Supporting Information: Density functionals for nondynamical correlation constructed from an upper bound to the exact exchange energy density

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Gaussian, Inc, Wallingford, CT 06492, USA

SI-I. GAUSSIAN CITATION

Gaussian Development Version, Revision I.14+,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone,
G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich,
J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian,
J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young,
F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone,
T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega,
G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda,
J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai,
T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta,
F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin,
V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar,
J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi,
J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas,
J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2018.

SI-II. NOMENCLATURE

There is to our knowledge no unique rigorous universally acceptable separation of "dynamical" and "nondynamical" correlation. We will assume here that "nondynamical" correlation is relatively large in stretched covalent bonds and is negligible in atomic cores and in isolated atoms whose exact Kohn-Sham ground-state wavefunction is not nearly degenerate. The ground singlet state of H_2 stretched past the Coulson-Fischer point has significant nondynamical correlation. Isolated beryllium atom may or may not have significant nondynamical correlation. Isolated argon atom should have negligible nondynamical correlation. We will further assume that standard DFT "correlation" functionals model only dynamical correlation. With these assumptions, we may state that the PBE0 global hybrid models dynamical correlation with the PBE correlation functional, and models nondynamical correlation as 75% of the difference between PBE and HF exchange.

We note for completeness that the low-density limit of the uniform electron gas could be regarded as having large "nondynamical" correlation, and that local density approximation correlation functionals effectively describe this form of correlation.

We define "exact" exchange as the exchange energy obtained by substituting the exact Kohn-Sham orbitals, from the exact ground state of the noninteracting Kohn-Sham reference system of a noninteracting-v-representable system, into the Hartree-Fock exchange formula. We define "HF" or "Hartree-Fock" exchange as the exchange energy obtained by substituting **any** approximate orbitals, including those from a generalized Kohn-Sham ground-state density functional theory calculation using a finite basis set and an approximate exchange-correlation functional, into the Hartree-Fock exchange formula.

SI-III. ANALYTIC FORMULA FOR $F_{Hup}(y,x)$

$$
\begin{aligned}
F_{Hup}(y,x) = {} & \frac{1}{9\log^2\left(\frac{x^3}{8\pi}\right)} 2^{\frac{4\sqrt[3]{6}\pi^{2/3}\log\left(\frac{x^3}{8\pi}\right)}{x^2y^2}-7} \pi^{\frac{1}{3}\left(-\frac{4\sqrt[3]{6}\pi^{2/3}\log\left(\frac{8\pi}{x^3}\right)}{x^2y^2}-1\right)} x^{\frac{4\sqrt[3]{6}\pi^{2/3}\log\left(\frac{8\pi}{x^3}\right)}{x^2y^2}-5} \\
& \Bigg(8\pi^{7/6}\left(3x^2y^2 - 8\sqrt[3]{6}\pi^{2/3}\left(\log\left(\frac{x^3}{8\pi}\right)+2\right)\right) \\
& \Bigg(-\operatorname{erfc}\left(\frac{8\sqrt[3]{6}\pi^{2/3}\log\left(\frac{8\pi}{x^3}\right)+3x^2y^2}{4\ 6^{2/3}\sqrt[3]{\pi}xy}\right) \\
& -\operatorname{erfc}\left(\frac{8\sqrt[3]{6}\pi^{2/3}\log\left(\frac{x^3}{8\pi}\right)+3x^2y^2}{4\ 6^{2/3}\sqrt[3]{\pi}xy}\right) + 2\operatorname{erfc}\left(\frac{\sqrt[3]{\frac{3}{\pi}}xy}{4\ 2^{2/3}}\right)\Bigg) \\
& \exp\left(\frac{\left(8\sqrt[3]{6}\pi^{2/3}\log\left(\frac{x^3}{8\pi}\right)+3x^2y^2\right)^2}{96\sqrt[3]{6}\pi^{2/3}x^2y^2}\right) \\
& +\sqrt[6]{\pi}\Bigg(-8\sqrt[3]{6}\pi^{2/3}\left(-2x^3+\left(x^3+8\pi\right)\log\left(\frac{x^3}{8\pi}\right)+16\pi\right) \\
& -3x^2\left(x^3-8\pi\right)y^2\Bigg) \\
& \operatorname{erfc}\left(\frac{8\sqrt[3]{6}\pi^{2/3}\log\left(\frac{x^3}{8\pi}\right)+3x^2y^2}{4\ 6^{2/3}\sqrt[3]{\pi}xy}\right) \\
& \exp\left(\frac{\left(8\sqrt[3]{6}\pi^{2/3}\log\left(\frac{x^3}{8\pi}\right)+3x^2y^2\right)^2}{96\sqrt[3]{6}\pi^{2/3}x^2y^2}\right) \\
& +4\ 6^{2/3}x\left(x^3-8\pi\right)y + 4\ 6^{2/3}xy\Bigg(x^3 - 2^{\frac{2\sqrt[3]{6}\pi^{2/3}\log\left(\frac{8\pi}{x^3}\right)}{x^2y^2}+\frac{5}{2}} \\
& \pi^{\frac{1}{6}\left(\frac{4\sqrt[3]{6}\pi^{2/3}\log\left(\frac{8\pi}{x^3}\right)}{x^2y^2}+3\right)} x^{\frac{2\sqrt[3]{6}\pi^{2/3}\log\left(\frac{x^3}{8\pi}\right)}{x^2y^2}+\frac{3}{2}} + 8\pi\Bigg)\Bigg)^2
\end{aligned}
$$

