On the accuracy of DFT-SAPT, MP2, SCS-MP2, MP2C, and DFT+Disp methods for the interaction energies of endohedral complexes of the C_{60} fullerene with a rare gas atom. Supplementary material.

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TABLE I: Components of the DFT-SAPT interaction energy for the He@C_{60} complex. The total DFT-SAPT energy, as well as MP2, SCS-MP2, DFT+Disp, and MP2C interaction energies are also given. Energy values in kJ/mol, distances in Å. Note that for distances r>3.5 Å the complex is *exohedral*.

r	$E^{(1)}_{\mathrm{elst}}$	$E^{(1)}_{\mathrm{exch}}$	$E^{(2)}_{\mathrm{ind}}$	$E^{(2)}_{\mathrm{exch-ind}}$	$E^{(2)}_{\mathrm{disp}}$	$E^{(2)}_{\mathrm{exch-disp}}$	δE_{HF}	$E^{\mathrm{SAPT}}_{\mathrm{int}}$	$E^{\mathrm{MP2}}_{\mathrm{int}}$	$E^{\mathrm{SCS-MP2}}_{\mathrm{int}}$	$E^{\mathrm{DFT+Disp}}_{\mathrm{int}}$	$E^{\mathrm{MP2C}}_{\mathrm{int}}$
0.0	−1.17	5.10	−0.31	0.32	−10.75	0.45	−0.25	−6.61	−8.77	−6.07	−8.51	−7.07
0.2	−1.24	5.40	−0.35	0.36	−10.64	0.47	−0.28	−6.28	−8.66	−5.92	–	−7.09
0.4	−1.62	7.04	−0.48	0.49	−11.49	0.59	−0.39	−5.86	−8.24	−5.36	−7.91	−5.75
0.6	−2.41	10.29	−0.77	0.78	−12.73	0.81	−0.62	−4.66	−7.20	−4.09	–	−4.61
0.8	−3.89	16.29	−1.37	1.37	−14.78	1.18	−1.10	−2.30	−4.90	−1.44	−5.32	–
1.0	−6.69	27.34	−2.64	2.61	−17.83	1.78	−2.04	2.53	−0.11	3.82	–	2.82
1.2	−11.83	47.18	−5.26	5.13	−21.95	2.65	−3.81	12.10	9.37	13.94	7.58	12.68
1.4	−21.04	82.25	−10.66	10.12	−27.68	3.92	−6.88	30.02	27.34	32.75	–	31.21
2.0	−106.22	400.44	−78.07	58.89	−60.48	10.69	−17.77	207.49	207.10	216.77	–	–
5.0	−26.30	112.39	−16.59	15.03	−22.17	3.57	−8.91	57.01	56.52	59.88	–	–
6.0	−1.32	6.37	−0.52	0.56	−4.07	0.28	−0.65	0.65	0.40	1.24	–	1.17
7.0	−0.06	0.31	−0.02	0.02	−0.85	0.01	−0.03	−0.62	−0.75	−0.54	–	−0.22
8.0	0.00	0.01	0.00	0.00	−0.24	0.00	0.00	−0.23	−0.28	−0.21	–	−0.09
9.0	0.00	0.00	0.00	0.00	−0.09	0.00	0.00	−0.09	−0.11	−0.08	–	−0.03

TABLE II: Components of the DFT-SAPT interaction energy for the Ne@C_{60} complex. The total DFT-SAPT energy, as well as MP2, SCS-MP2, DFT+Disp, and MP2C interaction energies are also given. Energy values in kJ/mol, distances in Å.

