
    3.0806943     2        3.7700000
d-f
    35.0451235     2        5.3500000
    6.1112595     2        2.4918215
    21.0937760     2        7.5400000
    3.0806943     2        3.7700000
*
*
nb def2-TZVPP
# nb      (7s7p5d2f1g) / [6s4p3d2f1g]      {211111/4111/311/11/1}
*
  2 s
  12.000000000      -0.20219507530
  10.500000000      0.33640105939
  1 s
  3.9276062854      1.0000000000
  1 s
  0.85976543258      1.0000000000
  1 s
  0.39074087505      1.0000000000
  1 s
  0.86387259879E-01  1.0000000000
  1 s
  0.32906200326E-01  1.0000000000
  4 p
  9.2056285646      0.43347689874E-01
  4.8679632125      -0.21302479233
  1.2442155792      0.48102127136
  0.60390590312      0.53917858960
  1 p
  0.27967675553      1.0000000000
  1 p
  0.90000000000E-01  1.0000000000
  1 p
  0.30000000000E-01  1.0000000000
  3 d
  4.6170975867      -0.13574476955E-01
  1.5663438480      0.20374310496
  0.66952425826      0.42997453105
  1 d

```

```

0.27140946867      1.0000000000
  1 d
0.10054426592      1.0000000000
  1 f
0.91801000000      1.0000000000
  1 f
0.25820000000      1.0000000000
  1 g
0.46829000000      1.0000000000
*
nb def2-ecp
*
  ncore =      28          lmax =      3
#      coefficient      r^n      exponent
f
      -22.9295500      2          8.4900000
      -3.6663099      2          4.2500000
s-f
      165.1791435      2          8.9000000
      21.9929744      2          4.4300000
      22.9295500      2          8.4900000
      3.6663099      2          4.2500000
p-f
      111.7944145      2          7.7700000
      16.6334833      2          3.9600000
      22.9295500      2          8.4900000
      3.6663099      2          4.2500000
d-f
      38.1122488      2          6.0500000
      8.0391673      2          2.8400000
      22.9295500      2          8.4900000
      3.6663099      2          4.2500000
*
*
mo def2-TZVPP
# mo      (7s7p5d2f1g) / [6s4p3d2f1g]      {211111/4111/311/11/1}
*
  2 s
  14.000000000      -0.22490043406
  12.500000000      0.33151248555
  1 s
  4.0921501803      1.0000000000
  1 s
  0.97053602586      1.0000000000
  1 s
  0.44217620170      1.0000000000
  1 s
  0.92915024334E-01      1.0000000000
  1 s
  0.35016314389E-01      1.0000000000
  4 p
  8.8931117915      0.699944449475E-01
  5.4689112270      -0.23547141883
  1.3548473007      0.46315460007
  0.65494867461      0.48820184710
  1 p
  0.30428197472      1.0000000000
  1 p
  0.10000000000      1.0000000000
  1 p

```

```

0.330000000000E-01  1.0000000000
  3 d
  5.0044445497      -0.21587364862E-01
  1.7736823324      0.20958680086
0.76950591696      0.43730880599
  1 d
0.31530878939      1.0000000000
  1 d
0.11754374390      1.0000000000
  1 f
  1.1805100000      1.0000000000
  1 f
0.33348000000      1.0000000000
  1 g
0.64670000000      1.0000000000
*
mo def2-ecp
*
  ncore =    28          lmax =    3
#      coefficient      r^n      exponent
f
      -24.8051771      2          9.4500000
      -4.1537815      2          4.7200000
s-f
      180.1031085      2          9.7145938
      24.9972279      2          4.6805004
      24.8051771      2          9.4500000
      4.1537815      2          4.7200000
p-f
      123.7727523      2          8.1421366
      19.5302280      2          4.6259863
      24.8051771      2          9.4500000
      4.1537815      2          4.7200000
d-f
      48.3750223      2          6.6184148
      8.8920527      2          3.2487516
      24.8051771      2          9.4500000
      4.1537815      2          4.7200000
*
*
tc def2-TZVPP
# tc      (7s7p5d2f1g) / [6s4p3d2f1g]      {211111/4111/311/11/1}
*
  2 s
  15.000000000      -0.19945408941
  12.910581694      0.33689922245
  1 s
  4.4493321158      1.0000000000
  1 s
  1.0548409451      1.0000000000
  1 s
0.47909677246      1.0000000000
  1 s
0.99124162989E-01  1.0000000000
  1 s
0.36882799789E-01  1.0000000000
  4 p
  10.027138011      0.61481602710E-01
  5.8463419741      -0.23600729385
  1.4968345491      0.47746483995

```

```

0.72934632066      0.50731543496
 1 p
0.33913558879      1.00000000000
 1 p
0.11000000000      1.00000000000
 1 p
0.35000000000E-01  1.00000000000
 3 d
 5.0906268699      -0.32176405405E-01
 2.0156178510      0.21280802536
0.88113887240      0.44403309175
 1 d
0.36427094833      1.00000000000
 1 d
0.13678402297      1.00000000000
 1 f
 1.4406400000      1.00000000000
 1 f
0.40875000000      1.00000000000
 1 g
0.82510000000      1.00000000000
*
tc def2-ecp
*
  ncore =      28          lmax =      3
#   coefficient  r^n      exponent
f
  -26.5624475    2          10.4000000
  -4.5856805    2          5.2000000
s-f
  195.1591659   2          10.4223462
  28.0926033   2          5.0365160
  26.5624475    2          10.4000000
  4.5856805    2          5.2000000
p-f
  135.2845662   2          8.9504494
  21.8065043   2          4.8544394
  26.5624475    2          10.4000000
  4.5856805    2          5.2000000
d-f
  54.3297294    2          6.9456968
  11.1550679   2          3.9705849
  26.5624475    2          10.4000000
  4.5856805    2          5.2000000
*
*
ru def2-TZVPP
# ru      (7s7p5d2f1g) / [6s4p3d2f1g]      {211111/4111/311/11/1}
*
  2 s
  16.000000000    -0.20634002919
  13.910581694    0.33550437725
  1 s
  4.7967971407    1.00000000000
  1 s
  1.1555425594    1.00000000000
  1 s
  0.52455741182    1.00000000000
  1 s
  0.10734572646    1.00000000000

```

```

1 s
0.39432760192E-01 1.0000000000
4 p
11.187208671 0.53225073263E-01
6.2477688734 -0.22731662050
1.6279472859 0.47869486056
0.79326493538 0.50213311567
1 p
0.36707276865 1.0000000000
1 p
0.11500000000 1.0000000000
1 p
0.37000000000E-01 1.0000000000
3 d
5.7341846619 -0.35266111560E-01
2.2483686294 0.21802502222
0.98376978359 0.44709565013
1 d
0.40379445583 1.0000000000
1 d
0.14978618173 1.0000000000
1 f
1.7077900000 1.0000000000
1 f
0.48442000000 1.0000000000
1 g
1.0093000000 1.0000000000
*
ru def2-ecp
*
ncore = 28 lmax = 3
# coefficient r^n exponent
f
-28.3406163 2 11.3600000
-4.9446292 2 5.6800000
s-f
209.8229712 2 11.1052693
30.6547264 2 5.4147454
28.3406163 2 11.3600000
4.9446292 2 5.6800000
p-f
146.3361823 2 9.7712707
24.1278772 2 5.0739908
28.3406163 2 11.3600000
4.9446292 2 5.6800000
d-f
67.5158967 2 7.6714231
9.8701041 2 4.1365647
28.3406163 2 11.3600000
4.9446292 2 5.6800000
*
*
rh def2-TZVPP
# rh (7s7p6d2f1g) / [6s4p3d2f1g] {211111/4111/411/11/1}
*
2 s
17.000000000 -0.16690803139
13.910581694 0.34235001652
1 s
5.2481265288 1.0000000000

```

```

1 s
1.2262575928      1.0000000000
1 s
0.53930216349    1.0000000000
1 s
0.10130730377    1.0000000000
1 s
0.37124139005E-01  1.0000000000
4 p
11.767103631     0.59494859388E-01
6.7485133083     -0.23735853477
1.7502679834     0.49019334303
0.84321166133    0.50623933751
1 p
0.38295544759    1.0000000000
1 p
0.11500000000    1.0000000000
1 p
0.37000000000E-01  1.0000000000
4 d
19.857830136     0.66960778187E-02
10.061378139     -0.21981738213E-01
2.2619546477     0.37918706236
0.97098845035    0.67289976592
1 d
0.38391195297    1.0000000000
1 d
0.13537026904    1.0000000000
1 f
1.9750700000     1.0000000000
1 f
0.56009000000    1.0000000000
1 g
1.1935000000     1.0000000000
*
rh def2-ecp
*
ncore = 28      lmax = 3
#      coefficient  r^n      exponent
f
      -30.0934557   2        12.3100000
      -5.2184819   2         6.1600000
s-f
      225.3477535   2         11.7200000
      32.8231890    2         5.8200000
      30.0934557   2         12.3100000
      5.2184819    2         6.1600000
p-f
      158.7094116   2         10.4200000
      26.4441005    2         5.4500000
      30.0934557   2         12.3100000
      5.2184819    2         6.1600000
d-f
      62.7586257    2         8.8200000
      10.9787195    2         3.8700000
      30.0934557   2         12.3100000
      5.2184819    2         6.1600000
*
*
pd def2-TZVPP

```

pd (7s7p6d2f1g) / [6s4p3d2f1g] {211111/4111/411/11/1}

```

*
  2 s
18.000000000 -0.16605388598
14.662134308 0.34899955055
  1 s
  5.6388709265 1.0000000000
  1 s
  1.3198953252 1.0000000000
  1 s
0.57817908509 1.0000000000
  1 s
0.10352166239 1.0000000000
  1 s
0.37548442674E-01 1.0000000000
  4 p
  12.552899300 0.61728998206E-01
  7.2444496380 -0.24178626753
  1.8905941078 0.49453200915
0.90737168760 0.50454362626
  1 p
0.40877210813 1.0000000000
  1 p
0.11500000000 1.0000000000
  1 p
0.37000000000E-01 1.0000000000
  4 d
  22.357457575 0.39559479546E-02
  10.682526382 -0.14039011601E-01
  2.4858232550 0.24219476776
  1.0735333903 0.42580283281
  1 d
0.42613842853 1.0000000000
  1 d
0.15046355385 1.0000000000
  1 f
  2.2424600000 1.0000000000
  1 f
0.63575000000 1.0000000000
  1 g
  1.3777000000 1.0000000000

```

*
pd def2-ecp

```

*
ncore = 28 lmax = 3
# coefficient r^n exponent
f
-31.9295543 2 13.2700000
-5.3982169 2 6.6300000
s-f
240.2290403 2 12.4300000
35.1719435 2 6.1707594
31.9295543 2 13.2700000
5.3982169 2 6.6300000
p-f
170.4172760 2 11.0800000
28.4721329 2 5.8295541
31.9295543 2 13.2700000
5.3982169 2 6.6300000
d-f

```

69.0138449	2	9.5100000
11.7508616	2	4.1397811
31.9295543	2	13.2700000
5.3982169	2	6.6300000

*
*

ag def2-TZVPP

ag (7s7p6d2f1g) / [6s4p3d2f1g] {211111/4111/411/11/1}

*

2 s		
19.000000000	-0.16600104141	
15.428199933	0.35665095918	
1 s		
6.0553507268	1.0000000000	
1 s		
1.4162368935	1.0000000000	
1 s		
0.61758635858	1.0000000000	
1 s		
0.10474197431	1.0000000000	
1 s		
0.37685106264E-01	1.0000000000	
4 p		
13.188180180	0.66928737147E-01	
7.7952789138	-0.24735235409	
2.0351571912	0.49154280216	
0.98093914842	0.49741609006	
1 p		
0.44451179958	1.0000000000	
1 p		
0.13000000000	1.0000000000	
1 p		
0.41200000000E-01	1.0000000000	
4 d		
25.784397351	0.35645063082E-02	
11.396636755	-0.12984262784E-01	
2.7345581361	0.24108826548	
1.1873583605	0.42412330744	
1 d		
0.47316910566	1.0000000000	
1 d		
0.16746017986	1.0000000000	
1 f		
2.5100300000	1.0000000000	
1 f		
0.71142000000	1.0000000000	
1 g		
1.5619000000	1.0000000000	

*

ag def2-ecp

*

ncore =	28	lmax =	3
#	coefficient	r^n	exponent
f	-33.6899201	2	14.2200000
	-5.5311202	2	7.1100000
s-f	255.1393645	2	13.1300000
	36.8661215	2	6.5100000
	33.6899201	2	14.2200000

	5.5311202	2	7.1100000
p-f	182.1818687	2	11.7400000
	30.3577515	2	6.2000000
	33.6899201	2	14.2200000
	5.5311202	2	7.1100000
d-f	73.7192609	2	10.2100000
	12.5021171	2	4.3800000
	33.6899201	2	14.2200000
	5.5311202	2	7.1100000

*

*

cd def2-TZVPP

cd (7s7p6d2f1g) / [6s4p3d2f1g] {211111/4111/411/11/1}

*

2 s		
20.000000000	-0.17401196927	
16.309051661	0.37137277194	
1 s		
6.4512709901	1.0000000000	
1 s		
1.5350047390	1.0000000000	
1 s		
0.68983631523	1.0000000000	
1 s		
0.13475720977	1.0000000000	
1 s		
0.47416874527E-01	1.0000000000	
4 p		
14.000681404	0.69333062793E-01	
8.3094019872	-0.25420103681	
2.2020058122	0.49200980368	
1.0779246137	0.49702118131	
1 p		
0.50111879846	1.0000000000	
1 p		
0.16000000000	1.0000000000	
1 p		
0.51600000000E-01	1.0000000000	
4 d		
30.380789793	0.32545123835E-02	
11.474551578	-0.14212074843E-01	
3.0507394903	0.24961756436	
1.3622028524	0.44905635176	
1 d		
0.56399409888	1.0000000000	
1 d		
0.20916686535	1.0000000000	
1 f		
2.8400100000	1.0000000000	
1 f		
0.82048000000	1.0000000000	
1 g		
1.7896000000	1.0000000000	

*

cd def2-ecp

*

ncore =	28	lmax =	3
# coefficient	r^n	exponent	

```

f
      -35.4766256    2      15.1847957
      -5.6176768    2      7.5923978
s-f
      270.0094832    2      13.8358689
      38.7673080     2      6.8572704
      35.4766256     2      15.1847957
      5.6176768      2      7.5923978
p-f
      193.8296294    2      12.4049710
      31.8965252     2      6.5677995
      35.4766256     2      15.1847957
      5.6176768      2      7.5923978
d-f
      79.1936470     2      10.8969253
      13.2308267     2      4.6411649
      35.4766256     2      15.1847957
      5.6176768      2      7.5923978
*
*
in def2-TZVPP
# in      (10s9p8d2f) / [6s5p3d2f]      {421111/33111/611/11}
*
  4 s
  847.79276774      0.12432052471E-03
  72.041054824      0.23600367607E-02
  41.061316522      -0.85588299453E-02
  12.407609713      0.62952032489
  2 s
  11.640316941      1.5543429200
  6.3695642727      0.67492488361
  1 s
  1.7063236353      1.0000000000
  1 s
  0.78666967936      1.0000000000
  1 s
  0.16965196873      1.0000000000
  1 s
  0.62074858667E-01  1.0000000000
  3 p
  268.28136685      0.11542193636E-03
  14.781553782      0.77779830292E-01
  8.8041476194      -0.28332389472
  3 p
  2.3717277227      0.47896111744
  1.1927065422      0.48293819961
  0.58352812041      0.16843883728
  1 p
  0.23280968310      1.0000000000
  1 p
  0.88674065208E-01  1.0000000000
  1 p
  0.33598828267E-01  1.0000000000
  6 d
  94.282575063      0.43652729696E-03
  19.716431102      0.63918753088
  19.600106824      -0.64663115577
  3.5643186737      0.21187579614
  1.7017801400      0.42129321741
  0.76456615531      0.38418127707

```

```

1 d
0.31826765584      1.0000000000
1 d
0.10000000000     1.0000000000
1 f
0.26415991000     1.0000000000
1 f
0.90000000000     1.0000000000
*
in def2-ecp
*
ncore =      28      lmax =      3
#      coefficient  r^n      exponent
f
      -13.7280780    2      12.5390560
      -18.2068660    2      12.5525610
s-f
      281.1223500    2      15.3928220
      61.9014700    2      8.0558640
      13.7280780    2      12.5390560
      18.2068660    2      12.5525610
p-f
      67.4621540    2      13.9286720
      134.9492500   2      13.3472340
      14.7461400    2      7.6141320
      29.6392620    2      7.3183650
      13.7280780    2      12.5390560
      18.2068660    2      12.5525610
d-f
      35.4932540    2      14.0347150
      53.1787730    2      14.5116160
      9.1772810     2      5.5505500
      12.3924100    2      5.0594150
      13.7280780    2      12.5390560
      18.2068660    2      12.5525610
*
*
sn def2-TZVPP
# sn      (10s9p8d2f) / [6s5p3d2f]      {421111/33111/611/11}
*
4 s
1577.0715931      0.17042767713E-03
235.26601078      0.81467057272E-03
38.206330645      -0.39057904293E-02
13.097031765      0.53245922343
2 s
11.681492759      1.5435287275
5.9647604361      0.76421510041
1 s
1.8891070740      1.0000000000
1 s
0.88514080630      1.0000000000
1 s
0.20500105152      1.0000000000
1 s
0.76748551032E-01  1.0000000000
3 p
221.55767496      0.31125177983E-03
21.084021433      0.31108097016E-01
8.7600138521      -0.27571560918

```

```

3 p
2.5912909722      0.45912328666
1.3426801157      0.49682867217
0.67732735829     0.18962377821
1 p
0.29418756752     1.00000000000
1 p
0.11863762052     1.00000000000
1 p
0.46215750632E-01 1.00000000000
6 d
108.33210154      0.46561853277E-03
23.703936630      0.54063163067E-01
22.339843906      -0.58928768877E-01
4.0874834028      0.19588500896
1.9737354146      0.42301799185
0.90158257692     0.39252716176
1 d
0.38237153649     1.00000000000
1 d
0.12000000000     1.00000000000
1 f
0.29392848500     1.00000000000
1 f
1.00000000000     1.00000000000
*
sn def2-ecp
*
ncore = 28          lmax = 3
# coefficient      r^n          exponent
f
-12.5763330       2            12.2823480
-16.5959440       2            12.2721500
s-f
279.9886820       2            17.4204140
62.3778100        2            7.6311550
12.5763330        2            12.2823480
16.5959440        2            12.2721500
p-f
66.1625230        2            16.1310240
132.1743960       2            15.6280770
16.3394170        2            7.3256080
32.4889590        2            6.9425190
12.5763330        2            12.2823480
16.5959440        2            12.2721500
d-f
36.3874410        2            15.5149760
54.5078410        2            15.1881600
8.6968230         2            5.4560240
12.8402080        2            5.3631050
12.5763330        2            12.2823480
16.5959440        2            12.2721500
*
*
sb def2-TZVPP
# sb (10s9p8d2f) / [6s5p3d2f] {421111/33111/611/11}
*
4 s
1612.4199933      0.28540380783E-03
238.84452097      0.13393778746E-02

```

23.998118809	-0.49388154574E-01
15.193124213	0.43392227254
2 s	
11.736409733	0.92125519965
6.5259774794	0.79235280226
1 s	
2.0247451872	1.0000000000
1 s	
0.97113418587	1.0000000000
1 s	
0.24254333998	1.0000000000
1 s	
0.92206608177E-01	1.0000000000
3 p	
215.68393354	0.26051823221E-03
16.374479088	0.73728000195E-01
9.7216283345	-0.27230028128
3 p	
2.7982643154	0.46472692374
1.4711045033	0.50364242075
0.75165385301	0.18706666294
1 p	
0.33168699849	1.0000000000
1 p	
0.13931606366	1.0000000000
1 p	
0.56399307526E-01	1.0000000000
6 d	
115.90312253	0.53140915051E-03
30.474233720	0.59411139166E-02
18.228418239	-0.10563706947E-01
4.3291456646	0.20348177341
2.1294818496	0.42748378928
0.99682636692	0.38539560809
1 d	
0.43347239863	1.0000000000
1 d	
0.14000000000	1.0000000000
1 f	
0.32369706000	1.0000000000
1 f	
1.10000000000	1.0000000000

*

sb def2-ecp

*

#	ncore = 28	lmax = 3	coefficient	r^n	exponent
f			-15.3668010	2	14.4449780
			-20.2961380	2	14.4492950
s-f			281.0715810	2	16.3308650
			61.7166040	2	8.5565420
			15.3668010	2	14.4449780
			20.2961380	2	14.4492950
p-f			67.4573800	2	14.4703370
			134.9335030	2	13.8161940
			14.7163440	2	8.4249240
			29.5185120	2	8.0927280

```

15.3668010      2      14.4449780
20.2961380      2      14.4492950
d-f
35.4478150      2      14.8863310
53.1434660      2      15.1463190
9.1792230       2      5.9082670
13.2402530      2      5.5943220
15.3668010      2      14.4449780
20.2961380      2      14.4492950
*
*
te def2-TZVPP
# te      (11s9p8d2f) / [6s5p3d2f]      {521111/33111/611/11}
*
5 s
6213.2001650    0.17392073280E-03
920.89640017    0.11933589842E-02
199.28042708    0.36256556777E-02
24.774233098    -0.59791033012E-01
14.838199169    0.95943203263
2 s
12.278761954    0.75942429936
6.3807845532    0.35331689542
1 s
2.2228405205    1.0000000000
1 s
1.0776043442    1.0000000000
1 s
0.28136649025    1.0000000000
1 s
0.10781573341    1.0000000000
3 p
204.29400852    0.40605406751E-03
18.208759358    0.60255451613E-01
9.9211024302    -0.27491671277
3 p
3.1441528685    0.43154849974
1.7220884031    0.55403079110
0.89098945714    0.24087311227
1 p
0.39804719568    1.0000000000
1 p
0.16538785242    1.0000000000
1 p
0.65082695586E-01 1.0000000000
6 d
121.51055249    0.63490629024E-03
32.968794396    0.61811936324E-02
19.249862451    -0.88929825218E-02
4.7198407254    0.20159884764
2.3428061416    0.42976049013
1.1135379412    0.38247126751
1 d
0.49200061510    1.0000000000
1 d
0.16000000000    1.0000000000
1 f
0.38255757000    1.0000000000
1 f
1.85000000000    1.0000000000

```

```

*
te def2-ecp
*
ncore = 28          lmax = 3
# coefficient      r^n      exponent
f
    -15.7454500    2        15.2061680
    -20.7424480    2        15.2017020
s-f
    281.0458430    2        16.8144730
    61.6206560    2        8.7935260
    15.7454500    2        15.2061680
    20.7424480    2        15.2017020
p-f
    67.4494640    2        14.8778010
    134.9043040   2        14.2697310
    14.6895470    2        8.7244350
    29.4150630    2        8.2915150
    15.7454500    2        15.2061680
    20.7424480    2        15.2017020
d-f
    35.4320570    2        15.2050080
    53.1356870    2        15.2258480
    9.0698020     2        6.0717690
    13.1223040    2        5.8047600
    15.7454500    2        15.2061680
    20.7424480    2        15.2017020
*
*
i def2-TZVPP
# i      (11s10p8d2f) / [6s5p3d2f]      {521111/34111/611/11}
*
5 s
5899.5791533      0.24188269271E-03
898.54238765      0.15474041742E-02
200.37237912      0.42836684457E-02
31.418053840      -0.39417936275E-01
15.645987838      0.96086691992
2 s
11.815741857      0.75961524091
6.4614458287      0.42495501835
1 s
2.3838067579      1.0000000000
1 s
1.1712089662      1.0000000000
1 s
0.32115875757      1.0000000000
1 s
0.12387919364      1.0000000000
3 p
197.30030547      0.73951226905E-03
20.061411349      0.66168450008E-01
9.7631460485      -0.28554662348
4 p
12.984316904      -0.49096186164E-01
3.6199503008      0.38914432482
2.0232273090      0.65610817262
1.0367490559      0.31803551647
1 p
0.45937816000      1.0000000000

```

```

1 p
0.19116532928      1.0000000000
1 p
0.74878813023E-01  1.0000000000
6 d
119.12671745      0.82596039573E-03
33.404240134      0.68377675770E-02
17.805918203      -0.10308158997E-01
4.8990510353      0.22670457658
2.4516753106      0.44180113937
1.1820693432      0.36775472225
1 d
0.52923110068      1.0000000000
1 d
0.17000000000      1.0000000000
1 f
0.44141808000      1.0000000000
1 f
2.18000000000      1.0000000000
*
i def2-ecp
*
ncore =      28      lmax =      3
#      coefficient      r^n      exponent
f
      -21.8420400      2      19.4586090
      -28.4681910      2      19.3492600
      -0.2437130      2      4.8237670
      -0.3208040      2      4.8843150
s-f
      49.9942930      2      40.0158350
      281.0253170      2      17.4297470
      61.5733260      2      9.0054840
      21.8420400      2      19.4586090
      28.4681910      2      19.3492600
      0.2437130      2      4.8237670
      0.3208040      2      4.8843150
p-f
      67.4428410      2      15.3554660
      134.8811370      2      14.9718330
      14.6750510      2      8.9601640
      29.3756660      2      8.2590960
      21.8420400      2      19.4586090
      28.4681910      2      19.3492600
      0.2437130      2      4.8237670
      0.3208040      2      4.8843150
d-f
      35.4395290      2      15.0689080
      53.1760570      2      14.5553220
      9.0671950      2      6.7186470
      13.2069370      2      6.4563930
      0.0893350      2      1.1917790
      0.0523800      2      1.2911570
      21.8420400      2      19.4586090
      28.4681910      2      19.3492600
      0.2437130      2      4.8237670
      0.3208040      2      4.8843150
*
*
xe def2-TZVPP

```


xe (11s10p8d2f) / [6s5p3d2f] {521111/34111/611/11}

```
*
  5 s
  6420.2481656      0.25092173886E-03
  983.54530664     0.16251948178E-02
  219.43881364     0.46037106451E-02
  23.012587807    -0.14698707182
  18.048324490     0.57524870348
  2 s
  11.752550163     0.66038420156
  6.2390917199     0.38470524721
  1 s
  2.6257211320     1.0000000000
  1 s
  1.2905042943     1.0000000000
  1 s
  0.36204185060    1.0000000000
  1 s
  0.14069888091    1.0000000000
  3 p
  193.81432545     0.95394802497E-03
  21.725228086     0.57393353332E-01
  9.8891605641     -0.27974266640
  4 p
  13.960683826     -0.50950157807E-01
  4.0928947097     0.36669211800
  2.2546815460     0.72619456861
  1.1546596184     0.35555871740
  1 p
  0.52321923128    1.0000000000
  1 p
  0.21945569800    1.0000000000
  1 p
  0.86158996836E-01 1.0000000000
  6 d
  135.60300038     0.81873543290E-03
  38.727062692     0.60897654151E-02
  15.377328089     -0.92782985596E-02
  5.2602537686     0.22890785589
  2.6590627424     0.44434407051
  1.2938205124     0.36029482992
  1 d
  0.58050830139    1.0000000000
  1 d
  0.18000000000    1.0000000000
  1 f
  0.49652793000    1.0000000000
  1 f
  2.50000000000    1.0000000000
```

*
xe def2-ecp
*

```
ncore = 28          lmax = 3
# coefficient r^n    exponent
f          -23.0892950  2      20.8815570
           -30.0744750  2      20.7834430
           -0.2882270   2      5.2533890
           -0.3869240   2      5.3611880
```

s-f

	49.9979620	2	40.0051840
	281.0133030	2	17.8122140
	61.5382550	2	9.3041500
	23.0892950	2	20.8815570
	30.0744750	2	20.7834430
	0.2882270	2	5.2533890
	0.3869240	2	5.3611880
p-f			
	67.4391420	2	15.7017720
	134.8747110	2	15.2586080
	14.6633000	2	9.2921840
	29.3547300	2	8.5590030
	23.0892950	2	20.8815570
	30.0744750	2	20.7834430
	0.2882270	2	5.2533890
	0.3869240	2	5.3611880
d-f			
	35.4369080	2	15.1856000
	53.1957720	2	14.2845000
	9.0462320	2	7.1218890
	13.2236810	2	6.9919630
	0.0848530	2	0.6239460
	0.0441550	2	0.6472840
	23.0892950	2	20.8815570
	30.0744750	2	20.7834430
	0.2882270	2	5.2533890
	0.3869240	2	5.3611880
*			
*			
cs def2-TZVPP			
# cs	(7s6p3d1f) / [5s3p3d1f]		{31111/411/111/1}
*			
3 s			
	5.8778113443	0.12859994983	
	4.3631538286	-0.34632569725	
	1.8048475155	0.69930637051	
1 s			
	0.37485237136	1.0000000000	
1 s			
	0.16384858778	1.0000000000	
1 s			
	0.27230462048E-01	1.0000000000	
1 s			
	0.11991533212E-01	1.0000000000	
4 p			
	4.2751856154	0.45723074174E-01	
	1.9656663360	-0.25019961976	
	0.47689195212	0.55660850066	
	0.21529749588	0.58218553406	
1 p			
	0.91450850296E-01	1.0000000000	
1 p			
	0.17592078473E-01	1.0000000000	
1 d			
	0.27941471548	0.15040680034	
1 d			
	0.62419809739E-01	0.36150912942	
1 d			
	0.15987870156E-01	1.0000000000	
1 f			

```

0.58777000000      0.0000000000
*
cs def2-ecp
*
ncore =      46      lmax =      3
# coefficient r^n      exponent
f      -28.8843090      2      3.1232690
s-f      84.5477300      2      4.0797500
      16.6541730      2      2.4174060
      28.8843090      2      3.1232690
p-f      157.0490590      2      5.5140800
      26.4233070      2      2.1603160
      28.8843090      2      3.1232690
d-f      13.1727530      2      1.8074100
      3.3428330      2      0.8581820
      28.8843090      2      3.1232690
*
*
ba def2-TZVPP
# ba      (7s7p5d1f) / [6s4p3d1f]      {211111/4111/311/1}
*
2 s
6.0000000000      -0.56587174838
4.9822082226      0.97514768535
1 s
2.1451943914      1.0000000000
1 s
0.41486174100      1.0000000000
1 s
0.19214757016      1.0000000000
1 s
0.48465890337E-01      1.0000000000
1 s
0.20138298948E-01      1.0000000000
4 p
5.5000000000      -0.44586312998
4.9017938336      0.67755479813
2.6142685062      -0.46010554954
0.47903394983      0.68749608021
1 p
0.19415138747      1.0000000000
1 p
0.34917622027E-01      1.0000000000
1 p
0.16320065666E-01      1.0000000000
3 d
0.96631500000      -0.90893800000
0.89382800000      0.94724000000
0.27319500000      0.32205700000
1 d
0.10389100000      1.0000000000
1 d
0.35578000000E-01      1.0000000000
1 f
0.65760000000      0.0000000000
*

```

```

ba def2-ecp
*
  ncore =    46          lmax =    3
#      coefficient      r^n      exponent
f
  -33.4731740      2      3.5894650
s-f
  427.8458160      2      9.5269860
  204.4175300      2      4.4875100
  33.4731740      2      3.5894650
p-f
  293.6058640      2      8.3159300
  294.1933160      2      4.2922170
  33.4731740      2      3.5894650
d-f
  112.5504020      2      5.9161080
  181.7826210      2      2.8748420
  33.4731740      2      3.5894650
*
*
la def2-TZVPP
# la      (7s7p5d2f1g) / [6s4p3d2f1g]      {211111/4111/311/11/1}
*
  2 s
  5.0873990000      -0.44174952534
  4.2709780000      0.85812466843
  1 s
  2.1823656045      1.0000000000
  1 s
  0.48966533785      1.0000000000
  1 s
  0.23301675348      1.0000000000
  1 s
  0.55719523051E-01      1.0000000000
  1 s
  0.22854708808E-01      1.0000000000
  4 p
  6.0000000000      -0.11397960924E-01
  3.6808191615      0.14675038550
  2.3265462081      -0.35581819167
  0.64342629633      0.45834955229
  1 p
  0.33584281962      1.0000000000
  1 p
  0.16519051916      1.0000000000
  1 p
  0.35400000000E-01      1.0000000000
  3 d
  1.2675288018      -0.17569274035
  0.89395340284      0.25139922933
  0.33095767339      0.44603267053
  1 d
  0.13461377501      1.0000000000
  1 d
  0.51441629839E-01      1.0000000000
  1 f
  0.38941000000      1.0000000000
  1 f
  0.12043000000      1.0000000000
  1 g

```

```

0.17907000000      1.0000000000
*
la def2-ecp
*
ncore =      46      lmax =      3
# coefficient  r^n      exponent
f      -36.0100160    2      4.0286000
s-f      91.9321770    2      3.3099000
      -3.7887640    2      1.6550000
      36.0100160    2      4.0286000
p-f      63.7594860    2      2.8368000
      -0.6479580    2      1.4184000
      36.0100160    2      4.0286000
d-f      36.1161730    2      2.0213000
      0.2191140    2      1.0107000
      36.0100160    2      4.0286000
*
*
hf def2-TZVPP
# hf      (9s7p5d2f1g) / [6s4p3d2f1g]      {411111/4111/311/11/1}
*
4 s
24.000000000      0.19369448644
16.000000000      -3.5064630782
14.400000000      4.3082581000
10.304504667      -0.91045809742
1 s
3.8426510824      1.0000000000
1 s
0.93296029049      1.0000000000
1 s
0.42615320942      1.0000000000
1 s
0.93366560195E-01  1.0000000000
1 s
0.35532895141E-01  1.0000000000
4 p
17.000000000      -0.30316491880E-01
11.738072097      0.10139279686
4.9203967161      -0.28227924657
1.1251726138      0.52032008501
1 p
0.54220114055      1.0000000000
1 p
0.25659447877      1.0000000000
1 p
0.65000000000E-01  1.0000000000
3 d
3.9820623229      -0.42446023944E-01
1.3077987772      0.18409232564
0.53272310298      0.41484423516
1 d
0.20564954488      1.0000000000
1 d
0.73099858787E-01  1.0000000000
1 f

```

```

0.53104000000      1.0000000000
  1 f
0.16537000000      1.0000000000
  1 g
0.29036000000      1.0000000000
*
hf def2-ecp
*
  ncore =    60      lmax =    3
#      coefficient  r^n      exponent
f
      10.0467225    2        1.7857698
s-f
      1499.2847107  2        14.7699590
      40.2821014   2        7.3849794
      -10.0467225  2        1.7857698
p-f
      397.7330053   2        9.8494895
      19.3164059   2        4.9247445
      -10.0467225  2        1.7857698
d-f
      101.3298053   2        6.0967564
      5.8734382    2        3.0483782
      -10.0467225  2        1.7857698
*
*
ta def2-TZVPP
# ta      (9s7p5d2f1g) / [6s4p3d2f1g]      {4111111/4111/311/11/1}
*
  4 s
  24.473650944      0.20590322488
  18.721372549      -0.74670795514
  11.500000000      3.4071363897
  10.350000000      -2.8175487609
  1 s
  3.8436180089      1.0000000000
  1 s
  1.0202266016      1.0000000000
  1 s
  0.46774781869     1.0000000000
  1 s
  0.10323186670     1.0000000000
  1 s
  0.38674461203E-01 1.0000000000
  4 p
  17.000000000      -0.32577305616E-01
  12.008186536      0.10336287365
  5.0278760583      -0.28526521696
  1.1937124184      0.51790141155
  1 p
  0.57889707053     1.0000000000
  1 p
  0.27225198801     1.0000000000
  1 p
  0.65000000000E-01 1.0000000000
  3 d
  3.9738796278      -0.52799310714E-01
  1.4528884813      0.18558319471
  0.61042908544     0.42959071631
  1 d

```

```

0.24216276510      1.0000000000
  1 d
0.87909318337E-01  1.0000000000
  1 f
0.67066000000     1.0000000000
  1 f
0.21031000000     1.0000000000
  1 g
0.40165000000     1.0000000000
*
ta def2-ecp
*
  ncore =      60          lmax =      3
#      coefficient      r^n      exponent
f
      12.0179609      2          2.0178811
s-f
      1345.8806470      2          14.5464077
      36.7668062      2          7.2732038
      -12.0179609      2          2.0178811
p-f
      378.4253015      2          9.9355653
      22.2930909      2          4.9677824
      -12.0179609      2          2.0178811
d-f
      104.8839557      2          6.3473769
      8.7558481      2          3.1736885
      -12.0179609      2          2.0178811
*
*
w def2-TZVPP
# w      (8s7p6d2f1g) / [6s4p3d2f1g]      {311111/4111/411/11/1}
*
  3 s
  30.000000000      0.32246483410
  27.000000000      -0.46692257214
  13.078045684      0.42699563776
  1 s
  4.8100449717      1.0000000000
  1 s
0.98497804263      1.0000000000
  1 s
0.44910485344      1.0000000000
  1 s
0.11448352920      1.0000000000
  1 s
0.41720421956E-01  1.0000000000
  4 p
  17.000000000      -0.37817768433E-01
  12.431973432      0.10905673845
  5.1586217658      -0.29399955020
  1.2801454812      0.51560726697
  1 p
0.62856790898      1.0000000000
  1 p
0.29380423553      1.0000000000
  1 p
0.65000000000E-01  1.0000000000
  4 d
  7.4064737315      0.86993963018E-01

```

```

5.9026268603      -0.17667540011
1.2984756750      0.55145697030
0.57153508541    0.95313596535
 1 d
0.23845526606    1.00000000000
 1 d
0.91144267331E-01 1.00000000000
 1 f
0.80824000000    1.00000000000
 1 f
0.25524000000    1.00000000000
 1 g
0.51293000000    1.00000000000
*
w def2-ecp
*
  ncore =    60          lmax =    3
#   coefficient   r^n      exponent
f
      14.1525795     2         2.2588885
s-f
      1192.3958823   2         14.3228564
      32.5229332    2         7.1614281
      -14.1525795   2         2.2588885
p-f
      359.0319671    2         10.0216411
      24.0303802    2         5.0108204
      -14.1525795   2         2.2588885
d-f
      108.3013490    2         6.5979974
      10.9825283    2         3.2989987
      -14.1525795   2         2.2588885
*
*
re def2-TZVPP
# re      (8s7p6d2f1g) / [6s4p3d2f1g]      {311111/4111/411/11/1}
*
  3 s
30.000000000      0.31780717811
27.000000000     -0.46492321332
13.078045684      0.45723641305
 1 s
5.0352712861     1.00000000000
 1 s
1.0482706438     1.00000000000
 1 s
0.47708773413    1.00000000000
 1 s
0.12225857255    1.00000000000
 1 s
0.44007400609E-01 1.00000000000
 4 p
18.000000000     -0.26890962397E-01
12.318606250     0.99711498502E-01
5.3719234505     -0.29289398145
1.3506646748     0.51466301434
 1 p
0.66212816808    1.00000000000
 1 p
0.31071385193    1.00000000000

```



```

1 p
0.700000000000E-01  1.0000000000
4 d
7.7352877672      0.83901798556E-01
6.0949443610     -0.17722258734
1.3871105497      0.55238259692
0.62324027854     0.91980111239
1 d
0.26517328547     1.0000000000
1 d
0.10321096849     1.0000000000
1 f
0.94386000000     1.0000000000
1 f
0.30018000000     1.0000000000
1 g
0.62422000000     1.0000000000
*
re def2-ecp
*
ncore = 60          lmax = 3
# coefficient      r^n      exponent
f
      16.4498523    2          2.5086506
s-f
      1038.9515723  2          14.0993051
      29.5617383   2          7.0496525
      -16.4498523  2          2.5086506
p-f
      339.5435096   2          10.1077169
      24.9136965   2          5.0538583
      -16.4498523  2          2.5086506
d-f
      111.6996527   2          6.8486179
      12.6243293   2          3.4243090
      -16.4498523  2          2.5086506
*
*
os def2-TZVPP
# os      (8s7p6d2f1g) / [6s4p3d2f1g]      {311111/4111/411/11/1}
*
3 s
30.000000000      0.32213004804
27.000000000      -0.47922918137
13.524730005      0.47465946837
1 s
5.2402883472      1.0000000000
1 s
1.1306661245      1.0000000000
1 s
0.51689966917     1.0000000000
1 s
0.13222953545     1.0000000000
1 s
0.47220318801E-01 1.0000000000
4 p
15.500000000      0.16016463376
14.000000000      -0.23201520402
5.5458290420      0.29772587274
1.4139502215      -0.54253238176

```

```

1 p
0.68136686765      1.0000000000
1 p
0.30911452647      1.0000000000
1 p
0.520000000000E-01  1.0000000000
4 d
8.2945059487      0.69648222110E-01
6.3060397430      -0.16444229630
1.4890109110      0.55154541033
0.67315390607      0.88461370291
1 d
0.28590805222      1.0000000000
1 d
0.11058012051      1.0000000000
1 f
1.0672900000      1.0000000000
1 f
0.34222000000      1.0000000000
1 g
0.75489000000      1.0000000000
*
os def2-ecp
*
ncore =      60      lmax =      3
# coefficient r^n      exponent
f
      18.9094570      2      2.7670751
s-f
      885.4057191      2      13.8757539
      25.9670401      2      6.9378769
      -18.9094570      2      2.7670751
p-f
      320.0839019      2      10.1937926
      26.1487649      2      5.0968962
      -18.9094570      2      2.7670751
d-f
      115.0448431      2      7.0992385
      13.6225746      2      3.5496192
      -18.9094570      2      2.7670751
*
*
ir def2-TZVPP
# ir      (8s7p6d2f1g) / [6s4p3d2f1g]      {311111/4111/411/11/1}
*
3 s
30.000000000      0.30797903228
27.000000000      -0.46726361781
13.961973911      0.47161003146
1 s
5.3956977802      1.0000000000
1 s
1.2149128721      1.0000000000
1 s
0.55885743756      1.0000000000
1 s
0.14097974313      1.0000000000
1 s
0.50021924989E-01  1.0000000000
4 p

```

```

15.902664143      -0.16290720099
14.415830698      0.23483212987
5.7597608991     -0.30305337176
1.5008913108     0.55512982069
 1 p
0.72348035957     1.00000000000
 1 p
0.32785980328     1.00000000000
 1 p
0.560000000000E-01 1.00000000000
 4 d
 8.6321692504     0.75000099949E-01
 6.5898192302     -0.17326965173
 1.5808379663     0.55065196913
0.71827834905     0.85273641436
 1 d
0.30571851998     1.00000000000
 1 d
0.11827071879     1.00000000000
 1 f
 1.1885700000     1.00000000000
 1 f
0.38426000000     1.00000000000
 1 g
0.88556000000     1.00000000000
*
ir def2-ecp
*
  ncore =    60      lmax =    3
#      coefficient  r^n      exponent
f
      21.5310311    2        3.0340719
s-f
      732.2691998    2        13.6522026
      26.4847209    2         6.8261013
      -21.5310311    2         3.0340719
p-f
      299.4894736    2        10.2798684
      26.4662335    2         5.1399341
      -21.5310311    2         3.0340719
d-f
      124.4575945    2         7.3498590
      14.0359952    2         3.6749295
      -21.5310311    2         3.0340719
*
*
pt def2-TZVPP
# pt      (8s7p6d2f1g) / [6s4p3d2f1g]      {311111/4111/411/11/1}
*
 3 s
30.000000000     0.27148263900
27.000000000     -0.42226758774
14.408318564     0.44361581995
 1 s
 5.5335788010     1.00000000000
 1 s
 1.2986438223     1.00000000000
 1 s
0.58759393108     1.00000000000
 1 s

```

```

0.13845587261      1.0000000000
 1 s
0.49204459888E-01  1.0000000000
 4 p
15.500000000      -0.15672718629
14.000000000      0.23853412989
 6.1161212339     -0.31041379733
 1.5715586385     0.56473525089
 1 p
0.75132510781     1.0000000000
 1 p
0.33306466812     1.0000000000
 1 p
0.57000000000E-01  1.0000000000
 4 d
 8.3207937611     0.62945798646E-01
 7.4207226520     -0.90271847072E-01
 1.6570410639     0.16812526416
0.73943569960     0.25045416970
 1 d
0.30510856008     1.0000000000
 1 d
0.11350405268     1.0000000000
 1 f
 1.3077100000     1.0000000000
 1 f
0.42630000000     1.0000000000
 1 g
 1.0162300000     1.0000000000
*
pt def2-ecp
*
  ncore =      60          lmax =      3
#      coefficient  r^n      exponent
f
      24.3143757      2          3.3095686
s-f
      579.2238609      2          13.4286513
      29.6694906      2          6.7143256
      -24.3143757      2          3.3095686
p-f
      280.8607742      2          10.3659442
      26.7453820      2          5.1829721
      -24.3143757      2          3.3095686
d-f
      120.3964443      2          7.6004795
      15.8109206      2          3.8002397
      -24.3143757      2          3.3095686
*
*
au def2-TZVPP
# au      (8s7p6d2f1g) / [6s4p3d2f1g]      {311111/4111/411/11/1}
*
  3 s
30.000000000      0.20749231108
27.000000000      -0.33267893394
14.746824331      0.38302817958
 1 s
5.6017248938     1.0000000000
 1 s

```

```

1.3874162443      1.0000000000
 1 s
0.62923031957    1.0000000000
 1 s
0.14027517613    1.0000000000
 1 s
0.49379413761E-01  1.0000000000
 4 p
15.500000000     0.15001711880
14.000000000     -0.23609813183
 6.4227368205    0.31458896948
 1.6595601681    -0.57279670446
 1 p
0.79402913993    1.0000000000
 1 p
0.35125155397    1.0000000000
 1 p
0.45000000000E-01  1.0000000000
 4 d
 9.5524098656    0.40145559502E-01
 7.2698886937    -0.93690906606E-01
 1.7746496789    0.31746282317
0.79960541055    0.46795192483
 1 d
0.33252279372    1.0000000000
 1 d
0.12445133105    1.0000000000
 1 f
 1.4246900000    1.0000000000
 1 f
0.46834000000    1.0000000000
 1 g
 1.1469000000    1.0000000000
*
au def2-ecp
*
  ncore =      60      lmax =      3
#      coefficient  r^n      exponent
f
      30.4900889    2      4.7898200
      5.1710738    2      2.3949100
s-f
      426.8466792   2      13.2051000
      37.0070829   2      6.6025500
      -30.4900889   2      4.7898200
      -5.1710738    2      2.3949100
p-f
      261.1995804   2      10.4520200
      26.9624960    2      5.2260100
      -30.4900889   2      4.7898200
      -5.1710738    2      2.3949100
d-f
      124.7906656   2      7.8511000
      16.3007257    2      3.9255500
      -30.4900889   2      4.7898200
      -5.1710738    2      2.3949100
*
*
hg def2-TZVPP
# hg      (8s8p6d2f1g) / [6s5p3d2f1g]      {311111/41111/411/11/1}

```