SI-IV. ATOMIC TOTAL ENERGIES

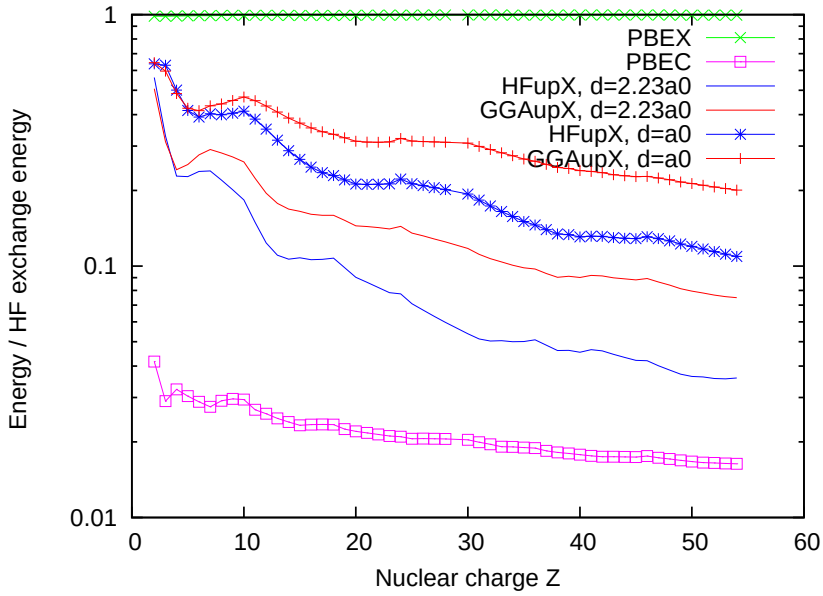

Figure SI-1 above shows the ratio of various exchange and correlation energies to HF exchange. Calculations treat atoms He-Xe, and use UHF/3-21G orbitals and densities. PBE exchange almost perfectly captures HF exchange, whereas the upper bounds to HF and PBE exchange both decay as nuclear charge Z increases. Individual energies are tabulated below.

# Atom	Z	HFX	PBEc	PBEx	HFupX,d=2.23a0	HFupX,d=a0	PBEupX,d=2.23a0	PBEupX,d=a0
He	2	-1.028537	-0.042882	-1.013462	-0.578561	-0.655824	-0.521787	-0.662222
Li	3	-1.779299	-0.051689	-1.753557	-0.585231	-1.118882	-0.555510	-1.061155
Be	4	-2.667237	-0.086285	-2.633427	-0.607976	-1.335744	-0.644657	-1.294664
B	5	-3.755723	-0.114136	-3.714897	-0.852455	-1.561477	-0.951176	-1.592580
C	6	-5.061499	-0.146116	-5.010785	-1.204631	-1.982240	-1.401732	-2.101892
N	7	-6.598949	-0.181770	-6.531750	-1.576230	-2.662267	-1.920348	-2.864639
O	8	-8.209740	-0.239120	-8.146048	-1.803774	-3.282980	-2.312684	-3.625025
F	9	-10.048111	-0.297713	-9.981050	-2.022403	-4.074991	-2.729262	-4.578401
Ne	10	-12.132591	-0.357502	-12.053067	-2.223408	-5.014471	-3.146090	-5.702435
Na	11	-13.981449	-0.374919	-13.886277	-2.085961	-5.366732	-3.124222	-6.356268
Mg	12	-15.991944	-0.413598	-15.887680	-1.977108	-5.602172	-3.116978	-6.931784
Al	13	-18.076103	-0.448032	-17.954113	-1.996240	-5.720726	-3.208413	-7.406062
Si	14	-20.283208	-0.486138	-20.142618	-2.160853	-5.833124	-3.418036	-7.870838
P	15	-22.626618	-0.526838	-22.462388	-2.442753	-6.017386	-3.732931	-8.385393
S	16	-25.004924	-0.585507	-24.827549	-2.652309	-6.183925	-4.019724	-8.861527
Cl	17	-27.513423	-0.645272	-27.319676	-2.924538	-6.468689	-4.382492	-9.417244
Ar	18	-30.163304	-0.706151	-29.946977	-3.242588	-6.909340	-4.801024	-10.078164
K	19	-32.628237	-0.733497	-32.409697	-3.218404	-7.188015	-4.962904	-10.573730
Ca	20	-35.142878	-0.774240	-34.932005	-3.169257	-7.454125	-5.079715	-11.025285
Sc	21	-37.976587	-0.824728	-37.785435	-3.273896	-8.029359	-5.459018	-11.818965
Ti	22	-41.001368	-0.876876	-40.813771	-3.370743	-8.678958	-5.833501	-12.748197
V	23	-44.164794	-0.931585	-43.978224	-3.459273	-9.375036	-6.201590	-13.769049
Cr	24	-47.961942	-1.005753	-47.749459	-3.716664	-10.638721	-6.894794	-15.433873
Mn	25	-50.964103	-1.047582	-50.751062	-3.609236	-10.834247	-6.889120	-16.009098
Fe	26	-54.389455	-1.120529	-54.199099	-3.633780	-11.360532	-7.168611	-17.023225
Co	27	-57.985070	-1.193258	-57.804573	-3.660490	-11.897728	-7.434332	-18.085509
Ni	28	-61.726784	-1.267460	-61.553708	-3.688136	-12.433372	-7.698201	-19.192509
Zn	30	-69.696976	-1.419233	-69.505339	-3.748144	-13.486626	-8.190401	-21.474383
Ga	31	-73.555412	-1.464773	-73.309283	-3.771792	-13.465692	-8.195209	-22.008374

Ge	32	-77.457140	-1.513734	-77.168595	-3.898930	-13.439504	-8.293956	-22.526698
As	33	-81.629027	-1.561394	-81.330051	-4.123912	-13.459230	-8.475445	-23.032579
Se	34	-85.464520	-1.633117	-85.096597	-4.276295	-13.446076	-8.620318	-23.490364
Br	35	-89.700862	-1.702427	-89.289117	-4.493441	-13.493627	-8.828048	-23.926765
Kr	36	-93.753462	-1.771101	-93.310388	-4.773631	-13.662645	-9.131842	-24.497767
Rb	37	-97.830071	-1.801300	-97.363912	-4.741504	-13.655702	-9.146488	-24.826511
Sr	38	-101.854696	-1.849366	-101.385352	-4.702565	-13.673137	-9.188888	-25.142330
Y	39	-105.403090	-1.894358	-105.047865	-4.873571	-14.046393	-9.608255	-25.764607
Zr	40	-109.870125	-1.952591	-109.502725	-4.992900	-14.347698	-9.895157	-26.326795
Nb	41	-114.649896	-2.017855	-114.265660	-5.335744	-15.067897	-10.523504	-27.271697
Mo	42	-119.282940	-2.080898	-118.876234	-5.483334	-15.659810	-10.902506	-28.073730
Tc	43	-123.968977	-2.164673	-123.489837	-5.526799	-16.093086	-11.136412	-28.639520
Ru	44	-128.689374	-2.242795	-128.199153	-5.576085	-16.600217	-11.440153	-29.411163
Rh	45	-133.498169	-2.321101	-132.994515	-5.633105	-17.168982	-11.764193	-30.262761
Pd	46	-138.722233	-2.437425	-138.188909	-5.831617	-18.165460	-12.380110	-31.521903
Ag	47	-143.487087	-2.478719	-142.937266	-5.760817	-18.450767	-12.404366	-32.132545
Cd	48	-148.291262	-2.534621	-147.736391	-5.724876	-18.693693	-12.464521	-32.723274
In	49	-153.537200	-2.591350	-152.867883	-5.702075	-18.801676	-12.479982	-33.175790
Sn	50	-158.481762	-2.647311	-157.784707	-5.772678	-18.973613	-12.609789	-33.726394
Sb	51	-163.544189	-2.704763	-162.809178	-5.924264	-19.139833	-12.786597	-34.279639
Te	52	-168.527218	-2.776688	-167.772355	-6.018061	-19.242497	-12.928051	-34.781580
I	53	-173.593578	-2.848652	-172.822321	-6.181012	-19.366005	-13.124463	-35.301695
Xe	54	-178.739781	-2.921147	-177.944498	-6.409838	-19.527341	-13.382036	-35.855231