r	$E^{(1)}_{\mathrm{elst}}$	$E^{(1)}_{\mathrm{exch}}$	$E^{(2)}_{\mathrm{ind}}$	$E^{(2)}_{\mathrm{exch-ind}}$	$E^{(2)}_{\mathrm{disp}}$	$E^{(2)}_{\mathrm{exch-disp}}$	δE_{HF}	$E^{\mathrm{SAPT}}_{\mathrm{int}}$	$E^{\mathrm{MP2}}_{\mathrm{int}}$	$E^{\mathrm{SCS-MP2}}_{\mathrm{int}}$	$E^{\mathrm{DFT+Disp}}_{\mathrm{int}}$	$E^{\mathrm{MP2C}}_{\mathrm{int}}$
0.0	−4.35	13.17	−4.00	4.14	−22.11	1.59	−0.38	−11.95	−17.05	−11.46	−23.41	−10.82
0.2	−4.82	14.62	−4.51	4.68	−23.43	1.96	−0.43	−11.93	−16.64	−10.95	–	−10.40
0.4	−6.26	19.15	−6.94	7.54	−24.57	2.27	−0.59	−9.39	−15.11	−9.13	−21.67	−8.53
0.6	−9.25	28.49	−9.43	9.82	−27.56	2.99	−0.94	−5.88	−11.48	−5.01	–	−4.49
0.8	−14.90	46.01	−15.88	16.48	−32.23	4.28	−1.66	2.10	−3.71	3.48	−10.93	3.98
1.0	−25.35	78.10	−28.70	29.66	−38.60	6.32	−3.02	18.41	12.06	20.20	–	20.85
1.2	−44.66	136.52	−54.02	55.32	−47.81	9.73	−5.24	49.85	42.52	51.91	37.68	52.89
1.4	−79.38	239.54	−107.33	108.43	−61.05	15.30	−7.87	107.63	98.73	109.78	–	111.35
2.0	−405.03	1157.09	−644.51	580.51	−140.33	55.69	−9.82	593.60	155.18	162.30	–	–
5.0	−99.72	307.70	−145.38	144.04	−51.50	16.12	44.49	215.75	632.25	652.32	–	–
6.0	−5.08	16.13	−6.78	7.14	−8.64	1.16	−0.95	2.98	2.23	3.99	–	3.49
7.0	−0.24	0.74	−0.32	0.34	−1.60	0.06	−0.03	−1.05	−1.38	−0.97	–	−1.03
8.0	−0.01	0.03	−0.01	0.01	−0.42	0.00	0.00	−0.40	−0.51	−0.38	–	−0.38
9.0	0.01	0.00	0.00	0.00	−0.15	0.00	0.00	−0.14	−0.20	−0.15	–	−0.14

TABLE III: Components of the DFT-SAPT interaction energy for the Ar@C_{60} complex. The total DFT-SAPT energy, as well as MP2, SCS-MP2, DFT+Disp, and MP2C interaction energies are also given. Energy values in kJ/mol, distances in Å.

r	$E^{(1)}_{\mathrm{elst}}$	$E^{(1)}_{\mathrm{exch}}$	$E^{(2)}_{\mathrm{ind}}$	$E^{(2)}_{\mathrm{exch-ind}}$	$E^{(2)}_{\mathrm{disp}}$	$E^{(2)}_{\mathrm{exch-disp}}$	δE_{HF}	$E^{\mathrm{SAPT}}_{\mathrm{int}}$	$E^{\mathrm{MP2}}_{\mathrm{int}}$	$E^{\mathrm{SCS-MP2}}_{\mathrm{int}}$	$E^{\mathrm{DFT+Disp}}_{\mathrm{int}}$	$E^{\mathrm{MP2C}}_{\mathrm{int}}$
0.0	−29.92	78.51	−32.59	31.98	−91.95	13.19	−2.18	−32.97	−71.29	−45.83	−40.69	−33.36
0.2	−32.48	85.03	−36.16	35.44	−93.83	13.85	−2.38	−30.54	−69.25	−43.48	–	−31.09
0.4	−40.86	106.37	−49.17	47.94	−99.54	15.90	−2.98	−22.34	−62.16	−35.38	−29.61	−22.12
0.6	−57.41	148.45	−73.89	71.52	−109.58	19.55	−3.87	−5.24	−46.71	−18.23	–	−3.75
0.8	−86.92	223.02	−122.68	117.14	−125.33	25.42	−4.25	26.41	−16.45	14.55	–	–
1.0	−137.84	350.37	−215.92	201.20	−147.28	33.95	−0.92	83.56	39.83	74.30	–	94.90
1.2	−224.04	562.74	−390.15	349.57	−179.38	46.36	16.18	181.28	140.43	179.55	194.87	205.25
1.4	−367.11	908.66	−696.17	590.36	−221.64	62.12	73.32	349.55	313.14	358.47	–	392.07
2.0	−1485.32	3487.40	−3465.52	2155.45	−449.72	131.37	1271.64	1645.30	1622.17	1703.53		–
5.0	−414.34	1099.78	−911.44	743.46	−184.42	56.38	121.75	511.17	516.79	546.91	–	–
6.0	−25.17	73.61	−44.32	43.22	−34.46	6.70	−3.00	16.60	10.17	17.84	–	19.03
7.0	−1.21	3.72	−1.83	1.81	−7.26	0.52	−0.18	−4.41	−6.77	−4.74	–	−4.51
8.0	−0.05	0.17	−0.08	0.08	−1.93	0.03	−0.02	−1.81	−2.60	−1.98	–	−1.81