```

*
  3 s
48.013786990      0.58008164912E-02
21.239875095     -0.17328165235
15.876100879      0.36416685034
  1 s
5.5180531820      1.00000000000
  1 s
1.5099145479      1.00000000000
  1 s
0.70683482159     1.00000000000
  1 s
0.16266265576     1.00000000000
  1 s
0.56960589112E-01 1.00000000000
  4 p
17.500000000      -0.86457187331E-01
15.252594855      0.15327318234
6.4404715169     -0.30274955249
1.8180159920      0.54361285026
  1 p
0.90067981801     1.00000000000
  1 p
0.41304540122     1.00000000000
  1 p
0.11845702655     1.00000000000
  1 p
0.36087619349E-01 1.00000000000
  4 d
10.028197701      0.39922353165E-01
7.5920661493     -0.94774230522E-01
1.9144256118      0.31164157463
0.88641552102     0.45567078406
  1 d
0.38154235320     1.00000000000
  1 d
0.14880740086     1.00000000000
  1 f
1.5521700000      1.00000000000
  1 f
0.52431000000     1.00000000000
  1 g
1.2895000000      1.00000000000

```

```

*
hg def2-ecp

```

```

*
  ncore =    60      lmax =    3
#      coefficient  r^n      exponent
f
      30.3649964    2        3.8857911
s-f
      275.7372117   2        12.9815487
      49.0892125    2        6.4907744
      -30.3649964   2        3.8857911
p-f
      241.5400740    2        10.5380958
      27.3965908    2        5.2690479
      -30.3649964   2        3.8857911
d-f
      127.8670076    2        8.1017205

```

16.6083115	2	4.0508603
-30.3649964	2	3.8857911

*

*

t1 def2-TZVPP

t1 (10s9p8d2f) / [6s5p3d2f] {421111/33111/611/11}

*

4	s		
729.65038145		0.13672829828E-03	
46.665548707		0.60443439951E-02	
20.970448726		-0.20022066697	
14.149588677		0.40801678488	
2	s		
20.730134285		-0.71861135918E-01	
6.1527631309		0.98057508445	
1	s		
1.5757324480		1.0000000000	
1	s		
0.74980169458		1.0000000000	
1	s		
0.19536816194		1.0000000000	
1	s		
0.70878767298E-01		1.0000000000	
3	p		
15.383852616		0.61717949180	
14.814929544		-0.72859235151	
6.7261253658		0.40438195364	
3	p		
1.9626182149		0.43157661160	
1.0331857851		0.39230403853	
0.53837445996		0.14007406820	
1	p		
0.24446611676		1.0000000000	
1	p		
0.90785377260E-01		1.0000000000	
1	p		
0.33401321498E-01		1.0000000000	
6	d		
57.606819928		0.16054811114E-03	
9.7368866667		0.24456562496E-01	
6.9256201679		-0.69914775031E-01	
2.1396230731		0.19496269490	
1.0836187110		0.29731629705	
0.52356298209		0.23728708102	
1	d		
0.23842309375		1.0000000000	
1	d		
0.95000000000E-01		1.0000000000	
1	f		
0.28435000000		1.0000000000	
1	f		
0.95000000000		1.0000000000	

*

t1 def2-ecp

*

ncore =	60	lmax =	3
#	coefficient	r^n	exponent
f	15.8254880	2	5.6263990
	21.1040210	2	5.5489520

	2.9151270	2	2.8749460
	3.8969030	2	2.8214510
s-f			
	281.2846630	2	12.1678050
	62.4342510	2	8.2949090
	-15.8254880	2	5.6263990
	-21.1040210	2	5.5489520
	-2.9151270	2	2.8749460
	-3.8969030	2	2.8214510
p-f			
	4.6334080	2	7.1514920
	9.3417560	2	5.1728650
	72.2992530	2	9.8910720
	144.5580370	2	9.0033910
	-15.8254880	2	5.6263990
	-21.1040210	2	5.5489520
	-2.9151270	2	2.8749460
	-3.8969030	2	2.8214510
d-f			
	35.9430390	2	7.1302180
	53.9095930	2	6.9269060
	10.3819390	2	5.4175700
	15.5838220	2	5.1386810
	-15.8254880	2	5.6263990
	-21.1040210	2	5.5489520
	-2.9151270	2	2.8749460
	-3.8969030	2	2.8214510

*

*

pb def2-TZVPP

pb (10s9p8d2f) / [6s5p3d2f] {421111/331111/611/11}

*

4	s	
591.61124370		0.22126521076E-03
46.757232559		0.56961959130E-02
20.746462696		-0.21374063831
14.610796419		0.40502620616
2	s	
20.222637612		-0.83541883299E-01
6.4767324865		0.97910892388
1	s	
1.6600600927		1.0000000000
1	s	
0.80431655001		1.0000000000
1	s	
0.22627039020		1.0000000000
1	s	
0.84014530665E-01		1.0000000000
3	p	
15.189102118		0.61952303583
14.693144415		-0.72498497086
6.8705890048		0.37680007984
3	p	
2.2021426123		0.40196284806
1.2209125119		0.46058131862
0.63367559815		0.19367655397
1	p	
0.28202837058		1.0000000000
1	p	
0.11333375666		1.0000000000


```

1 p
0.43948707430E-01 1.0000000000
6 d
61.315369628 0.33870800787E-03
12.372195840 0.13788683942E-01
6.9254944983 -0.75979608103E-01
2.3319539939 0.28113784298
1.2108730003 0.44474512269
0.60090478506 0.35326874351
1 d
0.28135869813 1.0000000000
1 d
0.11500000000 1.0000000000
1 f
0.28962000000 1.0000000000
1 f
1.00000000000 1.0000000000
*
pb def2-ecp
*
ncore = 60 lmax = 3
# coefficient r^n exponent
f
12.2098920 2 3.8875120
16.1902910 2 3.8119630
s-f
281.2854990 2 12.2963030
62.5202170 2 8.6326340
-12.2098920 2 3.8875120
-16.1902910 2 3.8119630
p-f
72.2768970 2 10.2417900
144.5910830 2 8.9241760
4.7586930 2 6.5813420
9.9406210 2 6.2554030
-12.2098920 2 3.8875120
-16.1902910 2 3.8119630
d-f
35.8485070 2 7.7543360
53.7243420 2 7.7202810
10.1152560 2 4.9702640
14.8337310 2 4.5637890
-12.2098920 2 3.8875120
-16.1902910 2 3.8119630
*
*
bi def2-TZVPP
# bi (10s9p8d2f) / [6s5p3d2f] {421111/33111/611/11}
*
4 s
716.41435310 0.31254307133E-03
83.806059047 0.17624768946E-02
21.116962853 -0.21910983437
15.491448187 0.40411224931
2 s
23.239855029 -0.68255758685E-01
6.6474255000 0.97888046471
1 s
1.7617744005 1.0000000000
1 s

```

0.87252866000	1.0000000000
1 s	
0.25618895997	1.0000000000
1 s	
0.97073913006E-01	1.0000000000
3 p	
15.249644669	0.74560356000
14.846176053	-0.85578637338
7.0636826784	0.40149159592
3 p	
2.5881255616	0.35542729633
1.5020208499	0.63976991890
0.76732724388	0.32332773839
1 p	
0.32797648982	1.0000000000
1 p	
0.13820335991	1.0000000000
1 p	
0.55137330969E-01	1.0000000000
6 d	
66.404481948	0.38102878348E-03
13.858426961	0.10746152442E-01
7.0654519000	-0.71947646845E-01
2.5252144035	0.26195974989
1.3419585000	0.42594750000
0.68340941000	0.33680325627
1 d	
0.32934755420	1.0000000000
1 d	
0.14000000000	1.0000000000
1 f	
0.31271000000	1.0000000000
1 f	
1.05000000000	1.0000000000

*

bi def2-ecp

*

#	ncore = 60	lmax = 3	coefficient	r^n	exponent
f			13.7133830	2	4.2145460
			18.1943080	2	4.1334000
s-f			283.2642270	2	13.0430900
			62.4719590	2	8.2216820
			-13.7133830	2	4.2145460
			-18.1943080	2	4.1334000
p-f			72.0014990	2	10.4677770
			144.0022770	2	9.1189010
			5.0079450	2	6.7547910
			9.9915500	2	6.2525920
			-13.7133830	2	4.2145460
			-18.1943080	2	4.1334000
d-f			36.3962590	2	8.0814740
			54.5976640	2	7.8905950
			9.9842940	2	4.9555560
			14.9814850	2	4.7045590
			-13.7133830	2	4.2145460

```

-18.1943080      2      4.1334000
*
*
po def2-TZVPP
# po      (11s10p8d2f) / [6s5p3d2f]      {521111/34111/611/11}
*
  5 s
6744.8211765      0.76891556363E-04
744.41892532      0.71284827354E-03
131.04029309      0.22057583958E-02
19.662021030      -0.64364713744
16.623025609      0.91997150546
  2 s
23.094002965      -0.70404410177E-01
6.9707398381      0.97886540086
  1 s
1.8497377593      1.0000000000
  1 s
0.93082999263      1.0000000000
  1 s
0.28673026462      1.0000000000
  1 s
0.10979212169      1.0000000000
  3 p
253.99024497      0.83876362116E-04
9.8712718748      0.24572710458
7.4489893496      -0.44297763661
  4 p
8.9027395407      -0.13798250445
5.7414667465      0.26304005326
1.9896329823      0.66225846161
0.94703210822      0.39547051892
  1 p
0.37071136280      1.0000000000
  1 p
0.15554706086      1.0000000000
  1 p
0.61173720818E-01  1.0000000000
  6 d
67.943077046      0.48919125336E-03
14.914219894      0.10157120776E-01
7.2973948305      -0.69943263066E-01
2.6826784400      0.26244730680
1.4374143009      0.42702361494
0.73903797417      0.32502435477
  1 d
0.35838153281      1.0000000000
  1 d
0.15000000000      1.0000000000
  1 f
0.33275000000      1.0000000000
  1 f
1.40000000000      1.0000000000
*
po def2-ecp
*
ncore =      60      lmax =      3
#      coefficient      r^n      exponent
f
      17.4282950      2      5.0132700

```

	23.3803530	2	4.9846400
	0.1633920	2	1.3267600
	0.3245660	2	1.5287580
s-f			
	283.2447060	2	13.2772270
	62.3964610	2	8.3995180
	-17.4282950	2	5.0132700
	-23.3803530	2	4.9846400
	-0.1633920	2	1.3267600
	-0.3245660	2	1.5287580
p-f			
	71.9917160	2	10.6656820
	143.9718710	2	9.2837530
	4.9496150	2	6.8727490
	9.7404990	2	6.3261500
	-17.4282950	2	5.0132700
	-23.3803530	2	4.9846400
	-0.1633920	2	1.3267600
	-0.3245660	2	1.5287580
d-f			
	36.3783830	2	8.2148660
	54.5627150	2	8.0086960
	9.8894990	2	5.0552270
	14.6938770	2	4.7825530
	-17.4282950	2	5.0132700
	-23.3803530	2	4.9846400
	-0.1633920	2	1.3267600
	-0.3245660	2	1.5287580
*			
*			
at def2-TZVPP			
# at	(11s10p8d2f) / [6s5p3d2f]		{5211111/341111/611/11}
*			
5 s			
	3635.9809356	0.12571463494E-03	
	537.64129823	0.75950883820E-03	
	91.600030756	0.25790982348E-02	
	20.200005804	-0.54772187699	
	16.893873824	0.78417507786	
2 s			
	18.177216938	-0.13023627002	
	7.2317852082	0.96473566747	
1 s			
	1.9496199739	1.0000000000	
1 s			
	0.99226695236	1.0000000000	
1 s			
	0.31957178881	1.0000000000	
1 s			
	0.12342539809	1.0000000000	
3 p			
	216.81518928	0.16975297090E-03	
	10.592298115	0.22683755793	
	7.4596585430	-0.47336848377	
4 p			
	8.9484156471	-0.15012953475	
	5.9694592464	0.27048141788	
	2.1099088209	0.63671217722	
	1.0236370373	0.38057472615	
1 p			

```

0.42186356565      1.0000000000
 1 p
0.17757132268      1.0000000000
 1 p
0.69670886939E-01  1.0000000000
 6 d
 70.619633393      0.59974022914E-03
 16.212096478      0.93445952839E-02
 7.3607401479      -0.70748413897E-01
 2.9309052592      0.24037366077
 1.6085414823      0.41841372624
0.84194162715      0.32832651044
 1 d
0.41335677957      1.0000000000
 1 d
0.17400000000      1.0000000000
 1 f
0.37408000000      1.0000000000
 1 f
 1.80000000000      1.0000000000
*
at def2-ecp
*
ncore =    60          lmax =    3
#      coefficient    r^n      exponent
f
      19.8701980      2          5.8121630
      26.4164520      2          5.7537150
      0.9949700      2          2.5134720
      1.4907010      2          2.5362610
s-f
      49.9571580      2          30.2008320
      283.2103710     2          13.6123060
      62.2810520      2          8.5293400
      -19.8701980     2          5.8121630
      -26.4164520     2          5.7537150
      -0.9949700      2          2.5134720
      -1.4907010      2          2.5362610
p-f
      71.9823710      2          10.8540650
      143.9035320     2          9.4682290
      4.8717590       2          7.0311140
      8.9830590       2          6.1438580
      -19.8701980     2          5.8121630
      -26.4164520     2          5.7537150
      -0.9949700      2          2.5134720
      -1.4907010      2          2.5362610
d-f
      36.3632370      2          8.3135150
      54.5489700      2          7.9989650
      9.7762850       2          5.1799660
      14.2647550      2          4.9422260
      -19.8701980     2          5.8121630
      -26.4164520     2          5.7537150
      -0.9949700      2          2.5134720
      -1.4907010      2          2.5362610
*
*
rn def2-TZVPP
# rn      (11s10p8d2f) / [6s5p3d2f]      {521111/34111/611/11}

```

```

*
  5 s
5187.7442468      0.16097034848E-03
768.14491207     0.10508214789E-02
159.35182065     0.27375438093E-02
21.863432724    -0.55045904905
18.388689978     0.78321373922
  2 s
24.816226448    -0.82636797204E-01
7.2923301677     1.0926256000
  1 s
2.0850437166     1.0000000000
  1 s
1.0915245945     1.0000000000
  1 s
0.34915708428    1.0000000000
  1 s
0.13648422952    1.0000000000
  3 p
194.68918723     0.26265814046E-03
11.210013525     0.19952302621
7.5298316489    -0.45994479561
  4 p
9.0845000304    -0.23093917426
6.2631489717     0.39747614192
2.2545193734     0.83026693838
1.1180666918     0.51467013112
  1 p
0.47444492594    1.0000000000
  1 p
0.20172354616    1.0000000000
  1 p
0.79503144392E-01 1.0000000000
  6 d
75.302723665     0.73590238429E-03
17.965913830     0.89490827389E-02
7.3741298033    -0.76641663693E-01
3.2296258578     0.22975404602
1.7937840508     0.43991495311
0.94633319732    0.35259395198
  1 d
0.46860482223    1.0000000000
  1 d
0.20000000000    1.0000000000
  1 f
0.41806000000    1.0000000000
  1 f
2.10000000000    1.0000000000

```

```

*
rn def2-ecp
*
ncore =      60          lmax =      3
#      coefficient      r^n      exponent
f
      21.7972900        2          6.3485710
      28.9468050        2          6.2959490
      1.4473650         2          2.8821180
      2.1779640         2          2.9080480
s-f
      49.9655510        2          30.1512420

```

	283.0700000	2	14.5212410
	62.0028700	2	8.0520380
	-21.7972900	2	6.3485710
	-28.9468050	2	6.2959490
	-1.4473650	2	2.8821180
	-2.1779640	2	2.9080480
p-f			
	71.9691190	2	11.0099420
	143.8605590	2	9.6176250
	4.7147610	2	7.3360080
	9.0130650	2	6.4062530
	-21.7972900	2	6.3485710
	-28.9468050	2	6.2959490
	-1.4473650	2	2.8821180
	-2.1779640	2	2.9080480
d-f			
	36.3683650	2	8.3692200
	54.5517610	2	8.1169750
	9.6344870	2	5.3536560
	14.3879020	2	5.0972120
	-21.7972900	2	6.3485710
	-28.9468050	2	6.2959490
	-1.4473650	2	2.8821180
	-2.1779640	2	2.9080480

*

=====
def2-QZVP
=====

*

h def2-QZVP

h (7s3p2d1f) / [4s3p2d1f] {4111/111/11/1}

*

4	s		
190.69169000		0.70815167000E-03	
28.605532000		0.54678827000E-02	
6.5095943000		0.27966605000E-01	
1.8412455000		0.10764538000	
1	s		
0.59853725000		1.00000000000	
1	s		
0.21397624000		1.00000000000	
1	s		
0.80316286000E-01		1.00000000000	
1	p		
2.29200000000		1.00000000000	
1	p		
0.83800000000		1.00000000000	
1	p		
0.29200000000		1.00000000000	
1	d		
2.06200000000		1.00000000000	
1	d		
0.66200000000		1.00000000000	
1	f		
1.39700000000		1.00000000000	

*

*

he def2-QZVP

he (8s3p2d1f) / [4s3p2d1f] {5111/111/11/1}

*

```

5 s
1144.6470809      0.35861578618E-03
171.64596667     0.27725434466E-02
39.066056254     0.14241892216E-01
11.051401989     0.55457352277E-01
3.5725574473     0.16170511810
1 s
1.2429415962     0.33177883833
1 s
0.44807668730   0.42014033068
1 s
0.16411579128   0.18652273014
1 p
5.9940000000     1.0000000000
1 p
1.7450000000     1.0000000000
1 p
0.56000000000   1.0000000000
1 d
4.2990000000     1.0000000000
1 d
1.2230000000     1.0000000000
1 f
2.6800000000     1.0000000000
*
*
li def2-QZVP
# li      (15s6p2d1f) / [6s4p2d1f]      {921111/3111/11/1}
*
9 s
14853.977085     0.42711388815E-04
2225.2236477     0.33235310800E-03
504.88739008     0.17518436649E-02
142.45847548     0.73477995850E-02
46.315599580     0.25899837683E-01
16.655335474     0.76670682431E-01
6.4331186199     0.18276075765
2.6027043858     0.32655434038
1.0897245405     0.37000429828
2 s
4.4236595971     0.11120987921
1.2356394990     0.79987335862
1 s
0.46067470602    1.0000000000
1 s
0.96617166955E-01 1.0000000000
1 s
0.45915452296E-01 1.0000000000
1 s
0.21140048730E-01 1.0000000000
3 p
3.2605109206     0.86504749023E-02
0.65003043115    0.47614123736E-01
0.16941671073    0.21001138000
1 p
0.55732343767E-01 1.0000000000
1 p
0.20489959241E-01 1.0000000000
1 p
3.3270000000     1.0000000000

```



```

1 d
0.230000000000      1.000000000000
1 d
0.757000000000E-01  1.000000000000
1 f
0.135000000000      1.000000000000
*
*
be def2-QZVP
# be      (15s7p2d1f) / [7s4p2d1f]      {8211111/4111/11/1}
*
8 s
29646.704407        0.37943320869E-04
4428.7614354        0.29605352634E-03
1005.4701332        0.15572477356E-02
284.15339578        0.65323195769E-02
92.504356461        0.23116861005E-01
33.311016058        0.69458515249E-01
12.911553314        0.17014371331
5.2665497361        0.31682711374
2 s
22.995386380        0.81791122747E-01
6.6236354176        0.80000038023
1 s
2.2289595003        1.000000000000
1 s
0.95302433451        1.000000000000
1 s
0.24651602436        1.000000000000
1 s
0.10153895315        1.000000000000
1 s
0.41551374604E-01   1.000000000000
4 p
14.099789445        0.38508871145E-02
3.1803188482        0.24152380771E-01
0.90489220496        0.97926925156E-01
0.30411585508        0.29470380030
1 p
0.11302606657        1.000000000000
1 p
0.42831733691E-01   1.000000000000
1 p
6.40000000000        1.000000000000
1 d
0.360000000000      1.000000000000
1 d
0.900000000000E-01  1.000000000000
1 f
0.290000000000      1.000000000000
*
*
b def2-QZVP
# b      (15s8p3d2f1g) / [7s4p3d2f1g]      {8211111/5111/111/11/1}
*
8 s
46447.667056        0.38388681014E-04
6957.6889042        0.29836770197E-03
1583.4428403        0.15645478806E-02
448.46601009        0.65476770742E-02

```

146.28639262	0.23139008388E-01
52.784386084	0.69615799357E-01
20.519396170	0.17119636876
8.4185659258	0.31913191837
2 s	
36.510018312	0.78990617244E-01
10.541854005	0.78926384265
1 s	
3.6004091387	1.0000000000
1 s	
1.5617023749	1.0000000000
1 s	
0.44997370775	1.0000000000
1 s	
0.18075230237	1.0000000000
1 s	
0.71596696319E-01	1.0000000000
5 p	
72.240462760	0.86539170411E-03
16.807707208	0.68762067365E-02
5.2259410747	0.30976687148E-01
1.8508350671	0.10432357913
0.72206782663	0.26164137577
1 p	
0.29491018056	1.0000000000
1 p	
0.12201141839	1.0000000000
1 p	
0.49865393625E-01	1.0000000000
1 d	
1.1100000000	1.0000000000
1 d	
0.4020000000	1.0000000000
1 d	
0.1450000000	1.0000000000
1 f	
0.8820000000	1.0000000000
1 f	
0.3110000000	1.0000000000
1 g	
0.6730000000	1.0000000000
*	
*	
c def2-QZVP	
# c (15s8p3d2f1g) / [7s4p3d2f1g]	{8211111/5111/111/11/1}
*	
8 s	
67025.071029	0.38736308501E-04
10039.986538	0.30107917575E-03
2284.9316911	0.15787918095E-02
647.14122130	0.66087087195E-02
211.09472335	0.23367123250E-01
76.177643862	0.70420716898E-01
29.633839163	0.17360344953
12.187785081	0.32292305648
2 s	
53.026006299	0.74897404492E-01
15.258502776	0.76136220983
1 s	
5.2403957464	1.0000000000

1 s		
2.2905022379	1.0000000000	
1 s		
0.69673283006	1.0000000000	
1 s		
0.27599337363	1.0000000000	
1 s		
0.10739884389	1.0000000000	
5 p		
105.12555082	0.84647553844E-03	
24.884461066	0.66274038534E-02	
7.8637230826	0.30120390419E-01	
2.8407001835	0.99951435476E-01	
1.1227137335	0.23826299282	
1 p		
0.46050725555	1.0000000000	
1 p		
0.18937530913	1.0000000000	
1 p		
0.75983791611E-01	1.0000000000	
1 d		
1.8480000000	1.0000000000	
1 d		
0.64900000000	1.0000000000	
1 d		
0.22800000000	1.0000000000	
1 f		
1.4190000000	1.0000000000	
1 f		
0.48500000000	1.0000000000	
1 g		
1.0110000000	1.0000000000	
*		
*		
n def2-QZVP		
# n (15s8p3d2f1g) / [7s4p3d2f1g]	{8211111/5111/111/11/1}	
*		
8 s		
90726.889210	0.39257887368E-04	
13590.528801	0.30513316455E-03	
3092.9883781	0.16000560446E-02	
875.99876362	0.66982937306E-02	
285.74469982	0.23690078765E-01	
103.11913417	0.71455405268E-01	
40.128556777	0.17632774876	
16.528095704	0.32677592815	
2 s		
69.390960983	0.80052094386E-01	
20.428200596	0.78268063538	
1 s		
7.1292587972	1.0000000000	
1 s		
3.1324304893	1.0000000000	
1 s		
0.98755778723	1.0000000000	
1 s		
0.38765721307	1.0000000000	
1 s		
0.14909883075	1.0000000000	
5 p		

150.05742670	-0.86216165986E-03	
35.491599483	-0.68571273236E-02	
11.247864223	-0.31795688855E-01	
4.0900305195	-0.10537396822	
1.6220573146	-0.24519708041	
1 p		
0.66442261530	1.0000000000	
1 p		
0.27099770070	1.0000000000	
1 p		
0.10688749984	1.0000000000	
1 d		
2.8370000000	1.0000000000	
1 d		
0.96800000000	1.0000000000	
1 d		
0.33500000000	1.0000000000	
1 f		
2.0270000000	1.0000000000	
1 f		
0.68500000000	1.0000000000	
1 g		
1.4270000000	1.0000000000	
*		
*		
o def2-QZVP		
# o (15s8p3d2f1g) / [7s4p3d2f1g]	{82111111/5111/111/11/1}	
*		
8 s		
116506.46908	0.40383857939E-04	
17504.349724	0.31255139004E-03	
3993.4513230	0.16341473495E-02	
1133.0063186	0.68283224757E-02	
369.99569594	0.24124410221E-01	
133.62074349	0.72730206154E-01	
52.035643649	0.17934429892	
21.461939313	0.33059588895	
2 s		
89.835051252	0.96468652996E-01	
26.428010844	0.94117481120	
1 s		
9.2822824649	1.0000000000	
1 s		
4.0947728533	1.0000000000	
1 s		
1.3255349078	1.0000000000	
1 s		
0.51877230787	1.0000000000	
1 s		
0.19772676454	1.0000000000	
5 p		
191.15255810	0.25115697705E-02	
45.233356739	0.20039240864E-01	
14.353465922	0.93609064762E-01	
5.2422371832	0.30618127124	
2.0792418599	0.67810501439	
1 p		
0.84282371424	1.0000000000	
1 p		
0.33617694891	1.0000000000	

```

1 p
0.12863997974      1.00000000000
1 d
3.77500000000     1.00000000000
1 d
1.30000000000     1.00000000000
1 d
0.44400000000     1.00000000000
1 f
2.66600000000     1.00000000000
1 f
0.85900000000     1.00000000000
1 g
1.84600000000     1.00000000000
*
*
f def2-QZVP
# f      (15s8p3d2f1g) / [7s4p3d2f1g]      {82111111/5111/111/11/1}
*
8 s
132535.97345      0.47387482743E-04
19758.112588      0.37070120897E-03
4485.1996947      0.19450784713E-02
1273.8151020      0.80573291994E-02
418.93831236      0.27992880781E-01
152.55721985      0.82735120175E-01
59.821524823      0.19854169012
24.819076932      0.34860632233
2 s
100.74446673      0.10505068816
30.103728290      0.94068472434
1 s
10.814283272      1.00000000000
1 s
4.8172886770      1.00000000000
1 s
1.6559334213      1.00000000000
1 s
0.64893519582      1.00000000000
1 s
0.24778104545      1.00000000000
5 p
240.96654114      0.30389933451E-02
57.020699781      0.24357738582E-01
18.126952120      0.11442925768
6.6457404621      0.37064659853
2.6375722892      0.79791551766
1 p
1.0638217200      1.00000000000
1 p
0.41932562750      1.00000000000
1 p
0.15747588299      1.00000000000
1 d
5.01400000000     1.00000000000
1 d
1.72500000000     1.00000000000
1 d
0.58600000000     1.00000000000
1 f

```

```

3.5620000000      1.0000000000
 1 f
1.1480000000      1.0000000000
 1 g
2.3760000000      1.0000000000
*
*
ne def2-QZVP
# ne      (15s9p3d2f1g) / [7s4p3d2f1g]      {82111111/6111/111/11/1}
*
 8 s
160676.27955      0.47387482743E-04
23953.195039      0.37070120897E-03
5437.5063711      0.19450784713E-02
1544.2741024      0.80573291994E-02
507.88814269      0.27992880781E-01
184.94847750      0.82735120175E-01
72.522952039      0.19854169012
30.088713575      0.34860632233
 2 s
120.68434940      0.10400597014
36.074294857      0.91999988986
 1 s
13.052091210      1.0000000000
 1 s
5.7974783353      1.0000000000
 1 s
2.0478626895      1.0000000000
 1 s
0.80214571994      1.0000000000
 1 s
0.30548672205      1.0000000000
 6 p
498.43397466      0.43118261050E-03
118.14109217      0.36206397703E-02
38.032529735      0.18245344081E-01
14.183731950      0.65133035572E-01
5.7864190721      0.16708915089
2.4599622160      0.29268019613
 1 p
1.0421999498      1.0000000000
 1 p
0.42987748916      1.0000000000
 1 p
0.16889708453      1.0000000000
 1 d
6.4710000000      1.0000000000
 1 d
2.2130000000      1.0000000000
 1 d
0.74700000000      1.0000000000
 1 f
4.6570000000      1.0000000000
 1 f
1.5240000000      1.0000000000
 1 g
2.9830000000      1.0000000000
*
*
na def2-QZVP

```

```

# na      (20s12p3d1f) / [9s5p3d1f]      {(10)31111111/81111/111/1}
*
10 s
379852.20081      0.20671384468E-04
56886.006378      0.16070466617E-03
12942.701838      0.84462905848E-03
3664.3017904      0.35519026029E-02
1194.7417499      0.12754034468E-01
430.98192917      0.39895462742E-01
167.83169424      0.10720154498
69.306669040      0.23339516913
29.951170886      0.36333077287
13.380791097      0.30544770974
3 s
121.74011283      0.36142427284E-01
37.044143387      0.28820961687
13.995422624      0.79337384869
1 s
5.9827797428      1.0000000000
1 s
2.4830455118      1.0000000000
1 s
1.0452506187      1.0000000000
1 s
0.43875640383      1.0000000000
1 s
0.65595633185E-01      1.0000000000
1 s
0.30561925072E-01      1.0000000000
1 s
0.15509064018E-01      1.0000000000
8 p
690.77627017      0.37478518415E-03
163.82806121      0.31775441030E-02
52.876460769      0.16333581338E-01
19.812270493      0.59754902585E-01
8.1320378784      0.15879328812
3.4969068377      0.29049363260
1.5117244146      0.36368131139
0.64479294912      0.28195867334
1 p
0.26145823312      1.0000000000
1 p
0.11704726116      1.0000000000
1 p
0.40494747666E-01      1.0000000000
1 p
0.15666707355E-01      1.0000000000
1 d
2.9000000000      1.0000000000
1 d
0.2300000000      1.0000000000
1 d
0.75700000000E-01      1.0000000000
1 f
0.1350000000      1.0000000000
*
*
mg def2-QZVP
# mg      (20s12p4d1f) / [9s5p4d1f]      {(10)31111111/81111/1111/1}

```

*

10 s	
605967.78753	0.14430176617E-04
90569.094692	0.11249871807E-03
20574.252844	0.59264972450E-03
5818.6284865	0.24988770424E-02
1895.6296075	0.90230775141E-02
683.45941021	0.28579919806E-01
266.18219762	0.79064453923E-01
110.11220010	0.18269337814
47.777041234	0.32157193967
21.542166149	0.35028259389
3 s	
174.12136378	0.22931111278E-01
53.484972498	0.19151777552
20.500213307	0.61155711055
1 s	
9.8056826922	1.0000000000
1 s	
3.5402989348	1.0000000000
1 s	
1.5450850046	1.0000000000
1 s	
0.66540195432	1.0000000000
1 s	
0.14355439071	1.0000000000
1 s	
0.66624673468E-01	1.0000000000
1 s	
0.29772648266E-01	1.0000000000
8 p	
893.20460829	0.34958267428E-03
211.78258286	0.29811890111E-02
68.443200537	0.15517845758E-01
25.727265349	0.57578659557E-01
10.606634281	0.15610307853
4.5934126484	0.29230912580
2.0100469807	0.37219024072
0.87384841536	0.27578088891
1 p	
0.35615076666	1.0000000000
1 p	
0.18995954356	1.0000000000
1 p	
0.74580135669E-01	1.0000000000
1 p	
0.29221641309E-01	1.0000000000
1 d	
3.8100000000	1.0000000000
1 d	
0.6500000000	1.0000000000
1 d	
0.2000000000	1.0000000000
1 d	
0.52000000000E-01	1.0000000000
1 f	
0.1600000000	1.0000000000

*

*

al def2-QZVP

a1 (20s14p4d2f1g) / [9s6p4d2f1g] {(10)
31111111/821111/1111/11/1}

*

10 s	
754550.78265	0.13421335886E-04
112999.38922	0.10433210786E-03
25715.831759	0.54841772080E-03
7283.6030283	0.23089081391E-02
2376.0008796	0.83309974593E-02
857.65468087	0.26417963653E-01
334.38922598	0.73443646426E-01
138.48504731	0.17184039139
60.150368808	0.31041980030
27.127610860	0.35669190596
3 s	
225.36500065	0.21522039783E-01
69.341968124	0.18531780493
26.619335712	0.63533181245
1 s	
12.349420671	1.0000000000
1 s	
4.5878785994	1.0000000000
1 s	
2.0571338103	1.0000000000
1 s	
0.90864549395	1.0000000000
1 s	
0.24226988038	1.0000000000
1 s	
0.11248136869	1.0000000000
1 s	
0.48156492817E-01	1.0000000000
8 p	
1489.6119522	0.20177122443E-03
353.01399267	0.17508109203E-02
114.40764069	0.94424704664E-02
43.312186111	0.36868004006E-01
18.027322216	0.10892874007
7.9675432403	0.23265901004
3.6090399541	0.34643587076
1.6456081630	0.33440809866
2 p	
34.731187489	0.17823073020E-01
1.2553083630	-0.59991263926
1 p	
0.73635534282	1.0000000000
1 p	
0.24686465559	1.0000000000
1 p	
0.94821971828E-01	1.0000000000
1 p	
0.36214165654E-01	1.0000000000
1 d	
1.9700000000	1.0000000000
1 d	
0.4370000000	1.0000000000
1 d	
0.1950000000	1.0000000000
1 d	
0.8000000000E-01	1.0000000000

```

1 f
0.15400000000 1.0000000000
1 f
0.40100000000 1.0000000000
1 g
0.35700000000 1.0000000000
*
*
si def2-QZVP
# si (20s14p4d2f1g) / [9s6p4d2f1g] {(10)}
31111111/821111/1111/11/1}
*
10 s
918070.69565 0.12658787192E-04
137485.25386 0.98408387461E-04
31287.772714 0.51731398244E-03
8861.6105697 0.21785441933E-02
2890.6943156 0.78656853716E-02
1043.4063979 0.24987553674E-01
406.80160276 0.69761818844E-01
168.48360207 0.16473362733
73.185628823 0.30285602647
32.998485420 0.36007260439
3 s
278.78751325 0.20185463814E-01
85.910228722 0.17720406747
32.992604031 0.63587860906
1 s
15.033693254 1.0000000000
1 s
5.7257514773 1.0000000000
1 s
2.6146521029 1.0000000000
1 s
1.1757833152 1.0000000000
1 s
0.35432330868 1.0000000000
1 s
0.16248335806 1.0000000000
1 s
0.68332457181E-01 1.0000000000
8 p
1775.8850516 0.20186971126E-03
420.83786849 0.17544314655E-02
136.42290243 0.95039532290E-02
51.700991737 0.37325741590E-01
21.559456002 0.11085396329
9.5559200095 0.23756407046
4.3529819473 0.35295783750
2.0096964381 0.32885931947
2 p
46.418153780 0.25858819154E-01
1.9076417796 -0.59874865899
1 p
0.92337221587 1.0000000000
1 p
0.34515720370 1.0000000000
1 p
0.13656834761 1.0000000000
1 p

```

```

0.52987060586E-01  1.0000000000
  1 d
  2.6450000000    1.0000000000
  1 d
0.608000000000    1.0000000000
  1 d
0.272000000000    1.0000000000
  1 d
0.113000000000    1.0000000000
  1 f
0.212000000000    1.0000000000
  1 f
0.541000000000    1.0000000000
  1 g
0.461000000000    1.0000000000
*
*
p def2-QZVP
# p      (20s14p4d2f1g) / [9s6p4d2f1g]      {(10)
31111111/821111/1111/11/1}
*
  10 s
  1090561.7138     0.12142449664E-04
  163316.39461     0.94395292614E-04
  37166.607451     0.49622262177E-03
  10526.880945     0.20900040747E-02
  3433.9976028     0.75489230025E-02
  1239.5360480     0.24010423937E-01
  483.27456199     0.67231473697E-01
  200.16911586     0.15978669881
  86.960394829     0.29735906782
  39.211283369     0.36187171850
  3 s
  336.75883662     0.19154721050E-01
  103.72179793     0.17134079100
  39.771861240     0.63689655985
  1 s
  17.888612952     1.0000000000
  1 s
  6.9644556879     1.0000000000
  1 s
  3.2198092087     1.0000000000
  1 s
  1.4669943979     1.0000000000
  1 s
0.47765437532     1.0000000000
  1 s
0.21637789241     1.0000000000
  1 s
0.90235894336E-01  1.0000000000
  8 p
  2019.6711374     0.21359172406E-03
  478.60125090     0.18568771399E-02
  155.14942504     0.10070690115E-01
  58.816356575     0.39605153679E-01
  24.544512785     0.11736067844
  10.883571061     0.24950540642
  4.9624791285     0.36421287984
  2.3002912343     0.31764127123
  2 p

```

59.371345016	0.39432918004
3.0694590986	-6.3522960431
1 p	
1.0634401739	1.0000000000
1 p	
0.45022152161	1.0000000000
1 p	
0.18267271344	1.0000000000
1 p	
0.71610333771E-01	1.0000000000
1 d	
3.3430000000	1.0000000000
1 d	
0.8070000000	1.0000000000
1 d	
0.3650000000	1.0000000000
1 d	
0.1540000000	1.0000000000
1 f	
0.2800000000	1.0000000000
1 f	
0.7030000000	1.0000000000
1 g	
0.5970000000	1.0000000000
*	
*	
s def2-QZVP	
# s (20s14p4d2f1g) / [9s6p4d2f1g]	{(10)}
31111111/821111/1111/11/1}	
*	
10 s	
1273410.9023	0.11767088246E-04
190697.83007	0.91478610166E-04
43397.885330	0.48090078640E-03
12291.809677	0.20257193592E-02
4009.7420824	0.73190096406E-02
1447.3531030	0.23300499900E-01
564.30102913	0.65386213610E-01
233.74506243	0.15614449910
101.56402814	0.29318563787
45.805907187	0.36287914289
3 s	
394.27281503	0.18753305081E-01
121.72249591	0.16870726663
46.754125963	0.63806830653
1 s	
20.923008254	1.0000000000
1 s	
8.2685567800	1.0000000000
1 s	
3.8629345671	1.0000000000
1 s	
1.7794684781	1.0000000000
1 s	
0.61064260103	1.0000000000
1 s	
0.27412269445	1.0000000000
1 s	
0.11325939107	1.0000000000
8 p	

2189.8930459	0.23912552864E-03
518.94596592	0.20772032158E-02
168.19560151	0.11242420571E-01
63.745282788	0.44069933941E-01
26.597033077	0.12918778608
11.774251449	0.26910820167
5.3534379024	0.37855928620
2.4701911802	0.29692134655
2 p	
82.120288349	-0.39420318847E-01
4.9523532869	0.64048403090
1 p	
1.0828262029	1.0000000000
1 p	
0.49271277356	1.0000000000
1 p	
0.20483450942	1.0000000000
1 p	
0.80743615716E-01	1.0000000000
1 d	
4.1590000000	1.0000000000
1 d	
1.0190000000	1.0000000000
1 d	
0.4640000000	1.0000000000
1 d	
0.1940000000	1.0000000000
1 f	
0.3350000000	1.0000000000
1 f	
0.8690000000	1.0000000000
1 g	
0.6830000000	1.0000000000
*	
*	
c1 def2-QZVP	
# c1 (20s14p4d2f1g) / [9s6p4d2f1g]	{(10)}
31111111/821111/1111/11/1}	
*	
10 s	
1467459.0095	0.11478257194E-04
219756.16433	0.89234299775E-04
50010.770301	0.46911086186E-03
14164.823918	0.19762446133E-02
4620.746525	0.71419937783E-02
1667.8991635	0.22753219445E-01
650.29199265	0.63959782953E-01
269.38037376	0.15331059238
117.06752106	0.28986952417
52.811766843	0.36348071452
3 s	
461.42769988	0.18019457578E-01
142.12665355	0.16489442314
54.437838768	0.63891587584
1 s	
24.160770219	1.0000000000
1 s	
9.7083540306	1.0000000000
1 s	
4.5640696733	1.0000000000

1 s		
2.1194744832	1.0000000000	
1 s		
0.75722365394	1.0000000000	
1 s		
0.33747224597	1.0000000000	
1 s		
0.13860775149	1.0000000000	
8 p		
2501.9457890	0.24242618410E-03	
592.88059285	0.21079961749E-02	
192.18089186	0.11432693869E-01	
72.875710488	0.44956698060E-01	
30.436358370	0.13197476145	
13.490178902	0.27493639225	
6.1478071413	0.38347236372	
2.8450944820	0.28871943885	
2 p		
105.39397936	-0.34311760144E-01	
6.7369738513	0.64060818902	
1 p		
1.2421095772	1.0000000000	
1 p		
0.55669714254	1.0000000000	
1 p		
0.23387801464	1.0000000000	
1 p		
0.93164490890E-01	1.0000000000	
1 d		
5.1910000000	1.0000000000	
1 d		
1.2760000000	1.0000000000	
1 d		
0.5830000000	1.0000000000	
1 d		
0.2430000000	1.0000000000	
1 f		
0.4230000000	1.0000000000	
1 f		
1.0890000000	1.0000000000	
1 g		
0.8270000000	1.0000000000	
*		
*		
ar def2-QZVP		
# ar (20s14p4d2f1g) / [9s6p4d2f1g]	{(10)	
31111111/821111/1111/11/1}		
*		
10 s		
1673421.9494	0.11245990413E-04	
250601.75373	0.87428115798E-04	
57030.912120	0.45961641275E-03	
16153.303915	0.19363890742E-02	
5269.4109288	0.69994046497E-02	
1902.0315541	0.22312068196E-01	
741.57677159	0.62808077697E-01	
307.20901906	0.15101140997	
133.52786203	0.28713661177	
60.253381291	0.36385490107	
3 s		

522.02426206	0.18071323116E-01
161.51290469	0.16449219884
62.126369433	0.63897334899
1 s	
27.590930012	1.0000000000
1 s	
11.175528881	1.0000000000
1 s	
5.2959065137	1.0000000000
1 s	
2.4782798895	1.0000000000
1 s	
0.91262095059	1.0000000000
1 s	
0.40426067549	1.0000000000
1 s	
0.16562886306	1.0000000000
8 p	
2868.4504581	0.24010435121E-03
679.71869590	0.20904788665E-02
220.36758824	0.11369316839E-01
83.620439734	0.44901977398E-01
34.964322657	0.13237156770
15.525131784	0.27709277600
7.0992979806	0.38613979646
3.3021336602	0.28492925372
2 p	
128.78765667	-0.30509457751E-01
8.4357867977	0.64101621070
1 p	
1.4618661855	1.0000000000
1 p	
0.64658010096	1.0000000000
1 p	
0.27229295755	1.0000000000
1 p	
0.10905182449	1.0000000000
1 d	
6.3150000000	1.0000000000
1 d	
1.5620000000	1.0000000000
1 d	
0.7150000000	1.0000000000
1 d	
0.2970000000	1.0000000000
1 f	
0.5430000000	1.0000000000
1 f	
1.3250000000	1.0000000000
1 g	
1.0070000000	1.0000000000
*	
*	
k def2-QZVP	
# k (24s18p4d1f) / [11s6p4d1f] {(11)4111111111/951111/1111/1}	
*	
11 s	
2022075.1391	0.10144874011E-04
303044.65568	0.78783500963E-04
69013.938490	0.41380919674E-03

19559.244615	0.17427571893E-02
6383.8934901	0.63004086126E-02
2305.3502858	0.20125347032E-01
899.14418101	0.56966060520E-01
372.59500133	0.13882654093
161.97635247	0.27132285414
73.085553853	0.36383620662
33.595644762	0.24724464776
4 s	
685.49855365	0.44367463797E-02
211.66163373	0.42502718169E-01
80.851405131	0.18467742018
35.108667236	0.29353173891
1 s	
14.409437283	1.0000000000
1 s	
6.8697147262	1.0000000000
1 s	
3.2121883687	1.0000000000
1 s	
1.2610484365	1.0000000000
1 s	
0.61438946301	1.0000000000
1 s	
0.27264370973	1.0000000000
1 s	
0.77173005207E-01	1.0000000000
1 s	
0.40918397569E-01	1.0000000000
1 s	
0.17055762425E-01	1.0000000000
9 p	
3469.6649718	0.21340225970E-03
822.02356107	0.18637844836E-02
266.58406636	0.10211431546E-01
101.28048161	0.40799604728E-01
42.429490761	0.12257473393
18.912083912	0.26405833679
8.7017779030	0.38227164575
4.0854567599	0.29998812383
1.8667286060	0.78007265591E-01
5 p	
27.544639057	-0.58222994163E-02
9.2098893609	-0.26787531329E-01
1.7232877425	0.30666847665
0.77969303735	0.66927944165
0.34379047862	0.60376468615
1 p	
0.14346681918	1.0000000000
1 p	
0.68000000000E-01	1.0000000000
1 p	
0.32000000000E-01	1.0000000000
1 p	
0.15300000000E-01	1.0000000000
1 d	
1.7000000000	1.0000000000
1 d	
0.5100000000	1.0000000000
1 d	


```

0.180000000000      1.000000000000
  1 d
0.540000000000E-01  1.000000000000
  1 f
0.267000000000      1.000000000000
*
*
ca def2-QZVP
# ca      (24s18p6d1f) / [11s6p4d1f]      {(11)4111111111/951111/3111/1}
*
  11 s
2433075.4304      0.91625196182E-05
364160.43015      0.71271617974E-04
82898.747637      0.37433706369E-03
23499.730540      0.15762862250E-02
7671.2245985      0.57026102580E-02
2770.2330687      0.18255738108E-01
1080.6807550      0.51906421035E-01
448.04894531      0.12791238579
194.92007727      0.25586635231
88.039793338      0.36028678275
40.645696719      0.26838462020
  4 s
779.53331918      -0.18403005509E-01
241.18856300      -0.17649440544
92.403869324      -0.77662799584
39.786090342      -1.3352155444
  1 s
18.195864278      1.000000000000
  1 s
8.3321457067      1.000000000000
  1 s
3.9190196209      1.000000000000
  1 s
1.6667099493      1.000000000000
  1 s
0.80891084908      1.000000000000
  1 s
0.36174199934      1.000000000000
  1 s
0.82379874526E-01  1.000000000000
  1 s
0.47947864375E-01  1.000000000000
  1 s
0.22308112408E-01  1.000000000000
  9 p
4064.2232796      0.19780891021E-03
962.91550624      0.17307465902E-02
312.34501046      0.95298721105E-02
118.76056036      0.38387459783E-01
49.816153133      0.11679256218
22.259679401      0.25637225097
10.286094124      0.37986193747
4.8606982416      0.30805760637
2.2525682942      0.85755999942E-01
  5 p
31.467555443      -0.42441487483E-02
10.657589056      -0.19579425947E-01
2.050555426      0.21237507422
0.94362089228      0.46277871121

