Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information for

On the σ, π and δ hole interactions: a molecular orbital overview

V. Angarov, S. Kozuch

FI

I	0.000000	0.000000	0.276060
F	0.000000	0.000000	-1.625686

NCH

N	0.000000	0.000000	0.649744
C	0.000000	0.000000	-0.497279
H	0.000000	0.000000	-1.564535

FI – NCH

N	0.000000	0.000000	-2.192127
C	0.000000	0.000000	-3.335815
H	0.000000	0.000000	-4.403814
I	0.000000	0.000000	0.361019
F	0.000000	0.000000	2.292177

$H_2C=O$

C	-0.000000	0.000000	-0.527028
H	0.000000	0.938017	-1.109367
H	-0.000000	-0.938017	-1.109367
O	0.000000	-0.000000	0.672613

$H_2C=O$ – NCH / C_{2v}

C	0.000000	0.000000	1.555359
O	0.000000	0.000000	2.756780
H	-0.000000	0.933331	0.966613
H	-0.000000	-0.933331	0.966613
N	0.000000	-0.000000	-1.730450
C	0.000000	-0.000000	-2.876997
H	0.000000	-0.000000	-3.944490

$H_2C=O$ – NCH / C_s

C	-0.771819	-1.380276	0.000000
O	0.044419	-2.261767	0.000000
H	-1.168210	-0.950038	0.935325
H	-1.168210	-0.950038	-0.935325
N	0.000000	1.573842	0.000000
C	0.833486	2.361092	0.000000
H	1.611067	3.092417	0.000000

$H_2C=O$ – NCH / C_s – H bond

C	0.442796	-2.381483	-0.000000
O	0.817392	-1.238423	-0.000000
H	-0.628283	-2.641382	-0.000000
H	1.158383	-3.219163	-0.000000
N	-0.984820	2.729308	0.000000
C	-0.472046	1.702380	0.000000
H	-0.000000	0.737393	0.000000

$H_2C=CH_2$

C	-0.000000	-0.000000	0.662335
C	0.000000	-0.000000	-0.662335
H	0.000000	0.921990	1.230869
H	-0.000000	-0.921990	1.230869
H	0.000000	0.921990	-1.230869
H	-0.000000	-0.921990	-1.230869

$F_2C=CF_2$

C	-0.000000	-0.000000	0.660064
C	0.000000	-0.000000	-0.660064
F	0.000000	1.094504	1.380618
F	-0.000000	-1.094504	1.380618
F	0.000000	1.094504	-1.380618
F	-0.000000	-1.094504	-1.380618

$F_2C=CF_2$ – NCH

C	-0.462191	-0.696349	0.000259
C	-1.298580	0.323689	0.000027
N	2.389650	0.487626	-0.000538
C	3.506613	0.746115	-0.000609
H	4.546153	0.987162	0.000932
F	-0.008987	-1.253776	1.094628
F	-0.009226	-1.254437	-1.093888
F	-1.754606	0.885491	1.095069
F	-1.754821	0.884803	-1.095279

MeI

C	0.000000	0.000000	-1.803497
H	0.000000	1.031161	-2.138498
H	0.893012	-0.515581	-2.138498
H	-0.893012	-0.515581	-2.138498
I	0.000000	0.000000	0.325216

CN^-

N	0.000000	0.000000	0.541405
C	0.000000	0.000000	-0.631639

MeI – CN^-

C	0.000000	0.000000	2.503422
H	-0.000000	1.026951	2.864530
H	-0.889365	-0.513475	2.864530
H	0.889365	-0.513475	2.864530
I	0.000000	0.000000	0.311120
C	0.000000	0.000000	-2.455948
N	0.000000	0.000000	-3.623972

$F_2C=O$

C	0.000000	0.000000	0.139775
F	-0.000000	1.057198	-0.629630
F	-0.000000	-1.057198	-0.629630
O	0.000000	0.000000	1.311837

$F_2C=O$ – CN^-

C	0.381860	0.188185	0.000000
F	0.793221	-0.633464	1.098117
F	0.793221	-0.633464	-1.098117
O	0.793221	1.343026	0.000000
C	-1.142308	-0.005323	0.000000
N	-2.294438	-0.062717	0.000000

BrI

I	0.000000	0.000000	0.981466
Br	0.000000	0.000000	-1.486220

BrI – CN^-

I	0.000000	0.000000	0.656538
Br	0.000000	0.000000	-2.255900
C	0.000000	0.000000	2.772930
N	0.000000	0.000000	3.931771

H_2C=Te

C	0.000000	0.000000	-1.660748
H	0.000000	0.920183	-2.233768
H	-0.000000	-0.920183	-2.233768
Te	0.000000	-0.000000	0.277539