SI-V. MGAE ATOMIZATION ENERGIES AND ERRORS

LH-HF

HCl	107.50	102.45	5.05
C4H8_cyc	1149.37	1193.36	-43.99
P2	117.59	92.35	25.24
SiH2_3B1	131.48	136.65	-5.17
N2	228.48	193.67	34.81
NH2NH2	438.60	435.89	2.71
C4H10_iso	1303.40	1343.04	-39.64
H2S	183.91	178.50	5.41
PH3	242.27	240.56	1.71
C4H6_tra	1012.73	1029.66	-16.93
C4H5N	1071.93	1106.45	-34.52
C3H4_pro	705.06	709.47	-4.41
C4H6_cyc	1001.97	1033.36	-31.39
CH2CH	446.09	452.57	-6.48
SiH3	228.01	230.40	-2.39
C2F4	591.06	609.26	-18.20
SH	87.00	86.27	0.73
CH3	307.88	315.64	-7.76
NH	83.10	80.24	2.86
CF4	477.93	501.85	-23.92
CH2CO	532.73	527.80	4.93
CCH	265.31	257.32	7.99
CH3SH	474.49	478.86	-4.37
C2H4O	651.11	665.18	-14.07
C2H5O	699.05	717.48	-18.43
CH3NO2	601.82	590.30	11.52
SO2	260.63	227.76	32.87
C5H8_spi	1284.73	1339.60	-54.87
C5H5N	1238.14	1268.13	-29.99
CH2OH	410.08	417.23	-7.15
CH2_1A1	181.46	185.74	-4.28
HCOOCH3	785.90	795.56	-9.66
C4H9_t	1199.70	1242.00	-42.30

CCl4	316.19	308.36	7.83
CH3COCH3	978.46	996.93	-18.47
CH3CH2OH	810.77	828.02	-17.25
C4H6_bic	987.56	1026.38	-38.82
ClF	62.79	46.52	16.27
C4H4O	994.33	1022.57	-28.24
SiCl4	388.73	376.61	12.12
SiH2_1A1	152.22	149.46	2.76
NO	152.75	127.03	25.72
NF3	205.67	181.71	23.96
F2	39.03	5.66	33.37
CHCl3	345.79	343.20	2.59
CH3COOH	803.68	813.34	-9.66
HCOCOH	633.99	625.31	8.68
C4H4S	963.65	983.84	-20.19
C2H5	603.93	623.72	-19.79
CO	259.74	240.97	18.77
CH3OCH3	798.46	818.17	-19.71
CH3NH2	582.31	590.45	-8.14
H2O	232.98	223.47	9.51
ClO	65.45	50.43	15.02
C3H6	853.68	883.74	-30.06
CH3CHO	677.44	683.18	-5.74
C4H8_iso	1158.97	1188.02	-29.05
CH3OH	513.54	518.63	-5.09
SC	171.76	144.46	27.30
SiH4	324.95	324.60	0.35
CH3Cl	396.44	400.08	-3.64
C2Cl4	469.82	469.24	0.58
HCOOH	501.53	498.10	3.43
AlF3	430.95	399.22	31.73
C3H4_all	703.47	708.67	-5.20
NH3	298.02	292.26	5.76
C2H4	563.69	569.12	-5.43
C2H5OCH3	1095.62	1127.64	-32.02
C4H10_anti	1301.68	1342.11	-40.43
HOCl	166.24	149.60	16.64
Si2	76.38	68.56	7.82
Si2H6	535.89	536.66	-0.77
C3H4_cyc	683.01	697.99	-14.98
OH	107.22	101.99	5.23
NH2	182.59	177.62	4.97
CH3CO	581.99	584.21	-2.22
HCO	279.43	268.97	10.46
CN	181.36	148.68	32.68
C3H8	1007.14	1036.04	-28.90
HCN	313.43	290.01	23.42
CH3CHCH2	860.88	878.47	-17.59
H2O2	269.03	246.80	22.23
H2	109.49	105.25	4.24
BF3	470.96	473.66	-2.70
CH	84.23	82.14	2.09
ClF3	127.31	87.92	39.39
CH3CN	616.02	607.03	8.99
Cl2	59.75	47.88	11.87
C2H6	712.98	730.06	-17.08
CH2_3B1	190.75	199.79	-9.04
C2H2	405.53	396.16	9.37
CH4	420.43	425.70	-5.27
CF3CN	641.17	640.01	1.16
H2CO	374.67	367.42	7.25
CH3CHCH3	901.02	932.75	-31.73
AlCl3	312.64	295.27	17.37