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```

0.42709067504      0.39177495728
 1 p
0.17788187209      1.00000000000
 1 p
0.860000000000E-01  1.00000000000
 1 p
0.415000000000E-01  1.00000000000
 1 p
0.200000000000E-01  1.00000000000
 3 d
16.924012098      0.35543971560E-01
4.4655403330      0.18133698335
1.4347576200      0.48002060116
 1 d
0.46552376784      1.00000000000
 1 d
0.14097711082      1.00000000000
 1 d
0.41467009281E-01  1.00000000000
 1 f
0.32100000000      1.00000000000
*
*
sc def2-QZVP
# sc      (24s18p9d3f1g) / [11s6p5d3f1g]      {(11)
4111111111/951111/51111/111/1}
*
 11 s
2855231.1264      0.84862794535E-05
427433.34221      0.65998092974E-04
97233.218545      0.34740968058E-03
27496.222846      0.14694099525E-02
8948.7324409      0.53410667286E-02
3221.0397292      0.17200652511E-01
1252.0534077      0.49287065332E-01
517.26093376      0.12273534550
224.33127242      0.24910183844
101.10551671      0.35884366997
46.684957855      0.27782811319
 4 s
947.75965484      0.36123019249E-02
293.07262846      0.35616224567E-01
111.70230657      0.16664064248
47.756215212      0.32531051399
 1 s
21.121984009      1.00000000000
 1 s
9.7765922198      1.00000000000
 1 s
4.5982699340      1.00000000000
 1 s
1.9928487767      1.00000000000
 1 s
0.95939954457      1.00000000000
 1 s
0.42566790070      1.00000000000
 1 s
0.98132196006E-01  1.00000000000
 1 s
0.56894222237E-01  1.00000000000

```

```

1 s
0.25369907195E-01 1.0000000000
9 p
4611.4680242 0.19180655992E-03
1092.4666458 0.16801897753E-02
354.41923265 0.92763338425E-02
134.83390286 0.37537202735E-01
56.610873926 0.11493045217
25.336605518 0.25446811084
11.741313238 0.37993352765
5.5697268625 0.30948776388
2.5949954062 0.86972259257E-01
5 p
35.951198081 -0.55780446917E-02
12.301020232 -0.25933825208E-01
2.3876557755 0.27489094204
1.1031823600 0.59208047142
0.50008479496 0.49113471853
1 p
0.20796508799 1.0000000000
1 p
0.10100000000 1.0000000000
1 p
0.48000000000E-01 1.0000000000
1 p
0.23000000000E-01 1.0000000000
5 d
73.531179748 0.22506354976E-02
21.764759639 0.16377610133E-01
7.9233701690 0.63330446952E-01
3.1847889778 0.17056208548
1.3427790019 0.30119020299
1 d
0.56149574983 1.0000000000
1 d
0.22764073650 1.0000000000
1 d
0.85211221793E-01 1.0000000000
1 d
0.35000000000E-01 1.0000000000
1 f
1.4810000000 1.0000000000
1 f
0.34500000000 1.0000000000
1 f
0.11000000000 1.0000000000
1 g
0.24700000000 1.0000000000
*
*
ti def2-QZVP
# ti (24s18p9d3f1g) / [11s6p5d3f1g] {(11)}
4111111111/951111/51111/111/1}
*
11 s
3070548.8651 0.86954016630E-05
460777.88643 0.67452737727E-04
104901.22889 0.35477293028E-03
29695.861199 0.14977525588E-02
9678.8892688 0.54309912055E-02

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3490.1877912	0.17439360524E-01
1359.2217621	0.49835634640E-01
562.42721208	0.12379633943
244.22296250	0.25057490943
110.16668710	0.35934609007
50.881903357	0.27594242664
4 s	
965.95430789	0.41773927781E-02
299.27072059	0.40277148567E-01
114.83772939	0.17898686817
49.477578954	0.31783043543
1 s	
22.982839977	1.0000000000
1 s	
10.518305037	1.0000000000
1 s	
4.9774390567	1.0000000000
1 s	
2.1339846838	1.0000000000
1 s	
1.0342457284	1.0000000000
1 s	
0.46199774995	1.0000000000
1 s	
0.10621264194	1.0000000000
1 s	
0.54340347374E-01	1.0000000000
1 s	
0.25110217385E-01	1.0000000000
9 p	
5169.6755427	0.18802523596E-03
1225.0961638	0.16473458826E-02
397.60051934	0.91104554321E-02
151.36154684	0.36987450926E-01
63.613321773	0.11376329624
28.514560307	0.25345208574
13.248003298	0.38019402704
6.3048807760	0.30989136346
2.9493525821	0.87418944007E-01
5 p	
40.738772213	-0.73233793267E-02
14.062358461	-0.34282591082E-01
2.7460680961	0.35655009250
1.2713688141	0.76112035427
0.57610015545	0.62716743237
1 p	
0.23981820724	1.0000000000
1 p	
0.11000000000	1.0000000000
1 p	
0.50000000000E-01	1.0000000000
1 p	
0.23000000000E-01	1.0000000000
5 d	
89.589880075	0.21223030030E-02
26.591412960	0.15911819913E-01
9.7739715702	0.62875243121E-01
3.9625083655	0.17144170807
1.6890532654	0.30565506624
1 d	

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0.71539771469      1.0000000000
  1 d
0.29366677748      1.0000000000
  1 d
0.11079094851      1.0000000000
  1 d
0.45000000000E-01  1.0000000000
  1 f
  2.0930000000      1.0000000000
  1 f
0.56200000000      1.0000000000
  1 f
0.19100000000      1.0000000000
  1 g
0.63400000000      1.0000000000
*
*
v def2-QZVP
# v      (24s18p9d3f1g) / [11s6p5d3f1g]      {(11)}
4111111111/951111/51111/111/1}
*
  11 s
  3360380.0382      0.87027840678E-05
  502646.73178      0.67786024965E-04
  114247.22867      0.35699229090E-03
  32321.972630      0.15075507352E-02
  10532.947271      0.54664377528E-02
  3798.3004439      0.17547310839E-01
  1479.6094715      0.50106594778E-01
  612.57405507      0.12431296066
  266.22103326      0.25117026883
  120.21980126      0.35926015903
  55.591180848      0.27505075685
  4 s
  1082.4768635      0.39326847695E-02
  334.94462061      0.38298477998E-01
  128.31559026      0.17259908827
  55.311589616      0.31287423870
  1 s
  25.108383036      1.0000000000
  1 s
  11.667553242      1.0000000000
  1 s
  5.5372073270      1.0000000000
  1 s
  2.3781007618      1.0000000000
  1 s
  1.1506947329      1.0000000000
  1 s
0.51283991040      1.0000000000
  1 s
0.11625711449      1.0000000000
  1 s
0.58272785598E-01  1.0000000000
  1 s
0.26662312245E-01  1.0000000000
  9 p
  5782.8035005      0.18344743045E-03
  1369.9392282      0.16095217453E-02
  444.53147129      0.89242268749E-02

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169.25617556	0.36375182379E-01
71.168730031	0.11246803294
31.933358374	0.25226107794
14.865336779	0.38039695005
7.0921740091	0.31068797325
3.3281157846	0.88141200458E-01
5 p	
45.842906017	-0.56661391945E-02
15.940339016	-0.26718979445E-01
3.1257155025	0.27354632707
1.4485867558	0.57972883053
0.65577902825	0.476011110515
1 p	
0.27311626644	1.0000000000
1 p	
0.12200000000	1.0000000000
1 p	
0.55000000000E-01	1.0000000000
1 p	
0.25000000000E-01	1.0000000000
5 d	
103.95047414	0.21007158819E-02
30.901688665	0.16015244877E-01
11.420321145	0.64127456940E-01
4.6573272292	0.17488905695
1.9963682623	0.31003778048
1 d	
0.84967249531	1.0000000000
1 d	
0.34953221876	1.0000000000
1 d	
0.13165588233	1.0000000000
1 d	
0.52000000000E-01	1.0000000000
1 f	
2.9330000000	1.0000000000
1 f	
0.8310000000	1.0000000000
1 f	
0.2570000000	1.0000000000
1 g	
1.0090000000	1.0000000000
*	
*	
cr def2-QZVP	
# cr (24s18p9d3f1g) / [11s6p5d3f1g]	{(11)}
4111111111/951111/51111/111/1}	
*	
11 s	
3637838.6820	0.87693297699E-05
544864.46100	0.68169050223E-04
123997.55079	0.35844590272E-03
35116.733166	0.15117006948E-02
11455.702298	0.54731929774E-02
4135.9906712	0.17539430107E-01
1613.2513581	0.50004870927E-01
668.77932380	0.12393518958
291.01365155	0.25039606407
131.57328167	0.35870470429
60.924567928	0.27581148880

4	s	
1196.2899601		0.77368642037E-02
369.76947592		0.75837835399E-01
141.54426084		0.34435148637
60.999228765		0.63249297923
1	s	
27.599113358		1.0000000000
1	s	
12.882112056		1.0000000000
1	s	
6.1247513721		1.0000000000
1	s	
2.6332895309		1.0000000000
1	s	
1.2708482289		1.0000000000
1	s	
0.56483575923		1.0000000000
1	s	
0.12596808943		1.0000000000
1	s	
0.62045607277E-01		1.0000000000
1	s	
0.28144312720E-01		1.0000000000
9	p	
6395.8781792		0.18104788151E-03
1515.1701574		0.15893658935E-02
491.70538681		0.88258739429E-02
187.28416675		0.36068946983E-01
78.800346444		0.11189649648
35.396291693		0.25202239843
16.509278879		0.38082266430
7.8947396863		0.31035222437
3.7136414465		0.87980310362E-01
5	p	
51.259312534		-0.60542038165E-02
17.934932523		-0.28761764001E-01
3.5257174218		0.29087768170
1.6339163906		0.61267525056
0.73852413834		0.50126035018
1	p	
0.30752368193		1.0000000000
1	p	
0.13500000000		1.0000000000
1	p	
0.59000000000E-01		1.0000000000
1	p	
0.26000000000E-01		1.0000000000
5	d	
118.24986288		0.21012757435E-02
35.193935700		0.16212269500E-01
13.057816022		0.65581852668E-01
5.3485602844		0.17849601449
2.3004233713		0.31376763016
1	d	
0.98114328305		1.0000000000
1	d	
0.40334183206		1.0000000000
1	d	
0.15135589551		1.0000000000
1	d	

```

0.600000000000E-01  1.0000000000
  1 f
3.7330000000  1.0000000000
  1 f
1.1470000000  1.0000000000
  1 f
0.3660000000  1.0000000000
  1 g
1.3820000000  1.0000000000
*
*
mn def2-QZVP
# mn      (24s18p10d3f1g) / [11s6p5d3f1g]      {(11)}
4111111111/951111/61111/111/1}
*
  11 s
4289357.6441      0.79360554972E-05
636361.00285     0.62542986761E-04
143637.27569     0.33226388724E-03
40406.345432     0.14130009568E-02
13104.363417     0.51560918319E-02
4705.0664255     0.16659574919E-01
1825.7125432     0.47908083403E-01
753.33816229     0.11994903752
326.47253285     0.24550296959
147.10300670     0.35822739571
67.987226869     0.28295764442
  4 s
1300.7266717     0.76025154141E-02
402.72027544     0.74365109808E-01
154.38971348     0.33780474819
66.443384613     0.62779331746
  1 s
30.975316006     1.0000000000
  1 s
14.222980890     1.0000000000
  1 s
6.7598265074     1.0000000000
  1 s
2.9087083287     1.0000000000
  1 s
1.3966507792     1.0000000000
  1 s
0.61792624091     1.0000000000
  1 s
0.13439483715     1.0000000000
  1 s
0.65195053803E-01  1.0000000000
  1 s
0.29415713624E-01  1.0000000000
  9 p
6483.2629658     0.20479778890E-03
1556.7134859     0.17525750185E-02
509.73925460     0.95798802458E-02
195.28408089     0.38681362983E-01
82.542547525     0.11832401588
37.212076731     0.26168459627
17.425804462     0.38400628821
8.3691376962     0.29704166759
3.9409000444     0.78263290323E-01

```



```

5 p
57.202741010 -0.47749099800E-02
20.090935947 -0.22989729915E-01
3.9357553763 0.23197065881
1.8181984012 0.48435204043
0.81881535281 0.39159479004
1 p
0.34038359193 1.0000000000
1 p
0.15000000000 1.0000000000
1 p
0.63000000000E-01 1.0000000000
1 p
0.27000000000E-01 1.0000000000
6 d
200.40254535 0.89549560240E-03
59.898225773 0.76257630942E-02
22.810570167 0.34523224226E-01
9.5874142097 0.10552676975
4.2933710910 0.22575377683
1.9537618373 0.32766533667
1 d
0.87378873598 1.0000000000
1 d
0.37597748904 1.0000000000
1 d
0.14811547592 1.0000000000
1 d
0.60000000000E-01 1.0000000000
1 f
4.3530000000 1.0000000000
1 f
1.3260000000 1.0000000000
1 f
0.40800000000 1.0000000000
1 g
1.7550000000 1.0000000000
*
*
fe def2-QZVP
# fe (24s18p10d3f1g) / [11s6p5d3f1g] {(11)}
4111111111/951111/61111/111/1}
*
11 s
4313154.4338 0.86712290122E-05
645875.08253 0.67423150519E-04
146981.87698 0.35448747955E-03
41630.615044 0.14948285557E-02
13580.620109 0.54136698440E-02
4902.0620613 0.17362460824E-01
1911.2900837 0.49566574059E-01
791.99837852 0.12309089705
344.54799181 0.24936705764
155.78722730 0.35858414677
72.179380315 0.27738221642
4 s
1417.9125091 0.74871631942E-02
439.23184195 0.73337584435E-01
168.51006820 0.33383143870
72.776269412 0.62022524641

```

1 s	
32.752961774	1.0000000000
1 s	
15.434336101	1.0000000000
1 s	
7.3639318205	1.0000000000
1 s	
3.1698832880	1.0000000000
1 s	
1.5243708395	1.0000000000
1 s	
0.67496281152	1.0000000000
1 s	
0.14718566032	1.0000000000
1 s	
0.70082216629E-01	1.0000000000
1 s	
0.31208269419E-01	1.0000000000
9 p	
7709.0587627	0.17711229843E-03
1826.4666323	0.15560056795E-02
592.84368362	0.86629536960E-02
225.93763245	0.35565954156E-01
95.164758890	0.11098847278
42.823132375	0.25177796624
20.036286581	0.38166911079
9.6159346283	0.30963598261
4.5393538787	0.87558276626E-01
5 p	
62.997519003	-0.50910388724E-02
22.262748731	-0.24540463235E-01
4.3900064942	0.24345605487
2.0328913928	0.50781898425
0.91592621576	0.41214895672
1 p	
0.38036653507	1.0000000000
1 p	
0.16000000000	1.0000000000
1 p	
0.67000000000E-01	1.0000000000
1 p	
0.28000000000E-01	1.0000000000
6 d	
218.33430163	0.93700006628E-03
65.256292616	0.80008769378E-02
24.866944817	0.36305286587E-01
10.473399301	0.11057189871
4.6947005007	0.23219588596
2.1315982534	0.32922859685
1 d	
0.94748004605	1.0000000000
1 d	
0.40346488831	1.0000000000
1 d	
0.15687414728	1.0000000000
1 d	
0.62000000000E-01	1.0000000000
1 f	
5.1030000000	1.0000000000
1 f	

```

1.5980000000      1.0000000000
 1 f
0.5050000000      1.0000000000
 1 g
2.1280000000      1.0000000000
*
*
co def2-QZVP
# co      (24s18p10d3f1g) / [11s6p5d3f1g]      {(11)
4111111111/951111/61111/111/1}
*
 11 s
4658206.5032      0.86609506454E-05
697560.87453      0.67336300186E-04
158759.87124      0.35399044899E-03
44969.099379      0.14926384309E-02
14670.714247      0.54053095095E-02
5295.8947250      0.17335233605E-01
2065.0581167      0.49486641301E-01
855.90627750      0.12289351961
372.48747255      0.24903230028
168.50576608      0.35838320259
78.128761566      0.27777974150
 4 s
1534.5149885      0.74464372833E-02
475.52976096      0.72993601986E-01
182.54836839      0.33243104986
78.916467177      0.61900490005
 1 s
35.500865522      1.0000000000
 1 s
16.790414486      1.0000000000
 1 s
8.0240232510      1.0000000000
 1 s
3.4571682964      1.0000000000
 1 s
1.6599835391      1.0000000000
 1 s
0.73380022453      1.0000000000
 1 s
0.15878613103      1.0000000000
 1 s
0.74535659476E-01  1.0000000000
 1 s
0.32867351695E-01  1.0000000000
 9 p
8425.4331352      0.17491775490E-03
1995.8758452      0.15378901702E-02
647.76765681      0.85752453448E-02
246.88261214      0.35295266911E-01
104.00952246      0.11050007672
46.827478138      0.25160924538
21.934444535      0.38209003019
10.540499528      0.30947119879
4.9820419385      0.87436873012E-01
 5 p
69.270787130      -0.61172424428E-02
24.583977935      -0.29655043898E-01
4.8562258878      0.29163333190

```

2.2480916102	0.60629408335
1.0114285977	0.49057440018
1 p	
0.41919905455	1.0000000000
1 p	
0.17500000000	1.0000000000
1 p	
0.73000000000E-01	1.0000000000
1 p	
0.30000000000E-01	1.0000000000
6 d	
237.58450966	0.97593282671E-03
71.086896302	0.83432571945E-02
27.119080683	0.37958471100E-01
11.448239054	0.11522936171
5.1391806672	0.23843467913
2.3323492099	0.33205699955
1 d	
1.0338662062	0.33276836067
1 d	
0.43785146294	0.22769290932
1 d	
0.16895004948	0.74634129160E-01
1 d	
0.66000000000E-01	1.0000000000
1 f	
5.9750000000	1.0000000000
1 f	
1.9030000000	1.0000000000
1 f	
0.59400000000	1.0000000000
1 g	
2.5000000000	1.0000000000
*	
*	
ni def2-QZVP	
# ni (24s18p10d3f1g) / [11s6p5d3f1g]	{(11)}
4111111111/951111/61111/111/1}	
*	
11 s	
5037649.9532	0.86072778771E-05
754246.39418	0.66935354750E-04
171644.16010	0.35190801168E-03
48617.230286	0.14839082715E-02
15860.961795	0.53736344264E-02
5726.0018653	0.17233376287E-01
2232.9547317	0.49211476915E-01
925.49649101	0.12232504536
402.75336913	0.24829251588
182.19422856	0.35825476194
84.494109788	0.27881865553
4 s	
1678.0564586	0.82462870895E-02
519.21358326	0.81505940361E-01
198.95881607	0.37495727651
85.901180703	0.70841743832
1 s	
38.435760123	1.0000000000
1 s	
18.252349351	1.0000000000

1 s	
8.7283616939	1.0000000000
1 s	
3.7616245662	1.0000000000
1 s	
1.8028217338	1.0000000000
1 s	
0.79507140513	1.0000000000
1 s	
0.17031720284	1.0000000000
1 s	
0.78971236177E-01	1.0000000000
1 s	
0.34503486750E-01	1.0000000000
9 p	
9156.5701453	0.17346418360E-03
2169.0239526	0.15257220493E-02
703.98918991	0.85163281036E-02
268.36293215	0.35117466952E-01
113.10288796	0.11020275383
50.955539222	0.25162601670
23.896708209	0.38246389853
11.498241522	0.30907230267
5.4410908056	0.87194377415E-01
5 p	
75.938560736	-0.74635546629E-02
27.037350184	-0.36453401627E-01
5.3404687432	0.35633549406
2.4700181361	0.73774121992
1.1095029064	0.59439383024
1 p	
0.45899767101	1.0000000000
1 p	
0.18700000000	1.0000000000
1 p	
0.76200000000E-01	1.0000000000
1 p	
0.31000000000E-01	1.0000000000
6 d	
258.11131142	0.23726274275E-02
77.254891371	0.20330132784E-01
29.500240033	0.92748486665E-01
12.477446945	0.28082284560
5.6070455111	0.57392657880
2.5427744163	0.78766058527
1 d	
1.1238296774	0.77868790423
1 d	
0.47361171459	0.52932234348
1 d	
0.18161858319	0.17478168242
1 d	
0.71000000000E-01	1.0000000000
1 f	
6.7580000000	1.0000000000
1 f	
2.1740000000	1.0000000000
1 f	
0.6810000000	1.0000000000
1 g	

```

2.8720000000      1.0000000000
*
*
cu def2-QZVP
# cu      (24s18p10d3f1g) / [11s6p5d3f1g]      {(11)}
4111111111/951111/61111/111/1}
*
11 s
5056467.8898      0.93501916365E-05
759457.83835      0.72323443222E-04
173524.88497      0.37813833845E-03
49327.259988      0.15870129862E-02
16144.149930      0.57220685294E-02
5844.5964680      0.18268390048E-01
2284.6812739      0.51893720863E-01
948.88232514      0.12796192366
413.66215455      0.25629891036
187.38942059      0.36064416138
86.872771648      0.26833664660
4 s
1744.0598287      0.88587079141E-02
540.93295513      0.86522785813E-01
207.99736224      0.38932285258
90.475793036      0.69777199902
1 s
38.869687699      1.0000000000
1 s
18.974829147      1.0000000000
1 s
9.0953644635      1.0000000000
1 s
3.8330020174      1.0000000000
1 s
1.8198891499      1.0000000000
1 s
0.79068098393      1.0000000000
1 s
0.14914142106      1.0000000000
1 s
0.72448090592E-01  1.0000000000
1 s
0.30959925368E-01  1.0000000000
9 p
9720.4614555      0.17828803512E-03
2302.7557452      0.15678108633E-02
747.48498314      0.87470094509E-02
285.00132623      0.36044549301E-01
120.15121609      0.11287209053
54.145261156      0.25647377341
25.406033563      0.38512918379
12.224331465      0.30316512356
5.7638720668      0.81677218969E-01
5 p
83.210837217      -0.63530359993E-02
29.694779129      -0.31383834666E-01
5.8248516206      0.30930039753
2.6746181180      0.63583925938
1.1841836775      0.50946045967
1 p
0.48043583535      1.0000000000

```

```

1 p
0.18700000000 1.0000000000
1 p
0.76200000000E-01 1.0000000000
1 p
0.31000000000E-01 1.0000000000
6 d
249.54025080 0.12432881244E-02
74.683914534 0.10456901995E-01
28.392717116 0.46451241249E-01
11.955968430 0.13541359729
5.3210744624 0.25852899978
2.3661189459 0.33168127635
1 d
1.0131863994 1.0000000000
1 d
0.40710035940 1.0000000000
1 d
0.14742541032 1.0000000000
1 d
0.71000000000E-01 1.0000000000
1 f
6.9620000000 1.0000000000
1 f
2.2330000000 1.0000000000
1 f
0.70400000000 1.0000000000
1 g
3.2450000000 1.0000000000
*
*
zn def2-QZVP
# zn (24s18p10d3f1g) / [11s6p5d3f1g] {(11)}
4111111111/951111/61111/111/1}
*
11 s
5742307.1507 0.86864381562E-05
861450.78790 0.67364668570E-04
196346.05866 0.35349715135E-03
55682.870737 0.14884153943E-02
18183.902394 0.53840916617E-02
6569.6448019 0.17252738209E-01
2563.5613276 0.49238679132E-01
1063.1147176 0.12235812174
462.89771078 0.24835390245
209.52821049 0.35830632832
97.240787991 0.27880259960
4 s
1929.2689992 0.83077002177E-02
598.07122307 0.81882590163E-01
229.69667336 0.37588060221
99.416819228 0.71067260445
1 s
44.241101421 1.0000000000
1 s
21.194367113 1.0000000000
1 s
10.158731597 1.0000000000
1 s
4.3746176158 1.0000000000

```

1 s	
2.0901489071	1.0000000000
1 s	
0.91869136437	1.0000000000
1 s	
0.19278660606	1.0000000000
1 s	
0.87329915171E-01	1.0000000000
1 s	
0.37552217126E-01	1.0000000000
9 p	
10690.445107	0.17142867222E-03
2532.3159340	0.15088012830E-02
821.94295003	0.84368777910E-02
313.42757800	0.34898103208E-01
132.18314247	0.10993617353
59.620554387	0.25207277070
28.019488868	0.38325657524
13.511704850	0.30787091255
6.4053711253	0.86411696761E-01
5 p	
89.981131918	-0.96262847843E-02
32.241767106	-0.47509407258E-01
6.3809448581	0.45834100431
2.9477928353	0.94473799128
1.3200854955	0.75923464871
1 p	
0.54424674445	1.0000000000
1 p	
0.25799971797	1.0000000000
1 p	
0.92863192359E-01	1.0000000000
1 p	
0.34059341410E-01	1.0000000000
6 d	
305.22298937	0.27359792434E-02
91.468273202	0.23585229776E-01
34.986985968	0.10858422440
14.849415187	0.32843594226
6.6858545707	0.66180235634
3.0309412620	0.89165339320
1 d	
1.3355050671	1.0000000000
1 d	
0.55883176392	1.0000000000
1 d	
0.21180799287	1.0000000000
1 d	
0.83000000000E-01	1.0000000000
1 f	
8.0200000000	1.0000000000
1 f	
2.6140000000	1.0000000000
1 f	
0.83600000000	1.0000000000
1 g	
3.6170000000	1.0000000000

*

*

ga def2-QZVP

ga (24s19p10d2f1g) / [11s7p4d2f1g] {(11)
4111111111/9241111/7111/11/1}

*

11 s	
6623802.0274	0.79091326051E-05
987904.07075	0.61835727406E-04
224132.05899	0.32636322451E-03
63315.192943	0.13810365049E-02
20611.312702	0.50153772104E-02
7429.1672482	0.16130936803E-01
2894.2071720	0.46240827188E-01
1198.9915786	0.11579099571
521.82003812	0.23834840794
236.27549237	0.35374255971
109.98395671	0.29055721918
4 s	
2101.2587253	0.83039611523E-02
650.97022519	0.82254127688E-01
250.22438356	0.38021717478
108.17616625	0.74503594690
1 s	
51.057486710	1.0000000000
1 s	
23.647474527	1.0000000000
1 s	
11.361701144	1.0000000000
1 s	
5.0178135897	1.0000000000
1 s	
2.4102674998	1.0000000000
1 s	
1.0741046685	1.0000000000
1 s	
0.25745075831	1.0000000000
1 s	
0.12175227548	1.0000000000
1 s	
0.52360599017E-01	1.0000000000
9 p	
14711.750483	0.11130990649E-03
3482.1451716	0.98495921142E-03
1130.2186655	0.55854182058E-02
431.54093448	0.23682413047E-01
182.41723648	0.78211587173E-01
82.706753603	0.19503829929
39.228128772	0.34131988495
19.201979939	0.35718665135
9.5056966689	0.16395955052
2 p	
92.615613022	-0.85848284169E-01
33.750148165	-0.39435019538
4 p	
7.3482283015	0.37941606569
3.7813384844	0.71306291866
2.3145183128	0.43210001481
0.80346859715	0.25838122797
1 p	
1.5423710087	1.0000000000
1 p	
0.32910239639	1.0000000000

```

1 p
0.11834088831      1.0000000000
1 p
0.41627877699E-01  1.0000000000
7 d
363.49565218      0.87402299276E-03
109.01749589      0.76751934098E-02
41.866430715      0.36388975341E-01
17.879279894      0.11325183017
8.1201893671      0.23770881294
3.7360611356      0.33306060389
1.6826812549      0.33130613756
1 d
0.72655790500     0.21895437571
1 d
0.28498585079     1.0000000000
1 d
0.11200000000     1.0000000000
1 f
0.18100000000     1.0000000000
1 f
0.47100000000     1.0000000000
1 g
0.40320000000     1.0000000000
*
*
ge def2-QZVP
# ge      (24s19p10d2f1g) / [11s7p4d2f1g]      {(11)
4111111111/9241111/7111/11/1}
*
11 s
7233056.0346      0.76638751457E-05
1082886.1731      0.59603601369E-04
246481.46959      0.31319088031E-03
69862.426955      0.13194051561E-02
22815.809662      0.47736099191E-02
8246.5369297      0.15319250467E-01
3219.9367257      0.43900870673E-01
1336.5743706      0.11028573632
582.87737501      0.22912630489
264.59511360      0.34779259246
123.77823320      0.29968722223
4 s
2311.1055804      0.75033084731E-02
716.27089868      0.74778386626E-01
275.45330910      0.35092882302
118.93292565      0.72055989686
1 s
58.435699085      1.0000000000
1 s
26.261575973      1.0000000000
1 s
12.664880671      1.0000000000
1 s
5.7269548505      1.0000000000
1 s
2.7555023203      1.0000000000
1 s
1.2432886754      1.0000000000
1 s

```

```

0.33107183846      1.0000000000
 1 s
0.15964081368      1.0000000000
 1 s
0.68463178923E-01  1.0000000000
 9 p
16555.711074       0.10199370391E-03
3914.9903745       0.90504190546E-03
1269.4766518       0.51558490762E-02
484.35437789       0.22010335708E-01
204.64985822       0.73434798827E-01
92.791032094       0.18608955294
44.055060255       0.33330981945
21.601319931       0.36229776246
10.732169233       0.17765186263
 2 p
100.88933962      -0.11146182144
36.640254741      -0.52324324314
 4 p
 8.0343224115     0.31484763263
 4.5613438333     0.38737744790
 3.1794882223     0.50034353638
0.92612041457     0.22656707948
 1 p
 1.7977040907     1.0000000000
 1 p
0.41386865432     1.0000000000
 1 p
0.15830798709     1.0000000000
 1 p
0.57877035911E-01 1.0000000000
 7 d
 420.99565921     0.78212192196E-03
126.36209818       0.69560123831E-02
48.661473548       0.33712188323E-01
20.880325527       0.10717291194
9.5418229355       0.23161030141
4.4353653868       0.33390954301
2.0285421942       0.33720676378
 1 d
0.89484935267     0.21702473265
 1 d
0.35786074334     1.0000000000
 1 d
0.14000000000     1.0000000000
 1 f
0.54920000000     1.0000000000
 1 f
0.21900000000     1.0000000000
 1 g
0.46810000000     1.0000000000
*
*
as def2-QZVP
# as      (24s20p10d2f1g) / [11s7p4d2f1g]      {(11)4111111111/(10)
511111/7111/11/1}
*
 11 s
 8217482.6198     0.70590618422E-05
1230500.3720     0.54880889611E-04

```

280225.86648	0.28809164698E-03
79482.509415	0.12129779464E-02
25963.783351	0.43914559880E-02
9381.4010193	0.14125362961E-01
3660.4911972	0.40657915618E-01
1518.2356024	0.10300382633
661.80098920	0.21730077101
300.58642127	0.33995751412
141.11137296	0.31088634077
4 s	
2577.0870580	0.70752991980E-02
798.07872277	0.71383615256E-01
306.57574948	0.34287024634
132.27558802	0.74361403413
1 s	
67.448702235	1.0000000000
1 s	
29.209180441	1.0000000000
1 s	
14.156509326	1.0000000000
1 s	
6.5561506682	1.0000000000
1 s	
3.1392847238	1.0000000000
1 s	
1.4294631050	1.0000000000
1 s	
0.41103390885	1.0000000000
1 s	
0.20032453310	1.0000000000
1 s	
0.85669928850E-01	1.0000000000
10 p	
25198.504278	0.54758168372E-04
5972.5601381	0.48572462452E-03
1941.9123183	0.27908085625E-02
743.59381104	0.12201505962E-01
315.63828052	0.42666285138E-01
143.96878925	0.11870919141
69.068683164	0.24909407023
34.254305629	0.36061356903
17.371746759	0.29392241832
8.7634555628	0.97829057366E-01
5 p	
228.49024582	-0.24900140765E-02
86.313555488	-0.19482515843E-01
36.751366267	-0.61495071038E-01
8.5365149464	0.47258065062
4.1935128599	1.0236065079
1 p	
2.0464980417	1.0000000000
1 p	
0.98000000000	1.0000000000
1 p	
0.40534340618	1.0000000000
1 p	
0.16655070471	1.0000000000
1 p	
0.65981706123E-01	1.0000000000
7 d	

```

479.32599612      0.71722800196E-03
143.96064855      0.64419223046E-02
55.548909224      0.31776498964E-01
23.927581006      0.10276249168
10.988194172      0.22710952843
5.1489356262      0.33477474118
2.3836810892      0.34175986071
  1 d
1.0688204667      0.21462891644
  1 d
0.43305693742      1.0000000000
  1 d
0.17000000000      1.0000000000
  1 f
0.26400000000      1.0000000000
  1 f
0.64400000000      1.0000000000
  1 g
0.54650000000      1.0000000000
*
*
se def2-QZVP
# se      (24s20p10d2f1g) / [11s7p4d2f1g]      {(11)4111111111/(10)
511111/7111/11/1}
*
  11 s
9520446.7743      0.63309690150E-05
1424984.0802      0.49267697990E-04
324127.57682      0.25920249744E-03
91774.876950      0.10943145743E-02
29932.725725      0.39706139067E-02
10804.617905      0.12801187916E-01
4214.0134779      0.36980379417E-01
1747.8116633      0.94461349896E-01
762.12160878      0.20274705434
346.45604141      0.32878956424
163.11569304      0.32300252609
  4 s
2614.5153067      0.79113928518E-02
818.68552756      0.77187739408E-01
318.63398991      0.35672061949
139.04844125      0.75846750004
  1 s
78.348734788      1.0000000000
  1 s
31.704290663      1.0000000000
  1 s
15.505859269      1.0000000000
  1 s
7.3227423625      1.0000000000
  1 s
3.4969483549      1.0000000000
  1 s
1.6121546085      1.0000000000
  1 s
0.49587158541      1.0000000000
  1 s
0.24092138175      1.0000000000
  1 s
0.10231739397      1.0000000000

```

```

10 p
25360.215615      0.60531790911E-04
5993.7896610     0.53987774437E-03
1943.0741755     0.31130456170E-02
742.35316156    0.13599674694E-01
314.62114597    0.47298958377E-01
143.34748044    0.12981487726
68.673617552    0.26569982215
34.013554117    0.36723195311
17.198099621    0.27478356345
8.5830329629    0.79256169683E-01
 5 p
236.58209146    -0.12271649354E-02
90.576183214    -0.92584627774E-02
39.086689301    -0.28428728384E-01
9.3084344018    0.21201102192
4.6169923084    0.47117589805
 1 p
2.2653477506    1.0000000000
 1 p
1.0800000000    1.0000000000
 1 p
0.47939328581   1.0000000000
 1 p
0.19619983845   1.0000000000
 1 p
0.76256339275E-01 1.0000000000
 7 d
539.48700124    0.66722955533E-03
162.13394435    0.60399330928E-02
62.661795641    0.30238666507E-01
27.077272889    0.99267892065E-01
12.483003929    0.22358036310
5.8864623136    0.33574682762
2.7519131105    0.34554856483
 1 d
1.2500769617    0.21216654622
 1 d
0.51172841843   1.0000000000
 1 d
0.2000000000    1.0000000000
 1 f
0.2840000000    1.0000000000
 1 f
0.7097000000    1.0000000000
 1 g
0.5730000000    1.0000000000
*
*
br def2-QZVP
# br      (24s20p10d2f1g) / [11s7p4d2f1g]      {(11)4111111111/(10)
511111/7111/11/1}
*
11 s
10629044.264    0.59322104325E-05
1591918.2739    0.46118980689E-04
362333.98437    0.24244612378E-03
102643.11141    0.10231422748E-02
33489.846668    0.37121984175E-02
12091.247190    0.11978107933E-01

```

4716.1908789	0.34682692842E-01
1956.1598080	0.89068331264E-01
853.08595848	0.19330124567
387.96633666	0.32071144956
182.85156613	0.32996797574
4 s	
3240.4086421	0.65905194070E-02
1000.4631935	0.68439609656E-01
383.37301682	0.34495478668
166.03929698	0.82315542085
1 s	
87.919906994	1.0000000000
1 s	
35.675840068	1.0000000000
1 s	
17.543657842	1.0000000000
1 s	
8.4473660433	1.0000000000
1 s	
3.9666180616	1.0000000000
1 s	
1.8356815987	1.0000000000
1 s	
0.59084778776	1.0000000000
1 s	
0.28863218421	1.0000000000
1 s	
0.12153380537	1.0000000000
10 p	
26566.476579	0.62073657410E-04
6290.5088566	0.55131636217E-03
2043.3178410	0.31680110980E-02
781.67221007	0.13816597290E-01
331.51078945	0.48018539681E-01
151.09198667	0.13162015183
72.395278166	0.26860052203
35.869510844	0.36827391093
18.139906191	0.27108612944
9.0466688944	0.76215338633E-01
5 p	
253.71822146	-0.13729169381E-02
97.250818058	-0.10393811185E-01
42.034897960	-0.32204214612E-01
9.9685673555	0.24224770086
4.9395854745	0.53557868398
1 p	
2.4382845475	1.0000000000
1 p	
1.1800000000	1.0000000000
1 p	
0.51047564965	1.0000000000
1 p	
0.21215851928	1.0000000000
1 p	
0.83943604990E-01	1.0000000000
7 d	
601.44434484	0.62783723765E-03
180.85718640	0.57205157153E-02
69.986806340	0.29002521527E-01
30.324710300	0.96446989766E-01

14.027909238	0.22065825870
6.6511702082	0.33657642375
3.1354168338	0.34872040582
1 d	
1.4393591843	0.20984536473
1 d	
0.59350441438	1.0000000000
1 d	
0.23000000000	1.0000000000
1 f	
0.34070000000	1.0000000000
1 f	
0.82570000000	1.0000000000
1 g	
0.64910000000	1.0000000000
*	
*	
kr def2-QZVP	
# kr (24s20p10d2f1g) / [11s7p4d2f1g]	{(11)4111111111/(10)}
511111/7111/11/1}	
*	
11 s	
11713823.008	0.56915790360E-05
1755253.3979	0.44214471278E-04
399717.41924	0.23227813842E-03
113285.79260	0.97973661050E-03
36977.205293	0.35537627541E-02
13355.036580	0.11468673282E-01
5210.9012988	0.33241627469E-01
2162.1137020	0.85620725674E-01
943.29291023	0.18708766876
429.20724331	0.31497583326
202.40720840	0.33406191042
4 s	
3260.4985521	0.73091509287E-02
1011.1069716	0.74040355445E-01
392.44359273	0.35414962222
173.21702132	0.80188286115
1 s	
96.619988467	1.0000000000
1 s	
38.158284867	1.0000000000
1 s	
18.959517570	1.0000000000
1 s	
9.2505996199	1.0000000000
1 s	
4.3486517621	1.0000000000
1 s	
2.0380324209	1.0000000000
1 s	
0.69110152540	1.0000000000
1 s	
0.33506065143	1.0000000000
1 s	
0.14074441124	1.0000000000
10 p	
28609.335767	0.60526369543E-04
6773.1236364	0.53786288403E-03
2199.8011079	0.30935356550E-02

841.50201590	0.13514318412E-01
356.92110288	0.47090086910E-01
162.71174351	0.12960370449
78.004264994	0.26607435646
38.682579997	0.36775851233
19.589158685	0.27406903542
9.7990863417	0.78773352304E-01
5 p	
261.37786869	-0.16397212361E-02
100.09932146	-0.12034797573E-01
44.012139363	-0.34891485263E-01
10.854010739	0.25212650561
5.4351930182	0.57400781830
1 p	
2.7062805542	1.0000000000
1 p	
1.3195633408	1.0000000000
1 p	
0.58004455967	1.0000000000
1 p	
0.24329976264	1.0000000000
1 p	
0.96823725087E-01	1.0000000000
7 d	
665.35057386	0.59588702935E-03
200.17995366	0.54594260457E-02
77.545085570	0.27980992479E-01
33.677854345	0.94119165910E-01
15.624928334	0.21825215619
7.4427867423	0.33739971242
3.5336073535	0.35141418853
1 d	
1.6363725142	0.20756718931
1 d	
0.67845684728	1.0000000000
1 d	
0.27000000000	1.0000000000
1 f	
0.41300000000	1.0000000000
1 f	
0.95570000000	1.0000000000
1 g	
0.73950000000	1.0000000000
*	
*	
rb def2-QZVP	
# rb (8s8p5d1f) / [7s5p4d1f] {2111111/41111/2111/1}	
*	
2 s	
7.4744618040	0.26999390986
6.7296180594	-0.42624989529
1 s	
2.7822883445	1.0000000000
1 s	
0.53494544647	1.0000000000
1 s	
0.22522959349	1.0000000000
1 s	
0.50765580412E-01	1.0000000000
1 s	

```

0.26940281781E-01  1.0000000000
  1 s
0.13051395489E-01  1.0000000000
  4 p
  5.9998960731      0.54568549670E-01
  3.2040784712      -0.26447792498
0.86991979950      0.50033505958
0.44104169728      0.75243449327
  1 p
0.22139898232      1.0000000000
  1 p
0.10679039696      1.0000000000
  1 p
0.33292658822E-01  1.0000000000
  1 p
0.12847003750E-01  1.0000000000
  2 d
  4.6530655240      -0.11653388661E-02
0.44914033653      0.15584297068
  1 d
0.10089577190      0.48262396029
  1 d
0.27432280711E-01  1.0000000000
  1 d
0.95353625581E-02  1.0000000000
  1 f
0.85245000000      0.00000000000
*
rb def2-ecp
*
  ncore =      28          lmax =      3
#      coefficient      r^n          exponent
f
      -12.3169000      2          3.8431140
s-f
      89.5001980      2          5.0365510
      0.4937610      2          1.9708490
      12.3169000      2          3.8431140
p-f
      58.5689740      2          4.2583410
      0.4317910      2          1.4707090
      12.3169000      2          3.8431140
d-f
      26.2248980      2          3.0231270
      0.9628390      2          0.6503830
      12.3169000      2          3.8431140
*
*
sr def2-QZVP
# sr      (8s8p5d1f) / [7s5p4d1f]      {2111111/41111/2111/1}
*
  2 s
  11.000000000      -0.26157031021
  9.90000000000      0.36446668395
  1 s
  2.8771178206      1.0000000000
  1 s
0.63364987829      1.0000000000
  1 s
0.28588739731      1.0000000000

```

```

1 s
0.61938540840E-01 1.0000000000
1 s
0.31237518881E-01 1.0000000000
1 s
0.16266139051E-01 1.0000000000
4 p
7.6233499793 0.71548409039E-01
3.6643075442 -0.44232262175
0.97809648234 0.55690782709
0.77815253363 0.63437348922
1 p
0.40666316828 1.0000000000
1 p
0.18725455934 1.0000000000
1 p
0.56304594427E-01 1.0000000000
1 p
0.21826701680E-01 1.0000000000
2 d
4.3003648126 -0.43567751655E-02
0.84876551534 0.13176477946
1 d
0.29200562252 0.27410245307
1 d
0.94733990946E-01 1.0000000000
1 d
0.30479894317E-01 1.0000000000
1 f
0.99540000000 0.0000000000
*
sr def2-ecp
*
ncore = 28 lmax = 3
# coefficient r^n exponent
f -15.8059920 2 4.6339750
s-f 135.4794300 2 7.4000740
17.5344630 2 3.6063790
15.8059920 2 4.6339750
p-f 88.3597090 2 6.4848680
15.3943720 2 3.2880530
15.8059920 2 4.6339750
d-f 29.8889870 2 4.6228410
6.6594140 2 2.2469040
15.8059920 2 4.6339750
*
*
y def2-QZVP
# y (8s8p7d3f1g) / [7s5p4d3f1g] {2111111/41111/4111/111/1}
*
2 s
12.000000000 -0.27445870024
10.800000000 0.37995468727
1 s
3.1007372195 1.0000000000
1 s

```

0.74155427570	1.0000000000
1 s	
0.34176775775	1.0000000000
1 s	
0.79428797018E-01	1.0000000000
1 s	
0.43308336524E-01	1.0000000000
1 s	
0.21593224872E-01	1.0000000000
4 p	
8.0336135138	0.73041700172E-01
4.0181723477	-0.41610436192
1.1052105890	0.55451897342
0.83219316692	0.62307196069
1 p	
0.44762676666	1.0000000000
1 p	
0.20523347112	1.0000000000
1 p	
0.55045561759E-01	1.0000000000
1 p	
0.22603027453E-01	1.0000000000
4 d	
13.755105347	0.23830583863E-02
3.9629908552	-0.25068021047E-01
1.3427449755	0.22348991872
0.62579248108	0.55237929771
1 d	
0.27632363958	1.0000000000
1 d	
0.11706987754	1.0000000000
1 d	
0.46601501035E-01	1.0000000000
1 f	
0.76291000000	1.0000000000
1 f	
0.26515000000	1.0000000000
1 f	
0.92150000000E-01	1.0000000000
1 g	
0.11149000000	1.0000000000

*

y def2-ecp

*

#	ncore = 28	lmax = 3	exponent
f	coefficient	r^n	
	-19.1221981	2	6.5842120
	-2.4363754	2	3.2921060
s-f	135.1538441	2	7.4880494
	15.5524413	2	3.7440247
	19.1221981	2	6.5842120
	2.4363754	2	3.2921060
p-f	87.7849917	2	6.4453772
	11.5640660	2	3.2226886
	19.1221981	2	6.5842120
	2.4363754	2	3.2921060
d-f			

29.7010007	2	4.6584472
5.5399685	2	2.3292236
19.1221981	2	6.5842120
2.4363754	2	3.2921060

*
*

zr def2-QZVP

zr (8s8p7d3f1g) / [7s5p4d3f1g] {2111111/41111/4111/111/1}

*

2 s		
13.000000000	0.30219052022	
11.750000000	-0.41145056914	
1 s		
3.3679085035	1.0000000000	
1 s		
0.83813257389	1.0000000000	
1 s		
0.39094081796	1.0000000000	
1 s		
0.12165103956	1.0000000000	
1 s		
0.68995924030E-01	1.0000000000	
1 s		
0.28131941438E-01	1.0000000000	
4 p		
8.6639962104	0.73773984271E-01	
4.4109566148	-0.40022747074	
1.2360133871	0.54947233625	
0.87445820593	0.61937721413	
1 p		
0.47713887642	1.0000000000	
1 p		
0.21764845261	1.0000000000	
1 p		
0.57837163627E-01	1.0000000000	
1 p		
0.20242456645E-01	1.0000000000	
4 d		
14.106535710	0.29285547494E-02	
5.0597471810	-0.19680100129E-01	
1.4340490314	0.24763912308	
0.65933129072	0.53572735030	
1 d		
0.28894952351	1.0000000000	
1 d		
0.12160731860	1.0000000000	
1 d		
0.48470078407E-01	1.0000000000	
1 f		
1.1417100000	1.0000000000	
1 f		
0.3926100000	1.0000000000	
1 f		
0.1350100000	1.0000000000	
1 g		
0.28989000000	1.0000000000	