TABLE IV: Components of the DFT-SAPT interaction energy for the Kr@C_{60} complex. The total DFT-SAPT energy, as well as MP2, SCS-MP2, DFT+Disp, and MP2C interaction energies are also given. Energy values in kJ/mol, distances in Å.

r	$E^{(1)}_{\mathrm{elst}}$	$E^{(1)}_{\mathrm{exch}}$	$E^{(2)}_{\mathrm{ind}}$	$E^{(2)}_{\mathrm{exch-ind}}$	$E^{(2)}_{\mathrm{disp}}$	$E^{(2)}_{\mathrm{exch-disp}}$	δE_{HF}	$E^{\mathrm{SAPT}}_{\mathrm{int}}$	$E^{\mathrm{MP2}}_{\mathrm{int}}$	$E^{\mathrm{SCS-MP2}}_{\mathrm{int}}$	$E^{\mathrm{DFT+Disp}}_{\mathrm{int}}$	$E^{\mathrm{MP2C}}_{\mathrm{int}}$
0.0	−62.41	148.86	−86.65	84.46	−141.91	25.84	−2.75	−34.57	−91.14	−53.99	−54.99	−34.03
0.2	−67.16	159.93	−95.39	92.74	−144.14	26.79	−2.80	−30.04	−87.27	−49.69		−29.51
0.4	−82.59	195.82	−124.63	120.21	−153.01	30.19	−2.69	−16.70	−74.19	−35.31	−31.57	−14.67
0.8	−165.06	385.69	−302.15	280.37	−188.79	44.97	5.77	60.80	2.72	47.10	62.82	–
1.0	−252.75	584.93	−511.79	458.37	−222.40	58.38	30.06	144.80	91.16	140.01		169.88
1.2	−396.50	907.48	−885.40	752.19	−263.09	73.76	102.37	290.81	242.40	297.28	311.01	337.43
2.0	−2316.28	5032.91	−7332.84	4037.27	−599.65	157.37	3258.89	2237.67	2123.01	2241.76	–	608.69
5.0	−676.06	1660.62	−1960.32	1475.36	−257.95	76.48	426.59	744.72	768.47	809.94	–	–
6.0	−45.88	124.99	−109.39	104.46	−50.62	11.24	−2.41	32.39	24.40	35.38	–	38.33
7.0	−2.36	6.87	−4.48	4.41	−10.81	1.00	−0.33	−5.70	−9.46	−6.44	–	−5.91
8.0	−0.11	0.33	−0.19	0.18	−2.83	0.06	0.00	0.00	−3.88	−2.94	–	−2.64
9.0	0.00	0.02	−0.01	0.01	−0.97	0.00	0.00	0.00	−1.49	−1.14	–	–