SiF4	576.30	564.09	12.21
CO2	390.16	373.01	17.15
S2	104.25	90.37	13.88
SiO	193.06	158.55	34.51
PF3	365.01	354.98	10.03
C6H6	1368.10	1407.06	-38.96
C4H6_yne	1004.49	1021.57	-17.08
O2	120.83	101.05	19.78
BCl3	325.45	322.63	2.82
HF	141.63	133.71	7.92
PH2	153.20	155.57	-2.37
CHF3	458.73	474.46	-15.73
SO	126.48	109.87	16.61
LH-PBE			
HCl	107.50	107.11	0.39
C4H8_cyc	1149.37	1151.79	-2.42
P2	117.59	117.56	0.03
SiH2_3B1	131.48	134.56	-3.08
N2	228.48	229.11	-0.63
NH2NH2	438.60	436.14	2.46
C4H10_iso	1303.40	1302.25	1.15
H2S	183.91	182.56	1.35
PH3	242.27	239.20	3.07
C4H6_tra	1012.73	1019.91	-7.18
C4H5N	1071.93	1079.26	-7.33
C3H4_pro	705.06	710.78	-5.72
C4H6_cyc	1001.97	1006.65	-4.68
CH2CH	446.09	451.48	-5.39
SiH3	228.01	226.55	1.46
C2F4	591.06	585.62	5.44
SH	87.00	87.66	-0.66
CH3	307.88	308.52	-0.64
NH	83.10	86.71	-3.61
CF4	477.93	461.23	16.70
CH2CO	532.73	541.32	-8.59
CCH	265.31	270.34	-5.03
CH3SH	474.49	476.60	-2.11
C2H4O	651.11	651.33	-0.22
C2H5O	699.05	701.18	-2.13
CH3NO2	601.82	603.82	-2.00
SO2	260.63	257.13	3.50
C5H8_spi	1284.73	1291.03	-6.30
C5H5N	1238.14	1252.57	-14.43
CH2OH	410.08	409.15	0.93
CH2_1A1	181.46	184.08	-2.62
HCOOCH3	785.90	783.22	2.68
C4H9_t	1199.70	1204.06	-4.36
CCl4	316.19	327.24	-11.05
CH3COCH3	978.46	981.10	-2.64
CH3CH2OH	810.77	806.56	4.21
C4H6_bic	987.56	990.59	-3.03
ClF	62.79	63.64	-0.85
C4H4O	994.33	999.51	-5.18
SiCl4	388.73	400.54	-11.81
SiH2_1A1	152.22	149.33	2.89
NO	152.75	155.56	-2.81
NF3	205.67	210.74	-5.07
F2	39.03	41.03	-2.00
CHCl3	345.79	354.62	-8.83
CH3COOH	803.68	801.25	2.43
HCOCOH	633.99	636.53	-2.54
C4H4S	963.65	978.59	-14.94
C2H5	603.93	606.78	-2.85

CO	259.74	257.25	2.49
CH3OCH3	798.46	793.09	5.37
CH3NH2	582.31	580.34	1.97
H2O	232.98	228.10	4.88
ClO	65.45	72.64	-7.19
C3H6	853.68	855.60	-1.92
CH3CHO	677.44	678.66	-1.22
C4H8_iso	1158.97	1162.29	-3.32
CH3OH	513.54	508.68	4.86
SC	171.76	177.06	-5.30
SiH4	324.95	319.49	5.46
CH3Cl	396.44	398.16	-1.72
C2Cl4	469.82	488.80	-18.98
HCOOH	501.53	498.77	2.76
AlF3	430.95	432.48	-1.53
C3H4_all	703.47	713.12	-9.65
NH3	298.02	296.15	1.87
C2H4	563.69	565.27	-1.58
C2H5OCH3	1095.62	1090.89	4.73
C4H10_anti	1301.68	1301.42	0.26
HOCl	166.24	166.20	0.04
Si2	76.38	81.68	-5.30
Si2H6	535.89	532.06	3.83
C3H4_cyc	683.01	686.75	-3.74
OH	107.22	106.68	0.54
NH2	182.59	184.67	-2.08
CH3CO	581.99	588.14	-6.15
HCO	279.43	282.39	-2.96
CN	181.36	187.87	-6.51
C3H8	1007.14	1006.81	0.33
HCN	313.43	316.11	-2.68
CH3CHCH2	860.88	863.91	-3.03
H2O2	269.03	265.91	3.12
H2	109.49	104.18	5.31
BF3	470.96	468.18	2.78
CH	84.23	83.96	0.27
ClF3	127.31	138.12	-10.81
CH3CN	616.02	622.48	-6.46
Cl2	59.75	64.55	-4.80
C2H6	712.98	712.14	0.84
CH2_3B1	190.75	193.67	-2.92
C2H2	405.53	407.86	-2.33
CH4	420.43	418.96	1.47
CF3CN	641.17	637.94	3.23
H2CO	374.67	373.39	1.28
CH3CHCH3	901.02	905.45	-4.43
AlCl3	312.64	326.12	-13.48
SiF4	576.30	560.47	15.83
CO2	390.16	394.03	-3.87
S2	104.25	113.91	-9.66
SiO	193.06	195.42	-2.36
PF3	365.01	353.39	11.62
C6H6	1368.10	1383.42	-15.32
C4H6_yne	1004.49	1012.31	-7.82
O2	120.83	125.76	-4.93
BCl3	325.45	341.90	-16.45
HF	141.63	137.88	3.75
PH2	153.20	153.51	-0.31
CHF3	458.73	449.06	9.67
SO	126.48	131.68	-5.20
LH-PBE45			
HCl	107.50	103.39	4.11
C4H8_cyc	1149.37	1166.53	-17.16