*

zr def2-ecp

*

ncore = 28 lmax = 3

#	coefficient	r^n	exponent
f	-21.0937760	2	7.5400000
	-3.0806943	2	3.7700000
s-f	150.2675911	2	8.2000000
	18.9762165	2	4.0897278
	21.0937760	2	7.5400000
	3.0806943	2	3.7700000
p-f	99.6221237	2	7.1100000
	14.1687333	2	3.5967980
	21.0937760	2	7.5400000
	3.0806943	2	3.7700000
d-f	35.0451235	2	5.3500000
	6.1112595	2	2.4918215
	21.0937760	2	7.5400000
	3.0806943	2	3.7700000
*			
*			
nb def2-QZVP			
# nb	(8s8p7d3f1g) / [7s5p4d3f1g]		{21111111/41111/4111/111/1}
*			
2 s	13.500000000	-0.32410606901	
	12.200000000	0.44773333772	
1 s	3.7169274051	1.0000000000	
1 s	0.90652488058	1.0000000000	
1 s	0.41577606051	1.0000000000	
1 s	0.11042511303	1.0000000000	
1 s	0.62821821279E-01	1.0000000000	
1 s	0.28016289999E-01	1.0000000000	
4 p	9.3098091725	0.73705483583E-01	
	4.8178682975	-0.38234456657	
	1.3632838380	0.54987821838	
	0.90647526151	0.61931035808	
1 p	0.50089563075	1.0000000000	
1 p	0.22793279437	1.0000000000	
1 p	0.60000000000E-01	1.0000000000	
1 p	0.20600000000E-01	1.0000000000	
4 d	17.364404474	0.26413526976E-02	
	5.3680385855	-0.20806369564E-01	
	1.6586089067	0.24555637053	
	0.78121461396	0.53651499644	
1 d	0.34874234803	1.0000000000	
1 d			

```

0.14844540532      1.0000000000
  1 d
0.59334919015E-01  1.0000000000
  1 f
1.5360500000      1.0000000000
  1 f
0.5227000000      1.0000000000
  1 f
0.1778700000      1.0000000000
  1 g
0.4682900000      1.0000000000
*
nb def2-ecp
*
  ncore =      28      lmax =      3
#      coefficient  r^n      exponent
f      -22.9295500   2      8.4900000
      -3.6663099   2      4.2500000
s-f    165.1791435   2      8.9000000
      21.9929744   2      4.4300000
      22.9295500   2      8.4900000
      3.6663099   2      4.2500000
p-f    111.7944145   2      7.7700000
      16.6334833   2      3.9600000
      22.9295500   2      8.4900000
      3.6663099   2      4.2500000
d-f    38.1122488   2      6.0500000
      8.0391673   2      2.8400000
      22.9295500   2      8.4900000
      3.6663099   2      4.2500000
*
*
mo def2-QZVP
# mo      (9s8p7d3f1g) / [7s5p4d3f1g]      {3111111/41111/4111/111/1}
*
  3 s
15.000000000      0.57082903143E-01
13.500000000      -0.66824799324
12.571764111      0.75521146249
  1 s
4.1304342348      1.0000000000
  1 s
0.96478113331      1.0000000000
  1 s
0.43736648981      1.0000000000
  1 s
0.11318605514      1.0000000000
  1 s
0.57579423658E-01  1.0000000000
  1 s
0.27018151462E-01  1.0000000000
  4 p
9.1087343439      0.10192125262
5.3495476626      -0.38460279534
1.4870196599      0.53457134734
0.90585473836      0.61724117143

```

```

1 p
0.50141240214      1.0000000000
1 p
0.23286318145      1.0000000000
1 p
0.620000000000E-01  1.0000000000
1 p
0.210000000000E-01  1.0000000000
4 d
17.215377137      0.30147475909E-02
5.8496916871      -0.28923836319E-01
1.8232967249      0.25398642015
0.86970233105      0.52725603860
1 d
0.39461697588      1.0000000000
1 d
0.17084141240      1.0000000000
1 d
0.69272819629E-01  1.0000000000
1 f
1.9462500000      1.0000000000
1 f
0.65545000000      1.0000000000
1 f
0.22074000000      1.0000000000
1 g
0.64670000000      1.0000000000
*
mo def2-ecp
*
ncore = 28          lmax = 3
# coefficient      r^n      exponent
f
-24.8051771      2          9.4500000
-4.1537815      2          4.7200000
s-f
180.1031085      2          9.7145938
24.9972279      2          4.6805004
24.8051771      2          9.4500000
4.1537815      2          4.7200000
p-f
123.7727523      2          8.1421366
19.5302280      2          4.6259863
24.8051771      2          9.4500000
4.1537815      2          4.7200000
d-f
48.3750223      2          6.6184148
8.8920527      2          3.2487516
24.8051771      2          9.4500000
4.1537815      2          4.7200000
*
*
tc def2-QZVP
# tc      (9s8p7d3f1g) / [7s5p4d3f1g]      {3111111/41111/4111/111/1}
*
3 s
15.000000000      -0.31349221639
13.500000000      0.44793618799
7.1022525122      0.20051786822E-01
1 s

```


4.4415995038	1.0000000000
1 s	
1.0660127848	1.0000000000
1 s	
0.48568559673	1.0000000000
1 s	
0.12654965451	1.0000000000
1 s	
0.66997954399E-01	1.0000000000
1 s	
0.29822104753E-01	1.0000000000
4 p	
10.298029968	0.83867175334E-01
5.7213792785	-0.36246957884
1.6296063991	0.53649463822
0.97528623230	0.61837212480
1 p	
0.53997625690	1.0000000000
1 p	
0.25172025379	1.0000000000
1 p	
0.64000000000E-01	1.0000000000
1 p	
0.21500000000E-01	1.0000000000
4 d	
18.617708386	0.27056783609E-02
5.8369803972	-0.35968645824E-01
2.0921979438	0.21334851537
1.0148117201	0.45713971996
1 d	
0.46154215497	1.0000000000
1 d	
0.19795071041	1.0000000000
1 d	
0.78619872304E-01	1.0000000000
1 f	
2.3724000000	1.0000000000
1 f	
0.79080000000	1.0000000000
1 f	
0.26360000000	1.0000000000
1 g	
0.82510000000	1.0000000000

*

tc def2-ecp

*

#	ncore = 28	coefficient	r^n	lmax = 3	exponent
f		-26.5624475	2		10.4000000
		-4.5856805	2		5.2000000
s-f		195.1591659	2		10.4223462
		28.0926033	2		5.0365160
		26.5624475	2		10.4000000
		4.5856805	2		5.2000000
p-f		135.2845662	2		8.9504494
		21.8065043	2		4.8544394
		26.5624475	2		10.4000000

```

          4.5856805      2          5.2000000
d-f      54.3297294      2          6.9456968
          11.1550679      2          3.9705849
          26.5624475      2         10.4000000
          4.5856805      2          5.2000000
*
*
ru def2-QZVP
# ru      (9s8p7d3f1g) / [7s5p4d3f1g]      {3111111/41111/4111/111/1}
*
      3 s
      15.000000000      0.40205707045
      13.500000000     -0.59417167365
      7.2130868530      0.12541032854
      1 s
      4.5405901225      1.00000000000
      1 s
      1.1904973723      1.00000000000
      1 s
      0.54307531590      1.00000000000
      1 s
      0.13700563039      1.00000000000
      1 s
      0.73396375028E-01  1.00000000000
      1 s
      0.31250715458E-01  1.00000000000
      4 p
      11.388100061      0.55871461629E-01
      6.1591005666     -0.25808446847
      1.7320431063      0.42924265341
      1.0194857402      0.43313353048
      1 p
      0.58131419111      1.00000000000
      1 p
      0.27290530268      1.00000000000
      1 p
      0.66000000000E-01  1.00000000000
      1 p
      0.22000000000E-01  1.00000000000
      4 d
      18.598247778      0.31556859652E-02
      6.7883773752     -0.34551060293E-01
      2.2470797667      0.217085666158
      1.0884195428      0.42834135307
      1 d
      0.49787892886      1.00000000000
      1 d
      0.21481968266      1.00000000000
      1 d
      0.85666751170E-01  1.00000000000
      1 f
      2.8246600000      1.00000000000
      1 f
      0.94314000000      1.00000000000
      1 f
      0.31491000000      1.00000000000
      1 g
      1.00930000000      1.00000000000
*

```

ru def2-ecp

```
*
# ncore = 28          lmax = 3
# coefficient      r^n      exponent
f      -28.3406163    2          11.3600000
      -4.9446292     2          5.6800000
s-f    209.8229712    2          11.1052693
      30.6547264     2          5.4147454
      28.3406163     2          11.3600000
      4.9446292     2          5.6800000
p-f    146.3361823    2          9.7712707
      24.1278772     2          5.0739908
      28.3406163     2          11.3600000
      4.9446292     2          5.6800000
d-f    67.5158967     2          7.6714231
      9.8701041     2          4.1365647
      28.3406163     2          11.3600000
      4.9446292     2          5.6800000
```

*
*

rh def2-QZVP

```
# rh      (9s8p7d3f1g) / [7s5p4d3f1g]      {31111111/41111/4111/111/1}
```

*

```
3 s
15.000000000    0.50258059140
13.500000000    -0.76433277918
7.4051116103   0.31145290674
1 s
4.5131696431   1.00000000000
1 s
1.3235977422   1.00000000000
1 s
0.60954144541   1.00000000000
1 s
0.18907192773   1.00000000000
1 s
0.89080450794E-01  1.00000000000
1 s
0.34131567514E-01  1.00000000000
4 p
11.839425278    0.59787418531E-01
6.6953652636    -0.24743454054
1.8333616287    0.42987003231
1.0267931770    0.42547313311
1 p
0.58071767020    1.00000000000
1 p
0.27907753269    1.00000000000
1 p
0.67108954625E-01  1.00000000000
1 p
0.22101542156E-01  1.00000000000
4 d
26.341167176    0.20623159685E-02
7.8709462705    -0.17239329053E-01
2.5989970939    0.17284839402
```

```

1.2613435752      0.36282102279
 1 d
0.57578407979    1.00000000000
 1 d
0.24725174897    1.00000000000
 1 d
0.97531210324E-01 1.00000000000
 1 f
 3.2739100000    1.00000000000
 1 f
 1.0949900000    1.00000000000
 1 f
0.36623000000    1.00000000000
 1 g
 1.1935000000    1.00000000000
*
rh def2-ecp
*
  ncore =      28      lmax =      3
#      coefficient  r^n      exponent
f
      -30.0934557    2      12.3100000
      -5.2184819    2      6.1600000
s-f
      225.3477535    2      11.7200000
      32.8231890    2      5.8200000
      30.0934557    2      12.3100000
      5.2184819    2      6.1600000
p-f
      158.7094116    2      10.4200000
      26.4441005    2      5.4500000
      30.0934557    2      12.3100000
      5.2184819    2      6.1600000
d-f
      62.7586257    2      8.8200000
      10.9787195    2      3.8700000
      30.0934557    2      12.3100000
      5.2184819    2      6.1600000
*
*
pd def2-QZVP
# pd      (9s8p7d3f1g) / [7s5p4d3f1g]      {3111111/41111/4111/111/1}
*
  3 s
15.262399331      0.44145727454
13.721983176      -0.70293005979
 4.8448286268      0.36095390108
 1 s
 8.7309326588      1.00000000000
 1 s
 1.4357564094      1.00000000000
 1 s
0.66088433720      1.00000000000
 1 s
0.20897212790      1.00000000000
 1 s
0.91936735872E-01 1.00000000000
 1 s
0.34733479706E-01 1.00000000000
 4 p

```

```

12.585237008      0.60002003747E-01
7.2058104839     -0.24022183118
1.9558705640      0.43424940067
1.0534418618      0.42084436088
  1 p
0.59809389552      1.00000000000
  1 p
0.30362411297      1.00000000000
  1 p
0.880000000000E-01  1.00000000000
  1 p
0.300000000000E-01  1.00000000000
  4 d
28.840985892      0.21131470308E-02
8.4584163440     -0.17913194955E-01
2.8648941754      0.17165507663
1.3966488847      0.36149251150
  1 d
0.63921677230      1.00000000000
  1 d
0.27502319836      1.00000000000
  1 d
0.10829940074      1.00000000000
  1 f
3.72000000000      1.00000000000
  1 f
1.24629000000      1.00000000000
  1 f
0.41754000000      1.00000000000
  1 g
1.37770000000      1.00000000000
*
pd def2-ecp
*
  ncore =      28          lmax =      3
# coefficient  r^n      exponent
f
  -31.9295543    2      13.2700000
  -5.3982169    2      6.6300000
s-f
  240.2290403    2      12.4300000
  35.1719435    2      6.1707594
  31.9295543    2      13.2700000
  5.3982169    2      6.6300000
p-f
  170.4172760    2      11.0800000
  28.4721329    2      5.8295541
  31.9295543    2      13.2700000
  5.3982169    2      6.6300000
d-f
  69.0138449    2      9.5100000
  11.7508616    2      4.1397811
  31.9295543    2      13.2700000
  5.3982169    2      6.6300000
*
*
ag def2-QZVP
# ag (10s8p7d3f1g) / [7s5p4d3f1g] {4111111/41111/4111/111/1}
*
  4 s

```

256.50898381	0.73215128094E-03
19.000000000	-0.14706983774
14.129749737	0.47914881797
9.4840599768	-0.26930801705
1 s	
5.5812682897	1.0000000000
1 s	
1.4763753299	1.0000000000
1 s	
0.66184584335	1.0000000000
1 s	
0.15382171742	1.0000000000
1 s	
0.79534248689E-01	1.0000000000
1 s	
0.32408624506E-01	1.0000000000
4 p	
13.350389537	0.62479151672E-01
7.7163302467	-0.24398688175
2.0864535219	0.45439758415
1.0577805733	0.47607485340
1 p	
0.52564427657	1.0000000000
1 p	
0.23694908895	1.0000000000
1 p	
0.66457980332E-01	1.0000000000
1 p	
0.21864839286E-01	1.0000000000
4 d	
32.147961274	0.34564677092E-02
9.0323725307	-0.28135297216E-01
3.1673540854	0.26999486025
1.5519381135	0.57666767772
1 d	
0.71310284000	1.0000000000
1 d	
0.30749741551	1.0000000000
1 d	
0.12094304210	1.0000000000
1 f	
4.1631100000	1.0000000000
1 f	
1.3971100000	1.0000000000
1 f	
0.46886000000	1.0000000000
1 g	
1.5619000000	1.0000000000
*	
ag def2-ecp	
*	
ncore = 28	lmax = 3
# coefficient r^n	exponent
f	
-33.6899201	2 14.2200000
-5.5311202	2 7.1100000
s-f	
255.1393645	2 13.1300000
36.8661215	2 6.5100000
33.6899201	2 14.2200000

	5.5311202	2	7.1100000
p-f	182.1818687	2	11.7400000
	30.3577515	2	6.2000000
	33.6899201	2	14.2200000
	5.5311202	2	7.1100000
d-f	73.7192609	2	10.2100000
	12.5021171	2	4.3800000
	33.6899201	2	14.2200000
	5.5311202	2	7.1100000

*
*

```
cd def2-QZVP
# cd (10s8p7d3f1g) / [7s5p4d3f1g] {4111111/41111/4111/111/1}
```

*

```
4 s
269.30016289 0.62688949336E-03
18.554269093 -0.43456616075
16.729943183 0.66043072415
11.768546646 -0.11793513277
1 s
6.1816604427 1.0000000000
1 s
1.5775743989 1.0000000000
1 s
0.71857981187 1.0000000000
1 s
0.16433138409 1.0000000000
1 s
0.76794158768E-01 1.0000000000
1 s
0.34377199848E-01 1.0000000000
4 p
14.107678180 0.70307291426E-01
8.2750040714 -0.26474818030
2.2507338323 0.47494851120
1.1914970238 0.46327020832
1 p
0.66041257699 1.0000000000
1 p
0.33804403770 1.0000000000
1 p
0.96004037879E-01 1.0000000000
1 p
0.33681030012E-01 1.0000000000
4 d
35.689192548 0.44455913982E-02
9.3407971610 -0.39185351747E-01
3.5922659140 0.31235972097
1.7980676976 0.71163739606
1 d
0.84830057791 1.0000000000
1 d
0.37846492753 1.0000000000
1 d
0.15420101631 1.0000000000
1 f
4.7689900000 1.0000000000
1 f
```

```

1.5981300000      1.0000000000
 1 f
0.5355500000      1.0000000000
 1 g
1.7896000000      1.0000000000
*
cd def2-ecp
*
  ncore =    28      lmax =    3
#      coefficient   r^n      exponent
f
      -35.4766256    2      15.1847957
      -5.6176768    2      7.5923978
s-f
      270.0094832    2      13.8358689
      38.7673080     2      6.8572704
      35.4766256     2      15.1847957
      5.6176768      2      7.5923978
p-f
      193.8296294    2      12.4049710
      31.8965252     2      6.5677995
      35.4766256     2      15.1847957
      5.6176768      2      7.5923978
d-f
      79.1936470     2      10.8969253
      13.2308267     2      4.6411649
      35.4766256     2      15.1847957
      5.6176768      2      7.5923978
*
*
in def2-QZVP
# in      (17s14p11d4f1g) / [7s6p4d4f1g]      {9131111/731111/8111/1111/1}
*
  9 s
8931.8400000      0.190000000000E-04
1352.2200000      0.131000000000E-03
303.393000000     0.478000000000E-03
45.122900000     0.117080000000E-01
28.182200000     -0.873300000000E-01
17.604800000     0.259577000000
6.94058000000   -0.628471000000
4.33377000000   -0.158718000000
1.98684000000   0.674404000000
 1 s
1.0438672413     1.000000000000
 3 s
20.245544208     0.29650296199E-01
11.072298416    -0.14745372687
2.4929238916    0.53232061960
 1 s
0.532444484157     1.000000000000
 1 s
0.21211307407     1.000000000000
 1 s
0.95475196519E-01  1.000000000000
 1 s
0.42357644919E-01  1.000000000000
 7 p
129.23300000     0.279000000000E-03
29.628400000    -0.617100000000E-02

```


18.521100000	0.46912000000E-01
8.2853600000	-0.23990400000
2.4993900000	0.42981100000
1.3221600000	0.48610100000
0.68870700000	0.22203700000
3 p	
13.248633034	-0.18203004609E-01
3.0240161259	0.31476939453
1.0805448379	0.71919648136
1 p	
0.33353581509	1.0000000000
1 p	
0.15403760449	1.0000000000
1 p	
0.65770424632E-01	1.0000000000
1 p	
0.27642180293E-01	1.0000000000
8 d	
131.81131820	0.22281463414E-03
37.030875816	0.19331306797E-02
11.378665218	-0.17870304080E-01
6.4488212086	0.22953424346E-01
3.4878752216	0.17536747821
1.9912337572	0.29288830616
1.1306610212	0.31018960851
0.63074842914	0.24247651565
1 d	
0.33856463907	1.0000000000
1 d	
0.17026198815	1.0000000000
1 d	
0.69200000000E-01	1.0000000000
1 f	
0.39210000000	1.0000000000
1 f	
0.15600000000	1.0000000000
1 f	
1.3983200000	1.0000000000
1 f	
4.1949600000	1.0000000000
1 g	
0.34190000000	1.0000000000

*

in def2-ecp

*

#	ncore = 28	lmax = 3	coefficient	r^n	exponent
f			-13.7280780	2	12.5390560
			-18.2068660	2	12.5525610
s-f			281.1223500	2	15.3928220
			61.9014700	2	8.0558640
			13.7280780	2	12.5390560
			18.2068660	2	12.5525610
p-f			67.4621540	2	13.9286720
			134.9492500	2	13.3472340
			14.7461400	2	7.6141320
			29.6392620	2	7.3183650

	13.7280780	2	12.5390560
	18.2068660	2	12.5525610
d-f	35.4932540	2	14.0347150
	53.1787730	2	14.5116160
	9.1772810	2	5.5505500
	12.3924100	2	5.0594150
	13.7280780	2	12.5390560
	18.2068660	2	12.5525610

*

*

sn def2-QZVP

sn (17s14p11d4f1g) / [7s6p4d4f1g] {9131111/731111/8111/1111/1}

*

9 s		
11606.900000	0.290000000000E-04	
1754.8000000	0.206000000000E-03	
397.17800000	0.807000000000E-03	
90.299000000	0.247100000000E-02	
31.489000000	-0.400250000000E-01	
19.668500000	0.16315200000	
7.0675900000	-0.55698300000	
4.4149000000	-0.16993200000	
2.1635600000	0.65102800000	
1 s		
1.1440977736	1.0000000000	
3 s		
20.197961274	0.22393937317E-01	
10.880108426	-0.14330764814	
2.7745387028	0.53278527074	
1 s		
0.58550056279	1.0000000000	
1 s		
0.25317089836	1.0000000000	
1 s		
0.11599461634	1.0000000000	
1 s		
0.52233584109E-01	1.0000000000	
7 p		
195.49500000	0.258000000000E-03	
18.256300000	0.443410000000E-01	
11.409400000	-0.10914200000	
6.9056700000	-0.13860600000	
2.9820600000	0.34374300000	
1.6084300000	0.51827100000	
0.83176700000	0.27870600000	
3 p		
13.304065745	-0.20694775410E-01	
3.4193503621	0.33654593033	
1.2382899573	0.71397757129	
1 p		
0.39265300321	1.0000000000	
1 p		
0.19313059747	1.0000000000	
1 p		
0.86443518729E-01	1.0000000000	
1 p		
0.37350684674E-01	1.0000000000	
8 d		
143.82134199	0.26165602862E-03	

```

41.039940764      0.21562117321E-02
11.508999207     -0.24771286642E-01
8.4312612820     0.29022163379E-01
4.0180001346     0.16171344601
2.3122021836     0.29213521578
1.3168562511     0.32241037254
0.73729126651    0.24629433031
  1 d
0.40109472811    1.00000000000
  1 d
0.20593354535    1.00000000000
  1 d
0.86600000000E-01 1.00000000000
  1 f
0.43150000000    1.00000000000
  1 f
0.17720000000    1.00000000000
  1 f
1.59154000000    1.00000000000
  1 f
4.7988893935     1.00000000000
  1 g
0.37740000000    1.00000000000
*
sn def2-ecp
*
  ncore =    28      lmax =    3
#      coefficient  r^n      exponent
f
      -12.5763330   2        12.2823480
      -16.5959440   2        12.2721500
s-f
      279.9886820   2        17.4204140
      62.3778100   2        7.6311550
      12.5763330   2        12.2823480
      16.5959440   2        12.2721500
p-f
      66.1625230   2        16.1310240
      132.1743960   2        15.6280770
      16.3394170   2        7.3256080
      32.4889590   2        6.9425190
      12.5763330   2        12.2823480
      16.5959440   2        12.2721500
d-f
      36.3874410   2        15.5149760
      54.5078410   2        15.1881600
      8.6968230    2        5.4560240
      12.8402080   2        5.3631050
      12.5763330   2        12.2823480
      16.5959440   2        12.2721500
*
*
sb def2-QZVP
# sb      (17s14p11d4f1g) / [7s6p4d4f1g]      {9131111/731111/8111/1111/1}
*
  9 s
12339.316555     0.38545231046E-04
1854.7043271     0.27702166404E-03
418.44441772     0.11161923778E-02
96.965111109     0.28828055377E-02

```

28.537960267	-0.60556405021E-01
17.862907144	0.27988835315
8.4541754812	-0.54748479396
5.2813981306	-0.30336289748
2.3194618632	0.68093278701
1 s	
1.2167512076	1.0000000000
3 s	
25.336266601	0.22414355064E-01
12.477043309	-0.14737811818
3.0723142741	0.53278468779
1 s	
0.60174774699	1.0000000000
1 s	
0.28323936354	1.0000000000
1 s	
0.13221765728	1.0000000000
1 s	
0.60986718951E-01	1.0000000000
7 p	
162.89300000	0.37500000000E-03
30.399600000	-0.47980000000E-02
19.000400000	0.54731000000E-01
9.3225600000	-0.25528400000
3.0166800000	0.34537700000
1.8621900000	0.40483300000
1.1033100000	0.32592200000
3 p	
12.665326113	-0.20694788562E-01
3.3473442879	0.26878411014
1.1722158971	0.72590523998
1 p	
0.58886745483	1.0000000000
1 p	
0.25014249608	1.0000000000
1 p	
0.11120161090	1.0000000000
1 p	
0.48206685448E-01	1.0000000000
8 d	
142.61790051	0.34691704136E-03
40.920334292	0.27417583490E-02
10.854520545	-0.33847404142E-01
8.3926457719	0.42753986065E-01
4.1806878019	0.16545099365
2.5346474124	0.26821979719
1.5175455555	0.31482077294
0.86799625994	0.25485913704
1 d	
0.47323070711	1.0000000000
1 d	
0.24111763234	1.0000000000
1 d	
0.10080000000	1.0000000000
1 f	
0.48490000000	1.0000000000
1 f	
0.20490000000	1.0000000000
1 f	
1.7880600000	1.0000000000

```

1 f
5.6265581363      1.0000000000
1 g
0.42340000000    1.0000000000
*
sb def2-ecp
*
ncore =      28      lmax =      3
#      coefficient  r^n      exponent
f
      -15.3668010    2      14.4449780
      -20.2961380    2      14.4492950
s-f
      281.0715810    2      16.3308650
      61.7166040    2      8.5565420
      15.3668010    2      14.4449780
      20.2961380    2      14.4492950
p-f
      67.4573800    2      14.4703370
      134.9335030    2      13.8161940
      14.7163440    2      8.4249240
      29.5185120    2      8.0927280
      15.3668010    2      14.4449780
      20.2961380    2      14.4492950
d-f
      35.4478150    2      14.8863310
      53.1434660    2      15.1463190
      9.1792230     2      5.9082670
      13.2402530    2      5.5943220
      15.3668010    2      14.4449780
      20.2961380    2      14.4492950
*
*
te def2-QZVP
# te      (17s14p11d4f1g) / [7s6p4d4f1g]      {9131111/731111/8111/1111/1}
*
9 s
15746.300000      0.540000000000E-04
2369.2500000      0.398000000000E-03
535.86000000      0.166200000000E-02
141.88500000      0.363600000000E-02
27.819700000      -0.584270000000E-01
17.387900000      0.366520000000
10.865600000      -0.397589000000
6.5688500000      -0.519175000000
2.4013900000      0.687652000000
1 s
1.2865441585      1.0000000000
3 s
29.383253023      0.30079778033E-01
15.946408003      -0.13631630929
3.6679902632      0.53467574034
1 s
0.63533594694      1.0000000000
1 s
0.29807786206      1.0000000000
1 s
0.14061248688      1.0000000000
1 s
0.65660655893E-01  1.0000000000

```

```

7 p
750.22200000      0.520000000000E-04
163.96100000      0.410000000000E-03
16.922700000      0.833870000000E-01
10.575500000      -0.26821200000
5.7046200000      -0.229320000000E-01
2.9802200000      0.49554800000
1.5197000000      0.51452200000
3 p
13.925457258      -0.21336842159E-01
4.2323766654      0.22433961554
1.4547630727      0.73198528158
1 p
0.75528783692      1.00000000000
1 p
0.31829451168      1.00000000000
1 p
0.13721830923      1.00000000000
1 p
0.57099171462E-01  1.00000000000
8 d
146.30727119      0.43816018982E-03
42.243859354      0.33559305599E-02
9.9155377745      -0.11157186771
8.9949643607      0.13269569633
4.1376628430      0.21574044755
2.3659339431      0.32583679541
1.3736141857      0.30685918052
0.79846379228      0.19445241192
1 d
0.45685175394      1.00000000000
1 d
0.25022747959      1.00000000000
1 d
0.11560000000      1.00000000000
1 f
0.51840000000      1.00000000000
1 f
0.21350000000      1.00000000000
1 f
1.9347800000      1.00000000000
1 f
5.8043400000      1.00000000000
1 g
0.42940000000      1.00000000000
*
te def2-ecp
*
ncore = 28      lmax = 3
#      coefficient      r^n      exponent
f
      -15.7454500      2      15.2061680
      -20.7424480      2      15.2017020
s-f
      281.0458430      2      16.8144730
      61.6206560      2      8.7935260
      15.7454500      2      15.2061680
      20.7424480      2      15.2017020
p-f
      67.4494640      2      14.8778010

```

	134.9043040	2	14.2697310
	14.6895470	2	8.7244350
	29.4150630	2	8.2915150
	15.7454500	2	15.2061680
	20.7424480	2	15.2017020
d-f			
	35.4320570	2	15.2050080
	53.1356870	2	15.2258480
	9.0698020	2	6.0717690
	13.1223040	2	5.8047600
	15.7454500	2	15.2061680
	20.7424480	2	15.2017020
*			
*			
i	def2-QZVP		
#	i	(17s14p11d4f1g) / [7s6p4d4f1g]	{9131111/731111/8111/1111/1}
*			
	9	s	
	16788.400000	0.410000000000E-04	
	2526.6400000	0.303000000000E-03	
	571.98400000	0.124700000000E-02	
	150.43400000	0.265900000000E-02	
	29.540500000	-0.531900000000E-01	
	18.457100000	0.34009600000	
	11.528600000	-0.35235500000	
	7.0828900000	-0.54138500000	
	2.5040500000	0.71574900000	
	1	s	
	1.3540144781	1.0000000000	
	3	s	
	25.058617933	0.40897754402E-01	
	15.621979372	-0.14269668187	
	3.3536325162	0.52916319279	
	1	s	
	0.67430472704	1.0000000000	
	1	s	
	0.32727136949	1.0000000000	
	1	s	
	0.15749364119	1.0000000000	
	1	s	
	0.74377727841E-01	1.0000000000	
	7	p	
	656.27400000	0.91000000000E-04	
	149.23200000	0.61300000000E-03	
	19.015300000	0.59923000000E-01	
	10.737800000	-0.24925800000	
	6.4420800000	-0.43750000000E-02	
	3.0920300000	0.51399900000	
	1.5787400000	0.50721300000	
	3	p	
	15.660511893	-0.22143803592E-01	
	4.9250669812	0.23518064355	
	1.6692319982	0.73153925548	
	1	p	
	0.77817898176	1.0000000000	
	1	p	
	0.35608843716	1.0000000000	
	1	p	
	0.15493242649	1.0000000000	
	1	p	

```

0.64666212492E-01  1.0000000000
  8 d
318.22407776      0.10951692560E-03
95.810227352     0.91919139268E-03
35.322295259     0.47916935207E-02
13.107447819     -0.16280459996E-01
6.2949152988     0.90889609141E-01
3.6826101201     0.27483543784
2.0858950647     0.36067901632
1.1644342344     0.28384002219
  1 d
0.63180613129    1.0000000000
  1 d
0.32215084697    1.0000000000
  1 d
0.13490000000    1.0000000000
  1 f
0.58780000000    1.0000000000
  1 f
0.25000000000    1.0000000000
  1 f
2.17800000000    1.0000000000
  1 f
6.4253613600     1.0000000000
  1 g
0.47390000000    1.0000000000

```

```

*
i def2-ecp
*

```

```

ncore = 28      lmax = 3
#      coefficient  r^n      exponent
f
      -21.8420400   2      19.4586090
      -28.4681910   2      19.3492600
      -0.2437130    2      4.8237670
      -0.3208040    2      4.8843150
s-f
      49.9942930    2      40.0158350
      281.0253170   2      17.4297470
      61.5733260    2      9.0054840
      21.8420400    2      19.4586090
      28.4681910    2      19.3492600
      0.2437130     2      4.8237670
      0.3208040     2      4.8843150
p-f
      67.4428410    2      15.3554660
      134.8811370   2      14.9718330
      14.6750510    2      8.9601640
      29.3756660    2      8.2590960
      21.8420400    2      19.4586090
      28.4681910    2      19.3492600
      0.2437130     2      4.8237670
      0.3208040     2      4.8843150
d-f
      35.4395290     2      15.0689080
      53.1760570     2      14.5553220
      9.0671950      2      6.7186470
      13.2069370     2      6.4563930
      0.0893350      2      1.1917790
      0.0523800      2      1.2911570

```


21.8420400	2	19.4586090
28.4681910	2	19.3492600
0.2437130	2	4.8237670
0.3208040	2	4.8843150

*
*

xe def2-QZVP

xe (17s14p11d4f1g) / [7s6p4d4f1g] {9131111/731111/8111/1111/1}

*

9 s	
18774.300000	0.680000000000E-04
2824.8100000	0.501000000000E-03
640.08800000	0.209700000000E-02
172.61600000	0.449300000000E-02
29.516900000	-0.471510000000E-01
18.444800000	0.374033000000
11.523800000	-0.512826000000
6.6189000000	-0.478624000000
2.9955200000	0.596471000000
1 s	
1.6532586536	1.000000000000
3 s	
27.052171835	0.11189611954
20.940622415	-0.24055422724
6.0024591071	0.51452076187
1 s	
0.87553889270	1.000000000000
1 s	
0.41033616654	1.000000000000
1 s	
0.19493585779	1.000000000000
1 s	
0.90171093041E-01	1.000000000000
7 p	
613.33100000	0.138000000000E-03
141.71000000	0.853000000000E-03
20.310600000	0.550240000000E-01
11.033100000	-0.252988000000
6.8951300000	0.974600000000E-02
3.2416600000	0.526797000000
1.6653500000	0.501832000000
3 p	
18.388908413	-0.24514446229E-01
6.1139045431	0.25265669670
1.8729815691	0.72938328969
1 p	
0.82004665991	1.000000000000
1 p	
0.39552648254	1.000000000000
1 p	
0.17445509815	1.000000000000
1 p	
0.73389992663E-01	1.000000000000
8 d	
315.66106865	0.14235585191E-03
95.553873651	0.11707875751E-02
35.451236301	0.58783160362E-02
13.153211283	-0.16764226287E-01
6.3847329564	0.11558421625
3.6968166410	0.30375919653

```

2.0976070364      0.36037726827
1.1951246616      0.24813434400
  1 d
0.68431725339      1.00000000000
  1 d
0.37710480204      1.00000000000
  1 d
0.16760000000      1.00000000000
  1 f
0.66190000000      1.00000000000
  1 f
0.29790000000      1.00000000000
  1 f
2.43230000000      1.00000000000
  1 f
7.2077391789      1.00000000000
  1 g
0.52780000000      1.00000000000
*
xe def2-ecp
*
  ncore =      28      lmax =      3
#      coefficient      r^n      exponent
f
      -23.0892950      2      20.8815570
      -30.0744750      2      20.7834430
      -0.2882270      2      5.2533890
      -0.3869240      2      5.3611880
s-f
      49.9979620      2      40.0051840
      281.0133030      2      17.8122140
      61.5382550      2      9.3041500
      23.0892950      2      20.8815570
      30.0744750      2      20.7834430
      0.2882270      2      5.2533890
      0.3869240      2      5.3611880
p-f
      67.4391420      2      15.7017720
      134.8747110      2      15.2586080
      14.6633000      2      9.2921840
      29.3547300      2      8.5590030
      23.0892950      2      20.8815570
      30.0744750      2      20.7834430
      0.2882270      2      5.2533890
      0.3869240      2      5.3611880
d-f
      35.4369080      2      15.1856000
      53.1957720      2      14.2845000
      9.0462320      2      7.1218890
      13.2236810      2      6.9919630
      0.0848530      2      0.6239460
      0.0441550      2      0.6472840
      23.0892950      2      20.8815570
      30.0744750      2      20.7834430
      0.2882270      2      5.2533890
      0.3869240      2      5.3611880
*
*
cs def2-QZVP
# cs      (8s7p5d1f) / [6s5p3d1f]      {311111/31111/311/1}

```

```

*
  3 s
  5.8684829520      0.12906631816
  4.3741038860     -0.34380446158
  1.7951201473      0.69937346606
  1 s
  0.37816941125     1.00000000000
  1 s
  0.16624693130     1.00000000000
  1 s
  0.27763176052E-01  1.00000000000
  1 s
  0.16113005842E-01  1.00000000000
  1 s
  0.10996108743E-01  1.00000000000
  3 p
  4.2749775718      0.45595316685E-01
  1.9639316240     -0.25031125651
  0.47666322385     0.55660114378
  1 p
  0.21736718772     1.00000000000
  1 p
  0.97276293828E-01  1.00000000000
  1 p
  0.26770518041E-01  1.00000000000
  1 p
  0.10845412222E-01  1.00000000000
  3 d
  2.0091044335     -0.34453182058E-02
  0.35778351451     0.22686596025
  0.11070568254     0.47180885981
  1 d
  0.33216214821E-01  1.00000000000
  1 d
  0.11409380652E-01  1.00000000000
  1 f
  0.58777000000     0.00000000000
*
cs def2-ecp
*
  ncore =      46          lmax =      3
#      coefficient      r^n      exponent
f      -28.8843090      2      3.1232690
s-f      84.5477300      2      4.0797500
      16.6541730      2      2.4174060
      28.8843090      2      3.1232690
p-f      157.0490590      2      5.5140800
      26.4233070      2      2.1603160
      28.8843090      2      3.1232690
d-f      13.1727530      2      1.8074100
      3.3428330      2      0.8581820
      28.8843090      2      3.1232690
*
*
ba def2-QZVP
# ba      (8s8p5d1f) / [7s5p3d1f]      {2111111/41111/311/1}

```

```

*
  2 s
  5.7000000000      1.3292982002
  5.2043612469     -1.7367497134
  1 s
  2.1475437282      1.0000000000
  1 s
  0.41033660537     1.0000000000
  1 s
  0.18393532770     1.0000000000
  1 s
  0.72521216545E-01  1.0000000000
  1 s
  0.34526334903E-01  1.0000000000
  1 s
  0.16157891872E-01  1.0000000000
  4 p
  5.6000000000      0.51385026013
  5.1104879274     -0.70529238864
  2.5006544803      0.42822329830
  0.51947995345     -0.57125984472
  1 p
  0.24536994841     1.0000000000
  1 p
  0.11256056700     1.0000000000
  1 p
  0.34917622027E-01  1.0000000000
  1 p
  0.16320065666E-01  1.0000000000
  3 d
  2.7000000000      0.14372069824
  2.3460740881     -0.19565347309
  0.39553542609     0.29963058552
  1 d
  0.12967935859     1.0000000000
  1 d
  0.40463066544E-01  1.0000000000
  1 f
  0.65760000000     0.0000000000

```

```

*
ba def2-ecp
*
ncore =      46          lmax =      3
#      coefficient      r^n      exponent
f      -33.4731740      2          3.5894650
s-f      427.8458160      2          9.5269860
          204.4175300      2          4.4875100
          33.4731740      2          3.5894650
p-f      293.6058640      2          8.3159300
          294.1933160      2          4.2922170
          33.4731740      2          3.5894650
d-f      112.5504020      2          5.9161080
          181.7826210      2          2.8748420
          33.4731740      2          3.5894650

```

```

*
*
```

```

la def2-QZVP
# la      (9s8p6d3f1g) / [7s5p4d3f1g]      {3111111/41111/3111/111/1}
*

```

```

  3 s
26.077272000      0.23198684846E-02
 5.7127838000    -0.29787719611
 4.4057848000    0.70022722515
  1 s
 2.1315325829    1.00000000000
  1 s
0.49385808956    1.00000000000
  1 s
0.23595687888    1.00000000000
  1 s
0.63593489661E-01 1.00000000000
  1 s
0.31545394754E-01 1.00000000000
  1 s
0.15777655296E-01 1.00000000000
  4 p
 6.0000000000    -0.11397960924E-01
 3.6808191615    0.14675038550
 2.3265462081    -0.35581819167
0.64342629633    0.45834955229
  1 p
0.33584281962    1.00000000000
  1 p
0.16519051916    1.00000000000
  1 p
0.56715971797E-01 1.00000000000
  1 p
0.22100824776E-01 1.00000000000
  3 d
 1.2000000000    -0.35803482414
 1.0239524401    0.40483734122
0.37508490282    0.37649639849
  1 d
0.17161940245    1.00000000000
  1 d
0.78780423402E-01 1.00000000000
  1 d
0.35000047794E-01 1.00000000000
  1 f
0.65580000000    1.00000000000
  1 f
0.25683000000    1.00000000000
  1 f
0.10058000000    1.00000000000
  1 g
0.17907000000    1.00000000000
*

```

```

la def2-ecp

```

```

*
  ncore =    46          lmax =    3
#   coefficient   r^n      exponent
f
  -36.0100160     2         4.0286000
s-f
   91.9321770     2         3.3099000
  -3.7887640     2         1.6550000

```

	36.0100160	2	4.0286000
p-f	63.7594860	2	2.8368000
	-0.6479580	2	1.4184000
	36.0100160	2	4.0286000
d-f	36.1161730	2	2.0213000
	0.2191140	2	1.0107000
	36.0100160	2	4.0286000
*			
*			
hf	def2-QZVP		
# hf	(10s8p6d3f1g) / [7s5p4d3f1g]		{41111111/41111/3111/111/1}
*			
	4 s		
	24.000000000	0.19369448644	
	16.000000000	-3.5064630782	
	14.400000000	4.3082581000	
	10.304504667	-0.91045809742	
	1 s		
	3.8372797792	1.0000000000	
	1 s		
	0.94649028050	1.0000000000	
	1 s		
	0.44397931299	1.0000000000	
	1 s		
	0.13656009445	1.0000000000	
	1 s		
	0.66549732509E-01	1.0000000000	
	1 s		
	0.28719110054E-01	1.0000000000	
	4 p		
	17.000000000	-0.30316491880E-01	
	11.738072097	0.10139279686	
	4.9203967161	-0.28227924657	
	1.1251726138	0.52032008501	
	1 p		
	0.54220114055	1.0000000000	
	1 p		
	0.25659447877	1.0000000000	
	1 p		
	0.10000000000	1.0000000000	
	1 p		
	0.41700000000E-01	1.0000000000	
	3 d		
	6.9644775309	0.90606952386E-01	
	5.7275227587	-0.16459899714	
	1.1503305416	0.51375718250	
	1 d		
	0.47559482991	0.97807169690	
	1 d		
	0.18774414759	1.0000000000	
	1 d		
	0.68439488104E-01	1.0000000000	
	1 f		
	0.80387000000	1.0000000000	
	1 f		
	0.31547000000	1.0000000000	
	1 f		
	0.12380000000	1.0000000000	

```

1 g
0.29036000000 1.0000000000
*
hf def2-ecp
*
ncore = 60 lmax = 3
# coefficient r^n exponent
f
10.0467225 2 1.7857698
s-f
1499.2847107 2 14.7699590
40.2821014 2 7.3849794
-10.0467225 2 1.7857698
p-f
397.7330053 2 9.8494895
19.3164059 2 4.9247445
-10.0467225 2 1.7857698
d-f
101.3298053 2 6.0967564
5.8734382 2 3.0483782
-10.0467225 2 1.7857698
*
*
ta def2-QZVP
# ta (10s8p6d3f1g) / [7s5p4d3f1g] {4111111/41111/3111/111/1}
*
4 s
24.473650944 0.20537515818
18.721372549 -0.74477445680
11.500000000 3.4067771001
10.350000000 -2.8222400335
1 s
3.8125414615 1.0000000000
1 s
1.0507430630 1.0000000000
1 s
0.49732275755 1.0000000000
1 s
0.15602650970 1.0000000000
1 s
0.75056442354E-01 1.0000000000
1 s
0.31632668803E-01 1.0000000000
4 p
17.000000000 -0.32577305616E-01
12.008186536 0.10336287365
5.0278760583 -0.28526521696
1.1937124184 0.51790141155
1 p
0.57889707053 1.0000000000
1 p
0.27225198801 1.0000000000
1 p
0.10000000000 1.0000000000
1 p
0.41700000000E-01 1.0000000000
3 d
7.1419762952 0.88606814221E-01
5.7696869171 -0.17156962221
1.2199483941 0.53547693505

```

```

1 d
0.52366034246      1.0000000000
1 d
0.21384808767      1.0000000000
1 d
0.80254256735E-01  1.0000000000
1 f
0.95070000000      1.0000000000
1 f
0.37386000000      1.0000000000
1 f
0.14702000000      1.0000000000
1 g
0.40165000000      1.0000000000
*
ta def2-ecp
*
ncore =      60      lmax =      3
#      coefficient  r^n      exponent
f
      12.0179609      2      2.0178811
s-f
      1345.8806470      2      14.5464077
      36.7668062      2      7.2732038
      -12.0179609      2      2.0178811
p-f
      378.4253015      2      9.9355653
      22.2930909      2      4.9677824
      -12.0179609      2      2.0178811
d-f
      104.8839557      2      6.3473769
      8.7558481      2      3.1736885
      -12.0179609      2      2.0178811
*
*
w def2-QZVP
# w      (10s8p6d3f1g) / [7s5p4d3f1g]      {4111111/41111/3111/111/1}
*
4 s
22.106487883      0.66320504570
18.958062620      -1.5576189160
13.128699049      2.1416485467
10.149417378      -1.1823364947
1 s
4.0160322414      1.0000000000
1 s
1.1234496158      1.0000000000
1 s
0.53500662821      1.0000000000
1 s
0.17127449658      1.0000000000
1 s
0.80452897876E-01  1.0000000000
1 s
0.33669872229E-01  1.0000000000
4 p
17.000000000      -0.37817768433E-01
12.431973432      0.10905673845
5.1586217658      -0.29399955020
1.2801454812      0.51560726697

```



```

1 p
0.62856790898      1.0000000000
1 p
0.29380423553      1.0000000000
1 p
0.10000000000      1.0000000000
1 p
0.41700000000E-01  1.0000000000
3 d
7.4064737315      0.86993963018E-01
5.9026268603      -0.17667540011
1.2984756750      0.55145697030
1 d
0.57153508541      1.0000000000
1 d
0.23845526606      1.0000000000
1 d
0.91144267331E-01  1.0000000000
1 f
1.0962400000      1.0000000000
1 f
0.43199000000      1.0000000000
1 f
0.17023000000      1.0000000000
1 g
0.51293000000      1.0000000000
*
w def2-ecp
*
ncore = 60          lmax = 3
# coefficient      r^n      exponent
f
14.1525795        2          2.2588885
s-f
1192.3958823      2          14.3228564
32.5229332        2          7.1614281
-14.1525795       2          2.2588885
p-f
359.0319671       2          10.0216411
24.0303802        2          5.0108204
-14.1525795       2          2.2588885
d-f
108.3013490       2          6.5979974
10.9825283        2          3.2989987
-14.1525795       2          2.2588885
*
*
re def2-QZVP
# re (10s8p6d3f1g) / [7s5p4d3f1g] {4111111/41111/3111/111/1}
*
4 s
24.000000000      0.26968047163
18.204262749      -1.3559378623
14.048192487      1.9003709759
9.5166786954      -0.75626964015
1 s
4.1714667981      1.0000000000
1 s
1.1944213976      1.0000000000
1 s