H_2C=Te – NCH / C_{2v}

C	-0.000000	0.000000	2.497580
H	-0.000000	0.918306	3.074745
H	-0.000000	-0.918306	3.074745
Te	-0.000000	0.000000	0.555490
N	0.000000	0.000000	-2.923376
C	0.000000	0.000000	-4.069924
H	0.000000	0.000000	-5.137295

H_2C=Te – NCH / C_s

C	0.546516	0.873859	0.000000
Te	0.571464	-1.093282	0.000000
N	-2.413603	1.652364	0.000000
C	-3.553710	1.531789	0.000000
H	-4.615025	1.419026	0.000000
F	0.546516	1.635066	1.051866
F	0.546516	1.635066	-1.051866

F_2C=Te

C	0.000000	-0.000000	-1.161465
F	-0.000000	1.052315	-1.928323
F	-0.000000	-1.052315	-1.928323
Te	-0.000000	0.000000	0.801511

F_2C=Te – NCH / C_{2v}

C	0.000000	0.000000	1.896510
F	0.000000	1.052078	2.669767
F	0.000000	-1.052078	2.669767
Te	-0.000000	0.000000	-0.075258
N	-0.000000	0.000000	-3.316520
C	-0.000000	0.000000	-4.462617
H	-0.000000	0.000000	-5.530100

F_2C=Te – NCH / C_s

C	0.546516	0.873859	0.000000
Te	0.571464	-1.093282	0.000000
N	-2.413603	1.652364	0.000000
C	-3.553710	1.531789	0.000000
H	-4.615025	1.419026	0.000000
F	0.546516	1.635066	1.051866
F	0.546516	1.635066	-1.051866

TFDTE

S	0.000000	1.353767	0.000000
S	-0.000000	-1.353767	0.000000
F	1.996611	-0.000000	1.067868
F	1.996611	0.000000	-1.067868
F	-1.996611	-0.000000	-1.067868
F	-1.996611	0.000000	1.067868
C	-1.191313	0.000000	0.000000
C	1.191313	-0.000000	0.000000

TFDTE – NCH

S	-0.892311	-0.488648	0.000000
S	1.815340	-0.482005	0.000000
F	0.469683	1.512649	1.068594
F	0.469683	1.512649	-1.068594
F	0.469683	-2.483660	-1.067972
F	0.469683	-2.483660	1.067972
C	0.463367	-1.673110	0.000000
C	0.457326	0.708796	0.000000
N	-2.323399	2.214265	0.000000
C	-2.912798	3.196952	0.000000
H	-3.460643	4.112973	0.000000

S_2O_2 / D_{2h}

S	0.000000	0.000000	1.220193
S	0.000000	0.000000	-1.220193
O	0.000000	1.147099	0.000000
O	-0.000000	-1.147099	0.000000

S_2O_2 / C_{2v}

S	-0.000000	1.179686	-0.129673
S	-0.000000	-1.179686	-0.129673
O	1.122055	-0.000000	0.259347
O	-1.122055	0.000000	0.259347

S_2O_2 – NCH /C_s

S	-0.159918	-0.866127	-0.000000
S	-1.651264	1.080879	-0.000000
O	-1.827086	-0.571623	-0.000000
O	0.000000	0.808558	0.000000
N	2.479709	-0.516935	0.000000
C	3.599190	-0.276935	0.000000
H	4.642499	-0.051362	0.000000

$S(CF_2)_2$ – NCH

S	1.101861	-0.695910	0.000000
C	-0.512356	-1.441176	0.000000
C	-0.512512	0.040626	0.000000
F	-0.929369	-2.088035	1.084010
F	-0.929369	-2.088035	-1.084010
F	-0.929369	0.683645	1.084156
F	-0.929369	0.683645	-1.084156
N	1.461283	2.560971	0.000000
C	1.653020	3.691070	0.000000
H	1.829623	4.743653	0.000000

$S(CF_2)_3$ – NCH

S	1.174503	-0.466403	0.000000
F	-0.295185	1.469138	1.076564
F	-0.295185	1.469138	-1.076564
F	-2.031274	-0.461736	-1.085783
F	-2.031274	-0.461736	1.085783
F	-0.295185	-2.398967	-1.076308
F	-0.295185	-2.398967	1.076308
C	-1.263458	-0.462420	0.000000
C	-0.212313	0.688390	0.000000
C	-0.214885	-1.612416	0.000000
N	2.466616	2.333746	0.000000
C	2.972206	3.362074	0.000000
H	3.441935	4.320601	0.000000

$S(CF_2)_4$ – NCH

S	−0.692161	−1.179105	−0.259427
F	0.783877	2.346009	0.407975
F	0.968914	1.301310	−1.492937
F	−1.554396	1.167078	−1.018228
F	−1.284198	0.968690	1.113269
F	1.412836	0.112578	1.748234
F	2.861381	0.340695	0.137747
F	1.487382	−2.247887	0.655091
F	1.682680	−1.450015	−1.338402
C	0.660890	1.167927	−0.198676
C	−0.784181	0.617946	−0.077176
C	1.581797	0.110223	0.421491
C	1.105934	−1.246211	−0.145487
N	−3.760096	−0.632699	0.046581
C	−4.881865	−0.509533	0.246120
H	−5.926503	−0.393659	0.432396