P2	117.59	107.28	10.31
SiH2_3B1	131.48	131.36	0.12
N2	228.48	221.38	7.10
NH2NH2	438.60	441.21	-2.61
C4H10_iso	1303.40	1313.21	-9.81
H2S	183.91	178.51	5.40
PH3	242.27	237.07	5.20
C4H6_tra	1012.73	1022.10	-9.37
C4H5N	1071.93	1099.08	-27.15
C3H4_pro	705.06	709.20	-4.14
C4H6_cyc	1001.97	1017.69	-15.72
CH2CH	446.09	450.66	-4.57
SiH3	228.01	222.48	5.53
C2F4	591.06	612.23	-21.17
SH	87.00	86.32	0.68
CH3	307.88	309.63	-1.75
NH	83.10	83.89	-0.79
CF4	477.93	495.64	-17.71
CH2CO	532.73	538.92	-6.19
CCH	265.31	265.08	0.23
CH3SH	474.49	472.92	1.57
C2H4O	651.11	660.53	-9.42
C2H5O	699.05	706.07	-7.02
CH3NO2	601.82	611.51	-9.69
SO2	260.63	249.99	10.64
C5H8_spi	1284.73	1313.57	-28.84
C5H5N	1238.14	1265.84	-27.70
CH2OH	410.08	414.49	-4.41
CH2_1A1	181.46	183.88	-2.42
HCOOCH3	785.90	794.75	-8.85
C4H9_t	1199.70	1214.75	-15.05
CCl4	316.19	314.30	1.89
CH3COCH3	978.46	988.02	-9.56
CH3CH2OH	810.77	815.26	-4.49
C4H6_bic	987.56	1009.03	-21.47
ClF	62.79	57.69	5.10
C4H4O	994.33	1017.14	-22.81
SiCl4	388.73	370.48	18.25
SiH2_1A1	152.22	146.39	5.83
NO	152.75	151.28	1.47
NF3	205.67	210.92	-5.25
F2	39.03	29.44	9.59
CHCl3	345.79	345.09	0.70
CH3COOH	803.68	812.02	-8.34
HCOCOH	633.99	639.02	-5.03
C4H4S	963.65	979.95	-16.30
C2H5	603.93	610.85	-6.92
CO	259.74	254.50	5.24
CH3OCH3	798.46	804.73	-6.27
CH3NH2	582.31	584.92	-2.61
H2O	232.98	226.53	6.45
ClO	65.45	63.08	2.37
C3H6	853.68	866.80	-13.12
CH3CHO	677.44	682.08	-4.64
C4H8_iso	1158.97	1169.16	-10.19
CH3OH	513.54	513.53	0.01
SC	171.76	161.66	10.10
SiH4	324.95	313.71	11.24
CH3Cl	396.44	395.19	1.25
C2Cl4	469.82	477.37	-7.55
HCOOH	501.53	505.18	-3.65
AlF3	430.95	401.22	29.73
C3H4_all	703.47	710.33	-6.86

NH3	298.02	294.87	3.15
C2H4	563.69	565.27	-1.58
C2H5OCH3	1095.62	1106.46	-10.84
C4H10_anti	1301.68	1312.39	-10.71
HOCl	166.24	160.13	6.11
Si2	76.38	72.58	3.80
Si2H6	535.89	518.68	17.21
C3H4_cyc	683.01	693.91	-10.90
OH	107.22	104.90	2.32
NH2	182.59	181.88	0.71
CH3CO	581.99	588.33	-6.34
HCO	279.43	280.41	-0.98
CN	181.36	171.84	9.52
C3H8	1007.14	1013.96	-6.82
HCN	313.43	308.09	5.34
CH3CHCH2	860.88	867.23	-6.35
H2O2	269.03	262.17	6.86
H2	109.49	104.65	4.84
BF3	470.96	469.03	1.93
CH	84.23	82.71	1.52
ClF3	127.31	120.93	6.38
CH3CN	616.02	617.34	-1.32
Cl2	59.75	55.15	4.60
C2H6	712.98	715.55	-2.57
CH2_3B1	190.75	194.65	-3.90
C2H2	405.53	403.32	2.21
CH4	420.43	418.67	1.76
CF3CN	641.17	654.82	-13.65
H2CO	374.67	373.75	0.92
CH3CHCH3	901.02	912.79	-11.77
AlCl3	312.64	292.04	20.60
SiF4	576.30	554.71	21.59
CO2	390.16	392.40	-2.24
S2	104.25	101.60	2.65
SiO	193.06	174.67	18.39
PF3	365.01	356.18	8.83
C6H6	1368.10	1395.24	-27.14
C4H6_yne	1004.49	1013.80	-9.31
O2	120.83	123.58	-2.75
BCl3	325.45	321.74	3.71
HF	141.63	136.27	5.36
PH2	153.20	153.37	-0.17
CHF3	458.73	469.98	-11.25
SO	126.48	123.84	2.64

SI-VI. HTBH REACTION BARRIERS AND ERRORS

TS7	1.70	3.65
TS2	4.90	9.94
TS11	3.10	4.11
TS19	38.40	47.02
TS9	1.42	6.23
TS12	10.50	14.88
TS13	16.76	18.60
TS12	12.87	17.91
TS15	8.00	14.16
TS2	21.20	26.26
TS8	3.20	11.91
TS14	9.57	19.49
TS18	14.50	19.67

```
        TS13     3.50    5.19
         TS5     9.60    8.25
         TS4     6.50   36.90
        TS10     7.90   48.53
        TS16     7.50   15.64
         TS3    15.30   16.73
        TS16    18.30   24.80
        TS17    10.40   17.47
         TS9    33.40   34.97
        TS15    22.40   27.00
         TS4    19.60   48.32
        TS19    38.40   47.02
        TS11    23.20   24.64
        TS10    13.47   56.46
         TS6    12.70   23.71
         TS3    12.10   11.82
        TS14     9.36   19.22
         TS7     7.06   11.32
        TS18    17.80   24.02
         TS1     5.70    5.70
         TS1     7.86    8.45
        TS17    17.40   25.50
         TS6     3.00   16.65
         TS5     9.60    8.25
         TS8    19.90   27.01
# Method LH-PBE HTBH errors
         TS7     1.70   -6.34
         TS2     4.90   -4.69
        TS11     3.10   -0.52
        TS19    38.40   32.99
         TS9     1.42  -11.37
        TS12    10.50    3.65
        TS13    16.76    9.18
        TS12    12.87    1.05
        TS15     8.00    0.12
         TS2    21.20   12.86
         TS8     3.20   -7.28
        TS14     9.57   -6.82
        TS18    14.50    5.88
        TS13     3.50   -0.07
         TS5     9.60    5.41
         TS4     6.50   -3.66
        TS10     7.90   -1.45
        TS16     7.50    2.03
         TS3    15.30   10.70
        TS16    18.30    9.77
        TS17    10.40    2.86
         TS9    33.40   22.72
        TS15    22.40   12.85
         TS4    19.60    7.47
        TS19    38.40   32.99
        TS11    23.20   17.92
        TS10    13.47    2.37
         TS6    12.70    0.35
         TS3    12.10    4.29
        TS14     9.36   -7.52
         TS7     7.06   -3.24
        TS18    17.80    6.92
         TS1     5.70    1.06
         TS1     7.86   -2.25
        TS17    17.40    8.88
         TS6     3.00   -9.75
         TS5     9.60    5.41
```