```

```

0.56755447797      1.0000000000
 1 s
0.17533854868      1.0000000000
 1 s
0.82014250464E-01  1.0000000000
 1 s
0.34607892740E-01  1.0000000000
 4 p
18.000000000      -0.26890962397E-01
12.318606250      0.99711498502E-01
 5.3719234505     -0.29289398145
 1.3506646748      0.51466301434
 1 p
0.66212816808      1.0000000000
 1 p
0.31071385193      1.0000000000
 1 p
0.10800000000      1.0000000000
 1 p
0.45000000000E-01  1.0000000000
 3 d
 7.7352877672     0.83901798556E-01
 6.0949443610     -0.17722258734
 1.3871105497     0.55238259692
 1 d
0.62324027854      1.0000000000
 1 d
0.26517328547      1.0000000000
 1 d
0.10321096849      1.0000000000
 1 f
 1.2406000000      1.0000000000
 1 f
0.48989000000      1.0000000000
 1 f
0.19345000000      1.0000000000
 1 g
0.62422000000      1.0000000000
*
re def2-ecp
*
  ncore =      60      lmax =      3
#      coefficient  r^n      exponent
f      16.4498523    2      2.5086506
s-f    1038.9515723   2      14.0993051
      29.5617383    2      7.0496525
      -16.4498523   2      2.5086506
p-f    339.5435096    2      10.1077169
      24.9136965    2      5.0538583
      -16.4498523   2      2.5086506
d-f    111.6996527    2      6.8486179
      12.6243293    2      3.4243090
      -16.4498523   2      2.5086506
*
*
os def2-QZVP

```

os (10s8p6d3f1g) / [7s5p4d3f1g] {4111111/41111/3111/111/1}

```
*
  4 s
24.000000000 0.24559132972
18.204262749 -1.3020204925
14.048192487 1.9114896000
9.5166786954 -0.83098846799
  1 s
4.2529406042 1.0000000000
  1 s
1.2999583502 1.0000000000
  1 s
0.61756850127 1.0000000000
  1 s
0.18785305474 1.0000000000
  1 s
0.87865523960E-01 1.0000000000
  1 s
0.37004242944E-01 1.0000000000
  4 p
15.500000000 0.16016463376
14.000000000 -0.23201520402
5.5458290420 0.29772587274
1.4139502215 -0.54253238176
  1 p
0.68136686765 1.0000000000
  1 p
0.30911452647 1.0000000000
  1 p
0.90000000000E-01 1.0000000000
  1 p
0.33000000000E-01 1.0000000000
  3 d
8.5557226523 0.55081304746E-01
6.1927250845 -0.15041777374
1.4916733698 0.55087247584
  1 d
0.67423241512 1.0000000000
  1 d
0.28635737076 1.0000000000
  1 d
0.11074292707 1.0000000000
  1 f
1.3802600000 1.0000000000
  1 f
0.55065000000 1.0000000000
  1 f
0.21968000000 1.0000000000
  1 g
0.75489000000 1.0000000000
```

*
os def2-ecp
*

```
ncore = 60 lmax = 3
# coefficient r^n exponent
f 18.9094570 2 2.7670751
s-f 885.4057191 2 13.8757539
25.9670401 2 6.9378769
```

	-18.9094570	2	2.7670751
p-f	320.0839019	2	10.1937926
	26.1487649	2	5.0968962
	-18.9094570	2	2.7670751
d-f	115.0448431	2	7.0992385
	13.6225746	2	3.5496192
	-18.9094570	2	2.7670751

*

*

ir def2-QZVP

ir (10s8p6d3f1g) / [7s5p4d3f1g] {4111111/41111/3111/111/1}

*

4	s		
23.465507222		0.71085679679	
20.657091116		-1.5723547785	
15.725107858		1.2938086001	
7.9297463605		-0.42980466966	
1	s		
4.5196120103		1.0000000000	
1	s		
1.3392891402		1.0000000000	
1	s		
0.63692276928		1.0000000000	
1	s		
0.19126770642		1.0000000000	
1	s		
0.87881999015E-01		1.0000000000	
1	s		
0.37643105533E-01		1.0000000000	
4	p		
15.902664143		-0.16290720099	
14.415830698		0.23483212987	
5.7597608991		-0.30305337176	
1.5008913108		0.55512982069	
1	p		
0.72348035957		1.0000000000	
1	p		
0.32785980328		1.0000000000	
1	p		
0.91000000000E-01		1.0000000000	
1	p		
0.35000000000E-01		1.0000000000	
3	d		
8.9686781612		0.29754685954E-01	
6.4456319498		-0.82246052942E-01	
1.5835819740		0.29212392062	
1	d		
0.71871917882		0.45371657855	
1	d		
0.30539233284		0.35080208829	
1	d		
0.11791405498		0.12106264000	
1	f		
1.5134800000		1.0000000000	
1	f		
0.61008000000		1.0000000000	
1	f		
0.24592000000		1.0000000000	

```

1 g
0.88556000000 1.0000000000
*
ir def2-ecp
*
ncore = 60 lmax = 3
# coefficient r^n exponent
f
21.5310311 2 3.0340719
s-f
732.2691998 2 13.6522026
26.4847209 2 6.8261013
-21.5310311 2 3.0340719
p-f
299.4894736 2 10.2798684
26.4662335 2 5.1399341
-21.5310311 2 3.0340719
d-f
124.4575945 2 7.3498590
14.0359952 2 3.6749295
-21.5310311 2 3.0340719
*
*
pt def2-QZVP
# pt (10s8p6d3f1g) / [7s5p4d3f1g] {4111111/41111/3111/111/1}
*
4 s
23.465507222 0.55150926143
20.657091116 -1.2690274107
15.725107858 1.1215145470
7.9297463605 -0.42250178029
1 s
4.6667116243 1.0000000000
1 s
1.4202522633 1.0000000000
1 s
0.66786671541 1.0000000000
1 s
0.19745059689 1.0000000000
1 s
0.92573920368E-01 1.0000000000
1 s
0.38895936899E-01 1.0000000000
4 p
15.500000000 -0.15672718629
14.000000000 0.23853412989
6.1161212339 -0.31041379733
1.5715586385 0.56473525089
1 p
0.75132510781 1.0000000000
1 p
0.33306466812 1.0000000000
1 p
0.91000000000E-01 1.0000000000
1 p
0.35000000000E-01 1.0000000000
3 d
8.3207937611 0.62945508668E-01
7.4207226520 -0.90271154330E-01
1.6570410639 0.16812340903

```

```

1 d
0.73943569960      1.0000000000
1 d
0.30508290090      1.0000000000
1 d
0.11350435924      1.0000000000
1 f
1.6402500000      1.0000000000
1 f
0.66813000000      1.0000000000
1 f
0.27215000000      1.0000000000
1 g
1.0162300000      1.0000000000
*
pt def2-ecp
*
ncore = 60          lmax = 3
# coefficient      r^n          exponent
f
24.3143757        2            3.3095686
s-f
579.2238609      2            13.4286513
29.6694906       2            6.7143256
-24.3143757      2            3.3095686
p-f
280.8607742      2            10.3659442
26.7453820       2            5.1829721
-24.3143757      2            3.3095686
d-f
120.3964443      2            7.6004795
15.8109206       2            3.8002397
-24.3143757      2            3.3095686
*
*
au def2-QZVP
# au (9s8p6d3f1g) / [7s5p4d3f1g] {31111111/41111/3111/111/1}
*
3 s
24.200000000      1.4645004443
22.000000000      -3.9770190496
20.000000000      2.7298033533
1 s
5.4043553001      1.0000000000
1 s
1.4532546773      1.0000000000
1 s
0.68294298420     1.0000000000
1 s
0.19002755303     1.0000000000
1 s
0.88155981740E-01 1.0000000000
1 s
0.37739555187E-01 1.0000000000
4 p
15.500000000      0.15001711880
14.000000000      -0.23609813183
6.4227368205      0.31458896948
1.6595601681      -0.57279670446
1 p

```

```

0.79402913993      1.0000000000
 1 p
0.35125155397      1.0000000000
 1 p
0.810000000000E-01  1.0000000000
 1 p
0.250000000000E-01  1.0000000000
 3 d
 8.6000000000      0.15361654684
 7.8531899379     -0.20443530663
 1.7650856798      0.30781811607
 1 d
0.79482263260      1.0000000000
 1 d
0.33085396360      1.0000000000
 1 d
0.12398535801      1.0000000000
 1 f
 1.7607400000      1.0000000000
 1 f
0.72482000000      1.0000000000
 1 f
0.29838000000      1.0000000000
 1 g
 1.1469000000      1.0000000000
*
au def2-ecp
*
  ncore =    60      lmax =    3
#      coefficient  r^n      exponent
f
      30.4900889    2        4.7898200
      5.1710738    2        2.3949100
s-f
      426.8466792   2        13.2051000
      37.0070829   2        6.6025500
     -30.4900889   2        4.7898200
      -5.1710738   2        2.3949100
p-f
      261.1995804   2        10.4520200
      26.9624960   2        5.2260100
     -30.4900889   2        4.7898200
      -5.1710738   2        2.3949100
d-f
      124.7906656   2        7.8511000
      16.3007257   2        3.9255500
     -30.4900889   2        4.7898200
      -5.1710738   2        2.3949100
*
*
hg def2-QZVP
# hg      (9s8p7d3f1g) / [7s5p4d3f1g]      {31111111/41111/4111/111/1}
*
  3 s
48.013786990      0.56241403333E-02
21.239875095     -0.17054083503
15.876100879      0.35940389661
 1 s
5.4865939429      1.0000000000
 1 s

```

1.5521766895	1.0000000000
1 s	
0.74742541187	1.0000000000
1 s	
0.20268838483	1.0000000000
1 s	
0.93376229211E-01	1.0000000000
1 s	
0.41248705609E-01	1.0000000000
4 p	
17.500000000	-0.86457187331E-01
15.252594855	0.15327318234
6.4404715169	-0.30274955249
1.8180159920	0.54361285026
1 p	
0.90067981801	1.0000000000
1 p	
0.41304540122	1.0000000000
1 p	
0.11845702655	1.0000000000
1 p	
0.36087619349E-01	1.0000000000
4 d	
11.888648987	0.13311219898E-01
6.7773660954	-0.73346199848E-01
2.0934941340	0.24155986719
1.0817087176	0.38865972362
1 d	
0.53329136060	1.0000000000
1 d	
0.24984101827	1.0000000000
1 d	
0.10879770063	1.0000000000
1 f	
1.8893800000	1.0000000000
1 f	
0.79569000000	1.0000000000
1 f	
0.33510000000	1.0000000000
1 g	
1.2895000000	1.0000000000

*

hg def2-ecp

*

#	ncore = 60	lmax = 3	coefficient	r^n	exponent
f			30.3649964	2	3.8857911
s-f			275.7372117	2	12.9815487
			49.0892125	2	6.4907744
			-30.3649964	2	3.8857911
p-f			241.5400740	2	10.5380958
			27.3965908	2	5.2690479
			-30.3649964	2	3.8857911
d-f			127.8670076	2	8.1017205
			16.6083115	2	4.0508603
			-30.3649964	2	3.8857911


```

*
*
t1 def2-QZVP
# t1      (17s14p10d4f1g) / [7s6p4d4f1g]      {9131111/731111/7111/1111/1}
*
  9 s
  9675.5500000      0.800000000000E-05
  1471.4800000      0.570000000000E-04
  323.648000000     0.227000000000E-03
  33.807900000      0.216660000000E-01
  21.131600000      -0.19589700000
  13.209100000      0.67362000000
  8.2561100000      -0.57167600000
  5.1001400000      -0.61234400000
  1.8194300000      0.75954400000
  1 s
0.96804610176      1.00000000000
  3 s
  13.432924081      0.16050252545
  11.126956705      -0.25827112953
  2.0351129325      0.52570088358
  1 s
0.47288027019      1.00000000000
  1 s
0.21703241765      1.00000000000
  1 s
0.99551664344E-01  1.00000000000
  1 s
0.44674475181E-01  1.00000000000
  7 p
  42.524000000      0.160500000000E-02
  21.395700000      -0.231590000000E-01
  13.373700000      0.11173800000
  6.6133700000      -0.34647200000
  2.0421700000      0.47507300000
  1.1144900000      0.48633500000
0.59800600000      0.20513900000
  3 p
  9.0557032031      -0.57376712693E-01
  3.9424773914      0.27305802340
  1.2382159385      0.72255078460
  1 p
0.29943260745      1.00000000000
  1 p
0.14250182360      1.00000000000
  1 p
0.61655072518E-01  1.00000000000
  1 p
0.26054870511E-01  1.00000000000
  7 d
  63.792149375      0.19539028558E-03
  10.854099697      0.17775848298E-01
  6.3885280565      -0.89213657526E-01
  2.4120875010      0.18424406191
  1.4246170706      0.30659722011
0.83496548780      0.31018961556
0.48634320397      0.23215648111
  1 d
0.27592111650      1.00000000000
  1 d

```

```

0.14737244064      1.0000000000
  1 d
0.677000000000E-01  1.0000000000
  1 f
0.426300000000     1.0000000000
  1 f
0.169000000000     1.0000000000
  1 f
1.0848100000       1.0000000000
  1 f
2.3083704534       1.0000000000
  1 g
0.369300000000     1.0000000000
*
tl def2-ecp
*
  ncore =    60      lmax =    3
#      coefficient  r^n      exponent
f
      15.8254880    2        5.6263990
      21.1040210    2        5.5489520
      2.9151270     2        2.8749460
      3.8969030     2        2.8214510
s-f
      281.2846630    2        12.1678050
      62.4342510    2        8.2949090
      -15.8254880    2        5.6263990
      -21.1040210    2        5.5489520
      -2.9151270     2        2.8749460
      -3.8969030     2        2.8214510
p-f
      4.6334080     2        7.1514920
      9.3417560     2        5.1728650
      72.2992530    2        9.8910720
      144.5580370   2        9.0033910
      -15.8254880    2        5.6263990
      -21.1040210    2        5.5489520
      -2.9151270     2        2.8749460
      -3.8969030     2        2.8214510
d-f
      35.9430390     2        7.1302180
      53.9095930     2        6.9269060
      10.3819390     2        5.4175700
      15.5838220     2        5.1386810
      -15.8254880    2        5.6263990
      -21.1040210    2        5.5489520
      -2.9151270     2        2.8749460
      -3.8969030     2        2.8214510
*
*
pb def2-QZVP
# pb      (17s14p10d4f1g) / [7s6p4d4f1g]      {9131111/731111/7111/1111/1}
*
  9 s
9368.3300000      0.140000000000E-04
1366.9300000      0.103000000000E-03
299.682000000     0.379000000000E-03
34.859700000      0.232740000000E-01
21.788900000      -0.20343600000
13.620000000      0.69921400000

```

8.5129500000	-0.60684100000
5.3033200000	-0.61139200000
1.9281600000	0.76522700000
1 s	
1.0373400312	1.0000000000
3 s	
13.559944213	0.15955164155
11.039620045	-0.26750615828
2.1371722788	0.52500552105
1 s	
0.51111685694	1.0000000000
1 s	
0.24673987563	1.0000000000
1 s	
0.11577976738	1.0000000000
1 s	
0.52874167812E-01	1.0000000000
7 p	
59.090100000	0.71600000000E-03
20.919700000	-0.21082000000E-01
13.077700000	0.12706100000
6.8991000000	-0.37228400000
2.1962700000	0.43566300000
1.3048600000	0.43573500000
0.77957200000	0.26094700000
3 p	
9.1373183134	-0.55319030476E-01
3.9570574249	0.27275707058
1.2246639098	0.72280340692
1 p	
0.42601564238	1.0000000000
1 p	
0.20378586294	1.0000000000
1 p	
0.88168647885E-01	1.0000000000
1 p	
0.37094701422E-01	1.0000000000
7 d	
66.348248961	0.28507140251E-03
13.455899798	0.93352787747E-02
6.5510273149	-0.75354763534E-01
2.6574136949	0.16674578725
1.6001278005	0.31208757936
0.93304454981	0.32900401823
0.54391365526	0.22655044022
1 d	
0.32059545270	1.0000000000
1 d	
0.17922304239	1.0000000000
1 d	
0.83200000000E-01	1.0000000000
1 f	
0.44130000000	1.0000000000
1 f	
0.17820000000	1.0000000000
1 f	
1.1606000000	1.0000000000
1 f	
2.5184938758	1.0000000000
1 g	

```

0.38810000000      1.0000000000
*
pb def2-ecp
*
ncore =      60      lmax =      3
# coefficient      r^n      exponent
f
      12.2098920      2      3.8875120
      16.1902910      2      3.8119630
s-f
      281.2854990      2      12.2963030
      62.5202170      2      8.6326340
      -12.2098920      2      3.8875120
      -16.1902910      2      3.8119630
p-f
      72.2768970      2      10.2417900
      144.5910830      2      8.9241760
      4.7586930      2      6.5813420
      9.9406210      2      6.2554030
      -12.2098920      2      3.8875120
      -16.1902910      2      3.8119630
d-f
      35.8485070      2      7.7543360
      53.7243420      2      7.7202810
      10.1152560      2      4.9702640
      14.8337310      2      4.5637890
      -12.2098920      2      3.8875120
      -16.1902910      2      3.8119630
*
*
bi def2-QZVP
# bi      (17s14p10d4f1g) / [7s6p4d4f1g]      {9131111/731111/7111/1111/1}
*
9 s
8131.0900000      0.290000000000E-04
1225.7700000      0.200000000000E-03
274.67200000      0.684000000000E-03
37.616400000      0.202180000000E-01
23.480400000      -0.15932600000
14.106500000      0.61172600000
8.8130500000      -0.54465300000
5.5077800000      -0.63688400000
2.0397700000      0.77169800000
1 s
1.0975227257      1.00000000000
3 s
13.614284474      0.15800789319
11.010881766      -0.27164962692
2.2630089550      0.52469330212
1 s
0.52344449532      1.00000000000
1 s
0.26734409206      1.00000000000
1 s
0.12836608814      1.00000000000
1 s
0.60097735551E-01      1.00000000000
7 p
99.591400000      0.346000000000E-03
19.896400000      -0.199760000000E-01

```

12.437600000	0.17544600000
7.774000000	-0.37955600000
4.839950000	-0.55262000000E-01
2.254780000	0.52888400000
1.180490000	0.52132400000
3 p	
9.6213214965	-0.52920356623E-01
4.1321350830	0.26705180214
1.2785827783	0.72824686940
1 p	
0.59423596262	1.00000000000
1 p	
0.25794168858	1.00000000000
1 p	
0.11273595358	1.00000000000
1 p	
0.47791974731E-01	1.00000000000
7 d	
69.632799181	0.35055800732E-03
14.888614968	0.81591735697E-02
6.5949628713	-0.83905319526E-01
4.1796107640	0.28034212952E-01
2.5697950152	0.20202314185
1.5601364822	0.33621249652
0.89210528768	0.34629017140
1 d	
0.48093728228	1.00000000000
1 d	
0.24233621968	1.00000000000
1 d	
0.10440000000	1.00000000000
1 f	
0.48030000000	1.00000000000
1 f	
0.20060000000	1.00000000000
1 f	
1.2625600000	1.00000000000
1 f	
2.7210175470	1.00000000000
1 g	
0.42030000000	1.00000000000
*	
bi def2-ecp	
*	
ncore = 60	lmax = 3
# coefficient r^n	exponent
f	
13.7133830	2 4.2145460
18.1943080	2 4.1334000
s-f	
283.2642270	2 13.0430900
62.4719590	2 8.2216820
-13.7133830	2 4.2145460
-18.1943080	2 4.1334000
p-f	
72.0014990	2 10.4677770
144.0022770	2 9.1189010
5.0079450	2 6.7547910
9.9915500	2 6.2525920
-13.7133830	2 4.2145460

```

-18.1943080      2      4.1334000
d-f
  36.3962590      2      8.0814740
  54.5976640      2      7.8905950
   9.9842940      2      4.9555560
  14.9814850      2      4.7045590
 -13.7133830      2      4.2145460
 -18.1943080      2      4.1334000
*
*
po def2-QZVP
# po      (17s14p10d4f1g) / [7s6p4d4f1g]      {9131111/731111/7111/1111/1}
*
  9 s
8913.2900000      0.470000000000E-04
1338.9800000      0.331000000000E-03
299.538000000      0.116100000000E-02
51.148900000      0.789900000000E-02
23.015600000      -0.14934700000
14.376500000      0.63824200000
8.98279000000      -0.61708300000
5.61292000000      -0.60519700000
2.16484000000      0.77608600000
  1 s
1.17538000000      1.00000000000
  3 s
14.787766907      0.15929033129
11.958781204      -0.27310166985
2.4798455066      0.52423698726
  1 s
0.55481477792      1.00000000000
  1 s
0.28581735198      1.00000000000
  1 s
0.13849439468      1.00000000000
  1 s
0.64954523837E-01  1.00000000000
  7 p
113.557000000      0.387000000000E-03
20.363900000      -0.182550000000E-01
12.727400000      0.17477600000
7.94984000000      -0.39870300000
4.96477000000      -0.318120000000E-01
2.30130000000      0.56604700000
1.19545000000      0.51022200000
  3 p
8.46813000000      -0.23853762000
7.7962017000      0.28579119000
0.66871758000      0.46050656000
  1 p
0.59152423927      1.00000000000
  1 p
0.24444843795      1.00000000000
  1 p
0.11018922460      1.00000000000
  1 p
0.48149776000E-01  1.00000000000
  7 d
73.649818245      0.43310334586E-03
16.743441686      0.69436968591E-02

```

```

5.8163048812      -0.83799240387
5.6493757173      0.79372183416
2.4547686106      0.29055549251
1.3909015593      0.38177920670
0.78934505572     0.29342954208
 1 d
0.44107648549     1.00000000000
 1 d
0.23631248810     1.00000000000
 1 d
0.10930000000     1.00000000000
 1 f
0.48940000000     1.00000000000
 1 f
0.20020000000     1.00000000000
 1 f
1.31220000000     1.00000000000
 1 f
2.8220658714      1.00000000000
 1 g
0.40740000000     1.00000000000
*
po def2-ecp
*
ncore =      60          lmax =      3
# coefficient  r^n      exponent
f
      17.4282950      2          5.0132700
      23.3803530      2          4.9846400
      0.1633920      2          1.3267600
      0.3245660      2          1.5287580
s-f
      283.2447060      2          13.2772270
      62.3964610      2          8.3995180
      -17.4282950      2          5.0132700
      -23.3803530      2          4.9846400
      -0.1633920      2          1.3267600
      -0.3245660      2          1.5287580
p-f
      71.9917160      2          10.6656820
      143.9718710      2          9.2837530
      4.9496150      2          6.8727490
      9.7404990      2          6.3261500
      -17.4282950      2          5.0132700
      -23.3803530      2          4.9846400
      -0.1633920      2          1.3267600
      -0.3245660      2          1.5287580
d-f
      36.3783830      2          8.2148660
      54.5627150      2          8.0086960
      9.8894990      2          5.0552270
      14.6938770      2          4.7825530
      -17.4282950      2          5.0132700
      -23.3803530      2          4.9846400
      -0.1633920      2          1.3267600
      -0.3245660      2          1.5287580
*
*
at def2-QZVP
# at      (17s14p10d4f1g) / [7s6p4d4f1g]      {9131111/731111/7111/1111/1}

```

*

9 s	
9090.2800000	0.350000000000E-04
1373.0700000	0.242000000000E-03
307.9500000	0.815000000000E-03
48.017600000	0.846500000000E-02
23.909900000	-0.14733300000
14.933400000	0.63241500000
9.3317100000	-0.61640600000
5.8320600000	-0.61925800000
2.2878700000	0.78512400000
1 s	
1.2537238008	1.00000000000
3 s	
14.805780876	0.15771473639
11.855783628	-0.28007490839
2.5818782360	0.52359428906
1 s	
0.61460691976	1.00000000000
1 s	
0.31486716636	1.00000000000
1 s	
0.15441669153	1.00000000000
1 s	
0.72866424566E-01	1.00000000000
7 p	
124.60200000	0.468000000000E-03
20.889900000	-0.161240000000E-01
13.058500000	0.17119600000
8.1606100000	-0.40887500000
5.0980800000	-0.164070000000E-01
2.3787600000	0.58817200000
1.2375500000	0.50099700000
3 p	
8.7977584321	-0.23832810213
8.0996431502	0.28585830834
0.67629719775	0.46050935965
1 p	
0.60785017930	1.00000000000
1 p	
0.26116561417	1.00000000000
1 p	
0.11948611257	1.00000000000
1 p	
0.52899086095E-01	1.00000000000
7 d	
76.152584155	0.54645145370E-03
17.982092186	0.70498116717E-02
5.8900316564	-0.59711331046
5.6001503121	0.56517203927
2.4782622062	0.32344318344
1.3928750256	0.39511263456
0.78560551382	0.27094838862
1 d	
0.44173978741	1.00000000000
1 d	
0.24984733563	1.00000000000
1 d	
0.12700000000	1.00000000000
1 f	


```

0.538900000000      1.0000000000
  1 f
0.228700000000      1.0000000000
  1 f
1.423720000000      1.0000000000
  1 f
  3.0086421207      1.0000000000
  1 g
0.436300000000      1.0000000000
*
at def2-ecp
*
  ncore =      60      lmax =      3
#      coefficient      r^n      exponent
f
      19.8701980      2      5.8121630
      26.4164520      2      5.7537150
      0.9949700      2      2.5134720
      1.4907010      2      2.5362610
s-f
      49.9571580      2      30.2008320
      283.2103710      2      13.6123060
      62.2810520      2      8.5293400
      -19.8701980      2      5.8121630
      -26.4164520      2      5.7537150
      -0.9949700      2      2.5134720
      -1.4907010      2      2.5362610
p-f
      71.9823710      2      10.8540650
      143.9035320      2      9.4682290
      4.8717590      2      7.0311140
      8.9830590      2      6.1438580
      -19.8701980      2      5.8121630
      -26.4164520      2      5.7537150
      -0.9949700      2      2.5134720
      -1.4907010      2      2.5362610
d-f
      36.3632370      2      8.3135150
      54.5489700      2      7.9989650
      9.7762850      2      5.1799660
      14.2647550      2      4.9422260
      -19.8701980      2      5.8121630
      -26.4164520      2      5.7537150
      -0.9949700      2      2.5134720
      -1.4907010      2      2.5362610
*
*
rn def2-QZVP
# rn      (17s14p11d4f1g) / [7s6p4d4f1g]      {9131111/731111/8111/1111/1}
*
  9 s
12715.600000      0.470000000000E-04
1913.300000      0.338000000000E-03
429.95600000      0.128000000000E-02
100.97800000      0.278200000000E-02
24.4708000000      -0.100421000000
15.2922000000      0.539824000000
9.5548300000      -0.573856000000
5.9666100000      -0.610000000000
2.3893900000      0.793253000000

```

1 s	
1.3276477516	1.0000000000
3 s	
17.195195341	0.16333005101
14.230303720	-0.27167744770
3.0760339153	0.52372666490
1 s	
0.69973866760	1.0000000000
1 s	
0.33174234887	1.0000000000
1 s	
0.16093431878	1.0000000000
1 s	
0.75883596172E-01	1.0000000000
7 p	
131.70800000	0.58500000000E-03
21.401600000	-0.14438000000E-01
13.382600000	0.17009500000
8.3688000000	-0.42250400000
5.2294500000	-0.17190000000E-02
2.4768500000	0.60115800000
1.3018000000	0.49278000000
3 p	
9.0768547920	-0.23950411879
8.3822367043	0.28554010268
0.70618692299	0.46017587936
1 p	
0.64553860374	1.0000000000
1 p	
0.28380500916	1.0000000000
1 p	
0.13160518578	1.0000000000
1 p	
0.58958259826E-01	1.0000000000
8 d	
183.73000000	0.12900000000E-03
54.689700000	0.94900000000E-03
16.425500000	0.10100000000E-01
7.3050000000	-0.87309000000E-01
4.2747700000	0.71452000000E-01
2.6114200000	0.29537800000
1.5667400000	0.35873100000
0.96097900000	0.25612000000
1 d	
0.59653500000	1.0000000000
1 d	
0.34202800000	1.0000000000
1 d	
0.15160000000	1.0000000000
1 f	
0.59400000000	1.0000000000
1 f	
0.26840000000	1.0000000000
1 f	
1.5556400000	1.0000000000
1 f	
3.2498641894	1.0000000000
1 g	
0.47630000000	1.0000000000

*

rn def2-ecp

```
*
ncore = 60          lmax = 3
# coefficient      r^n      exponent
f
    21.7972900      2          6.3485710
    28.9468050      2          6.2959490
    1.4473650       2          2.8821180
    2.1779640       2          2.9080480
s-f
    49.9655510      2          30.1512420
    283.0700000     2          14.5212410
    62.0028700      2          8.0520380
    -21.7972900     2          6.3485710
    -28.9468050     2          6.2959490
    -1.4473650      2          2.8821180
    -2.1779640      2          2.9080480
p-f
    71.9691190      2          11.0099420
    143.8605590     2          9.6176250
    4.7147610       2          7.3360080
    9.0130650       2          6.4062530
    -21.7972900     2          6.3485710
    -28.9468050     2          6.2959490
    -1.4473650      2          2.8821180
    -2.1779640      2          2.9080480
d-f
    36.3683650      2          8.3692200
    54.5517610      2          8.1169750
    9.6344870       2          5.3536560
    14.3879020      2          5.0972120
    -21.7972900     2          6.3485710
    -28.9468050     2          6.2959490
    -1.4473650      2          2.8821180
    -2.1779640      2          2.9080480
```

```
*
=====
def2-QZVPP
=====
```

```
*
h def2-QZVPP
# h      (7s3p2d1f) / [4s3p2d1f]      {4111/111/11/1}
*
```

```
4 s
190.69169000      0.70815167000E-03
28.605532000      0.54678827000E-02
6.5095943000      0.27966605000E-01
1.8412455000      0.10764538000
1 s
0.59853725000      1.00000000000
1 s
0.21397624000      1.00000000000
1 s
0.80316286000E-01  1.00000000000
1 p
2.29200000000      1.00000000000
1 p
0.83800000000      1.00000000000
1 p
0.29200000000      1.00000000000
```

```

1 d
2.0620000000      1.0000000000
1 d
0.662000000000   1.0000000000
1 f
1.3970000000     1.0000000000
*
*
he def2-QZVPP
# he      (8s3p2d1f) / [4s3p2d1f]      {5111/111/11/1}
*
5 s
1144.6470809     0.35861578618E-03
171.64596667     0.27725434466E-02
39.066056254     0.14241892216E-01
11.051401989     0.55457352277E-01
3.5725574473     0.16170511810
1 s
1.2429415962     0.33177883833
1 s
0.44807668730   0.42014033068
1 s
0.16411579128   0.18652273014
1 p
5.9940000000    1.0000000000
1 p
1.7450000000    1.0000000000
1 p
0.56000000000   1.0000000000
1 d
4.2990000000    1.0000000000
1 d
1.2230000000    1.0000000000
1 f
2.6800000000    1.0000000000
*
*
li def2-QZVPP
# li      (15s6p2d1f) / [6s4p2d1f]      {921111/3111/11/1}
*
9 s
14853.977085     0.42711388815E-04
2225.2236477     0.33235310800E-03
504.88739008     0.17518436649E-02
142.45847548     0.73477995850E-02
46.315599580     0.25899837683E-01
16.655335474     0.76670682431E-01
6.4331186199     0.18276075765
2.6027043858     0.32655434038
1.0897245405     0.37000429828
2 s
4.4236595971     0.11120987921
1.2356394990     0.79987335862
1 s
0.46067470602    1.0000000000
1 s
0.96617166955E-01 1.0000000000
1 s
0.45915452296E-01 1.0000000000
1 s

```

```

0.21140048730E-01  1.0000000000
  3 p
  3.2605109206      0.86504749023E-02
0.65003043115      0.47614123736E-01
0.16941671073      0.21001138000
  1 p
0.55732343767E-01  1.0000000000
  1 p
0.20489959241E-01  1.0000000000
  1 p
  3.3270000000      1.0000000000
  1 d
0.23000000000      1.0000000000
  1 d
0.75700000000E-01  1.0000000000
  1 f
0.13500000000      1.0000000000
*
*
be def2-QZVPP
# be      (15s7p2d1f) / [7s4p2d1f]      {8211111/4111/11/1}
*
  8 s
  29646.704407      0.37943320869E-04
  4428.7614354      0.29605352634E-03
  1005.4701332      0.15572477356E-02
  284.15339578      0.65323195769E-02
  92.504356461      0.23116861005E-01
  33.311016058      0.69458515249E-01
  12.911553314      0.17014371331
  5.2665497361      0.31682711374
  2 s
  22.995386380      0.81791122747E-01
  6.6236354176      0.80000038023
  1 s
  2.2289595003      1.0000000000
  1 s
0.95302433451      1.0000000000
  1 s
0.24651602436      1.0000000000
  1 s
0.10153895315      1.0000000000
  1 s
0.41551374604E-01  1.0000000000
  4 p
  14.099789445      0.38508871145E-02
  3.1803188482      0.24152380771E-01
0.90489220496      0.97926925156E-01
0.30411585508      0.29470380030
  1 p
0.11302606657      1.0000000000
  1 p
0.42831733691E-01  1.0000000000
  1 p
  6.4000000000      1.0000000000
  1 d
0.36000000000      1.0000000000
  1 d
0.90000000000E-01  1.0000000000
  1 f

```

```

0.290000000000      1.0000000000
*
*
b def2-QZVPP
# b      (15s8p3d2f1g) / [7s4p3d2f1g]      {8211111/5111/111/11/1}
*
      8 s
46447.667056      0.38388681014E-04
6957.6889042      0.29836770197E-03
1583.4428403      0.15645478806E-02
448.46601009      0.65476770742E-02
146.28639262      0.23139008388E-01
52.784386084      0.69615799357E-01
20.519396170      0.17119636876
8.4185659258      0.31913191837
      2 s
36.510018312      0.78990617244E-01
10.541854005      0.78926384265
      1 s
3.6004091387      1.0000000000
      1 s
1.5617023749      1.0000000000
      1 s
0.44997370775      1.0000000000
      1 s
0.18075230237      1.0000000000
      1 s
0.71596696319E-01  1.0000000000
      5 p
72.240462760      0.86539170411E-03
16.807707208      0.68762067365E-02
5.2259410747      0.30976687148E-01
1.8508350671      0.10432357913
0.72206782663      0.26164137577
      1 p
0.29491018056      1.0000000000
      1 p
0.12201141839      1.0000000000
      1 p
0.49865393625E-01  1.0000000000
      1 d
1.1100000000      1.0000000000
      1 d
0.4020000000      1.0000000000
      1 d
0.1450000000      1.0000000000
      1 f
0.8820000000      1.0000000000
      1 f
0.3110000000      1.0000000000
      1 g
0.6730000000      1.0000000000
*
*
c def2-QZVPP
# c      (15s8p3d2f1g) / [7s4p3d2f1g]      {8211111/5111/111/11/1}
*
      8 s
67025.071029      0.38736308501E-04
10039.986538      0.30107917575E-03

```

2284.9316911	0.15787918095E-02
647.14122130	0.66087087195E-02
211.09472335	0.23367123250E-01
76.177643862	0.70420716898E-01
29.633839163	0.17360344953
12.187785081	0.32292305648
2 s	
53.026006299	0.74897404492E-01
15.258502776	0.76136220983
1 s	
5.2403957464	1.0000000000
1 s	
2.2905022379	1.0000000000
1 s	
0.69673283006	1.0000000000
1 s	
0.27599337363	1.0000000000
1 s	
0.10739884389	1.0000000000
5 p	
105.12555082	0.84647553844E-03
24.884461066	0.66274038534E-02
7.8637230826	0.30120390419E-01
2.8407001835	0.99951435476E-01
1.1227137335	0.23826299282
1 p	
0.46050725555	1.0000000000
1 p	
0.18937530913	1.0000000000
1 p	
0.75983791611E-01	1.0000000000
1 d	
1.8480000000	1.0000000000
1 d	
0.64900000000	1.0000000000
1 d	
0.22800000000	1.0000000000
1 f	
1.4190000000	1.0000000000
1 f	
0.48500000000	1.0000000000
1 g	
1.0110000000	1.0000000000
*	
*	
n def2-QZVPP	
# n (15s8p3d2f1g) / [7s4p3d2f1g]	{82111111/5111/111/11/1}
*	
8 s	
90726.889210	0.39257887368E-04
13590.528801	0.30513316455E-03
3092.9883781	0.16000560446E-02
875.99876362	0.66982937306E-02
285.74469982	0.23690078765E-01
103.11913417	0.71455405268E-01
40.128556777	0.17632774876
16.528095704	0.32677592815
2 s	
69.390960983	0.80052094386E-01
20.428200596	0.78268063538

```

1 s
7.1292587972      1.0000000000
1 s
3.1324304893      1.0000000000
1 s
0.98755778723     1.0000000000
1 s
0.38765721307     1.0000000000
1 s
0.14909883075     1.0000000000
5 p
150.05742670      -0.86216165986E-03
35.491599483      -0.68571273236E-02
11.247864223      -0.31795688855E-01
4.0900305195      -0.10537396822
1.6220573146      -0.24519708041
1 p
0.66442261530     1.0000000000
1 p
0.27099770070     1.0000000000
1 p
0.10688749984     1.0000000000
1 d
2.83700000000     1.0000000000
1 d
0.96800000000     1.0000000000
1 d
0.33500000000     1.0000000000
1 f
2.02700000000     1.0000000000
1 f
0.68500000000     1.0000000000
1 g
1.42700000000     1.0000000000
*
*
o def2-QZVPP
# o      (15s8p3d2f1g) / [7s4p3d2f1g]      {8211111/5111/111/11/1}
*
8 s
116506.46908      0.40383857939E-04
17504.349724      0.31255139004E-03
3993.4513230      0.16341473495E-02
1133.0063186      0.68283224757E-02
369.99569594      0.24124410221E-01
133.62074349      0.72730206154E-01
52.035643649      0.17934429892
21.461939313      0.33059588895
2 s
89.835051252      0.96468652996E-01
26.428010844      0.94117481120
1 s
9.2822824649      1.0000000000
1 s
4.0947728533      1.0000000000
1 s
1.3255349078      1.0000000000
1 s
0.51877230787     1.0000000000
1 s

```


0.19772676454	1.0000000000	
5 p		
191.15255810	0.25115697705E-02	
45.233356739	0.20039240864E-01	
14.353465922	0.93609064762E-01	
5.2422371832	0.30618127124	
2.0792418599	0.67810501439	
1 p		
0.84282371424	1.0000000000	
1 p		
0.33617694891	1.0000000000	
1 p		
0.12863997974	1.0000000000	
1 d		
3.7750000000	1.0000000000	
1 d		
1.3000000000	1.0000000000	
1 d		
0.44400000000	1.0000000000	
1 f		
2.6660000000	1.0000000000	
1 f		
0.85900000000	1.0000000000	
1 g		
1.8460000000	1.0000000000	
*		
*		
f def2-QZVPP		
# f (15s8p3d2f1g) / [7s4p3d2f1g]		{8211111/5111/111/11/1}
*		
8 s		
132535.97345	0.47387482743E-04	
19758.112588	0.37070120897E-03	
4485.1996947	0.19450784713E-02	
1273.8151020	0.80573291994E-02	
418.93831236	0.27992880781E-01	
152.55721985	0.82735120175E-01	
59.821524823	0.19854169012	
24.819076932	0.34860632233	
2 s		
100.74446673	0.10505068816	
30.103728290	0.94068472434	
1 s		
10.814283272	1.0000000000	
1 s		
4.8172886770	1.0000000000	
1 s		
1.6559334213	1.0000000000	
1 s		
0.64893519582	1.0000000000	
1 s		
0.24778104545	1.0000000000	
5 p		
240.96654114	0.30389933451E-02	
57.020699781	0.24357738582E-01	
18.126952120	0.11442925768	
6.6457404621	0.37064659853	
2.6375722892	0.79791551766	
1 p		
1.0638217200	1.0000000000	

```

1 p
0.41932562750      1.0000000000
1 p
0.15747588299      1.0000000000
1 d
5.0140000000       1.0000000000
1 d
1.7250000000       1.0000000000
1 d
0.586000000000    1.0000000000
1 f
3.5620000000       1.0000000000
1 f
1.1480000000       1.0000000000
1 g
2.3760000000       1.0000000000
*
*
ne def2-QZVPP
# ne      (15s9p3d2f1g) / [7s4p3d2f1g]      {82111111/6111/111/11/1}
*
8 s
160676.27955       0.47387482743E-04
23953.195039       0.37070120897E-03
5437.5063711       0.19450784713E-02
1544.2741024       0.80573291994E-02
507.88814269       0.27992880781E-01
184.94847750       0.82735120175E-01
72.522952039       0.19854169012
30.088713575       0.34860632233
2 s
120.68434940       0.10400597014
36.074294857       0.91999988986
1 s
13.052091210       1.0000000000
1 s
5.7974783353       1.0000000000
1 s
2.0478626895       1.0000000000
1 s
0.80214571994       1.0000000000
1 s
0.30548672205       1.0000000000
6 p
498.43397466       0.43118261050E-03
118.14109217       0.36206397703E-02
38.032529735       0.18245344081E-01
14.183731950       0.65133035572E-01
5.7864190721       0.16708915089
2.4599622160       0.29268019613
1 p
1.0421999498       1.0000000000
1 p
0.42987748916       1.0000000000
1 p
0.16889708453       1.0000000000
1 d
6.4710000000       1.0000000000
1 d
2.2130000000       1.0000000000

```

```

1 d
0.74700000000 1.0000000000
1 f
4.65700000000 1.0000000000
1 f
1.52400000000 1.0000000000
1 g
2.98300000000 1.0000000000
*
*
na def2-QZVPP
# na (20s12p4d2f) / [9s5p4d2f] {(10)31111111/81111/1111/11}
*
10 s
379852.20081 0.20671384468E-04
56886.006378 0.16070466617E-03
12942.701838 0.84462905848E-03
3664.3017904 0.35519026029E-02
1194.7417499 0.12754034468E-01
430.98192917 0.39895462742E-01
167.83169424 0.10720154498
69.306669040 0.23339516913
29.951170886 0.36333077287
13.380791097 0.30544770974
3 s
121.74011283 0.36142427284E-01
37.044143387 0.28820961687
13.995422624 0.79337384869
1 s
5.9827797428 1.0000000000
1 s
2.4830455118 1.0000000000
1 s
1.0452506187 1.0000000000
1 s
0.43875640383 1.0000000000
1 s
0.65595633185E-01 1.0000000000
1 s
0.30561925072E-01 1.0000000000
1 s
0.15509064018E-01 1.0000000000
8 p
690.77627017 0.37478518415E-03
163.82806121 0.31775441030E-02
52.876460769 0.16333581338E-01
19.812270493 0.59754902585E-01
8.1320378784 0.15879328812
3.4969068377 0.29049363260
1.5117244146 0.36368131139
0.64479294912 0.28195867334
1 p
0.26145823312 1.0000000000
1 p
0.11704726116 1.0000000000
1 p
0.40494747666E-01 1.0000000000
1 p
0.15666707355E-01 1.0000000000
1 d

```

```

5.3000000000      1.0000000000
 1 d
1.5900000000      1.0000000000
 1 d
0.2300000000      1.0000000000
 1 d
0.7570000000E-01  1.0000000000
 1 f
4.2700000000      1.0000000000
 1 f
0.1350000000      1.0000000000
*
*
mg def2-QZVPP
# mg      (20s12p5d2f) / [9s5p5d2f]      {(10)31111111/81111/11111/11}
*
10 s
605967.78753      0.14430176617E-04
90569.094692      0.11249871807E-03
20574.252844      0.59264972450E-03
5818.6284865      0.24988770424E-02
1895.6296075      0.90230775141E-02
683.45941021      0.28579919806E-01
266.18219762      0.79064453923E-01
110.11220010      0.18269337814
47.777041234      0.32157193967
21.542166149      0.35028259389
 3 s
174.12136378      0.22931111278E-01
53.484972498      0.19151777552
20.500213307      0.61155711055
 1 s
9.8056826922      1.0000000000
 1 s
3.5402989348      1.0000000000
 1 s
1.5450850046      1.0000000000
 1 s
0.66540195432      1.0000000000
 1 s
0.14355439071      1.0000000000
 1 s
0.66624673468E-01  1.0000000000
 1 s
0.29772648266E-01  1.0000000000
 8 p
893.20460829      0.34958267428E-03
211.78258286      0.29811890111E-02
68.443200537      0.15517845758E-01
25.727265349      0.57578659557E-01
10.606634281      0.15610307853
4.5934126484      0.29230912580
2.0100469807      0.37219024072
0.87384841536      0.27578088891
 1 p
0.35615076666      1.0000000000
 1 p
0.18995954356      1.0000000000
 1 p
0.74580135669E-01  1.0000000000

```

```

1 p
0.29221641309E-01 1.0000000000
1 d
6.9300000000 1.0000000000
1 d
2.1000000000 1.0000000000
1 d
0.6500000000 1.0000000000
1 d
0.2000000000 1.0000000000
1 d
0.5200000000E-01 1.0000000000
1 f
5.6000000000 1.0000000000
1 f
0.1600000000 1.0000000000
*
*
al def2-QZVPP
# al (20s14p4d2f1g) / [9s6p4d2f1g] {(10)}
31111111/821111/1111/11/1}
*
10 s
754550.78265 0.13421335886E-04
112999.38922 0.10433210786E-03
25715.831759 0.54841772080E-03
7283.6030283 0.23089081391E-02
2376.0008796 0.83309974593E-02
857.65468087 0.26417963653E-01
334.38922598 0.73443646426E-01
138.48504731 0.17184039139
60.150368808 0.31041980030
27.127610860 0.35669190596
3 s
225.36500065 0.21522039783E-01
69.341968124 0.18531780493
26.619335712 0.63533181245
1 s
12.349420671 1.0000000000
1 s
4.5878785994 1.0000000000
1 s
2.0571338103 1.0000000000
1 s
0.90864549395 1.0000000000
1 s
0.24226988038 1.0000000000
1 s
0.11248136869 1.0000000000
1 s
0.48156492817E-01 1.0000000000
8 p
1489.6119522 0.20177122443E-03
353.01399267 0.17508109203E-02
114.40764069 0.94424704664E-02
43.312186111 0.36868004006E-01
18.027322216 0.10892874007
7.9675432403 0.23265901004
3.6090399541 0.34643587076
1.6456081630 0.33440809866