$S(CF_2)_5$ – NCH

S	1.110230	1.033298	0.052377
F	−2.043220	−0.943637	1.135999
F	−2.400791	−1.440907	−0.951201
F	−1.369755	0.844463	−1.781286
F	−2.847196	1.172171	−0.219229
F	−0.947124	1.549805	1.602258
F	−0.672293	2.813043	−0.141141
F	0.180868	−1.468791	−1.497875
F	−0.265956	−2.681491	0.251465
F	2.064864	−1.299984	0.368758
F	0.610228	−0.772853	1.888338
C	−1.588752	−0.792429	−0.111167
C	−1.619974	0.709066	−0.475772
C	−0.593757	1.555064	0.311948
C	−0.185053	−1.430742	−0.213527
C	0.904101	−0.676846	0.586265
N	4.369749	0.668833	−0.433559
C	5.476032	0.413268	−0.592369
H	6.505885	0.174744	−0.740159

SF_2

S	−0.000000	0.000000	0.547911
F	−0.000000	1.191769	−0.487032
F	−0.000000	−1.191769	−0.487032

SF_2 – NCH

S	−0.000000	−0.852075	0.000000
F	−1.324307	0.012667	−0.000000
F	−0.706023	−2.275969	0.000000
N	1.121246	1.806288	−0.000000
C	1.446120	2.904987	−0.000000
H	1.747537	3.928988	−0.000000

SHF

S	0.051060	−0.549901	0.000000
H	−1.276510	−0.692608	0.000000
F	0.051060	1.054558	0.000000

SHF – NCH

S	−0.000000	−0.830216	−0.000000
H	−1.228880	−0.317257	−0.000000
F	−0.466396	−2.378754	−0.000000
N	0.174617	1.887634	0.000000
C	0.550361	2.969726	0.000000
H	0.901958	3.977703	0.000000

PF_3

P	0.000000	0.000000	0.500773
F	0.000000	1.353616	−0.278207
F	−1.172265	−0.676808	−0.278207
F	1.172265	−0.676808	−0.278207

PF_3 – NCH

P	−0.809157	0.000052	0.428939
F	−2.354919	−0.001528	0.155735
F	−0.455155	−1.174002	−0.540391
F	−0.457547	1.174849	−0.540321
N	2.335724	0.002212	0.284601
C	3.451066	−0.001023	0.020770
H	4.489471	−0.004003	−0.226106

$P(CF_2)_3CH$

P	0.000000	0.000000	1.340505
C	0.000000	1.270739	−0.084567
C	−1.100492	−0.635369	−0.084567
C	1.100492	−0.635369	−0.084567
C	0.000000	0.000000	−0.954201
F	1.252742	−1.959180	−0.200296
F	2.323071	−0.105317	−0.200296
F	1.070328	2.064497	−0.200296
F	−1.070328	2.064497	−0.200296
F	−2.323071	−0.105317	−0.200296
F	−1.252742	−1.959180	−0.200296
H	0.000000	0.000000	−2.044159

$P(CF_2)_3CH$ – NCH

P	−1.114004	−0.005933	0.000000
C	−0.329091	−1.746119	−0.000000
C	0.449814	−0.007617	1.099601
C	0.449814	−0.007617	−1.099601
C	0.982004	−0.944819	−0.000000
F	1.115870	1.141241	−1.257667
F	0.333727	−0.540830	−2.323590
F	−0.544016	−2.523717	−1.070869
F	−0.544016	−2.523717	1.070869
F	0.333727	−0.540830	2.323590
F	1.115870	1.141241	1.257667
H	1.978608	−1.387289	−0.000000
N	−0.882873	3.097488	0.000000
C	−0.697321	4.228273	0.000000
H	−0.520212	5.280777	0.000000

Mo_2

Mo	0.000000	0.000000	0.941318
Mo	0.000000	0.000000	−0.941318

Mo_2 – Rn / C_s

Mo	1.834312	2.028168	0.000000
Mo	0.000000	1.591359	0.000000
Rn	−0.895827	−1.767676	0.000000

Mo_2 – Rn / $C_{\infty v}$

Mo	0.000000	0.000000	−1.559141
Mo	0.000000	0.000000	−3.443543
Rn	0.000000	0.000000	2.443171

Tc_2

Tc	0.000000	0.000000	0.951634
Tc	0.000000	0.000000	−0.951634

Tc_2 – Rn

Tc	0.000000	1.431305	0.000000
Tc	1.837285	1.949245	0.000000
Rn	−0.918643	−1.690275	0.000000