TS8	19.90	8.84

LH-PBE45

TS7	1.70	-0.36
TS2	4.90	3.37
TS11	3.10	1.23
TS19	38.40	38.05
TS9	1.42	-0.53
TS12	10.50	9.50
TS13	16.76	14.84
TS12	12.87	9.04
TS15	8.00	8.29
TS2	21.20	20.56
TS8	3.20	3.27
TS14	9.57	7.61
TS18	14.50	12.79
TS13	3.50	2.15
TS5	9.60	5.91
TS4	6.50	5.84
TS10	7.90	7.55
TS16	7.50	10.08
TS3	15.30	13.03
TS16	18.30	17.04
TS17	10.40	10.40
TS9	33.40	31.42
TS15	22.40	19.53
TS4	19.60	18.46
TS19	38.40	38.05
TS11	23.20	22.28
TS10	13.47	11.66
TS6	12.70	12.34
TS3	12.10	8.46
TS14	9.36	9.15
TS7	7.06	5.30
TS18	17.80	16.60
TS1	5.70	3.36
TS1	7.86	4.45
TS17	17.40	18.49
TS6	3.00	3.53
TS5	9.60	5.91
TS8	19.90	20.17

SI-VII. TOTAL ATOMIC ENERGIES AND ERRORS

Results are tablulated as reference and computed values in kcal/mol per electron.

LHup-HF

S	-15613.6129403	-15613.7205949
Mg	-10461.2631670	-10464.5775555
F	-6953.7744136	-6956.6515912
N	-4893.6059425	-4895.2050654
Ne	-8090.9568907	-8093.8695206
C	-3958.0161712	-3957.6669873
Li	-1564.1845639	-1561.9705920
Be	-2300.9769350	-2298.9047106
Cl	-16985.1318474	-16985.3643434
He	-911.1437940	-902.0171935
O	-5888.1804862	-5890.4494377
Al	-11698.0320990	-11700.2808482
Ar	-18390.9089794	-18391.7257540
Si	-12969.6801007	-12970.8475133
P	-14276.2176307	-14276.4503806

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          B   -3094.1125474  -3092.5660192
          H    -313.7547500   -313.3656497
         Na   -9256.0275381  -9260.4812122
LHup-PBE
          S  -15613.6129403 -15609.3222458
         Mg  -10461.2631670 -10455.8103355
          F   -6953.7744136  -6951.0304185
          N   -4893.6059425  -4892.1273205
         Ne   -8090.9568907  -8086.8914457
          C   -3958.0161712  -3956.7558598
         Li   -1564.1845639  -1566.6969383
         Be   -2300.9769350  -2297.9502563
         Cl  -16985.1318474 -16980.6909118
         He    -911.1437940   -919.9783460
          O   -5888.1804862  -5886.4002937
         Al  -11698.0320990 -11692.9151314
         Ar  -18390.9089794 -18386.2955190
         Si  -12969.6801007 -12965.0341597
          P  -14276.2176307 -14271.8805968
          B   -3094.1125474  -3092.0967353
          H    -313.7547500   -321.5692061
         Na   -9256.0275381  -9250.8835203
LHup-PBE45
          S  -15613.6129403 -15608.0787837
         Mg  -10461.2631670 -10457.8102399
          F   -6953.7744136  -6948.8610777
          N   -4893.6059425  -4888.1048857
         Ne   -8090.9568907  -8085.8549957
          C   -3958.0161712  -3952.1283330
         Li   -1564.1845639  -1558.4486078
         Be   -2300.9769350  -2294.8594257
         Cl  -16985.1318474 -16979.3302221
         He    -911.1437940   -899.7867087
          O   -5888.1804862  -5883.0874077
         Al  -11698.0320990 -11694.2945350
         Ar  -18390.9089794 -18385.0680352
         Si  -12969.6801007 -12965.3045140
          P  -14276.2176307 -14270.9992682
          B   -3094.1125474  -3088.1096424
          H    -313.7547500   -309.9679636
         Na   -9256.0275381  -9252.5184019
```

SI-VIII. IP21, EA12, PA5 RESULTS

```
# Method LH-HF IP errors
          S   238.3  237.0  267.8
         PH   234.1  234.7  245.0
         Pd   192.2  183.6  234.9
         Mo   163.7  146.3  149.4
         Ru   169.9  151.4  153.9
         Cu   178.2  157.0  157.5
         S2   216.0  223.8  248.7
          C   259.7  266.3  282.0
         OH   298.9  290.7  362.4
         SH   238.4  234.2  260.0
         Cl   299.3  294.2  321.7
        FeC   175.0  169.4  172.8
          O   313.7  305.6  394.9
         Si   188.1  189.2  195.2
         O2   278.9  294.8  365.3
```

```
           P   242.8  240.0  248.0
          Cr   156.0  141.8  143.7
         PH2   226.3  227.0  240.6
          Rh   172.1  128.8  154.6
         Cl2   265.3  264.4  292.7
          Zn   216.6  192.2  196.0
# Method LH-HF EA errors
          Cl    84.2   69.2  -64.7
          SH    53.8   39.9   -0.0
           S    47.9   37.8  -53.0
          PH    23.2   14.1  -42.4
           O    33.8    5.6 -107.1
          Si    32.3   28.3   16.8
          O2    10.8  -13.2 -103.1
           P    16.9   11.7  -45.5
         PH2    29.4   17.0  -39.9
          S2    38.5   30.8  -37.4
           C    29.2   20.2    0.7
         Cl2    55.6   44.5    3.1
          OH    42.3   10.7  -83.1
# Method LH-HF PA errors
         HCl   143.5
        SiH4   157.2
          H2   109.8
         H2O   183.1
         NH3   225.1
         H2S   180.7
         PH3   202.4
        C2H2   170.2
# Method LH-PBE IP errors
           S   238.3  246.6  173.0
          PH   234.1  245.6  157.1
          Pd   192.2  202.7  100.8
          Mo   163.7  177.8  110.9
          Ru   169.9  184.4  118.0
          Cu   178.2  200.6  113.1
          S2   216.0  227.5  147.3
           C   259.7  271.9  153.3
          OH   298.9  312.1  200.8
          SH   238.4  246.8  166.5
          Cl   299.3  308.2  214.6
         FeC   175.0  192.5  124.6
           O   313.7  332.7  218.9
          Si   188.1  195.0  115.9
          O2   278.9  293.2  167.3
           P   242.8  251.4  160.1
          Cr   156.0  174.6   87.3
         PH2   226.3  239.0  153.3
          Rh   172.1  186.3  118.3
         Cl2   265.3  269.1  183.8
          Zn   216.6  227.8  148.8
# Method LH-PBE EA errors
          Cl    84.2   94.7   -8.1
          SH    53.8   61.3   14.8
           S    47.9   56.3   -0.9
          PH    23.2   28.2   10.2
           O    33.8   47.4  -41.1
          Si    32.3   39.1  103.8
          O2    10.8   23.0  -40.9
           P    16.9   22.8    3.2
         PH2    29.4   33.7   10.5
          S2    38.5   44.1   32.9
           C    29.2   42.7  131.0
```