```

```

2 p
34.731187489      0.17823073020E-01
1.2553083630     -0.59991263926
1 p
0.73635534282    1.00000000000
1 p
0.24686465559    1.00000000000
1 p
0.94821971828E-01 1.00000000000
1 p
0.36214165654E-01 1.00000000000
1 d
1.97000000000    1.00000000000
1 d
0.43700000000    1.00000000000
1 d
0.19500000000    1.00000000000
1 d
0.80000000000E-01 1.00000000000
1 f
0.15400000000    1.00000000000
1 f
0.40100000000    1.00000000000
1 g
0.35700000000    1.00000000000
*
*
si def2-QZVPP
# si      (20s14p4d2f1g) / [9s6p4d2f1g]      {(10)}
31111111/821111/1111/11/1}
*
10 s
918070.69565      0.12658787192E-04
137485.25386      0.98408387461E-04
31287.772714      0.51731398244E-03
8861.6105697      0.21785441933E-02
2890.6943156      0.78656853716E-02
1043.4063979      0.24987553674E-01
406.80160276      0.69761818844E-01
168.48360207      0.16473362733
73.185628823      0.30285602647
32.998485420      0.36007260439
3 s
278.78751325      0.20185463814E-01
85.910228722      0.17720406747
32.992604031      0.63587860906
1 s
15.033693254      1.00000000000
1 s
5.7257514773      1.00000000000
1 s
2.6146521029      1.00000000000
1 s
1.1757833152      1.00000000000
1 s
0.35432330868      1.00000000000
1 s
0.16248335806      1.00000000000
1 s
0.68332457181E-01 1.00000000000

```

```

      8 p
1775.8850516      0.20186971126E-03
420.83786849     0.17544314655E-02
136.42290243     0.95039532290E-02
51.700991737     0.37325741590E-01
21.559456002     0.11085396329
9.5559200095     0.23756407046
4.3529819473     0.35295783750
2.0096964381     0.32885931947
      2 p
46.418153780     0.25858819154E-01
1.9076417796     -0.59874865899
      1 p
0.92337221587     1.0000000000
      1 p
0.34515720370     1.0000000000
      1 p
0.13656834761     1.0000000000
      1 p
0.52987060586E-01 1.0000000000
      1 d
2.6450000000     1.0000000000
      1 d
0.60800000000     1.0000000000
      1 d
0.27200000000     1.0000000000
      1 d
0.11300000000     1.0000000000
      1 f
0.21200000000     1.0000000000
      1 f
0.54100000000     1.0000000000
      1 g
0.46100000000     1.0000000000
*
*
p def2-QZVPP
# p      (20s14p4d2f1g) / [9s6p4d2f1g]      {(10)
31111111/821111/1111/11/1}
*
      10 s
1090561.7138     0.12142449664E-04
163316.39461     0.94395292614E-04
37166.607451     0.49622262177E-03
10526.880945     0.20900040747E-02
3433.9976028     0.75489230025E-02
1239.5360480     0.24010423937E-01
483.27456199     0.67231473697E-01
200.16911586     0.15978669881
86.960394829     0.29735906782
39.211283369     0.36187171850
      3 s
336.75883662     0.19154721050E-01
103.72179793     0.17134079100
39.771861240     0.63689655985
      1 s
17.888612952     1.0000000000
      1 s
6.9644556879     1.0000000000
      1 s

```

3.2198092087	1.0000000000	
1 s		
1.4669943979	1.0000000000	
1 s		
0.47765437532	1.0000000000	
1 s		
0.21637789241	1.0000000000	
1 s		
0.90235894336E-01	1.0000000000	
8 p		
2019.6711374	0.21359172406E-03	
478.60125090	0.18568771399E-02	
155.14942504	0.10070690115E-01	
58.816356575	0.39605153679E-01	
24.544512785	0.11736067844	
10.883571061	0.24950540642	
4.9624791285	0.36421287984	
2.3002912343	0.31764127123	
2 p		
59.371345016	0.39432918004	
3.0694590986	-6.3522960431	
1 p		
1.0634401739	1.0000000000	
1 p		
0.45022152161	1.0000000000	
1 p		
0.18267271344	1.0000000000	
1 p		
0.71610333771E-01	1.0000000000	
1 d		
3.3430000000	1.0000000000	
1 d		
0.80700000000	1.0000000000	
1 d		
0.36500000000	1.0000000000	
1 d		
0.15400000000	1.0000000000	
1 f		
0.28000000000	1.0000000000	
1 f		
0.70300000000	1.0000000000	
1 g		
0.59700000000	1.0000000000	
*		
*		
s def2-QZVPP		
# s (20s14p4d2f1g) / [9s6p4d2f1g]		{(10)}
31111111/821111/1111/11/1}		
*		
10 s		
1273410.9023	0.11767088246E-04	
190697.83007	0.91478610166E-04	
43397.885330	0.48090078640E-03	
12291.809677	0.20257193592E-02	
4009.7420824	0.73190096406E-02	
1447.3531030	0.23300499900E-01	
564.30102913	0.65386213610E-01	
233.74506243	0.15614449910	
101.56402814	0.29318563787	
45.805907187	0.36287914289	

3 s		
394.27281503	0.18753305081E-01	
121.72249591	0.16870726663	
46.754125963	0.63806830653	
1 s		
20.923008254	1.0000000000	
1 s		
8.2685567800	1.0000000000	
1 s		
3.8629345671	1.0000000000	
1 s		
1.7794684781	1.0000000000	
1 s		
0.61064260103	1.0000000000	
1 s		
0.27412269445	1.0000000000	
1 s		
0.11325939107	1.0000000000	
8 p		
2189.8930459	0.23912552864E-03	
518.94596592	0.20772032158E-02	
168.19560151	0.11242420571E-01	
63.745282788	0.44069933941E-01	
26.597033077	0.12918778608	
11.774251449	0.26910820167	
5.3534379024	0.37855928620	
2.4701911802	0.29692134655	
2 p		
82.120288349	-0.39420318847E-01	
4.9523532869	0.64048403090	
1 p		
1.0828262029	1.0000000000	
1 p		
0.49271277356	1.0000000000	
1 p		
0.20483450942	1.0000000000	
1 p		
0.80743615716E-01	1.0000000000	
1 d		
4.1590000000	1.0000000000	
1 d		
1.0190000000	1.0000000000	
1 d		
0.46400000000	1.0000000000	
1 d		
0.19400000000	1.0000000000	
1 f		
0.33500000000	1.0000000000	
1 f		
0.86900000000	1.0000000000	
1 g		
0.68300000000	1.0000000000	
*		
*		
c1 def2-QZVPP		
# c1 (20s14p4d2f1g) / [9s6p4d2f1g]	{(10)	
31111111/821111/1111/11/1}		
*		
10 s		
1467459.0095	0.11478257194E-04	

219756.16433	0.89234299775E-04
50010.770301	0.46911086186E-03
14164.823918	0.19762446133E-02
4620.7465525	0.71419937783E-02
1667.8991635	0.22753219445E-01
650.29199265	0.63959782953E-01
269.38037376	0.15331059238
117.06752106	0.28986952417
52.811766843	0.36348071452
3 s	
461.42769988	0.18019457578E-01
142.12665355	0.16489442314
54.437838768	0.63891587584
1 s	
24.160770219	1.0000000000
1 s	
9.7083540306	1.0000000000
1 s	
4.5640696733	1.0000000000
1 s	
2.1194744832	1.0000000000
1 s	
0.75722365394	1.0000000000
1 s	
0.33747224597	1.0000000000
1 s	
0.13860775149	1.0000000000
8 p	
2501.9457890	0.24242618410E-03
592.88059285	0.21079961749E-02
192.18089186	0.11432693869E-01
72.875710488	0.44956698060E-01
30.436358370	0.13197476145
13.490178902	0.27493639225
6.1478071413	0.38347236372
2.8450944820	0.28871943885
2 p	
105.39397936	-0.34311760144E-01
6.7369738513	0.64060818902
1 p	
1.2421095772	1.0000000000
1 p	
0.55669714254	1.0000000000
1 p	
0.23387801464	1.0000000000
1 p	
0.93164490890E-01	1.0000000000
1 d	
5.1910000000	1.0000000000
1 d	
1.2760000000	1.0000000000
1 d	
0.5830000000	1.0000000000
1 d	
0.2430000000	1.0000000000
1 f	
0.4230000000	1.0000000000
1 f	
1.0890000000	1.0000000000
1 g	

```

0.82700000000      1.0000000000
*
*
ar def2-QZVPP
# ar      (20s14p4d2f1g) / [9s6p4d2f1g]      {(10)
31111111/821111/1111/11/1}
*
10 s
1673421.9494      0.11245990413E-04
250601.75373      0.87428115798E-04
57030.912120      0.45961641275E-03
16153.303915      0.19363890742E-02
5269.4109288      0.69994046497E-02
1902.0315541      0.22312068196E-01
741.57677159      0.62808077697E-01
307.20901906      0.15101140997
133.52786203      0.28713661177
60.253381291      0.36385490107
3 s
522.02426206      0.18071323116E-01
161.51290469      0.16449219884
62.126369433      0.63897334899
1 s
27.590930012      1.0000000000
1 s
11.175528881      1.0000000000
1 s
5.2959065137      1.0000000000
1 s
2.4782798895      1.0000000000
1 s
0.91262095059      1.0000000000
1 s
0.40426067549      1.0000000000
1 s
0.16562886306      1.0000000000
8 p
2868.4504581      0.24010435121E-03
679.71869590      0.20904788665E-02
220.36758824      0.11369316839E-01
83.620439734      0.44901977398E-01
34.964322657      0.13237156770
15.525131784      0.27709277600
7.0992979806      0.38613979646
3.3021336602      0.28492925372
2 p
128.78765667      -0.30509457751E-01
8.4357867977      0.64101621070
1 p
1.4618661855      1.0000000000
1 p
0.64658010096      1.0000000000
1 p
0.27229295755      1.0000000000
1 p
0.10905182449      1.0000000000
1 d
6.3150000000      1.0000000000
1 d
1.5620000000      1.0000000000

```

```

1 d
0.71500000000 1.0000000000
1 d
0.29700000000 1.0000000000
1 f
0.54300000000 1.0000000000
1 f
1.3250000000 1.0000000000
1 g
1.0070000000 1.0000000000
*
*
k def2-QZVPP
# k (24s18p4d3f) / [11s6p4d3f] {(11)4111111111/951111/1111/111}
*
11 s
2022075.1391 0.10144874011E-04
303044.65568 0.78783500963E-04
69013.938490 0.41380919674E-03
19559.244615 0.17427571893E-02
6383.8934901 0.63004086126E-02
2305.3502858 0.20125347032E-01
899.14418101 0.56966060520E-01
372.59500133 0.13882654093
161.97635247 0.27132285414
73.085553853 0.36383620662
33.595644762 0.24724464776
4 s
685.49855365 0.44367463797E-02
211.66163373 0.42502718169E-01
80.851405131 0.18467742018
35.108667236 0.29353173891
1 s
14.409437283 1.0000000000
1 s
6.8697147262 1.0000000000
1 s
3.2121883687 1.0000000000
1 s
1.2610484365 1.0000000000
1 s
0.61438946301 1.0000000000
1 s
0.27264370973 1.0000000000
1 s
0.77173005207E-01 1.0000000000
1 s
0.40918397569E-01 1.0000000000
1 s
0.17055762425E-01 1.0000000000
9 p
3469.6649718 0.21340225970E-03
822.02356107 0.18637844836E-02
266.58406636 0.10211431546E-01
101.28048161 0.40799604728E-01
42.429490761 0.12257473393
18.912083912 0.26405833679
8.7017779030 0.38227164575
4.0854567599 0.29998812383
1.8667286060 0.78007265591E-01

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```

5 p
27.544639057 -0.58222994163E-02
9.2098893609 -0.26787531329E-01
1.7232877425 0.30666847665
0.77969303735 0.66927944165
0.34379047862 0.60376468615
1 p
0.14346681918 1.0000000000
1 p
0.68000000000E-01 1.0000000000
1 p
0.32000000000E-01 1.0000000000
1 p
0.15300000000E-01 1.0000000000
1 d
1.7000000000 1.0000000000
1 d
0.5100000000 1.0000000000
1 d
0.1800000000 1.0000000000
1 d
0.54000000000E-01 1.0000000000
1 f
2.3700000000 1.0000000000
1 f
0.7900000000 1.0000000000
1 f
0.90000000000E-01 1.0000000000
*
*
ca def2-QZVPP
# ca (24s18p6d3f) / [11s6p4d3f] {(11)4111111111/951111/3111/111}
*
11 s
2433075.4304 0.91625196182E-05
364160.43015 0.71271617974E-04
82898.747637 0.37433706369E-03
23499.730540 0.15762862250E-02
7671.2245985 0.57026102580E-02
2770.2330687 0.18255738108E-01
1080.6807550 0.51906421035E-01
448.04894531 0.12791238579
194.92007727 0.25586635231
88.039793338 0.36028678275
40.645696719 0.26838462020
4 s
779.53331918 -0.18403005509E-01
241.18856300 -0.17649440544
92.403869324 -0.77662799584
39.786090342 -1.3352155444
1 s
18.195864278 1.0000000000
1 s
8.3321457067 1.0000000000
1 s
3.9190196209 1.0000000000
1 s
1.6667099493 1.0000000000
1 s
0.80891084908 1.0000000000

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1 s
0.36174199934      1.0000000000
1 s
0.82379874526E-01  1.0000000000
1 s
0.47947864375E-01  1.0000000000
1 s
0.22308112408E-01  1.0000000000
9 p
4064.2232796      0.19780891021E-03
962.91550624      0.17307465902E-02
312.34501046      0.95298721105E-02
118.76056036      0.38387459783E-01
49.816153133      0.11679256218
22.259679401      0.25637225097
10.286094124      0.37986193747
4.8606982416      0.30805760637
2.2525682942      0.85755999942E-01
5 p
31.467555443      -0.42441487483E-02
10.657589056      -0.19579425947E-01
2.0505555426      0.21237507422
0.94362089228      0.46277871121
0.42709067504      0.39177495728
1 p
0.17788187209      1.0000000000
1 p
0.86000000000E-01  1.0000000000
1 p
0.41500000000E-01  1.0000000000
1 p
0.20000000000E-01  1.0000000000
3 d
16.924012098      0.35543971560E-01
4.4655403330      0.18133698335
1.4347576200      0.48002060116
1 d
0.46552376784      1.0000000000
1 d
0.14097711082      1.0000000000
1 d
0.41467009281E-01  1.0000000000
1 f
2.6500000000      1.0000000000
1 f
0.79400000000      1.0000000000
1 f
0.13000000000      1.0000000000
*
*
sc def2-QZVPP
# sc      (24s18p9d3f2g) / [11s6p5d3f2g]      {(11)}
4111111111/951111/51111/111/11}
*
11 s
2855231.1264      0.84862794535E-05
427433.34221      0.65998092974E-04
97233.218545      0.34740968058E-03
27496.222846      0.14694099525E-02
8948.7324409      0.53410667286E-02

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3221.0397292	0.17200652511E-01
1252.0534077	0.49287065332E-01
517.26093376	0.12273534550
224.33127242	0.24910183844
101.10551671	0.35884366997
46.684957855	0.27782811319
4 s	
947.75965484	0.36123019249E-02
293.07262846	0.35616224567E-01
111.70230657	0.16664064248
47.756215212	0.32531051399
1 s	
21.121984009	1.0000000000
1 s	
9.7765922198	1.0000000000
1 s	
4.5982699340	1.0000000000
1 s	
1.9928487767	1.0000000000
1 s	
0.95939954457	1.0000000000
1 s	
0.42566790070	1.0000000000
1 s	
0.98132196006E-01	1.0000000000
1 s	
0.56894222237E-01	1.0000000000
1 s	
0.25369907195E-01	1.0000000000
9 p	
4611.4680242	0.19180655992E-03
1092.4666458	0.16801897753E-02
354.41923265	0.92763338425E-02
134.83390286	0.37537202735E-01
56.610873926	0.11493045217
25.336605518	0.25446811084
11.741313238	0.37993352765
5.5697268625	0.30948776388
2.5949954062	0.86972259257E-01
5 p	
35.951198081	-0.55780446917E-02
12.301020232	-0.25933825208E-01
2.3876557755	0.27489094204
1.1031823600	0.59208047142
0.50008479496	0.49113471853
1 p	
0.20796508799	1.0000000000
1 p	
0.10100000000	1.0000000000
1 p	
0.48000000000E-01	1.0000000000
1 p	
0.23000000000E-01	1.0000000000
5 d	
73.531179748	0.22506354976E-02
21.764759639	0.16377610133E-01
7.9233701690	0.63330446952E-01
3.1847889778	0.17056208548
1.3427790019	0.30119020299
1 d	

```

0.56149574983      1.0000000000
  1 d
0.22764073650      1.0000000000
  1 d
0.85211221793E-01  1.0000000000
  1 d
0.35000000000E-01  1.0000000000
  1 f
  1.4810000000      1.0000000000
  1 f
0.34500000000      1.0000000000
  1 f
0.11000000000      1.0000000000
  1 g
0.53100000000      1.0000000000
  1 g
0.13300000000      1.0000000000
*
*
ti def2-QZVPP
# ti      (24s18p9d3f2g) / [11s6p5d3f2g]      {(11)
4111111111/951111/51111/111/11}
*
  11 s
3070548.8651      0.86954016630E-05
460777.88643      0.67452737727E-04
104901.22889      0.35477293028E-03
29695.861199      0.14977525588E-02
9678.8892688      0.54309912055E-02
3490.1877912      0.17439360524E-01
1359.2217621      0.49835634640E-01
562.42721208      0.12379633943
244.22296250      0.25057490943
110.16668710      0.35934609007
50.881903357      0.27594242664
  4 s
965.95430789      0.41773927781E-02
299.27072059      0.40277148567E-01
114.83772939      0.17898686817
49.477578954      0.31783043543
  1 s
22.982839977      1.0000000000
  1 s
10.518305037      1.0000000000
  1 s
4.9774390567      1.0000000000
  1 s
2.1339846838      1.0000000000
  1 s
1.0342457284      1.0000000000
  1 s
0.46199774995      1.0000000000
  1 s
0.10621264194      1.0000000000
  1 s
0.54340347374E-01  1.0000000000
  1 s
0.25110217385E-01  1.0000000000
  9 p
5169.6755427      0.18802523596E-03

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1225.0961638	0.16473458826E-02	
397.60051934	0.91104554321E-02	
151.36154684	0.36987450926E-01	
63.613321773	0.11376329624	
28.514560307	0.25345208574	
13.248003298	0.38019402704	
6.3048807760	0.30989136346	
2.9493525821	0.87418944007E-01	
5 p		
40.738772213	-0.73233793267E-02	
14.062358461	-0.34282591082E-01	
2.7460680961	0.35655009250	
1.2713688141	0.76112035427	
0.57610015545	0.62716743237	
1 p		
0.23981820724	1.0000000000	
1 p		
0.11000000000	1.0000000000	
1 p		
0.50000000000E-01	1.0000000000	
1 p		
0.23000000000E-01	1.0000000000	
5 d		
89.589880075	0.21223030030E-02	
26.591412960	0.15911819913E-01	
9.7739715702	0.62875243121E-01	
3.9625083655	0.17144170807	
1.6890532654	0.30565506624	
1 d		
0.71539771469	1.0000000000	
1 d		
0.29366677748	1.0000000000	
1 d		
0.11079094851	1.0000000000	
1 d		
0.45000000000E-01	1.0000000000	
1 f		
2.0930000000	1.0000000000	
1 f		
0.56200000000	1.0000000000	
1 f		
0.19100000000	1.0000000000	
1 g		
1.0040000000	1.0000000000	
1 g		
0.26800000000	1.0000000000	
*		
*		
v def2-QZVPP		
# v (24s18p9d3f2g) / [11s6p5d3f2g]	{(11)}	
4111111111/951111/51111/111/11}		
*		
11 s		
3360380.0382	0.87027840678E-05	
502646.73178	0.67786024965E-04	
114247.22867	0.35699229090E-03	
32321.972630	0.15075507352E-02	
10532.947271	0.54664377528E-02	
3798.3004439	0.17547310839E-01	
1479.6094715	0.50106594778E-01	

612.57405507	0.12431296066
266.22103326	0.25117026883
120.21980126	0.35926015903
55.591180848	0.27505075685
4 s	
1082.4768635	0.39326847695E-02
334.94462061	0.38298477998E-01
128.31559026	0.17259908827
55.311589616	0.31287423870
1 s	
25.108383036	1.0000000000
1 s	
11.667553242	1.0000000000
1 s	
5.5372073270	1.0000000000
1 s	
2.3781007618	1.0000000000
1 s	
1.1506947329	1.0000000000
1 s	
0.51283991040	1.0000000000
1 s	
0.11625711449	1.0000000000
1 s	
0.58272785598E-01	1.0000000000
1 s	
0.26662312245E-01	1.0000000000
9 p	
5782.8035005	0.18344743045E-03
1369.9392282	0.16095217453E-02
444.53147129	0.89242268749E-02
169.25617556	0.36375182379E-01
71.168730031	0.11246803294
31.933358374	0.25226107794
14.865336779	0.38039695005
7.0921740091	0.31068797325
3.3281157846	0.88141200458E-01
5 p	
45.842906017	-0.56661391945E-02
15.940339016	-0.26718979445E-01
3.1257155025	0.27354632707
1.4485867558	0.57972883053
0.65577902825	0.47601110515
1 p	
0.27311626644	1.0000000000
1 p	
0.12200000000	1.0000000000
1 p	
0.55000000000E-01	1.0000000000
1 p	
0.25000000000E-01	1.0000000000
5 d	
103.95047414	0.21007158819E-02
30.901688665	0.16015244877E-01
11.420321145	0.64127456940E-01
4.6573272292	0.17488905695
1.9963682623	0.31003778048
1 d	
0.84967249531	1.0000000000
1 d	

```

0.34953221876      1.0000000000
 1 d
0.13165588233      1.0000000000
 1 d
0.52000000000E-01  1.0000000000
 1 f
 2.9330000000      1.0000000000
 1 f
0.83100000000      1.0000000000
 1 f
0.25700000000      1.0000000000
 1 g
 1.8560000000      1.0000000000
 1 g
0.45500000000      1.0000000000
*
*
cr def2-QZVPP
# cr      (24s18p9d3f2g) / [11s6p5d3f2g]      {(11)
4111111111/951111/51111/111/11}
*
 11 s
3637838.6820      0.87693297699E-05
544864.46100      0.68169050223E-04
123997.55079      0.35844590272E-03
35116.733166      0.15117006948E-02
11455.702298      0.54731929774E-02
4135.9906712      0.17539430107E-01
1613.2513581      0.50004870927E-01
668.77932380      0.12393518958
291.01365155      0.25039606407
131.57328167      0.35870470429
60.924567928      0.27581148880
 4 s
1196.2899601      0.77368642037E-02
369.76947592      0.75837835399E-01
141.54426084      0.34435148637
60.999228765      0.63249297923
 1 s
27.599113358      1.0000000000
 1 s
12.882112056      1.0000000000
 1 s
 6.1247513721      1.0000000000
 1 s
 2.6332895309      1.0000000000
 1 s
 1.2708482289      1.0000000000
 1 s
0.56483575923      1.0000000000
 1 s
0.12596808943      1.0000000000
 1 s
0.62045607277E-01  1.0000000000
 1 s
0.28144312720E-01  1.0000000000
 9 p
6395.8781792      0.18104788151E-03
1515.1701574      0.15893658935E-02
491.70538681      0.88258739429E-02

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187.28416675	0.36068946983E-01	
78.800346444	0.11189649648	
35.396291693	0.25202239843	
16.509278879	0.38082266430	
7.8947396863	0.31035222437	
3.7136414465	0.87980310362E-01	
5 p		
51.259312534	-0.60542038165E-02	
17.934932523	-0.28761764001E-01	
3.5257174218	0.29087768170	
1.6339163906	0.61267525056	
0.73852413834	0.50126035018	
1 p		
0.30752368193	1.0000000000	
1 p		
0.13500000000	1.0000000000	
1 p		
0.59000000000E-01	1.0000000000	
1 p		
0.26000000000E-01	1.0000000000	
5 d		
118.24986288	0.21012757435E-02	
35.193935700	0.16212269500E-01	
13.057816022	0.65581852668E-01	
5.3485602844	0.17849601449	
2.3004233713	0.31376763016	
1 d		
0.98114328305	1.0000000000	
1 d		
0.40334183206	1.0000000000	
1 d		
0.15135589551	1.0000000000	
1 d		
0.60000000000E-01	1.0000000000	
1 f		
3.7330000000	1.0000000000	
1 f		
1.1470000000	1.0000000000	
1 f		
0.3660000000	1.0000000000	
1 g		
2.6570000000	1.0000000000	
1 g		
0.7190000000	1.0000000000	
*		
*		
mn def2-QZVPP		
# mn (24s18p10d4f2g) / [11s6p5d4f2g]	{(11)}	
4111111111/951111/61111/1111/11}		
*		
11 s		
4289357.6441	0.79360554972E-05	
636361.00285	0.62542986761E-04	
143637.27569	0.33226388724E-03	
40406.345432	0.14130009568E-02	
13104.363417	0.51560918319E-02	
4705.0664255	0.16659574919E-01	
1825.7125432	0.47908083403E-01	
753.33816229	0.11994903752	
326.47253285	0.24550296959	

147.10300670	0.35822739571
67.987226869	0.28295764442
4 s	
1300.7266717	0.76025154141E-02
402.72027544	0.74365109808E-01
154.38971348	0.33780474819
66.443384613	0.62779331746
1 s	
30.975316006	1.0000000000
1 s	
14.222980890	1.0000000000
1 s	
6.7598265074	1.0000000000
1 s	
2.9087083287	1.0000000000
1 s	
1.3966507792	1.0000000000
1 s	
0.61792624091	1.0000000000
1 s	
0.13439483715	1.0000000000
1 s	
0.65195053803E-01	1.0000000000
1 s	
0.29415713624E-01	1.0000000000
9 p	
6483.2629658	0.20479778890E-03
1556.7134859	0.17525750185E-02
509.73925460	0.95798802458E-02
195.28408089	0.38681362983E-01
82.542547525	0.11832401588
37.212076731	0.26168459627
17.425804462	0.38400628821
8.3691376962	0.29704166759
3.9409000444	0.78263290323E-01
5 p	
57.202741010	-0.47749099800E-02
20.090935947	-0.22989729915E-01
3.9357553763	0.23197065881
1.8181984012	0.48435204043
0.81881535281	0.39159479004
1 p	
0.34038359193	1.0000000000
1 p	
0.15000000000	1.0000000000
1 p	
0.63000000000E-01	1.0000000000
1 p	
0.27000000000E-01	1.0000000000
6 d	
200.40254535	0.89549560240E-03
59.898225773	0.76257630942E-02
22.810570167	0.34523224226E-01
9.5874142097	0.10552676975
4.2933710910	0.22575377683
1.9537618373	0.32766533667
1 d	
0.87378873598	1.0000000000
1 d	
0.37597748904	1.0000000000

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1 d
0.14811547592      1.0000000000
1 d
0.60000000000E-01  1.0000000000
1 f
4.3530000000      1.0000000000
1 f
1.3260000000      1.0000000000
1 f
0.40800000000     1.0000000000
1 f
0.12550000000     1.0000000000
1 g
3.3160000000      1.0000000000
1 g
0.92900000000     1.0000000000
*
*
fe def2-QZVPP
# fe      (24s18p10d4f2g) / [11s6p5d4f2g]      {(11)}
4111111111/951111/61111/1111/11}
*
11 s
4313154.4338      0.86712290122E-05
645875.08253      0.67423150519E-04
146981.87698      0.35448747955E-03
41630.615044      0.14948285557E-02
13580.620109      0.54136698440E-02
4902.0620613      0.17362460824E-01
1911.2900837      0.49566574059E-01
791.99837852      0.12309089705
344.54799181      0.24936705764
155.78722730      0.35858414677
72.179380315      0.27738221642
4 s
1417.9125091      0.74871631942E-02
439.23184195      0.73337584435E-01
168.51006820      0.33383143870
72.776269412      0.62022524641
1 s
32.752961774      1.0000000000
1 s
15.434336101      1.0000000000
1 s
7.3639318205      1.0000000000
1 s
3.1698832880      1.0000000000
1 s
1.5243708395      1.0000000000
1 s
0.67496281152      1.0000000000
1 s
0.14718566032      1.0000000000
1 s
0.70082216629E-01  1.0000000000
1 s
0.31208269419E-01  1.0000000000
9 p
7709.0587627      0.17711229843E-03
1826.4666323      0.15560056795E-02

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592.84368362	0.86629536960E-02	
225.93763245	0.35565954156E-01	
95.164758890	0.11098847278	
42.823132375	0.25177796624	
20.036286581	0.38166911079	
9.6159346283	0.30963598261	
4.5393538787	0.87558276626E-01	
5 p		
62.997519003	-0.50910388724E-02	
22.262748731	-0.24540463235E-01	
4.3900064942	0.24345605487	
2.0328913928	0.50781898425	
0.91592621576	0.41214895672	
1 p		
0.38036653507	1.0000000000	
1 p		
0.16000000000	1.0000000000	
1 p		
0.67000000000E-01	1.0000000000	
1 p		
0.28000000000E-01	1.0000000000	
6 d		
218.33430163	0.93700006628E-03	
65.256292616	0.80008769378E-02	
24.866944817	0.36305286587E-01	
10.473399301	0.11057189871	
4.6947005007	0.23219588596	
2.1315982534	0.32922859685	
1 d		
0.94748004605	1.0000000000	
1 d		
0.40346488831	1.0000000000	
1 d		
0.15687414728	1.0000000000	
1 d		
0.62000000000E-01	1.0000000000	
1 f		
5.1030000000	1.0000000000	
1 f		
1.5980000000	1.0000000000	
1 f		
0.50500000000	1.0000000000	
1 f		
0.15960000000	1.0000000000	
1 g		
3.9750000000	1.0000000000	
1 g		
1.1390000000	1.0000000000	
*		
*		
co def2-QZVPP		
# co (24s18p10d4f2g) / [11s6p5d4f2g]	{(11)}	
4111111111/951111/61111/1111/11}		
*		
11 s		
4658206.5032	0.86609506454E-05	
697560.87453	0.67336300186E-04	
158759.87124	0.35399044899E-03	
44969.099379	0.14926384309E-02	
14670.714247	0.54053095095E-02	

5295.8947250	0.17335233605E-01
2065.0581167	0.49486641301E-01
855.90627750	0.12289351961
372.48747255	0.24903230028
168.50576608	0.35838320259
78.128761566	0.27777974150
4 s	
1534.5149885	0.74464372833E-02
475.52976096	0.72993601986E-01
182.54836839	0.33243104986
78.916467177	0.61900490005
1 s	
35.500865522	1.0000000000
1 s	
16.790414486	1.0000000000
1 s	
8.0240232510	1.0000000000
1 s	
3.4571682964	1.0000000000
1 s	
1.6599835391	1.0000000000
1 s	
0.73380022453	1.0000000000
1 s	
0.15878613103	1.0000000000
1 s	
0.74535659476E-01	1.0000000000
1 s	
0.32867351695E-01	1.0000000000
9 p	
8425.4331352	0.17491775490E-03
1995.8758452	0.15378901702E-02
647.76765681	0.85752453448E-02
246.88261214	0.35295266911E-01
104.00952246	0.11050007672
46.827478138	0.25160924538
21.934444535	0.38209003019
10.540499528	0.30947119879
4.9820419385	0.87436873012E-01
5 p	
69.270787130	-0.61172424428E-02
24.583977935	-0.29655043898E-01
4.8562258878	0.29163333190
2.2480916102	0.60629408335
1.0114285977	0.49057440018
1 p	
0.41919905455	1.0000000000
1 p	
0.17500000000	1.0000000000
1 p	
0.73000000000E-01	1.0000000000
1 p	
0.30000000000E-01	1.0000000000
6 d	
237.58450966	0.97593282671E-03
71.086896302	0.83432571945E-02
27.119080683	0.37958471100E-01
11.448239054	0.11522936171
5.1391806672	0.23843467913
2.3323492099	0.33205699955

1	d		
1.0338662062		0.33276836067	
1	d		
0.43785146294		0.22769290932	
1	d		
0.16895004948		0.74634129160E-01	
1	d		
0.66000000000E-01		1.0000000000	
1	f		
5.9750000000		1.0000000000	
1	f		
1.9030000000		1.0000000000	
1	f		
0.59400000000		1.0000000000	
1	f		
0.18540000000		1.0000000000	
1	g		
4.6350000000		1.0000000000	
1	g		
1.3490000000		1.0000000000	
*			
*			
ni	def2-QZVPP		
# ni	(24s18p10d4f2g) / [11s6p5d4f2g]	{(11)}	
4111111111/951111/61111/1111/11}			
*			
11	s		
5037649.9532		0.86072778771E-05	
754246.39418		0.66935354750E-04	
171644.16010		0.35190801168E-03	
48617.230286		0.14839082715E-02	
15860.961795		0.53736344264E-02	
5726.0018653		0.17233376287E-01	
2232.9547317		0.49211476915E-01	
925.49649101		0.12232504536	
402.75336913		0.24829251588	
182.19422856		0.35825476194	
84.494109788		0.27881865553	
4	s		
1678.0564586		0.82462870895E-02	
519.21358326		0.81505940361E-01	
198.95881607		0.37495727651	
85.901180703		0.70841743832	
1	s		
38.435760123		1.0000000000	
1	s		
18.252349351		1.0000000000	
1	s		
8.7283616939		1.0000000000	
1	s		
3.7616245662		1.0000000000	
1	s		
1.8028217338		1.0000000000	
1	s		
0.79507140513		1.0000000000	
1	s		
0.17031720284		1.0000000000	
1	s		
0.78971236177E-01		1.0000000000	
1	s		

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0.34503486750E-01  1.0000000000
 9 p
9156.5701453      0.17346418360E-03
2169.0239526      0.15257220493E-02
703.98918991      0.85163281036E-02
268.36293215      0.35117466952E-01
113.10288796      0.11020275383
50.955539222      0.25162601670
23.896708209      0.38246389853
11.498241522      0.30907230267
5.4410908056      0.87194377415E-01
 5 p
75.938560736      -0.74635546629E-02
27.037350184      -0.36453401627E-01
5.3404687432      0.35633549406
2.4700181361      0.73774121992
1.1095029064      0.59439383024
 1 p
0.45899767101     1.0000000000
 1 p
0.18700000000     1.0000000000
 1 p
0.76200000000E-01 1.0000000000
 1 p
0.31000000000E-01 1.0000000000
 6 d
258.11131142      0.23726274275E-02
77.254891371      0.20330132784E-01
29.500240033      0.92748486665E-01
12.477446945      0.28082284560
5.6070455111      0.57392657880
2.5427744163      0.78766058527
 1 d
1.1238296774      0.77868790423
 1 d
0.47361171459     0.52932234348
 1 d
0.18161858319     0.17478168242
 1 d
0.71000000000E-01 1.0000000000
 1 f
6.7580000000      1.0000000000
 1 f
2.1740000000      1.0000000000
 1 f
0.6810000000      1.0000000000
 1 f
0.2130000000      1.0000000000
 1 g
5.2940000000      1.0000000000
 1 g
1.5580000000      1.0000000000
*
*
cu def2-QZVPP
# cu      (24s18p10d4f2g) / [11s6p5d4f2g]      {(11)
4111111111/951111/61111/1111/11}
*
 11 s
5056467.8898      0.93501916365E-05

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759457.83835	0.72323443222E-04
173524.88497	0.37813833845E-03
49327.259988	0.15870129862E-02
16144.149930	0.57220685294E-02
5844.5964680	0.18268390048E-01
2284.6812739	0.51893720863E-01
948.88232514	0.12796192366
413.66215455	0.25629891036
187.38942059	0.36064416138
86.872771648	0.26833664660
4 s	
1744.0598287	0.88587079141E-02
540.93295513	0.86522785813E-01
207.99736224	0.38932285258
90.475793036	0.69777199902
1 s	
38.869687699	1.0000000000
1 s	
18.974829147	1.0000000000
1 s	
9.0953644635	1.0000000000
1 s	
3.8330020174	1.0000000000
1 s	
1.8198891499	1.0000000000
1 s	
0.79068098393	1.0000000000
1 s	
0.14914142106	1.0000000000
1 s	
0.72448090592E-01	1.0000000000
1 s	
0.30959925368E-01	1.0000000000
9 p	
9720.4614555	0.17828803512E-03
2302.7557452	0.15678108633E-02
747.48498314	0.87470094509E-02
285.00132623	0.36044549301E-01
120.15121609	0.11287209053
54.145261156	0.25647377341
25.406033563	0.38512918379
12.224331465	0.30316512356
5.7638720668	0.81677218969E-01
5 p	
83.210837217	-0.63530359993E-02
29.694779129	-0.31383834666E-01
5.8248516206	0.30930039753
2.6746181180	0.63583925938
1.1841836775	0.50946045967
1 p	
0.48043583535	1.0000000000
1 p	
0.18700000000	1.0000000000
1 p	
0.76200000000E-01	1.0000000000
1 p	
0.31000000000E-01	1.0000000000
6 d	
249.54025080	0.12432881244E-02
74.683914534	0.10456901995E-01

28.392717116	0.46451241249E-01	
11.955968430	0.13541359729	
5.3210744624	0.25852899978	
2.3661189459	0.33168127635	
1 d		
1.0131863994	1.0000000000	
1 d		
0.40710035940	1.0000000000	
1 d		
0.14742541032	1.0000000000	
1 d		
0.71000000000E-01	1.0000000000	
1 f		
6.9620000000	1.0000000000	
1 f		
2.2330000000	1.0000000000	
1 f		
0.70400000000	1.0000000000	
1 f		
0.24000000000	1.0000000000	
1 g		
5.9530000000	1.0000000000	
1 g		
1.7680000000	1.0000000000	
*		
*		
zn def2-QZVPP		
# zn (24s18p10d4f2g) / [11s6p5d4f2g]	{(11)}	
4111111111/951111/61111/1111/11}		
*		
11 s		
5742307.1507	0.86864381562E-05	
861450.78790	0.67364668570E-04	
196346.05866	0.35349715135E-03	
55682.870737	0.14884153943E-02	
18183.902394	0.53840916617E-02	
6569.6448019	0.17252738209E-01	
2563.5613276	0.49238679132E-01	
1063.1147176	0.12235812174	
462.89771078	0.24835390245	
209.52821049	0.35830632832	
97.240787991	0.27880259960	
4 s		
1929.2689992	0.83077002177E-02	
598.07122307	0.81882590163E-01	
229.69667336	0.37588060221	
99.416819228	0.71067260445	
1 s		
44.241101421	1.0000000000	
1 s		
21.194367113	1.0000000000	
1 s		
10.158731597	1.0000000000	
1 s		
4.3746176158	1.0000000000	
1 s		
2.0901489071	1.0000000000	
1 s		
0.91869136437	1.0000000000	
1 s		

0.19278660606	1.0000000000
1 s	
0.87329915171E-01	1.0000000000
1 s	
0.37552217126E-01	1.0000000000
9 p	
10690.445107	0.17142867222E-03
2532.3159340	0.15088012830E-02
821.94295003	0.84368777910E-02
313.42757800	0.34898103208E-01
132.18314247	0.10993617353
59.620554387	0.25207277070
28.019488868	0.38325657524
13.511704850	0.30787091255
6.4053711253	0.86411696761E-01
5 p	
89.981131918	-0.96262847843E-02
32.241767106	-0.47509407258E-01
6.3809448581	0.45834100431
2.9477928353	0.94473799128
1.3200854955	0.75923464871
1 p	
0.54424674445	1.0000000000
1 p	
0.25799971797	1.0000000000
1 p	
0.92863192359E-01	1.0000000000
1 p	
0.34059341410E-01	1.0000000000
6 d	
305.22298937	0.27359792434E-02
91.468273202	0.23585229776E-01
34.986985968	0.10858422440
14.849415187	0.32843594226
6.6858545707	0.66180235634
3.0309412620	0.89165339320
1 d	
1.3355050671	1.0000000000
1 d	
0.55883176392	1.0000000000
1 d	
0.21180799287	1.0000000000
1 d	
0.83000000000E-01	1.0000000000
1 f	
8.0200000000	1.0000000000
1 f	
2.6140000000	1.0000000000
1 f	
0.83600000000	1.0000000000
1 f	
0.26730000000	1.0000000000
1 g	
6.6130000000	1.0000000000
1 g	
1.9780000000	1.0000000000
*	
*	
ga def2-QZVPP	
# ga (24s19p10d4f1g) / [11s7p4d4f1g] {(11)}	

4111111111/9241111/7111/1111/1}

*

11 s	
6623802.0274	0.79091326051E-05
987904.07075	0.61835727406E-04
224132.05899	0.32636322451E-03
63315.192943	0.13810365049E-02
20611.312702	0.50153772104E-02
7429.1672482	0.16130936803E-01
2894.2071720	0.46240827188E-01
1198.9915786	0.11579099571
521.82003812	0.23834840794
236.27549237	0.35374255971
109.98395671	0.29055721918
4 s	
2101.2587253	0.83039611523E-02
650.97022519	0.82254127688E-01
250.22438356	0.38021717478
108.17616625	0.74503594690
1 s	
51.057486710	1.0000000000
1 s	
23.647474527	1.0000000000
1 s	
11.361701144	1.0000000000
1 s	
5.0178135897	1.0000000000
1 s	
2.4102674998	1.0000000000
1 s	
1.0741046685	1.0000000000
1 s	
0.25745075831	1.0000000000
1 s	
0.12175227548	1.0000000000
1 s	
0.52360599017E-01	1.0000000000
9 p	
14711.750483	0.11130990649E-03
3482.1451716	0.98495921142E-03
1130.2186655	0.55854182058E-02
431.54093448	0.23682413047E-01
182.41723648	0.78211587173E-01
82.706753603	0.19503829929
39.228128772	0.34131988495
19.201979939	0.35718665135
9.5056966689	0.16395955052
2 p	
92.615613022	-0.85848284169E-01
33.750148165	-0.39435019538
4 p	
7.3482283015	0.37941606569
3.7813384844	0.71306291866
2.3145183128	0.43210001481
0.80346859715	0.25838122797
1 p	
1.5423710087	1.0000000000
1 p	
0.32910239639	1.0000000000
1 p	

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0.11834088831      1.0000000000
  1 p
0.41627877699E-01  1.0000000000
  7 d
363.49565218      0.87402299276E-03
109.01749589      0.76751934098E-02
41.866430715      0.36388975341E-01
17.879279894      0.11325183017
8.1201893671      0.23770881294
3.7360611356      0.33306060389
1.6826812549      0.33130613756
  1 d
0.72655790500      0.21895437571
  1 d
0.28498585079      1.0000000000
  1 d
0.11200000000      1.0000000000
  1 f
7.7947037670      1.0000000000
  1 f
2.2956705920      1.0000000000
  1 f
0.18100000000      1.0000000000
  1 f
0.47100000000      1.0000000000
  1 g
0.40320000000      1.0000000000
*
*
ge def2-QZVPP
# ge      (24s19p10d4f1g) / [11s7p4d4f1g]      {(11)
4111111111/9241111/7111/1111/1}
*
  11 s
7233056.0346      0.76638751457E-05
1082886.1731      0.59603601369E-04
246481.46959      0.31319088031E-03
69862.426955      0.13194051561E-02
22815.809662      0.47736099191E-02
8246.5369297      0.15319250467E-01
3219.9367257      0.43900870673E-01
1336.5743706      0.11028573632
582.87737501      0.22912630489
264.59511360      0.34779259246
123.77823320      0.29968722223
  4 s
2311.1055804      0.75033084731E-02
716.27089868      0.74778386626E-01
275.45330910      0.35092882302
118.93292565      0.72055989686
  1 s
58.435699085      1.0000000000
  1 s
26.261575973      1.0000000000
  1 s
12.664880671      1.0000000000
  1 s
5.7269548505      1.0000000000
  1 s
2.7555023203      1.0000000000

```

1 s	
1.2432886754	1.0000000000
1 s	
0.33107183846	1.0000000000
1 s	
0.15964081368	1.0000000000
1 s	
0.68463178923E-01	1.0000000000
9 p	
16555.711074	0.10199370391E-03
3914.9903745	0.90504190546E-03
1269.4766518	0.51558490762E-02
484.35437789	0.22010335708E-01
204.64985822	0.73434798827E-01
92.791032094	0.18608955294
44.055060255	0.33330981945
21.601319931	0.36229776246
10.732169233	0.17765186263
2 p	
100.88933962	-0.11146182144
36.640254741	-0.52324324314
4 p	
8.0343224115	0.31484763263
4.5613438333	0.38737744790
3.1794882223	0.50034353638
0.92612041457	0.22656707948
1 p	
1.7977040907	1.0000000000
1 p	
0.41386865432	1.0000000000
1 p	
0.15830798709	1.0000000000
1 p	
0.57877035911E-01	1.0000000000
7 d	
420.99565921	0.78212192196E-03
126.36209818	0.69560123831E-02
48.661473548	0.33712188323E-01
20.880325527	0.10717291194
9.5418229355	0.23161030141
4.4353653868	0.33390954301
2.0285421942	0.33720676378
1 d	
0.89484935267	0.21702473265
1 d	
0.35786074334	1.0000000000
1 d	
0.14000000000	1.0000000000
1 f	
8.9425329000	1.0000000000
1 f	
2.6920312990	1.0000000000
1 f	
0.54920000000	1.0000000000
1 f	
0.21900000000	1.0000000000
1 g	
0.46810000000	1.0000000000

*

*


```

as def2-QZVPP
# as      (24s20p10d4f1g) / [11s7p4d4f1g]      {(11)4111111111/(10)
511111/7111/1111/1}
*
  11 s
  8217482.6198      0.70590618422E-05
  1230500.3720      0.54880889611E-04
  280225.86648      0.28809164698E-03
  79482.509415      0.12129779464E-02
  25963.783351      0.43914559880E-02
  9381.4010193      0.14125362961E-01
  3660.4911972      0.40657915618E-01
  1518.2356024      0.10300382633
  661.80098920      0.21730077101
  300.58642127      0.33995751412
  141.11137296      0.31088634077
  4 s
  2577.0870580      0.70752991980E-02
  798.07872277      0.71383615256E-01
  306.57574948      0.34287024634
  132.27558802      0.74361403413
  1 s
  67.448702235      1.0000000000
  1 s
  29.209180441      1.0000000000
  1 s
  14.156509326      1.0000000000
  1 s
  6.5561506682      1.0000000000
  1 s
  3.1392847238      1.0000000000
  1 s
  1.4294631050      1.0000000000
  1 s
  0.41103390885      1.0000000000
  1 s
  0.20032453310      1.0000000000
  1 s
  0.85669928850E-01  1.0000000000
  10 p
  25198.504278      0.54758168372E-04
  5972.5601381      0.48572462452E-03
  1941.9123183      0.27908085625E-02
  743.59381104      0.12201505962E-01
  315.63828052      0.42666285138E-01
  143.96878925      0.11870919141
  69.068683164      0.24909407023
  34.254305629      0.36061356903
  17.371746759      0.29392241832
  8.7634555628      0.97829057366E-01
  5 p
  228.49024582      -0.24900140765E-02
  86.313555488      -0.19482515843E-01
  36.751366267      -0.61495071038E-01
  8.5365149464      0.47258065062
  4.1935128599      1.0236065079
  1 p
  2.0464980417      1.0000000000
  1 p
  0.98000000000      1.0000000000