```
         Cl2    55.6   71.7  106.9
          OH    42.3   52.3   -5.5
# Method LH-PBE PA errors
         HCl   136.7
        SiH4   156.9
          H2   104.9
         H2O   166.8
         NH3   208.1
         H2S   173.9
         PH3   191.3
        C2H2   157.7
# Method LH-PBEhyb IP errors
           S   238.3  235.4  201.7
          PH   234.1  231.6  183.4
          Pd   192.2  190.7  150.6
          Mo   163.7  157.5  122.9
          Ru   169.9  163.5  126.3
          Cu   178.2  172.3  130.5
          S2   216.0  216.9  179.8
           C   259.7  262.0  197.5
          OH   298.9  293.1  256.4
          SH   238.4  233.4  195.0
          Cl   299.3  292.4  246.7
         FeC   175.0  172.6  136.2
           O   313.7  310.9  281.1
          Si   188.1  186.1  142.0
          O2   278.9  283.4  242.9
           P   242.8  237.2  186.2
          Cr   156.0  154.3  118.4
         PH2   226.3  225.1  179.7
          Rh   172.1  165.0  126.8
         Cl2   265.3  255.8  218.8
          Zn   216.6  204.5  160.6
# Method LH-PBEhyb EA errors
          Cl    84.2   73.1  -34.4
          SH    53.8   44.0  -18.1
           S    47.9   41.2  -25.1
          PH    23.2   17.4  -16.2
           O    33.8   18.2  -71.7
          Si    32.3   29.1   59.7
          O2    10.8   -7.3  -72.2
           P    16.9   14.2  -19.3
         PH2    29.4   20.8  -14.6
          S2    38.5   30.1   -6.6
           C    29.2   25.0   64.7
         Cl2    55.6   49.4   53.5
          OH    42.3   22.9  -42.9
# Method LH-PBEhyb PA errors
         HCl   140.8
        SiH4   156.6
          H2   107.6
         H2O   176.6
         NH3   217.2
         H2S   176.5
         PH3   194.5
        C2H2   163.5
```

SI-IX. MGBL BOND LENGTHS

```
== Method HFPBE MGBL20 bond lengths
```

```
System  Reference  Computed
CH4 1.086 1.0716
N2 1.098 1.059
HCN-2 1.065 1.0514
NH3 1.012 0.9888
H2CO-1 1.203 1.166
CO2 1.160 1.1251
F2 1.412 1.2957
OH 0.970 0.9411
C2H2-1 1.203 1.1711
N2O-1 1.128 1.0746
N2O-2 1.184 1.1477
CO 1.128 1.0948
H2 0.741 0.7311
H2O 0.957 0.9309
C2H2-2 1.063 1.0486
H2CO-2 1.102 1.0843
HF 0.917 0.8884
Cl2 1.988 1.9301
HCN-1 1.153 1.116
MgS 2.143 2.091
== Method LH-HF MGBL20 bond lengths
System  Reference  Computed
CH4 1.086 1.0613
N2 1.098 1.0439
HCN-2 1.065 1.0475
NH3 1.012 0.9745
H2CO-1 1.203 1.1404
CO2 1.160 1.1048
F2 1.412 1.2439
OH 0.970 0.9267
C2H2-1 1.203 1.1574
N2O-1 1.128 1.0599
N2O-2 1.184 1.1173
CO 1.128 1.0762
H2 0.741 0.7411
H2O 0.957 0.916
C2H2-2 1.063 1.0444
H2CO-2 1.102 1.0766
HF 0.917 0.8741
Cl2 1.988 1.883
HCN-1 1.153 1.0994
MgS 2.143 2.0779
== Method LH-PBE MGBL20 bond lengths
System  Reference  Computed
CH4 1.086 1.0964
N2 1.098 1.1138
HCN-2 1.065 1.0735
NH3 1.012 1.0284
H2CO-1 1.203 1.2297
CO2 1.160 1.1862
F2 1.412 1.4583
OH 0.970 0.9917
C2H2-1 1.203 1.2118
N2O-1 1.128 1.1498
N2O-2 1.184 1.2158
CO 1.128 1.1513
H2 0.741 0.7374
H2O 0.957 0.978
C2H2-2 1.063 1.0682
H2CO-2 1.102 1.115
HF 0.917 0.9397
Cl2 1.988 2.0401
```

```
HCN-1 1.153 1.1681
MgS 2.143 2.1501
== Method LH-PBEhyb MGBL20 bond lengths
System  Reference  Computed
CH4 1.086 1.0815
N2 1.098 1.0723
HCN-2 1.065 1.0637
NH3 1.012 0.9983
H2CO-1 1.203 1.1722
CO2 1.160 1.1359
F2 1.412 1.3167
OH 0.970 0.9547
C2H2-1 1.203 1.1839
N2O-1 1.128 1.0963
N2O-2 1.184 1.1488
CO 1.128 1.1043
H2 0.741 0.7505
H2O 0.957 0.9421
C2H2-2 1.063 1.0603
H2CO-2 1.102 1.1
HF 0.917 0.9012
Cl2 1.988 1.9441
HCN-1 1.153 1.1286
MgS 2.143 2.1279
== Method PBE0 MGBL20 bond lengths
System  Reference  Computed
CH4 1.086 1.0886
N2 1.098 1.0896
HCN-2 1.065 1.0681
NH3 1.012 1.0115
H2CO-1 1.203 1.1958
CO2 1.160 1.1566
F2 1.412 1.3742
OH 0.970 0.9706
C2H2-1 1.203 1.1964
N2O-1 1.128 1.1179
N2O-2 1.184 1.1752
CO 1.128 1.1236
H2 0.741 0.7453
H2O 0.957 0.9576
C2H2-2 1.063 1.0642
H2CO-2 1.102 1.1072
HF 0.917 0.9176
Cl2 1.988 1.9863
HCN-1 1.153 1.1454
MgS 2.143 2.1386
== Method PBE45 MGBL20 bond lengths
System  Reference  Computed
CH4 1.086 1.0836
N2 1.098 1.0802
HCN-2 1.065 1.063
NH3 1.012 1.0046
H2CO-1 1.203 1.1867
CO2 1.160 1.1468
F2 1.412 1.349
OH 0.970 0.9617
C2H2-1 1.203 1.1888
N2O-1 1.128 1.1044
N2O-2 1.184 1.166
CO 1.128 1.1146
H2 0.741 0.7412
H2O 0.957 0.9495
C2H2-2 1.063 1.0596
```