```

```

1 p
0.40534340618      1.0000000000
1 p
0.16655070471      1.0000000000
1 p
0.65981706123E-01  1.0000000000
7 d
479.32599612      0.71722800196E-03
143.96064855      0.64419223046E-02
55.548909224      0.31776498964E-01
23.927581006      0.10276249168
10.988194172      0.22710952843
5.1489356262      0.33477474118
2.3836810892      0.34175986071
1 d
1.0688204667      0.21462891644
1 d
0.43305693742      1.0000000000
1 d
0.17000000000      1.0000000000
1 f
10.181096831      1.0000000000
1 f
3.1280704550      1.0000000000
1 f
0.26400000000      1.0000000000
1 f
0.64400000000      1.0000000000
1 g
0.54650000000      1.0000000000
*
*
se def2-QZVPP
# se      (24s20p10d4f1g) / [11s7p4d4f1g]      {(11)4111111111/(10)
511111/7111/1111/1}
*
11 s
9520446.7743      0.63309690150E-05
1424984.0802      0.49267697990E-04
324127.57682      0.25920249744E-03
91774.876950      0.10943145743E-02
29932.725725      0.39706139067E-02
10804.617905      0.12801187916E-01
4214.0134779      0.36980379417E-01
1747.8116633      0.94461349896E-01
762.12160878      0.20274705434
346.45604141      0.32878956424
163.11569304      0.32300252609
4 s
2614.5153067      0.79113928518E-02
818.68552756      0.77187739408E-01
318.63398991      0.35672061949
139.04844125      0.75846750004
1 s
78.348734788      1.0000000000
1 s
31.704290663      1.0000000000
1 s
15.505859269      1.0000000000
1 s

```

7.3227423625	1.0000000000
1 s	
3.4969483549	1.0000000000
1 s	
1.6121546085	1.0000000000
1 s	
0.49587158541	1.0000000000
1 s	
0.24092138175	1.0000000000
1 s	
0.10231739397	1.0000000000
10 p	
25360.215615	0.60531790911E-04
5993.7896610	0.53987774437E-03
1943.0741755	0.31130456170E-02
742.35316156	0.13599674694E-01
314.62114597	0.47298958377E-01
143.34748044	0.12981487726
68.673617552	0.26569982215
34.013554117	0.36723195311
17.198099621	0.27478356345
8.5830329629	0.79256169683E-01
5 p	
236.58209146	-0.12271649354E-02
90.576183214	-0.92584627774E-02
39.086689301	-0.28428728384E-01
9.3084344018	0.21201102192
4.6169923084	0.47117589805
1 p	
2.2653477506	1.0000000000
1 p	
1.0800000000	1.0000000000
1 p	
0.47939328581	1.0000000000
1 p	
0.19619983845	1.0000000000
1 p	
0.76256339275E-01	1.0000000000
7 d	
539.48700124	0.66722955533E-03
162.13394435	0.60399330928E-02
62.661795641	0.30238666507E-01
27.077272889	0.99267892065E-01
12.483003929	0.22358036310
5.8864623136	0.33574682762
2.7519131105	0.34554856483
1 d	
1.2500769617	0.21216654622
1 d	
0.51172841843	1.0000000000
1 d	
0.2000000000	1.0000000000
1 f	
11.333391939	1.0000000000
1 f	
3.5185505690	1.0000000000
1 f	
0.2840000000	1.0000000000
1 f	
0.7097000000	1.0000000000

```

1 g
0.57300000000 1.0000000000
*
*
br def2-QZVPP
# br (24s20p10d4f1g) / [11s7p4d4f1g] {(11)4111111111/(10)
511111/7111/1111/1}
*
11 s
10629044.264 0.59322104325E-05
1591918.2739 0.46118980689E-04
362333.98437 0.24244612378E-03
102643.11141 0.10231422748E-02
33489.846668 0.37121984175E-02
12091.247190 0.11978107933E-01
4716.1908789 0.34682692842E-01
1956.1598080 0.89068331264E-01
853.08595848 0.19330124567
387.96633666 0.32071144956
182.85156613 0.32996797574
4 s
3240.4086421 0.65905194070E-02
1000.4631935 0.68439609656E-01
383.37301682 0.34495478668
166.03929698 0.82315542085
1 s
87.919906994 1.0000000000
1 s
35.675840068 1.0000000000
1 s
17.543657842 1.0000000000
1 s
8.4473660433 1.0000000000
1 s
3.9666180616 1.0000000000
1 s
1.8356815987 1.0000000000
1 s
0.59084778776 1.0000000000
1 s
0.28863218421 1.0000000000
1 s
0.12153380537 1.0000000000
10 p
26566.476579 0.62073657410E-04
6290.5088566 0.55131636217E-03
2043.3178410 0.31680110980E-02
781.67221007 0.13816597290E-01
331.51078945 0.48018539681E-01
151.09198667 0.13162015183
72.395278166 0.26860052203
35.869510844 0.36827391093
18.139906191 0.27108612944
9.0466688944 0.76215338633E-01
5 p
253.71822146 -0.13729169381E-02
97.250818058 -0.10393811185E-01
42.034897960 -0.32204214612E-01
9.9685673555 0.24224770086
4.9395854745 0.53557868398

```

```

1 p
2.4382845475      1.0000000000
1 p
1.1800000000      1.0000000000
1 p
0.51047564965     1.0000000000
1 p
0.21215851928     1.0000000000
1 p
0.83943604990E-01 1.0000000000
7 d
601.44434484      0.62783723765E-03
180.85718640      0.57205157153E-02
69.986806340      0.29002521527E-01
30.324710300      0.96446989766E-01
14.027909238      0.22065825870
6.6511702082      0.33657642375
3.1354168338      0.34872040582
1 d
1.4393591843      0.20984536473
1 d
0.59350441438     1.0000000000
1 d
0.23000000000     1.0000000000
1 f
12.703062423      1.0000000000
1 f
4.0083455670      1.0000000000
1 f
0.34070000000     1.0000000000
1 f
0.82570000000     1.0000000000
1 g
0.64910000000     1.0000000000
*
*
kr def2-QZVPP
# kr      (24s20p10d4f1g) / [11s7p4d4f1g]      {(11)4111111111/(10)
511111/7111/1111/1}
*
11 s
11713823.008      0.56915790360E-05
1755253.3979      0.44214471278E-04
399717.41924      0.23227813842E-03
113285.79260      0.97973661050E-03
36977.205293      0.35537627541E-02
13355.036580      0.11468673282E-01
5210.9012988      0.33241627469E-01
2162.1137020      0.85620725674E-01
943.29291023      0.18708766876
429.20724331      0.31497583326
202.40720840      0.33406191042
4 s
3260.4985521      0.73091509287E-02
1011.1069716      0.74040355445E-01
392.44359273      0.35414962222
173.21702132      0.80188286115
1 s
96.619988467      1.0000000000
1 s

```

38.158284867	1.0000000000
1 s	
18.959517570	1.0000000000
1 s	
9.2505996199	1.0000000000
1 s	
4.3486517621	1.0000000000
1 s	
2.0380324209	1.0000000000
1 s	
0.69110152540	1.0000000000
1 s	
0.33506065143	1.0000000000
1 s	
0.14074441124	1.0000000000
10 p	
28609.335767	0.60526369543E-04
6773.1236364	0.53786288403E-03
2199.8011079	0.30935356550E-02
841.50201590	0.13514318412E-01
356.92110288	0.47090086910E-01
162.71174351	0.12960370449
78.004264994	0.26607435646
38.682579997	0.36775851233
19.589158685	0.27406903542
9.7990863417	0.78773352304E-01
5 p	
261.37786869	-0.16397212361E-02
100.09932146	-0.12034797573E-01
44.012139363	-0.34891485263E-01
10.854010739	0.25212650561
5.4351930182	0.57400781830
1 p	
2.7062805542	1.0000000000
1 p	
1.3195633408	1.0000000000
1 p	
0.58004455967	1.0000000000
1 p	
0.24329976264	1.0000000000
1 p	
0.96823725087E-01	1.0000000000
7 d	
665.35057386	0.59588702935E-03
200.17995366	0.54594260457E-02
77.545085570	0.27980992479E-01
33.677854345	0.94119165910E-01
15.624928334	0.21825215619
7.4427867423	0.33739971242
3.5336073535	0.35141418853
1 d	
1.6363725142	0.20756718931
1 d	
0.67845684728	1.0000000000
1 d	
0.27000000000	1.0000000000
1 f	
14.180116992	1.0000000000
1 f	
4.5393183680	1.0000000000

```

    1 f
    0.41300000000      1.0000000000
    1 f
    0.95570000000      1.0000000000
    1 g
    0.73950000000      1.0000000000
*
*
rb def2-QZVPP
# rb      (8s8p5d3f) / [7s5p4d3f]      {2111111/41111/2111/111}
*
    2 s
    7.4744618040      0.26999390986
    6.7296180594      -0.42624989529
    1 s
    2.7822883445      1.0000000000
    1 s
    0.53494544647      1.0000000000
    1 s
    0.22522959349      1.0000000000
    1 s
    0.50765580412E-01  1.0000000000
    1 s
    0.26940281781E-01  1.0000000000
    1 s
    0.13051395489E-01  1.0000000000
    4 p
    5.9998960731      0.54568549670E-01
    3.2040784712      -0.26447792498
    0.86991979950      0.50033505958
    0.44104169728      0.75243449327
    1 p
    0.22139898232      1.0000000000
    1 p
    0.10679039696      1.0000000000
    1 p
    0.33292658822E-01  1.0000000000
    1 p
    0.12847003750E-01  1.0000000000
    2 d
    4.6530655240      -0.11653388661E-02
    0.44914033653      0.15584297068
    1 d
    0.10089577190      0.48262396029
    1 d
    0.27432280711E-01  1.0000000000
    1 d
    0.95353625581E-02  1.0000000000
    1 f
    0.76580000000E-01  0.0000000000
    1 f
    0.48744000000      0.0000000000
    1 f
    1.18448000000      0.0000000000
*
rb def2-ecp
*
    ncore =      28      lmax =      3
#      coefficient      r^n      exponent
f

```

	-12.3169000	2	3.8431140
s-f	89.5001980	2	5.0365510
	0.4937610	2	1.9708490
	12.3169000	2	3.8431140
p-f	58.5689740	2	4.2583410
	0.4317910	2	1.4707090
	12.3169000	2	3.8431140
d-f	26.2248980	2	3.0231270
	0.9628390	2	0.6503830
	12.3169000	2	3.8431140

*

*

sr def2-QZVPP

sr (8s8p5d3f) / [7s5p4d3f] {21111111/411111/2111/111}

*

2 s		
11.000000000	-0.26157031021	
9.900000000	0.36446668395	
1 s		
2.8771178206	1.0000000000	
1 s		
0.63364987829	1.0000000000	
1 s		
0.28588739731	1.0000000000	
1 s		
0.61938540840E-01	1.0000000000	
1 s		
0.31237518881E-01	1.0000000000	
1 s		
0.16266139051E-01	1.0000000000	
4 p		
7.6233499793	0.71548409039E-01	
3.6643075442	-0.44232262175	
0.97809648234	0.55690782709	
0.77815253363	0.63437348922	
1 p		
0.40666316828	1.0000000000	
1 p		
0.18725455934	1.0000000000	
1 p		
0.56304594427E-01	1.0000000000	
1 p		
0.21826701680E-01	1.0000000000	
2 d		
4.3003648126	-0.43567751655E-02	
0.84876551534	0.13176477946	
1 d		
0.29200562252	0.27410245307	
1 d		
0.94733990946E-01	1.0000000000	
1 d		
0.30479894317E-01	1.0000000000	
1 f		
0.10940000000	0.0000000000	
1 f		
0.54080000000	0.0000000000	
1 f		


```

1.3460000000      0.0000000000
*
sr def2-ecp
*
ncore =      28          lmax =      3
#   coefficient   r^n      exponent
f      -15.8059920      2          4.6339750
s-f      135.4794300      2          7.4000740
          17.5344630      2          3.6063790
          15.8059920      2          4.6339750
p-f      88.3597090      2          6.4848680
          15.3943720      2          3.2880530
          15.8059920      2          4.6339750
d-f      29.8889870      2          4.6228410
          6.6594140      2          2.2469040
          15.8059920      2          4.6339750
*
*
y def2-QZVPP
# y      (8s8p7d3f2g) / [7s5p4d3f2g]      {2111111/41111/4111/111/11}
*
2 s
12.000000000      -0.27445870024
10.800000000      0.37995468727
1 s
3.1007372195      1.00000000000
1 s
0.74155427570      1.00000000000
1 s
0.34176775775      1.00000000000
1 s
0.79428797018E-01  1.00000000000
1 s
0.43308336524E-01  1.00000000000
1 s
0.21593224872E-01  1.00000000000
4 p
8.0336135138      0.73041700172E-01
4.0181723477      -0.41610436192
1.1052105890      0.55451897342
0.83219316692      0.62307196069
1 p
0.44762676666      1.00000000000
1 p
0.20523347112      1.00000000000
1 p
0.55045561759E-01  1.00000000000
1 p
0.22603027453E-01  1.00000000000
4 d
13.755105347      0.23830583863E-02
3.9629908552      -0.25068021047E-01
1.3427449755      0.22348991872
0.62579248108      0.55237929771
1 d
0.27632363958      1.00000000000

```

```

1 d
0.11706987754      1.0000000000
1 d
0.46601501035E-01  1.0000000000
1 f
0.76291000000      1.0000000000
1 f
0.26515000000      1.0000000000
1 f
0.92150000000E-01  1.0000000000
1 g
0.30250000000      1.0000000000
1 g
0.11474000000      1.0000000000
*
y def2-ecp
*
ncore =      28      lmax =      3
#      coefficient  r^n      exponent
f
      -19.1221981    2      6.5842120
      -2.4363754    2      3.2921060
s-f
      135.1538441    2      7.4880494
      15.5524413    2      3.7440247
      19.1221981    2      6.5842120
      2.4363754    2      3.2921060
p-f
      87.7849917    2      6.4453772
      11.5640660    2      3.2226886
      19.1221981    2      6.5842120
      2.4363754    2      3.2921060
d-f
      29.7010007    2      4.6584472
      5.5399685    2      2.3292236
      19.1221981    2      6.5842120
      2.4363754    2      3.2921060
*
*
zr def2-QZVPP
# zr      (8s8p7d3f2g) / [7s5p4d3f2g]      {21111111/41111/4111/111/11}
*
2 s
13.000000000      0.30219052022
11.750000000      -0.41145056914
1 s
3.3679085035      1.0000000000
1 s
0.83813257389      1.0000000000
1 s
0.39094081796      1.0000000000
1 s
0.12165103956      1.0000000000
1 s
0.68995924030E-01  1.0000000000
1 s
0.28131941438E-01  1.0000000000
4 p
8.6639962104      0.73773984271E-01
4.4109566148      -0.40022747074

```

```

1.2360133871      0.54947233625
0.87445820593    0.61937721413
  1 p
0.47713887642    1.00000000000
  1 p
0.21764845261    1.00000000000
  1 p
0.57837163627E-01  1.00000000000
  1 p
0.20242456645E-01  1.00000000000
  4 d
14.106535710     0.29285547494E-02
 5.0597471810    -0.19680100129E-01
 1.4340490314     0.24763912308
0.65933129072     0.53572735030
  1 d
0.28894952351    1.00000000000
  1 d
0.12160731860    1.00000000000
  1 d
0.48470078407E-01  1.00000000000
  1 f
 1.1417100000     1.00000000000
  1 f
0.39261000000     1.00000000000
  1 f
0.13501000000     1.00000000000
  1 g
0.53073000000     1.00000000000
  1 g
0.18969000000     1.00000000000
*
zr def2-ecp
*
  ncore =      28          lmax =      3
#   coefficient   r^n      exponent
f
  -21.0937760     2          7.5400000
  -3.0806943      2          3.7700000
s-f
  150.2675911     2          8.2000000
  18.9762165      2          4.0897278
  21.0937760      2          7.5400000
  3.0806943       2          3.7700000
p-f
  99.6221237      2          7.1100000
  14.1687333      2          3.5967980
  21.0937760      2          7.5400000
  3.0806943       2          3.7700000
d-f
  35.0451235      2          5.3500000
  6.1112595       2          2.4918215
  21.0937760      2          7.5400000
  3.0806943       2          3.7700000
*
*
nb def2-QZVPP
# nb      (8s8p7d3f2g) / [7s5p4d3f2g]      {2111111/41111/4111/111/11}
*
  2 s

```

13.500000000	-0.32410606901
12.200000000	0.44773333772
1 s	
3.7169274051	1.0000000000
1 s	
0.90652488058	1.0000000000
1 s	
0.41577606051	1.0000000000
1 s	
0.11042511303	1.0000000000
1 s	
0.62821821279E-01	1.0000000000
1 s	
0.28016289999E-01	1.0000000000
4 p	
9.3098091725	0.73705483583E-01
4.8178682975	-0.38234456657
1.3632838380	0.54987821838
0.90647526151	0.61931035808
1 p	
0.50089563075	1.0000000000
1 p	
0.22793279437	1.0000000000
1 p	
0.60000000000E-01	1.0000000000
1 p	
0.20600000000E-01	1.0000000000
4 d	
17.364404474	0.26413526976E-02
5.3680385855	-0.20806369564E-01
1.6586089067	0.24555637053
0.78121461396	0.53651499644
1 d	
0.34874234803	1.0000000000
1 d	
0.14844540532	1.0000000000
1 d	
0.59334919015E-01	1.0000000000
1 f	
1.5360500000	1.0000000000
1 f	
0.52270000000	1.0000000000
1 f	
0.17787000000	1.0000000000
1 g	
0.78318000000	1.0000000000
1 g	
0.26464000000	1.0000000000
*	
nb def2-ecp	
*	
ncore = 28	lmax = 3
# coefficient r^n	exponent
f	
-22.9295500	2 8.4900000
-3.6663099	2 4.2500000
s-f	
165.1791435	2 8.9000000
21.9929744	2 4.4300000
22.9295500	2 8.4900000

	3.6663099	2	4.2500000
p-f	111.7944145	2	7.7700000
	16.6334833	2	3.9600000
	22.9295500	2	8.4900000
	3.6663099	2	4.2500000
d-f	38.1122488	2	6.0500000
	8.0391673	2	2.8400000
	22.9295500	2	8.4900000
	3.6663099	2	4.2500000

*
*

mo def2-QZVPP
mo (9s8p7d3f2g) / [7s5p4d3f2g] {3111111/41111/4111/111/11}

*

3	s		
15.000000000		0.57082903143E-01	
13.500000000		-0.66824799324	
12.571764111		0.75521146249	
1	s		
4.1304342348		1.0000000000	
1	s		
0.96478113331		1.0000000000	
1	s		
0.43736648981		1.0000000000	
1	s		
0.11318605514		1.0000000000	
1	s		
0.57579423658E-01		1.0000000000	
1	s		
0.27018151462E-01		1.0000000000	
4	p		
9.1087343439		0.10192125262	
5.3495476626		-0.38460279534	
1.4870196599		0.53457134734	
0.90585473836		0.61724117143	
1	p		
0.50141240214		1.0000000000	
1	p		
0.23286318145		1.0000000000	
1	p		
0.62000000000E-01		1.0000000000	
1	p		
0.21000000000E-01		1.0000000000	
4	d		
17.215377137		0.30147475909E-02	
5.8496916871		-0.28923836319E-01	
1.8232967249		0.25398642015	
0.86970233105		0.52725603860	
1	d		
0.39461697588		1.0000000000	
1	d		
0.17084141240		1.0000000000	
1	d		
0.69272819629E-01		1.0000000000	
1	f		
1.9462500000		1.0000000000	
1	f		
0.65545000000		1.0000000000	

```

1 f
0.22074000000 1.0000000000
1 g
1.05980000000 1.0000000000
1 g
0.33958000000 1.0000000000
*
mo def2-ecp
*
ncore = 28 lmax = 3
# coefficient r^n exponent
f
-24.8051771 2 9.4500000
-4.1537815 2 4.7200000
s-f
180.1031085 2 9.7145938
24.9972279 2 4.6805004
24.8051771 2 9.4500000
4.1537815 2 4.7200000
p-f
123.7727523 2 8.1421366
19.5302280 2 4.6259863
24.8051771 2 9.4500000
4.1537815 2 4.7200000
d-f
48.3750223 2 6.6184148
8.8920527 2 3.2487516
24.8051771 2 9.4500000
4.1537815 2 4.7200000
*
*
tc def2-QZVPP
# tc (9s8p7d4f2g) / [7s5p4d4f2g] {3111111/41111/4111/1111/11}
*
3 s
15.000000000 -0.31349221639
13.500000000 0.44793618799
7.1022525122 0.20051786822E-01
1 s
4.4415995038 1.0000000000
1 s
1.0660127848 1.0000000000
1 s
0.48568559673 1.0000000000
1 s
0.12654965451 1.0000000000
1 s
0.66997954399E-01 1.0000000000
1 s
0.29822104753E-01 1.0000000000
4 p
10.298029968 0.83867175334E-01
5.7213792785 -0.36246957884
1.6296063991 0.53649463822
0.97528623230 0.61837212480
1 p
0.53997625690 1.0000000000
1 p
0.25172025379 1.0000000000
1 p

```

```

0.640000000000E-01  1.0000000000
 1 p
0.215000000000E-01  1.0000000000
 4 d
18.617708386      0.27056783609E-02
5.8369803972     -0.35968645824E-01
2.0921979438     0.21334851537
1.0148117201     0.45713971996
 1 d
0.46154215497    1.0000000000
 1 d
0.19795071041    1.0000000000
 1 d
0.78619872304E-01 1.0000000000
 1 f
2.3724000000     1.0000000000
 1 f
0.790800000000   1.0000000000
 1 f
0.263600000000   1.0000000000
 1 f
0.878700000000E-01 1.0000000000
 1 g
1.3606500000     1.0000000000
 1 g
0.41453000000    1.0000000000
*
tc def2-ecp
*
  ncore =    28      lmax =    3
#      coefficient  r^n      exponent
f
      -26.5624475   2      10.4000000
      -4.5856805   2      5.2000000
s-f
      195.1591659   2      10.4223462
      28.0926033   2      5.0365160
      26.5624475   2      10.4000000
      4.5856805    2      5.2000000
p-f
      135.2845662   2      8.9504494
      21.8065043   2      4.8544394
      26.5624475   2      10.4000000
      4.5856805    2      5.2000000
d-f
      54.3297294    2      6.9456968
      11.1550679    2      3.9705849
      26.5624475   2      10.4000000
      4.5856805    2      5.2000000
*
*
ru def2-QZVPP
# ru      (9s8p7d4f2g) / [7s5p4d4f2g]      {3111111/41111/4111/1111/11}
*
  3 s
15.000000000     0.40205707045
13.500000000     -0.59417167365
7.2130868530     0.12541032854
 1 s
4.5405901225     1.0000000000

```

```

1 s
1.1904973723      1.0000000000
1 s
0.54307531590    1.0000000000
1 s
0.13700563039    1.0000000000
1 s
0.73396375028E-01  1.0000000000
1 s
0.31250715458E-01  1.0000000000
4 p
11.388100061      0.55871461629E-01
6.1591005666     -0.25808446847
1.7320431063      0.42924265341
1.0194857402      0.43313353048
1 p
0.58131419111    1.0000000000
1 p
0.27290530268    1.0000000000
1 p
0.66000000000E-01  1.0000000000
1 p
0.22000000000E-01  1.0000000000
4 d
18.598247778     0.31556859652E-02
6.7883773752     -0.34551060293E-01
2.2470797667     0.21708566158
1.0884195428     0.42834135307
1 d
0.49787892886    1.0000000000
1 d
0.21481968266    1.0000000000
1 d
0.85666751170E-01  1.0000000000
1 f
2.8246600000     1.0000000000
1 f
0.94314000000    1.0000000000
1 f
0.31491000000    1.0000000000
1 f
0.10515000000    1.0000000000
1 g
1.7089400000     1.0000000000
1 g
0.53873000000    1.0000000000
*
ru def2-ecp
*
ncore = 28      lmax = 3
#      coefficient  r^n      exponent
f
      -28.3406163   2        11.3600000
      -4.9446292   2         5.6800000
s-f
      209.8229712   2        11.1052693
      30.6547264    2         5.4147454
      28.3406163   2        11.3600000
      4.9446292    2         5.6800000
p-f

```


	146.3361823	2	9.7712707
	24.1278772	2	5.0739908
	28.3406163	2	11.3600000
	4.9446292	2	5.6800000
d-f			
	67.5158967	2	7.6714231
	9.8701041	2	4.1365647
	28.3406163	2	11.3600000
	4.9446292	2	5.6800000
*			
*			
rh	def2-QZVPP		
# rh	(9s8p7d4f2g) / [7s5p4d4f2g]		{31111111/41111/4111/1111/11}
*			
	3 s		
	15.000000000	0.50258059140	
	13.500000000	-0.76433277918	
	7.4051116103	0.31145290674	
	1 s		
	4.5131696431	1.00000000000	
	1 s		
	1.3235977422	1.00000000000	
	1 s		
	0.60954144541	1.00000000000	
	1 s		
	0.18907192773	1.00000000000	
	1 s		
	0.89080450794E-01	1.00000000000	
	1 s		
	0.34131567514E-01	1.00000000000	
	4 p		
	11.839425278	0.59787418531E-01	
	6.6953652636	-0.24743454054	
	1.8333616287	0.42987003231	
	1.0267931770	0.42547313311	
	1 p		
	0.58071767020	1.00000000000	
	1 p		
	0.27907753269	1.00000000000	
	1 p		
	0.67108954625E-01	1.00000000000	
	1 p		
	0.22101542156E-01	1.00000000000	
	4 d		
	26.341167176	0.20623159685E-02	
	7.8709462705	-0.17239329053E-01	
	2.5989970939	0.17284839402	
	1.2613435752	0.36282102279	
	1 d		
	0.57578407979	1.00000000000	
	1 d		
	0.24725174897	1.00000000000	
	1 d		
	0.97531210324E-01	1.00000000000	
	1 f		
	3.2739100000	1.00000000000	
	1 f		
	1.0949900000	1.00000000000	
	1 f		
	0.36623000000	1.00000000000	

```

1 f
0.12249000000 1.0000000000
1 g
2.0298900000 1.0000000000
1 g
0.66294000000 1.0000000000
*
rh def2-ecp
*
ncore = 28 lmax = 3
# coefficient r^n exponent
f
-30.0934557 2 12.3100000
-5.2184819 2 6.1600000
s-f
225.3477535 2 11.7200000
32.8231890 2 5.8200000
30.0934557 2 12.3100000
5.2184819 2 6.1600000
p-f
158.7094116 2 10.4200000
26.4441005 2 5.4500000
30.0934557 2 12.3100000
5.2184819 2 6.1600000
d-f
62.7586257 2 8.8200000
10.9787195 2 3.8700000
30.0934557 2 12.3100000
5.2184819 2 6.1600000
*
*
pd def2-QZVPP
# pd (9s8p7d4f2g) / [7s5p4d4f2g] {3111111/41111/4111/1111/11}
*
3 s
15.262399331 0.44145727454
13.721983176 -0.70293005979
4.8448286268 0.36095390108
1 s
8.7309326588 1.0000000000
1 s
1.4357564094 1.0000000000
1 s
0.66088433720 1.0000000000
1 s
0.20897212790 1.0000000000
1 s
0.91936735872E-01 1.0000000000
1 s
0.34733479706E-01 1.0000000000
4 p
12.585237008 0.60002003747E-01
7.2058104839 -0.24022183118
1.9558705640 0.43424940067
1.0534418618 0.42084436088
1 p
0.59809389552 1.0000000000
1 p
0.30362411297 1.0000000000
1 p

```

```

0.880000000000E-01  1.0000000000
  1 p
0.300000000000E-01  1.0000000000
  4 d
  28.840985892      0.21131470308E-02
  8.4584163440     -0.17913194955E-01
  2.8648941754      0.17165507663
  1.3966488847      0.36149251150
  1 d
0.63921677230      1.0000000000
  1 d
0.27502319836      1.0000000000
  1 d
0.10829940074      1.0000000000
  1 f
  3.7200000000      1.0000000000
  1 f
  1.2462900000      1.0000000000
  1 f
0.41754000000      1.0000000000
  1 f
0.13989000000      1.0000000000
  1 g
  2.3234500000      1.0000000000
  1 g
0.78715000000      1.0000000000
*
pd def2-ecp
*
  ncore =    28      lmax =    3
#      coefficient  r^n      exponent
f
      -31.9295543   2      13.2700000
      -5.3982169   2      6.6300000
s-f
      240.2290403   2      12.4300000
      35.1719435    2      6.1707594
      31.9295543   2      13.2700000
      5.3982169    2      6.6300000
p-f
      170.4172760   2      11.0800000
      28.4721329    2      5.8295541
      31.9295543   2      13.2700000
      5.3982169    2      6.6300000
d-f
      69.0138449    2      9.5100000
      11.7508616    2      4.1397811
      31.9295543   2      13.2700000
      5.3982169    2      6.6300000
*
*
ag def2-QZVPP
# ag      (10s8p7d4f2g) / [7s5p4d4f2g]      {4111111/41111/4111/1111/11}
*
  4 s
  256.50898381      0.73215128094E-03
  19.000000000      -0.14706983774
  14.129749737      0.47914881797
  9.4840599768      -0.26930801705
  1 s

```

5.5812682897	1.0000000000
1 s	
1.4763753299	1.0000000000
1 s	
0.66184584335	1.0000000000
1 s	
0.15382171742	1.0000000000
1 s	
0.79534248689E-01	1.0000000000
1 s	
0.32408624506E-01	1.0000000000
4 p	
13.350389537	0.62479151672E-01
7.7163302467	-0.24398688175
2.0864535219	0.45439758415
1.0577805733	0.47607485340
1 p	
0.52564427657	1.0000000000
1 p	
0.23694908895	1.0000000000
1 p	
0.66457980332E-01	1.0000000000
1 p	
0.21864839286E-01	1.0000000000
4 d	
32.147961274	0.34564677092E-02
9.0323725307	-0.28135297216E-01
3.1673540854	0.26999486025
1.5519381135	0.57666767772
1 d	
0.71310284000	1.0000000000
1 d	
0.30749741551	1.0000000000
1 d	
0.12094304210	1.0000000000
1 f	
4.1631100000	1.0000000000
1 f	
1.3971100000	1.0000000000
1 f	
0.46886000000	1.0000000000
1 f	
0.15735000000	1.0000000000
1 g	
2.5896000000	1.0000000000
1 g	
0.91135000000	1.0000000000
*	
ag def2-ecp	
*	
ncore = 28	lmax = 3
# coefficient r^n exponent	
f	
-33.6899201 2 14.2200000	
-5.5311202 2 7.1100000	
s-f	
255.1393645 2 13.1300000	
36.8661215 2 6.5100000	
33.6899201 2 14.2200000	
5.5311202 2 7.1100000	

```

p-f
    182.1818687    2    11.7400000
    30.3577515    2    6.2000000
    33.6899201    2    14.2200000
    5.5311202     2    7.1100000

d-f
    73.7192609    2    10.2100000
    12.5021171    2    4.3800000
    33.6899201    2    14.2200000
    5.5311202     2    7.1100000

```

*

*

```

cd def2-QZVPP
# cd (10s8p7d4f2g) / [7s5p4d4f2g] {41111111/411111/41111/1111/11}
*

```

```

4 s
269.30016289    0.62688949336E-03
18.554269093   -0.43456616075
16.729943183    0.66043072415
11.768546646   -0.11793513277
1 s
6.1816604427    1.00000000000
1 s
1.5775743989    1.00000000000
1 s
0.71857981187    1.00000000000
1 s
0.16433138409    1.00000000000
1 s
0.76794158768E-01 1.00000000000
1 s
0.34377199848E-01 1.00000000000
4 p
14.107678180    0.70307291426E-01
8.2750040714   -0.26474818030
2.2507338323    0.47494851120
1.1914970238    0.46327020832
1 p
0.66041257699    1.00000000000
1 p
0.33804403770    1.00000000000
1 p
0.96004037879E-01 1.00000000000
1 p
0.33681030012E-01 1.00000000000
4 d
35.689192548    0.44455913982E-02
9.3407971610   -0.39185351747E-01
3.5922659140    0.31235972097
1.7980676976    0.71163739606
1 d
0.84830057791    1.00000000000
1 d
0.37846492753    1.00000000000
1 d
0.15420101631    1.00000000000
1 f
4.7689900000    1.00000000000
1 f
1.5981300000    1.00000000000

```

```

1 f
0.53555000000 1.0000000000
1 f
0.17947000000 1.0000000000
1 g
2.9414200000 1.0000000000
1 g
1.0371000000 1.0000000000
*
cd def2-ecp
*
ncore = 28 lmax = 3
# coefficient r^n exponent
f
-35.4766256 2 15.1847957
-5.6176768 2 7.5923978
s-f
270.0094832 2 13.8358689
38.7673080 2 6.8572704
35.4766256 2 15.1847957
5.6176768 2 7.5923978
p-f
193.8296294 2 12.4049710
31.8965252 2 6.5677995
35.4766256 2 15.1847957
5.6176768 2 7.5923978
d-f
79.1936470 2 10.8969253
13.2308267 2 4.6411649
35.4766256 2 15.1847957
5.6176768 2 7.5923978
*
*
in def2-QZVPP
# in (17s14p11d4f1g) / [7s6p4d4f1g] {9131111/731111/8111/1111/1}
*
9 s
8931.8400000 0.19000000000E-04
1352.2200000 0.13100000000E-03
303.39300000 0.47800000000E-03
45.122900000 0.11708000000E-01
28.182200000 -0.87330000000E-01
17.604800000 0.25957700000
6.9405800000 -0.62847100000
4.3337700000 -0.15871800000
1.9868400000 0.67440400000
1 s
1.0438672413 1.0000000000
3 s
20.245544208 0.29650296199E-01
11.072298416 -0.14745372687
2.4929238916 0.53232061960
1 s
0.53244484157 1.0000000000
1 s
0.21211307407 1.0000000000
1 s
0.95475196519E-01 1.0000000000
1 s
0.42357644919E-01 1.0000000000

```

7 p		
129.23300000	0.279000000000E-03	
29.628400000	-0.617100000000E-02	
18.521100000	0.469120000000E-01	
8.2853600000	-0.23990400000	
2.4993900000	0.42981100000	
1.3221600000	0.48610100000	
0.68870700000	0.22203700000	
3 p		
13.248633034	-0.18203004609E-01	
3.0240161259	0.31476939453	
1.0805448379	0.71919648136	
1 p		
0.33353581509	1.0000000000	
1 p		
0.15403760449	1.0000000000	
1 p		
0.65770424632E-01	1.0000000000	
1 p		
0.27642180293E-01	1.0000000000	
8 d		
131.81131820	0.22281463414E-03	
37.030875816	0.19331306797E-02	
11.378665218	-0.17870304080E-01	
6.4488212086	0.22953424346E-01	
3.4878752216	0.17536747821	
1.9912337572	0.29288830616	
1.1306610212	0.31018960851	
0.63074842914	0.24247651565	
1 d		
0.33856463907	1.0000000000	
1 d		
0.17026198815	1.0000000000	
1 d		
0.692000000000E-01	1.0000000000	
1 f		
0.39210000000	1.0000000000	
1 f		
0.15600000000	1.0000000000	
1 f		
1.3983200000	1.0000000000	
1 f		
4.1949600000	1.0000000000	
1 g		
0.34190000000	1.0000000000	

```

*
in def2-ecp
*
ncore = 28      lmax = 3
#      coefficient  r^n      exponent
f
      -13.7280780    2      12.5390560
      -18.2068660    2      12.5525610
s-f
      281.1223500    2      15.3928220
      61.9014700    2      8.0558640
      13.7280780    2      12.5390560
      18.2068660    2      12.5525610
p-f
      67.4621540    2      13.9286720

```

	134.9492500	2	13.3472340
	14.7461400	2	7.6141320
	29.6392620	2	7.3183650
	13.7280780	2	12.5390560
	18.2068660	2	12.5525610
d-f			
	35.4932540	2	14.0347150
	53.1787730	2	14.5116160
	9.1772810	2	5.5505500
	12.3924100	2	5.0594150
	13.7280780	2	12.5390560
	18.2068660	2	12.5525610

*

*

sn def2-QZVPP

sn (17s14p11d4f1g) / [7s6p4d4f1g] {9131111/731111/8111/1111/1}

*

9	s		
11606.900000		0.290000000000E-04	
1754.8000000		0.206000000000E-03	
397.17800000		0.807000000000E-03	
90.299000000		0.247100000000E-02	
31.489000000		-0.400250000000E-01	
19.668500000		0.16315200000	
7.0675900000		-0.55698300000	
4.4149000000		-0.16993200000	
2.1635600000		0.65102800000	
1	s		
1.1440977736		1.0000000000	
3	s		
20.197961274		0.22393937317E-01	
10.880108426		-0.14330764814	
2.7745387028		0.53278527074	
1	s		
0.58550056279		1.0000000000	
1	s		
0.25317089836		1.0000000000	
1	s		
0.11599461634		1.0000000000	
1	s		
0.52233584109E-01		1.0000000000	
7	p		
195.49500000		0.258000000000E-03	
18.256300000		0.443410000000E-01	
11.409400000		-0.10914200000	
6.9056700000		-0.13860600000	
2.9820600000		0.34374300000	
1.6084300000		0.51827100000	
0.83176700000		0.27870600000	
3	p		
13.304065745		-0.20694775410E-01	
3.4193503621		0.33654593033	
1.2382899573		0.71397757129	
1	p		
0.39265300321		1.0000000000	
1	p		
0.19313059747		1.0000000000	
1	p		
0.86443518729E-01		1.0000000000	
1	p		


```

0.37350684674E-01  1.0000000000
 8 d
143.82134199      0.26165602862E-03
41.039940764      0.21562117321E-02
11.508999207      -0.24771286642E-01
8.4312612820      0.29022163379E-01
4.0180001346      0.16171344601
2.3122021836      0.29213521578
1.3168562511      0.32241037254
0.73729126651     0.24629433031
 1 d
0.40109472811     1.0000000000
 1 d
0.20593354535     1.0000000000
 1 d
0.866000000000E-01 1.0000000000
 1 f
0.43150000000     1.0000000000
 1 f
0.17720000000     1.0000000000
 1 f
1.5915400000      1.0000000000
 1 f
4.7988893935      1.0000000000
 1 g
0.37740000000     1.0000000000
*
sn def2-ecp
*
  ncore =    28          lmax =    3
#      coefficient      r^n      exponent
f
      -12.5763330      2          12.2823480
      -16.5959440      2          12.2721500
s-f
      279.9886820      2          17.4204140
      62.3778100      2           7.6311550
      12.5763330      2          12.2823480
      16.5959440      2          12.2721500
p-f
      66.1625230      2          16.1310240
      132.1743960      2          15.6280770
      16.3394170      2           7.3256080
      32.4889590      2           6.9425190
      12.5763330      2          12.2823480
      16.5959440      2          12.2721500
d-f
      36.3874410      2          15.5149760
      54.5078410      2          15.1881600
      8.6968230      2           5.4560240
      12.8402080      2           5.3631050
      12.5763330      2          12.2823480
      16.5959440      2          12.2721500
*
*
sb def2-QZVPP
# sb      (17s14p11d4f1g) / [7s6p4d4f1g]      {9131111/731111/8111/1111/1}
*
  9 s
12339.316555      0.38545231046E-04

```

1854.7043271	0.27702166404E-03
418.44441772	0.11161923778E-02
96.965111109	0.28828055377E-02
28.537960267	-0.60556405021E-01
17.862907144	0.27988835315
8.4541754812	-0.54748479396
5.2813981306	-0.30336289748
2.3194618632	0.68093278701
1 s	
1.2167512076	1.0000000000
3 s	
25.336266601	0.22414355064E-01
12.477043309	-0.14737811818
3.0723142741	0.53278468779
1 s	
0.60174774699	1.0000000000
1 s	
0.28323936354	1.0000000000
1 s	
0.13221765728	1.0000000000
1 s	
0.60986718951E-01	1.0000000000
7 p	
162.89300000	0.37500000000E-03
30.399600000	-0.47980000000E-02
19.000400000	0.54731000000E-01
9.3225600000	-0.25528400000
3.0166800000	0.34537700000
1.8621900000	0.40483300000
1.1033100000	0.32592200000
3 p	
12.665326113	-0.20694788562E-01
3.3473442879	0.26878411014
1.1722158971	0.72590523998
1 p	
0.58886745483	1.0000000000
1 p	
0.25014249608	1.0000000000
1 p	
0.11120161090	1.0000000000
1 p	
0.48206685448E-01	1.0000000000
8 d	
142.61790051	0.34691704136E-03
40.920334292	0.27417583490E-02
10.854520545	-0.33847404142E-01
8.3926457719	0.42753986065E-01
4.1806878019	0.16545099365
2.5346474124	0.26821979719
1.5175455555	0.31482077294
0.86799625994	0.25485913704
1 d	
0.47323070711	1.0000000000
1 d	
0.24111763234	1.0000000000
1 d	
0.10080000000	1.0000000000
1 f	
0.48490000000	1.0000000000
1 f	

```

0.20490000000    1.0000000000
  1 f
1.7880600000    1.0000000000
  1 f
5.6265581363    1.0000000000
  1 g
0.42340000000    1.0000000000
*
sb def2-ecp
*
  ncore =    28          lmax =    3
#      coefficient      r^n          exponent
f
      -15.3668010      2          14.4449780
      -20.2961380      2          14.4492950
s-f
      281.0715810      2          16.3308650
      61.7166040      2          8.5565420
      15.3668010      2          14.4449780
      20.2961380      2          14.4492950
p-f
      67.4573800      2          14.4703370
      134.9335030      2          13.8161940
      14.7163440      2          8.4249240
      29.5185120      2          8.0927280
      15.3668010      2          14.4449780
      20.2961380      2          14.4492950
d-f
      35.4478150      2          14.8863310
      53.1434660      2          15.1463190
      9.1792230      2          5.9082670
      13.2402530      2          5.5943220
      15.3668010      2          14.4449780
      20.2961380      2          14.4492950
*
*
te def2-QZVPP
# te      (17s14p11d4f1g) / [7s6p4d4f1g]      {9131111/731111/8111/1111/1}
*
  9 s
15746.300000    0.540000000000E-04
2369.2500000    0.398000000000E-03
535.86000000    0.166200000000E-02
141.88500000    0.363600000000E-02
27.819700000    -0.584270000000E-01
17.387900000    0.366520000000
10.865600000    -0.397589000000
6.5688500000    -0.519175000000
2.4013900000    0.687652000000
  1 s
1.2865441585    1.0000000000
  3 s
29.383253023    0.30079778033E-01
15.946408003    -0.13631630929
3.6679902632    0.53467574034
  1 s
0.63533594694    1.0000000000
  1 s
0.29807786206    1.0000000000
  1 s

```

```

0.14061248688      1.0000000000
 1 s
0.65660655893E-01  1.0000000000
 7 p
750.22200000      0.52000000000E-04
163.96100000      0.41000000000E-03
16.922700000      0.83387000000E-01
10.575500000     -0.26821200000
 5.7046200000     -0.22932000000E-01
 2.9802200000      0.49554800000
 1.5197000000      0.51452200000
 3 p
13.925457258     -0.21336842159E-01
 4.2323766654      0.22433961554
 1.4547630727      0.73198528158
 1 p
0.75528783692     1.0000000000
 1 p
0.31829451168     1.0000000000
 1 p
0.13721830923     1.0000000000
 1 p
0.57099171462E-01  1.0000000000
 8 d
146.30727119      0.43816018982E-03
42.243859354      0.33559305599E-02
 9.9155377745     -0.11157186771
 8.9949643607      0.13269569633
 4.1376628430      0.21574044755
 2.3659339431      0.32583679541
 1.3736141857      0.30685918052
0.79846379228     0.19445241192
 1 d
0.45685175394     1.0000000000
 1 d
0.25022747959     1.0000000000
 1 d
0.11560000000     1.0000000000
 1 f
0.51840000000     1.0000000000
 1 f
0.21350000000     1.0000000000
 1 f
 1.9347800000      1.0000000000
 1 f
 5.8043400000      1.0000000000
 1 g
0.42940000000     1.0000000000
*
te def2-ecp
*
ncore =      28          lmax =      3
#      coefficient    r^n      exponent
f      -15.7454500     2        15.2061680
      -20.7424480     2        15.2017020
s-f    281.0458430     2        16.8144730
      61.6206560     2         8.7935260
      15.7454500     2        15.2061680

```

	20.7424480	2	15.2017020
p-f	67.4494640	2	14.8778010
	134.9043040	2	14.2697310
	14.6895470	2	8.7244350
	29.4150630	2	8.2915150
	15.7454500	2	15.2061680
	20.7424480	2	15.2017020
d-f	35.4320570	2	15.2050080
	53.1356870	2	15.2258480
	9.0698020	2	6.0717690
	13.1223040	2	5.8047600
	15.7454500	2	15.2061680
	20.7424480	2	15.2017020

*

*

i def2-QZVPP

i (17s14p11d4f1g) / [7s6p4d4f1g] {9131111/731111/8111/1111/1}

*

9 s		
16788.400000	0.410000000000E-04	
2526.6400000	0.303000000000E-03	
571.98400000	0.124700000000E-02	
150.43400000	0.265900000000E-02	
29.540500000	-0.531900000000E-01	
18.457100000	0.340096000000	
11.528600000	-0.352355000000	
7.0828900000	-0.541385000000	
2.5040500000	0.715749000000	
1 s		
1.3540144781	1.000000000000	
3 s		
25.058617933	0.40897754402E-01	
15.621979372	-0.14269668187	
3.3536325162	0.52916319279	
1 s		
0.67430472704	1.000000000000	
1 s		
0.32727136949	1.000000000000	
1 s		
0.15749364119	1.000000000000	
1 s		
0.74377727841E-01	1.000000000000	
7 p		
656.27400000	0.910000000000E-04	
149.23200000	0.613000000000E-03	
19.015300000	0.599230000000E-01	
10.737800000	-0.249258000000	
6.4420800000	-0.437500000000E-02	
3.0920300000	0.513999000000	
1.5787400000	0.507213000000	
3 p		
15.660511893	-0.22143803592E-01	
4.9250669812	0.23518064355	
1.6692319982	0.73153925548	
1 p		
0.77817898176	1.000000000000	
1 p		
0.35608843716	1.000000000000	

```

1 p
0.15493242649      1.0000000000
1 p
0.64666212492E-01  1.0000000000
8 d
318.22407776      0.10951692560E-03
95.810227352      0.91919139268E-03
35.322295259      0.47916935207E-02
13.107447819      -0.16280459996E-01
6.2949152988      0.90889609141E-01
3.6826101201      0.27483543784
2.0858950647      0.36067901632
1.1644342344      0.28384002219
1 d
0.63180613129     1.0000000000
1 d
0.32215084697     1.0000000000
1 d
0.13490000000     1.0000000000
1 f
0.58780000000     1.0000000000
1 f
0.25000000000     1.0000000000
1 f
2.17800000000     1.0000000000
1 f
6.4253613600      1.0000000000
1 g
0.47390000000     1.0000000000

```

```

*
i def2-ecp
*
ncore =      28          lmax =      3
#      coefficient      r^n      exponent
f
      -21.8420400      2          19.4586090
      -28.4681910      2          19.3492600
      -0.2437130      2           4.8237670
      -0.3208040      2           4.8843150
s-f
      49.9942930      2          40.0158350
      281.0253170      2          17.4297470
      61.5733260      2           9.0054840
      21.8420400      2          19.4586090
      28.4681910      2          19.3492600
      0.2437130      2           4.8237670
      0.3208040      2           4.8843150
p-f
      67.4428410      2          15.3554660
      134.8811370      2          14.9718330
      14.6750510      2           8.9601640
      29.3756660      2           8.2590960
      21.8420400      2          19.4586090
      28.4681910      2          19.3492600
      0.2437130      2           4.8237670
      0.3208040      2           4.8843150
d-f
      35.4395290      2          15.0689080
      53.1760570      2          14.5553220
      9.0671950      2           6.7186470

```

13.2069370	2	6.4563930
0.0893350	2	1.1917790
0.0523800	2	1.2911570
21.8420400	2	19.4586090
28.4681910	2	19.3492600
0.2437130	2	4.8237670
0.3208040	2	4.8843150

*
*

xe def2-QZVPP

xe (17s14p11d4f1g) / [7s6p4d4f1g] {9131111/731111/8111/1111/1}

*

9 s	
18774.300000	0.680000000000E-04
2824.8100000	0.501000000000E-03
640.08800000	0.209700000000E-02
172.61600000	0.449300000000E-02
29.516900000	-0.471510000000E-01
18.444800000	0.374033000000
11.523800000	-0.512826000000
6.6189000000	-0.478624000000
2.9955200000	0.596471000000
1 s	
1.6532586536	1.0000000000
3 s	
27.052171835	0.11189611954
20.940622415	-0.24055422724
6.0024591071	0.51452076187
1 s	
0.87553889270	1.0000000000
1 s	
0.41033616654	1.0000000000
1 s	
0.19493585779	1.0000000000
1 s	
0.90171093041E-01	1.0000000000
7 p	
613.33100000	0.138000000000E-03
141.71000000	0.853000000000E-03
20.310600000	0.550240000000E-01
11.033100000	-0.252988000000
6.8951300000	0.974600000000E-02
3.2416600000	0.526797000000
1.6653500000	0.501832000000
3 p	
18.388908413	-0.24514446229E-01
6.1139045431	0.25265669670
1.8729815691	0.72938328969
1 p	
0.82004665991	1.0000000000
1 p	
0.39552648254	1.0000000000
1 p	
0.17445509815	1.0000000000
1 p	
0.73389992663E-01	1.0000000000
8 d	
315.66106865	0.14235585191E-03
95.553873651	0.11707875751E-02
35.451236301	0.58783160362E-02

```

13.153211283      -0.16764226287E-01
6.3847329564      0.11558421625
3.6968166410      0.30375919653
2.0976070364      0.36037726827
1.1951246616      0.24813434400
 1 d
0.68431725339      1.00000000000
 1 d
0.37710480204      1.00000000000
 1 d
0.16760000000      1.00000000000
 1 f
0.66190000000      1.00000000000
 1 f
0.29790000000      1.00000000000
 1 f
2.43230000000      1.00000000000
 1 f
7.2077391789      1.00000000000
 1 g
0.52780000000      1.00000000000

```

```

*
xe def2-ecp

```

```

*
ncore =      28          lmax =      3
# coefficient  r^n      exponent
f
-23.0892950    2          20.8815570
-30.0744750    2          20.7834430
-0.2882270     2          5.2533890
-0.3869240     2          5.3611880
s-f
49.9979620    2          40.0051840
281.0133030   2          17.8122140
61.5382550    2          9.3041500
23.0892950    2          20.8815570
30.0744750    2          20.7834430
0.2882270     2          5.2533890
0.3869240     2          5.3611880
p-f
67.4391420    2          15.7017720
134.8747110   2          15.2586080
14.6633000    2          9.2921840
29.3547300    2          8.5590030
23.0892950    2          20.8815570
30.0744750    2          20.7834430
0.2882270     2          5.2533890
0.3869240     2          5.3611880
d-f
35.4369080    2          15.1856000
53.1957720    2          14.2845000
9.0462320     2          7.1218890
13.2236810    2          6.9919630
0.0848530     2          0.6239460
0.0441550     2          0.6472840
23.0892950    2          20.8815570
30.0744750    2          20.7834430
0.2882270     2          5.2533890
0.3869240     2          5.3611880

```

```

*
```



```

*
cs def2-QZVPP
# cs      (8s7p5d3f) / [6s5p3d3f]      {311111/31111/311/111}
*
  3 s
  5.8684829520      0.12906631816
  4.3741038860     -0.34380446158
  1.7951201473      0.69937346606
  1 s
  0.37816941125      1.00000000000
  1 s
  0.16624693130      1.00000000000
  1 s
  0.27763176052E-01  1.00000000000
  1 s
  0.16113005842E-01  1.00000000000
  1 s
  0.10996108743E-01  1.00000000000
  3 p
  4.2749775718      0.45595316685E-01
  1.9639316240     -0.25031125651
  0.47666322385      0.55660114378
  1 p
  0.21736718772      1.00000000000
  1 p
  0.97276293828E-01  1.00000000000
  1 p
  0.26770518041E-01  1.00000000000
  1 p
  0.10845412222E-01  1.00000000000
  3 d
  2.0091044335     -0.34453182058E-02
  0.35778351451      0.22686596025
  0.11070568254      0.47180885981
  1 d
  0.33216214821E-01  1.00000000000
  1 d
  0.11409380652E-01  1.00000000000
  1 f
  0.70000000000E-01  0.00000000000
  1 f
  0.34933000000      0.00000000000
  1 f
  0.84693000000      0.00000000000
*
cs def2-ecp
*
  ncore =    46      lmax =    3
#      coefficient  r^n      exponent
f
  -28.8843090      2      3.1232690
s-f
  84.5477300      2      4.0797500
  16.6541730      2      2.4174060
  28.8843090      2      3.1232690
p-f
  157.0490590     2      5.5140800
  26.4233070      2      2.1603160
  28.8843090      2      3.1232690
d-f

```

	13.1727530	2	1.8074100
	3.3428330	2	0.8581820
	28.8843090	2	3.1232690

*
*

ba def2-QZVPP
ba (8s8p5d3f) / [7s5p3d3f] {2111111/41111/311/111}

*
2 s
5.7000000000 1.3292982002
5.2043612469 -1.7367497134
1 s
2.1475437282 1.0000000000
1 s
0.41033660537 1.0000000000
1 s
0.18393532770 1.0000000000
1 s
0.72521216545E-01 1.0000000000
1 s
0.34526334903E-01 1.0000000000
1 s
0.16157891872E-01 1.0000000000
4 p
5.6000000000 0.51385026013
5.1104879274 -0.70529238864
2.5006544803 0.42822329830
0.51947995345 -0.57125984472
1 p
0.24536994841 1.0000000000
1 p
0.11256056700 1.0000000000
1 p
0.34917622027E-01 1.0000000000
1 p
0.16320065666E-01 1.0000000000
3 d
2.7000000000 0.14372069824
2.3460740881 -0.19565347309
0.39553542609 0.29963058552
1 d
0.12967935859 1.0000000000
1 d
0.40463066544E-01 1.0000000000
1 f
0.87880000000E-01 0.0000000000
1 f
0.36590000000 0.0000000000
1 f
0.87310000000 0.0000000000

*
ba def2-ecp
*
ncore = 46 lmax = 3
coefficient r^n exponent
f -33.4731740 2 3.5894650
s-f 427.8458160 2 9.5269860
204.4175300 2 4.4875100

	33.4731740	2	3.5894650
p-f	293.6058640	2	8.3159300
	294.1933160	2	4.2922170
	33.4731740	2	3.5894650
d-f	112.5504020	2	5.9161080
	181.7826210	2	2.8748420
	33.4731740	2	3.5894650

*

*

la def2-QZVPP

la (9s8p6d3f2g) / [7s5p4d3f2g] {31111111/41111/3111/111/11}

*

3	s		
26.077272000		0.23198684846E-02	
5.7127838000		-0.29787719611	
4.4057848000		0.70022722515	
1	s		
2.1315325829		1.0000000000	
1	s		
0.49385808956		1.0000000000	
1	s		
0.23595687888		1.0000000000	
1	s		
0.63593489661E-01		1.0000000000	
1	s		
0.31545394754E-01		1.0000000000	
1	s		
0.15777655296E-01		1.0000000000	
4	p		
6.0000000000		-0.11397960924E-01	
3.6808191615		0.14675038550	
2.3265462081		-0.35581819167	
0.64342629633		0.45834955229	
1	p		
0.33584281962		1.0000000000	
1	p		
0.16519051916		1.0000000000	
1	p		
0.56715971797E-01		1.0000000000	
1	p		
0.22100824776E-01		1.0000000000	
3	d		
1.2000000000		-0.35803482414	
1.0239524401		0.40483734122	
0.37508490282		0.37649639849	
1	d		
0.17161940245		1.0000000000	
1	d		
0.78780423402E-01		1.0000000000	
1	d		
0.35000047794E-01		1.0000000000	
1	f		
0.65580000000		1.0000000000	
1	f		
0.25683000000		1.0000000000	
1	f		
0.10058000000		1.0000000000	
1	g		

```

0.33218000000      1.0000000000
  1 g
0.13538000000      1.0000000000
*
la def2-ecp
*
  ncore =    46          lmax =    3
#   coefficient   r^n      exponent
f
  -36.0100160     2         4.0286000
s-f
  91.9321770     2         3.3099000
  -3.7887640     2         1.6550000
  36.0100160     2         4.0286000
p-f
  63.7594860     2         2.8368000
  -0.6479580     2         1.4184000
  36.0100160     2         4.0286000
d-f
  36.1161730     2         2.0213000
  0.2191140     2         1.0107000
  36.0100160     2         4.0286000
*
*
hf def2-QZVPP
# hf   (10s8p6d3f2g) / [7s5p4d3f2g]      {41111111/41111/3111/111/11}
*
  4 s
  24.000000000    0.19369448644
  16.000000000    -3.5064630782
  14.400000000    4.3082581000
  10.304504667    -0.91045809742
  1 s
  3.8372797792    1.0000000000
  1 s
  0.94649028050    1.0000000000
  1 s
  0.44397931299    1.0000000000
  1 s
  0.13656009445    1.0000000000
  1 s
  0.66549732509E-01  1.0000000000
  1 s
  0.28719110054E-01  1.0000000000
  4 p
  17.000000000    -0.30316491880E-01
  11.738072097    0.10139279686
  4.9203967161    -0.28227924657
  1.1251726138    0.52032008501
  1 p
  0.54220114055    1.0000000000
  1 p
  0.25659447877    1.0000000000
  1 p
  0.10000000000    1.0000000000
  1 p
  0.41700000000E-01  1.0000000000
  3 d
  6.9644775309    0.90606952386E-01
  5.7275227587    -0.16459899714

```

```

1.1503305416      0.51375718250
 1 d
0.47559482991    0.97807169690
 1 d
0.18774414759    1.00000000000
 1 d
0.68439488104E-01 1.00000000000
 1 f
0.80387000000    1.00000000000
 1 f
0.31547000000    1.00000000000
 1 f
0.12380000000    1.00000000000
 1 g
0.48820000000    1.00000000000
 1 g
0.18926000000    1.00000000000
*
hf def2-ecp
*
  ncore =      60      lmax =      3
#      coefficient  r^n      exponent
f
      10.0467225    2      1.7857698
s-f
      1499.2847107  2      14.7699590
      40.2821014   2      7.3849794
      -10.0467225  2      1.7857698
p-f
      397.7330053   2      9.8494895
      19.3164059   2      4.9247445
      -10.0467225  2      1.7857698
d-f
      101.3298053   2      6.0967564
      5.8734382    2      3.0483782
      -10.0467225  2      1.7857698
*
*
ta def2-QZVPP
# ta      (10s8p6d3f2g) / [7s5p4d3f2g]      {4111111/41111/3111/111/11}
*
  4 s
24.473650944      0.20537515818
18.721372549      -0.74477445680
11.500000000      3.4067771001
10.350000000      -2.8222400335
 1 s
 3.8125414615      1.00000000000
 1 s
 1.0507430630      1.00000000000
 1 s
0.49732275755      1.00000000000
 1 s
0.15602650970      1.00000000000
 1 s
0.75056442354E-01 1.00000000000
 1 s
0.31632668803E-01 1.00000000000
 4 p
17.000000000      -0.32577305616E-01

```

```

12.008186536      0.10336287365
5.0278760583     -0.28526521696
1.1937124184     0.51790141155
  1 p
0.57889707053    1.00000000000
  1 p
0.27225198801    1.00000000000
  1 p
0.10000000000    1.00000000000
  1 p
0.41700000000E-01 1.00000000000
  3 d
  7.1419762952    0.88606814221E-01
  5.7696869171    -0.17156962221
  1.2199483941    0.53547693505
  1 d
0.52366034246    1.00000000000
  1 d
0.21384808767    1.00000000000
  1 d
0.80254256735E-01 1.00000000000
  1 f
0.95070000000    1.00000000000
  1 f
0.37386000000    1.00000000000
  1 f
0.14702000000    1.00000000000
  1 g
0.65777000000    1.00000000000
  1 g
0.24314000000    1.00000000000
*
ta def2-ecp
*
  ncore =      60          lmax =      3
#   coefficient   r^n      exponent
f
      12.0179609      2          2.0178811
s-f
      1345.8806470      2          14.5464077
      36.7668062       2          7.2732038
      -12.0179609      2          2.0178811
p-f
      378.4253015      2          9.9355653
      22.2930909       2          4.9677824
      -12.0179609      2          2.0178811
d-f
      104.8839557      2          6.3473769
      8.7558481        2          3.1736885
      -12.0179609      2          2.0178811
*
*
w def2-QZVPP
# w      (10s8p6d3f2g) / [7s5p4d3f2g]      {4111111/41111/3111/111/11}
*
  4 s
22.106487883     0.66320504570
18.958062620     -1.5576189160
13.128699049     2.1416485467
10.149417378     -1.1823364947

```

1 s			
4.0160322414	1.0000000000		
1 s			
1.1234496158	1.0000000000		
1 s			
0.53500662821	1.0000000000		
1 s			
0.17127449658	1.0000000000		
1 s			
0.80452897876E-01	1.0000000000		
1 s			
0.33669872229E-01	1.0000000000		
4 p			
17.000000000	-0.37817768433E-01		
12.431973432	0.10905673845		
5.1586217658	-0.29399955020		
1.2801454812	0.51560726697		
1 p			
0.62856790898	1.0000000000		
1 p			
0.29380423553	1.0000000000		
1 p			
0.10000000000	1.0000000000		
1 p			
0.41700000000E-01	1.0000000000		
3 d			
7.4064737315	0.86993963018E-01		
5.9026268603	-0.17667540011		
1.2984756750	0.55145697030		
1 d			
0.57153508541	1.0000000000		
1 d			
0.23845526606	1.0000000000		
1 d			
0.91144267331E-01	1.0000000000		
1 f			
1.0962400000	1.0000000000		
1 f			
0.43199000000	1.0000000000		
1 f			
0.17023000000	1.0000000000		
1 g			
0.84089000000	1.0000000000		
1 g			
0.29702000000	1.0000000000		
*			
w def2-ecp			
*			
ncore =	60	lmax =	3
#	coefficient	r^n	exponent
f	14.1525795	2	2.2588885
s-f	1192.3958823	2	14.3228564
	32.5229332	2	7.1614281
	-14.1525795	2	2.2588885
p-f	359.0319671	2	10.0216411
	24.0303802	2	5.0108204
	-14.1525795	2	2.2588885

```

d-f
      108.3013490    2          6.5979974
      10.9825283    2          3.2989987
      -14.1525795    2          2.2588885
*
*
re def2-QZVPP
# re      (10s8p6d4f2g) / [7s5p4d4f2g]      {41111111/411111/3111/1111/11}
*
      4 s
      24.000000000    0.26968047163
      18.204262749    -1.3559378623
      14.048192487    1.9003709759
      9.5166786954    -0.75626964015
      1 s
      4.1714667981    1.0000000000
      1 s
      1.1944213976    1.0000000000
      1 s
      0.56755447797    1.0000000000
      1 s
      0.17533854868    1.0000000000
      1 s
      0.82014250464E-01  1.0000000000
      1 s
      0.34607892740E-01  1.0000000000
      4 p
      18.000000000    -0.26890962397E-01
      12.318606250    0.99711498502E-01
      5.3719234505    -0.29289398145
      1.3506646748    0.51466301434
      1 p
      0.66212816808    1.0000000000
      1 p
      0.31071385193    1.0000000000
      1 p
      0.10800000000    1.0000000000
      1 p
      0.45000000000E-01  1.0000000000
      3 d
      7.7352877672    0.83901798556E-01
      6.0949443610    -0.17722258734
      1.3871105497    0.55238259692
      1 d
      0.62324027854    1.0000000000
      1 d
      0.26517328547    1.0000000000
      1 d
      0.10321096849    1.0000000000
      1 f
      1.2406000000    1.0000000000
      1 f
      0.48989000000    1.0000000000
      1 f
      0.19345000000    1.0000000000
      1 f
      0.76390000000E-01  1.0000000000
      1 g
      1.0375800000    1.0000000000
      1 g

```



```

0.35090000000      1.0000000000
*
re def2-ecp
*
ncore =      60      lmax =      3
# coefficient  r^n      exponent
f
      16.4498523      2      2.5086506
s-f
      1038.9515723      2      14.0993051
      29.5617383      2      7.0496525
      -16.4498523      2      2.5086506
p-f
      339.5435096      2      10.1077169
      24.9136965      2      5.0538583
      -16.4498523      2      2.5086506
d-f
      111.6996527      2      6.8486179
      12.6243293      2      3.4243090
      -16.4498523      2      2.5086506
*
*
os def2-QZVPP
# os      (10s8p6d4f2g) / [7s5p4d4f2g]      {4111111/41111/3111/1111/11}
*
  4 s
24.000000000      0.24559132972
18.204262749      -1.3020204925
14.048192487      1.9114896000
9.5166786954      -0.83098846799
  1 s
4.2529406042      1.0000000000
  1 s
1.2999583502      1.0000000000
  1 s
0.61756850127      1.0000000000
  1 s
0.18785305474      1.0000000000
  1 s
0.87865523960E-01      1.0000000000
  1 s
0.37004242944E-01      1.0000000000
  4 p
15.500000000      0.16016463376
14.000000000      -0.23201520402
5.5458290420      0.29772587274
1.4139502215      -0.54253238176
  1 p
0.68136686765      1.0000000000
  1 p
0.30911452647      1.0000000000
  1 p
0.90000000000E-01      1.0000000000
  1 p
0.33000000000E-01      1.0000000000
  3 d
8.5557226523      0.55081304746E-01
6.1927250845      -0.15041777374
1.4916733698      0.55087247584
  1 d

```

```

0.67423241512      1.0000000000
  1 d
0.28635737076      1.0000000000
  1 d
0.11074292707      1.0000000000
  1 f
  1.3802600000      1.0000000000
    1 f
0.55065000000      1.0000000000
  1 f
0.21968000000      1.0000000000
  1 f
0.87640000000E-01  1.0000000000
  1 g
  1.2249700000      1.0000000000
    1 g
0.42803000000      1.0000000000
*
os def2-ecp
*
  ncore =    60      lmax =    3
#      coefficient  r^n      exponent
f
      18.9094570    2        2.7670751
s-f
      885.4057191    2        13.8757539
      25.9670401    2        6.9378769
      -18.9094570    2        2.7670751
p-f
      320.0839019    2        10.1937926
      26.1487649    2        5.0968962
      -18.9094570    2        2.7670751
d-f
      115.0448431    2        7.0992385
      13.6225746    2        3.5496192
      -18.9094570    2        2.7670751
*
*
ir def2-QZVPP
# ir      (10s8p6d4f2g) / [7s5p4d4f2g]      {4111111/41111/3111/1111/11}
*
  4 s
23.465507222      0.71085679679
20.657091116      -1.5723547785
15.725107858      1.2938086001
 7.9297463605     -0.42980466966
  1 s
 4.5196120103      1.0000000000
  1 s
 1.3392891402      1.0000000000
  1 s
0.63692276928      1.0000000000
  1 s
0.19126770642      1.0000000000
  1 s
0.87881999015E-01  1.0000000000
  1 s
0.37643105533E-01  1.0000000000
  4 p
15.902664143      -0.16290720099

```

```

14.415830698      0.23483212987
5.7597608991     -0.30305337176
1.5008913108     0.55512982069
  1 p
0.72348035957    1.00000000000
  1 p
0.32785980328    1.00000000000
  1 p
0.910000000000E-01  1.00000000000
  1 p
0.350000000000E-01  1.00000000000
  3 d
8.9686781612     0.29754685954E-01
6.4456319498    -0.82246052942E-01
1.5835819740     0.29212392062
  1 d
0.71871917882    0.45371657855
  1 d
0.30539233284    0.35080208829
  1 d
0.11791405498    0.12106264000
  1 f
1.5134800000     1.00000000000
  1 f
0.61008000000    1.00000000000
  1 f
0.24592000000    1.00000000000
  1 f
0.991300000000E-01  1.00000000000
  1 g
1.3977000000     1.00000000000
  1 g
0.50516000000    1.00000000000
*
ir def2-ecp
*
  ncore =      60      lmax =      3
#      coefficient      r^n      exponent
f
      21.5310311      2      3.0340719
s-f
      732.2691998      2      13.6522026
      26.4847209      2      6.8261013
      -21.5310311      2      3.0340719
p-f
      299.4894736      2      10.2798684
      26.4662335      2      5.1399341
      -21.5310311      2      3.0340719
d-f
      124.4575945      2      7.3498590
      14.0359952      2      3.6749295
      -21.5310311      2      3.0340719
*
*
pt def2-QZVPP
# pt      (10s8p6d4f2g) / [7s5p4d4f2g]      {4111111/41111/3111/1111/11}
*
  4 s
23.465507222     0.55150926143
20.657091116     -1.2690274107

```

15.725107858	1.1215145470
7.9297463605	-0.42250178029
1 s	
4.6667116243	1.0000000000
1 s	
1.4202522633	1.0000000000
1 s	
0.66786671541	1.0000000000
1 s	
0.19745059689	1.0000000000
1 s	
0.92573920368E-01	1.0000000000
1 s	
0.38895936899E-01	1.0000000000
4 p	
15.500000000	-0.15672718629
14.000000000	0.23853412989
6.1161212339	-0.31041379733
1.5715586385	0.56473525089
1 p	
0.75132510781	1.0000000000
1 p	
0.33306466812	1.0000000000
1 p	
0.91000000000E-01	1.0000000000
1 p	
0.35000000000E-01	1.0000000000
3 d	
8.3207937611	0.62945508668E-01
7.4207226520	-0.90271154330E-01
1.6570410639	0.16812340903
1 d	
0.73943569960	1.0000000000
1 d	
0.30508290090	1.0000000000
1 d	
0.11350435924	1.0000000000
1 f	
1.6402500000	1.0000000000
1 f	
0.66813000000	1.0000000000
1 f	
0.27215000000	1.0000000000
1 f	
0.11086000000	1.0000000000
1 g	
1.5557500000	1.0000000000
1 g	
0.58228000000	1.0000000000
*	
pt def2-ecp	
*	
ncore = 60	lmax = 3
# coefficient r^n	exponent
f	
24.3143757	2 3.3095686
s-f	
579.2238609	2 13.4286513
29.6694906	2 6.7143256
-24.3143757	2 3.3095686

```

p-f      280.8607742    2      10.3659442
          26.7453820    2      5.1829721
          -24.3143757    2      3.3095686
d-f      120.3964443    2      7.6004795
          15.8109206    2      3.8002397
          -24.3143757    2      3.3095686
*
*
au def2-QZVPP
# au      (9s8p6d4f2g) / [7s5p4d4f2g]      {31111111/411111/3111/1111/11}
*
  3 s
  24.200000000      1.4645004443
  22.000000000      -3.9770190496
  20.000000000      2.7298033533
  1 s
  5.4043553001      1.0000000000
  1 s
  1.4532546773      1.0000000000
  1 s
  0.68294298420      1.0000000000
  1 s
  0.19002755303      1.0000000000
  1 s
  0.88155981740E-01  1.0000000000
  1 s
  0.37739555187E-01  1.0000000000
  4 p
  15.500000000      0.15001711880
  14.000000000      -0.23609813183
  6.4227368205      0.31458896948
  1.6595601681      -0.57279670446
  1 p
  0.79402913993      1.0000000000
  1 p
  0.35125155397      1.0000000000
  1 p
  0.81000000000E-01  1.0000000000
  1 p
  0.25000000000E-01  1.0000000000
  3 d
  8.6000000000      0.15361654684
  7.8531899379      -0.20443530663
  1.7650856798      0.30781811607
  1 d
  0.79482263260      1.0000000000
  1 d
  0.33085396360      1.0000000000
  1 d
  0.12398535801      1.0000000000
  1 f
  1.7607400000      1.0000000000
  1 f
  0.72482000000      1.0000000000
  1 f
  0.29838000000      1.0000000000
  1 f
  0.12283000000      1.0000000000

```

```

1 g
1.6991700000      1.0000000000
1 g
0.6594100000      1.0000000000
*
au def2-ecp
*
ncore =      60      lmax =      3
#      coefficient      r^n      exponent
f
      30.4900889      2      4.7898200
      5.1710738      2      2.3949100
s-f
      426.8466792      2      13.2051000
      37.0070829      2      6.6025500
      -30.4900889      2      4.7898200
      -5.1710738      2      2.3949100
p-f
      261.1995804      2      10.4520200
      26.9624960      2      5.2260100
      -30.4900889      2      4.7898200
      -5.1710738      2      2.3949100
d-f
      124.7906656      2      7.8511000
      16.3007257      2      3.9255500
      -30.4900889      2      4.7898200
      -5.1710738      2      2.3949100
*
*
hg def2-QZVPP
# hg      (9s8p7d4f2g) / [7s5p4d4f2g]      {31111111/41111/4111/1111/11}
*
3 s
48.013786990      0.56241403333E-02
21.239875095      -0.17054083503
15.876100879      0.35940389661
1 s
5.4865939429      1.0000000000
1 s
1.5521766895      1.0000000000
1 s
0.74742541187      1.0000000000
1 s
0.20268838483      1.0000000000
1 s
0.93376229211E-01      1.0000000000
1 s
0.41248705609E-01      1.0000000000
4 p
17.500000000      -0.86457187331E-01
15.252594855      0.15327318234
6.4404715169      -0.30274955249
1.8180159920      0.54361285026
1 p
0.90067981801      1.0000000000
1 p
0.41304540122      1.0000000000
1 p
0.11845702655      1.0000000000
1 p

```

```

0.36087619349E-01  1.0000000000
 4 d
11.888648987      0.13311219898E-01
6.7773660954     -0.73346199848E-01
2.0934941340     0.24155986719
1.0817087176     0.38865972362
 1 d
0.53329136060    1.0000000000
 1 d
0.24984101827    1.0000000000
 1 d
0.10879770063    1.0000000000
 1 f
1.8893800000     1.0000000000
 1 f
0.79569000000    1.0000000000
 1 f
0.33510000000    1.0000000000
 1 f
0.14112000000    1.0000000000
 1 g
1.8358500000     1.0000000000
 1 g
0.72249000000    1.0000000000
*
hg def2-ecp
*
  ncore =    60      lmax =    3
#      coefficient  r^n      exponent
f
      30.3649964    2        3.8857911
s-f
      275.7372117   2        12.9815487
      49.0892125    2        6.4907744
      -30.3649964   2        3.8857911
p-f
      241.5400740    2        10.5380958
      27.3965908    2        5.2690479
      -30.3649964   2        3.8857911
d-f
      127.8670076    2        8.1017205
      16.6083115    2        4.0508603
      -30.3649964   2        3.8857911
*
*
t1 def2-QZVPP
# t1      (17s14p10d4f1g) / [7s6p4d4f1g]      {9131111/731111/7111/1111/1}
*
 9 s
9675.550000      0.80000000000E-05
1471.480000      0.57000000000E-04
323.6480000      0.22700000000E-03
33.807900000     0.21666000000E-01
21.131600000     -0.19589700000
13.209100000     0.67362000000
8.2561100000     -0.57167600000
5.1001400000     -0.61234400000
1.8194300000     0.75954400000
 1 s
0.96804610176    1.0000000000

```

```

3 s
13.432924081      0.16050252545
11.126956705     -0.25827112953
2.0351129325     0.52570088358
1 s
0.47288027019    1.00000000000
1 s
0.21703241765    1.00000000000
1 s
0.99551664344E-01 1.00000000000
1 s
0.44674475181E-01 1.00000000000
7 p
42.524000000     0.16050000000E-02
21.395700000     -0.23159000000E-01
13.373700000     0.11173800000
6.6133700000    -0.34647200000
2.0421700000     0.47507300000
1.1144900000     0.48633500000
0.59800600000    0.20513900000
3 p
9.0557032031    -0.57376712693E-01
3.9424773914     0.27305802340
1.2382159385     0.72255078460
1 p
0.29943260745    1.00000000000
1 p
0.14250182360    1.00000000000
1 p
0.61655072518E-01 1.00000000000
1 p
0.26054870511E-01 1.00000000000
7 d
63.792149375     0.19539028558E-03
10.854099697     0.17775848298E-01
6.3885280565     -0.89213657526E-01
2.4120875010     0.18424406191
1.4246170706     0.30659722011
0.83496548780    0.31018961556
0.48634320397    0.23215648111
1 d
0.27592111650    1.00000000000
1 d
0.14737244064    1.00000000000
1 d
0.67700000000E-01 1.00000000000
1 f
0.42630000000    1.00000000000
1 f
0.16900000000    1.00000000000
1 f
1.0848100000     1.00000000000
1 f
2.3083704534     1.00000000000
1 g
0.36930000000    1.00000000000
*
t1 def2-ecp
*
ncore =      60          lmax =      3

```


#	coefficient	r^n	exponent
f	15.8254880	2	5.6263990
	21.1040210	2	5.5489520
	2.9151270	2	2.8749460
	3.8969030	2	2.8214510
s-f	281.2846630	2	12.1678050
	62.4342510	2	8.2949090
	-15.8254880	2	5.6263990
	-21.1040210	2	5.5489520
	-2.9151270	2	2.8749460
	-3.8969030	2	2.8214510
p-f	4.6334080	2	7.1514920
	9.3417560	2	5.1728650
	72.2992530	2	9.8910720
	144.5580370	2	9.0033910
	-15.8254880	2	5.6263990
	-21.1040210	2	5.5489520
	-2.9151270	2	2.8749460
	-3.8969030	2	2.8214510
d-f	35.9430390	2	7.1302180
	53.9095930	2	6.9269060
	10.3819390	2	5.4175700
	15.5838220	2	5.1386810
	-15.8254880	2	5.6263990
	-21.1040210	2	5.5489520
	-2.9151270	2	2.8749460
	-3.8969030	2	2.8214510
*			
*			
pb def2-QZVPP			
# pb	(17s14p10d4f1g) / [7s6p4d4f1g]		{9131111/731111/7111/1111/1}
*			
9 s			
	9368.3300000	0.140000000000E-04	
	1366.9300000	0.103000000000E-03	
	299.68200000	0.379000000000E-03	
	34.859700000	0.232740000000E-01	
	21.788900000	-0.20343600000	
	13.620000000	0.69921400000	
	8.5129500000	-0.60684100000	
	5.3033200000	-0.61139200000	
	1.9281600000	0.76522700000	
1 s			
	1.0373400312	1.0000000000	
3 s			
	13.559944213	0.15955164155	
	11.039620045	-0.26750615828	
	2.1371722788	0.52500552105	
1 s			
	0.51111685694	1.0000000000	
1 s			
	0.24673987563	1.0000000000	
1 s			
	0.11577976738	1.0000000000	
1 s			
	0.52874167812E-01	1.0000000000	

7	p		
59.090100000		0.71600000000E-03	
20.919700000		-0.21082000000E-01	
13.077700000		0.12706100000	
6.8991000000		-0.37228400000	
2.1962700000		0.43566300000	
1.3048600000		0.43573500000	
0.77957200000		0.26094700000	
3	p		
9.1373183134		-0.55319030476E-01	
3.9570574249		0.27275707058	
1.2246639098		0.72280340692	
1	p		
0.42601564238		1.0000000000	
1	p		
0.20378586294		1.0000000000	
1	p		
0.88168647885E-01		1.0000000000	
1	p		
0.37094701422E-01		1.0000000000	
7	d		
66.348248961		0.28507140251E-03	
13.455899798		0.93352787747E-02	
6.5510273149		-0.75354763534E-01	
2.6574136949		0.16674578725	
1.6001278005		0.31208757936	
0.93304454981		0.32900401823	
0.54391365526		0.22655044022	
1	d		
0.32059545270		1.0000000000	
1	d		
0.17922304239		1.0000000000	
1	d		
0.83200000000E-01		1.0000000000	
1	f		
0.44130000000		1.0000000000	
1	f		
0.17820000000		1.0000000000	
1	f		
1.1606000000		1.0000000000	
1	f		
2.5184938758		1.0000000000	
1	g		
0.38810000000		1.0000000000	

*

pb def2-ecp

*

ncore =	60	lmax =	3
#	coefficient	r^n	exponent
f			
	12.2098920	2	3.8875120
	16.1902910	2	3.8119630
s-f			
	281.2854990	2	12.2963030
	62.5202170	2	8.6326340
	-12.2098920	2	3.8875120
	-16.1902910	2	3.8119630
p-f			
	72.2768970	2	10.2417900
	144.5910830	2	8.9241760

	4.7586930	2	6.5813420
	9.9406210	2	6.2554030
	-12.2098920	2	3.8875120
	-16.1902910	2	3.8119630
d-f			
	35.8485070	2	7.7543360
	53.7243420	2	7.7202810
	10.1152560	2	4.9702640
	14.8337310	2	4.5637890
	-12.2098920	2	3.8875120
	-16.1902910	2	3.8119630
*			
*			
bi	def2-QZVPP		
#	bi	(17s14p10d4f1g) / [7s6p4d4f1g]	{9131111/731111/7111/1111/1}
*			
	9	s	
	8131.0900000		0.290000000000E-04
	1225.7700000		0.200000000000E-03
	274.67200000		0.684000000000E-03
	37.616400000		0.202180000000E-01
	23.480400000		-0.15932600000
	14.106500000		0.61172600000
	8.8130500000		-0.54465300000
	5.5077800000		-0.63688400000
	2.0397700000		0.77169800000
	1	s	
	1.0975227257		1.0000000000
	3	s	
	13.614284474		0.15800789319
	11.010881766		-0.27164962692
	2.2630089550		0.52469330212
	1	s	
	0.52344449532		1.0000000000
	1	s	
	0.26734409206		1.0000000000
	1	s	
	0.12836608814		1.0000000000
	1	s	
	0.60097735551E-01		1.0000000000
	7	p	
	99.591400000		0.346000000000E-03
	19.896400000		-0.199760000000E-01
	12.437600000		0.17544600000
	7.7740000000		-0.37955600000
	4.8399500000		-0.552620000000E-01
	2.2547800000		0.52888400000
	1.1804900000		0.52132400000
	3	p	
	9.6213214965		-0.52920356623E-01
	4.1321350830		0.26705180214
	1.2785827783		0.72824686940
	1	p	
	0.59423596262		1.0000000000
	1	p	
	0.25794168858		1.0000000000
	1	p	
	0.11273595358		1.0000000000
	1	p	
	0.47791974731E-01		1.0000000000

```

7 d
69.632799181      0.35055800732E-03
14.888614968      0.81591735697E-02
6.5949628713     -0.83905319526E-01
4.1796107640      0.28034212952E-01
2.5697950152      0.20202314185
1.5601364822      0.33621249652
0.89210528768     0.34629017140
1 d
0.48093728228     1.00000000000
1 d
0.24233621968     1.00000000000
1 d
0.10440000000     1.00000000000
1 f
0.48030000000     1.00000000000
1 f
0.20060000000     1.00000000000
1 f
1.26256000000     1.00000000000
1 f
2.7210175470      1.00000000000
1 g
0.42030000000     1.00000000000
*
bi def2-ecp
*
ncore = 60          lmax = 3
# coefficient      r^n          exponent
f
      13.7133830    2            4.2145460
      18.1943080    2            4.1334000
s-f
      283.2642270   2            13.0430900
      62.4719590    2            8.2216820
      -13.7133830   2            4.2145460
      -18.1943080   2            4.1334000
p-f
      72.0014990    2            10.4677770
      144.0022770   2            9.1189010
      5.0079450     2            6.7547910
      9.9915500     2            6.2525920
      -13.7133830   2            4.2145460
      -18.1943080   2            4.1334000
d-f
      36.3962590    2            8.0814740
      54.5976640    2            7.8905950
      9.9842940     2            4.9555560
      14.9814850    2            4.7045590
      -13.7133830   2            4.2145460
      -18.1943080   2            4.1334000
*
*
po def2-QZVPP
# po (17s14p10d4f1g) / [7s6p4d4f1g] {9131111/731111/7111/1111/1}
*
9 s
8913.2900000      0.470000000000E-04
1338.9800000      0.331000000000E-03
299.538000000     0.116100000000E-02

```

51.148900000	0.789900000000E-02
23.015600000	-0.14934700000
14.376500000	0.63824200000
8.9827900000	-0.61708300000
5.6129200000	-0.60519700000
2.1648400000	0.77608600000
1 s	
1.1753800000	1.00000000000
3 s	
14.787766907	0.15929033129
11.958781204	-0.27310166985
2.4798455066	0.52423698726
1 s	
0.55481477792	1.00000000000
1 s	
0.28581735198	1.00000000000
1 s	
0.13849439468	1.00000000000
1 s	
0.64954523837E-01	1.00000000000
7 p	
113.55700000	0.387000000000E-03
20.363900000	-0.182550000000E-01
12.727400000	0.17477600000
7.9498400000	-0.39870300000
4.9647700000	-0.318120000000E-01
2.3013000000	0.56604700000
1.1954500000	0.51022200000
3 p	
8.4681300000	-0.23853762000
7.7962017000	0.28579119000
0.66871758000	0.46050656000
1 p	
0.59152423927	1.00000000000
1 p	
0.244444843795	1.00000000000
1 p	
0.11018922460	1.00000000000
1 p	
0.48149776000E-01	1.00000000000
7 d	
73.649818245	0.43310334586E-03
16.743441686	0.69436968591E-02
5.8163048812	-0.83799240387
5.6493757173	0.79372183416
2.4547686106	0.29055549251
1.3909015593	0.38177920670
0.78934505572	0.29342954208
1 d	
0.44107648549	1.00000000000
1 d	
0.23631248810	1.00000000000
1 d	
0.10930000000	1.00000000000
1 f	
0.48940000000	1.00000000000
1 f	
0.20020000000	1.00000000000
1 f	
1.31220000000	1.00000000000

```

1 f
2.8220658714      1.0000000000
1 g
0.40740000000    1.0000000000
*
po def2-ecp
*
ncore =      60      lmax =      3
#      coefficient  r^n      exponent
f
      17.4282950    2        5.0132700
      23.3803530    2        4.9846400
      0.1633920    2        1.3267600
      0.3245660    2        1.5287580
s-f
      283.2447060   2        13.2772270
      62.3964610   2        8.3995180
      -17.4282950  2        5.0132700
      -23.3803530  2        4.9846400
      -0.1633920  2        1.3267600
      -0.3245660  2        1.5287580
p-f
      71.9917160    2        10.6656820
      143.9718710   2        9.2837530
      4.9496150     2        6.8727490
      9.7404990     2        6.3261500
      -17.4282950  2        5.0132700
      -23.3803530  2        4.9846400
      -0.1633920  2        1.3267600
      -0.3245660  2        1.5287580
d-f
      36.3783830    2        8.2148660
      54.5627150    2        8.0086960
      9.8894990     2        5.0552270
      14.6938770    2        4.7825530
      -17.4282950  2        5.0132700
      -23.3803530  2        4.9846400
      -0.1633920  2        1.3267600
      -0.3245660  2        1.5287580
*
*
at def2-QZVPP
# at      (17s14p10d4f1g) / [7s6p4d4f1g]      {9131111/731111/7111/1111/1}
*
9 s
9090.2800000      0.350000000000E-04
1373.0700000      0.242000000000E-03
307.950000000     0.815000000000E-03
48.017600000      0.846500000000E-02
23.909900000      -0.14733300000
14.933400000      0.63241500000
9.3317100000      -0.61640600000
5.8320600000      -0.61925800000
2.2878700000      0.78512400000
1 s
1.2537238008      1.00000000000
3 s
14.805780876      0.15771473639
11.855783628      -0.28007490839
2.5818782360      0.52359428906

```

```

1 s
0.61460691976      1.0000000000
1 s
0.31486716636      1.0000000000
1 s
0.15441669153      1.0000000000
1 s
0.72866424566E-01  1.0000000000
7 p
124.60200000      0.468000000000E-03
20.889900000      -0.16124000000E-01
13.058500000      0.17119600000
8.1606100000      -0.40887500000
5.0980800000      -0.16407000000E-01
2.3787600000      0.58817200000
1.2375500000      0.50099700000
3 p
8.7977584321      -0.23832810213
8.0996431502      0.28585830834
0.67629719775      0.46050935965
1 p
0.60785017930      1.0000000000
1 p
0.26116561417      1.0000000000
1 p
0.11948611257      1.0000000000
1 p
0.52899086095E-01  1.0000000000
7 d
76.152584155      0.54645145370E-03
17.982092186      0.70498116717E-02
5.8900316564      -0.59711331046
5.6001503121      0.56517203927
2.4782622062      0.32344318344
1.3928750256      0.39511263456
0.78560551382      0.27094838862
1 d
0.44173978741      1.0000000000
1 d
0.24984733563      1.0000000000
1 d
0.12700000000      1.0000000000
1 f
0.53890000000      1.0000000000
1 f
0.22870000000      1.0000000000
1 f
1.4237200000      1.0000000000
1 f
3.0086421207      1.0000000000
1 g
0.43630000000      1.0000000000
*
at def2-ecp
*
ncore =      60      lmax =      3
#      coefficient      r^n      exponent
f
      19.8701980      2      5.8121630
      26.4164520      2      5.7537150

```

	0.9949700	2	2.5134720
	1.4907010	2	2.5362610
s-f			
	49.9571580	2	30.2008320
	283.2103710	2	13.6123060
	62.2810520	2	8.5293400
	-19.8701980	2	5.8121630
	-26.4164520	2	5.7537150
	-0.9949700	2	2.5134720
	-1.4907010	2	2.5362610
p-f			
	71.9823710	2	10.8540650
	143.9035320	2	9.4682290
	4.8717590	2	7.0311140
	8.9830590	2	6.1438580
	-19.8701980	2	5.8121630
	-26.4164520	2	5.7537150
	-0.9949700	2	2.5134720
	-1.4907010	2	2.5362610
d-f			
	36.3632370	2	8.3135150
	54.5489700	2	7.9989650
	9.7762850	2	5.1799660
	14.2647550	2	4.9422260
	-19.8701980	2	5.8121630
	-26.4164520	2	5.7537150
	-0.9949700	2	2.5134720
	-1.4907010	2	2.5362610

*
*

rn def2-QZVPP

rn (17s14p11d4f1g) / [7s6p4d4f1g] {9131111/731111/8111/1111/1}

*

9	s		
12715.600000		0.470000000000E-04	
1913.300000		0.338000000000E-03	
429.95600000		0.128000000000E-02	
100.97800000		0.278200000000E-02	
24.470800000		-0.10042100000	
15.292200000		0.53982400000	
9.5548300000		-0.57385600000	
5.9666100000		-0.61000000000	
2.3893900000		0.79325300000	
1	s		
1.3276477516		1.0000000000	
3	s		
17.195195341		0.16333005101	
14.230303720		-0.27167744770	
3.0760339153		0.52372666490	
1	s		
0.69973866760		1.0000000000	
1	s		
0.33174234887		1.0000000000	
1	s		
0.16093431878		1.0000000000	
1	s		
0.75883596172E-01		1.0000000000	
7	p		
131.70800000		0.58500000000E-03	
21.401600000		-0.14438000000E-01	

13.382600000	0.17009500000
8.368800000	-0.42250400000
5.229450000	-0.17190000000E-02
2.476850000	0.60115800000
1.301800000	0.49278000000
3 p	
9.0768547920	-0.23950411879
8.3822367043	0.28554010268
0.70618692299	0.46017587936
1 p	
0.64553860374	1.00000000000
1 p	
0.28380500916	1.00000000000
1 p	
0.13160518578	1.00000000000
1 p	
0.58958259826E-01	1.00000000000
8 d	
183.73000000	0.12900000000E-03
54.689700000	0.94900000000E-03
16.425500000	0.10100000000E-01
7.3050000000	-0.87309000000E-01
4.2747700000	0.71452000000E-01
2.6114200000	0.29537800000
1.5667400000	0.35873100000
0.96097900000	0.25612000000
1 d	
0.59653500000	1.00000000000
1 d	
0.34202800000	1.00000000000
1 d	
0.15160000000	1.00000000000
1 f	
0.59400000000	1.00000000000
1 f	
0.26840000000	1.00000000000
1 f	
1.5556400000	1.00000000000
1 f	
3.2498641894	1.00000000000
1 g	
0.47630000000	1.00000000000

*

rn def2-ecp

*

#	ncore = 60	lmax = 3	exponent
f	coefficient	r^n	
	21.7972900	2	6.3485710
	28.9468050	2	6.2959490
	1.4473650	2	2.8821180
	2.1779640	2	2.9080480
s-f			
	49.9655510	2	30.1512420
	283.0700000	2	14.5212410
	62.0028700	2	8.0520380
	-21.7972900	2	6.3485710
	-28.9468050	2	6.2959490
	-1.4473650	2	2.8821180
	-2.1779640	2	2.9080480

p-f

71.9691190	2	11.0099420
143.8605590	2	9.6176250
4.7147610	2	7.3360080
9.0130650	2	6.4062530
-21.7972900	2	6.3485710
-28.9468050	2	6.2959490
-1.4473650	2	2.8821180
-2.1779640	2	2.9080480

d-f

36.3683650	2	8.3692200
54.5517610	2	8.1169750
9.6344870	2	5.3536560
14.3879020	2	5.0972120
-21.7972900	2	6.3485710
-28.9468050	2	6.2959490
-1.4473650	2	2.8821180
-2.1779640	2	2.9080480

*

\$end