```
H2CO-2 1.102 1.1002
HF 0.917 0.9088
Cl2 1.988 1.9686
HCN-1 1.153 1.1365
MgS 2.143 2.125
== Method PBE MGBL20 bond lengths
System  Reference  Computed
CH4 1.086 1.0955
N2 1.098 1.103
HCN-2 1.065 1.0752
NH3 1.012 1.0211
H2CO-1 1.203 1.2087
CO2 1.160 1.1712
F2 1.412 1.412
OH 0.970 0.9832
C2H2-1 1.203 1.207
N2O-1 1.128 1.1376
N2O-2 1.184 1.1897
CO 1.128 1.1367
H2 0.741 0.7507
H2O 0.957 0.969
C2H2-2 1.063 1.0705
H2CO-2 1.102 1.1172
HF 0.917 0.9299
Cl2 1.988 2.0126
HCN-1 1.153 1.1583
MgS 2.143 2.1569
```

SI-X. COMPUTED SINGLET FISSION CHROMOPHORE EXCITED STATES

Results are tablulated as reference and computed values.

```
Method LH-HF molecule 1:
Singlet 1:    3.73    4.25
Singlet 2:    4.95    5.44
Triplet 1:    2.45   -1.70
Triplet 2:    4.87    3.64

Method LH-HF molecule 2:
Singlet 1:    4.47    5.02
Singlet 2:    5.37    5.40
Triplet 1:    2.76   -1.72
Triplet 2:    5.17    3.48

Method LH-HF molecule 3:
Singlet 1:    2.72    3.73
Singlet 2:    3.01    3.80
Triplet 1:    2.06   -1.98
Triplet 2:    2.72    0.43

Method LH-HF molecule 4:
Singlet 1:    2.86    3.73
Singlet 2:    3.38    4.21
Triplet 1:    2.04   -1.29
Triplet 2:    3.15    3.53

Method LH-HF molecule 5:
Singlet 1:    3.25    3.96
Singlet 2:    3.43    4.27
Triplet 1:    2.30   -1.31
Triplet 2:    3.19    3.57
```

```
Method LH-HF molecule 6:
Singlet 1:    1.85    2.79
Singlet 2:    2.93    3.80
Triplet 1:    1.38   -1.93
Triplet 2:    2.67   -0.44

Method LH-HF molecule 7:
Singlet 1:    2.22    3.27
Singlet 2:    2.93    3.75
Triplet 1:    1.68   -1.96
Triplet 2:    2.66   -0.25

Method LH-HF molecule 8:
Singlet 1:    2.13    2.98
Singlet 2:    2.98    3.80
Triplet 1:    1.59   -1.94
Triplet 2:    2.71   -0.45

Method LH-HF molecule 9:
Singlet 1:    3.02    3.69
Singlet 2:    3.61    4.33
Triplet 1:    2.09   -1.62
Triplet 2:    3.36    3.54

Method LH-HF molecule 10:
Singlet 1:    1.92    3.03
Singlet 2:    2.99    3.81
Triplet 1:    1.50   -1.82
Triplet 2:    2.73    0.25

Method LH-HF molecule 11:
Singlet 1:    2.47    3.31
Singlet 2:    3.05    3.91
Triplet 1:    1.88   -1.74
Triplet 2:    2.78    0.34

Method LH-PBE molecule 1:
Singlet 1:    3.73    3.37
Singlet 2:    4.95    4.25
Triplet 1:    2.45    1.97
Triplet 2:    4.87    4.07

Method LH-PBE molecule 2:
Singlet 1:    4.47    4.04
Singlet 2:    5.37    4.69
Triplet 1:    2.76    2.39
Triplet 2:    5.17    4.43

Method LH-PBE molecule 3:
Singlet 1:    2.72    1.87
Singlet 2:    3.01    2.50
Triplet 1:    2.06    1.23
Triplet 2:    2.72    2.03

Method LH-PBE molecule 4:
Singlet 1:    2.86    2.52
Singlet 2:    3.38    2.93
Triplet 1:    2.04    1.47
Triplet 2:    3.15    2.58

Method LH-PBE molecule 5:
Singlet 1:    3.25    2.94
Singlet 2:    3.43    3.01
```

```
Triplet 1:    2.30    1.81
Triplet 2:    3.19    2.64

Method LH-PBE molecule 6:
Singlet 1:    1.85    1.18
Singlet 2:    2.93    2.47
Triplet 1:    1.38    0.56
Triplet 2:    2.67    2.04

Method LH-PBE molecule 7:
Singlet 1:    2.22    1.45
Singlet 2:    2.93    2.40
Triplet 1:    1.68    0.83
Triplet 2:    2.66    1.96

Method LH-PBE molecule 8:
Singlet 1:    2.13    1.31
Singlet 2:    2.98    2.52
Triplet 1:    1.59    0.69
Triplet 2:    2.71    2.08

Method LH-PBE molecule 9:
Singlet 1:    3.02    2.67
Singlet 2:    3.61    3.17
Triplet 1:    2.09    1.52
Triplet 2:    3.36    2.82

Method LH-PBE molecule 10:
Singlet 1:    1.92    1.25
Singlet 2:    2.99    2.48
Triplet 1:    1.50    0.76
Triplet 2:    2.73    2.08

Method LH-PBE molecule 11:
Singlet 1:    2.47    1.71
Singlet 2:    3.05    2.61
Triplet 1:    1.88    1.07
Triplet 2:    2.78    2.18

Method LH-PBEhyb molecule 1:
Singlet 1:    3.73    3.70
Singlet 2:    4.95    4.95
Triplet 1:    2.45    1.45
Triplet 2:    4.87    4.70

Method LH-PBEhyb molecule 2:
Singlet 1:    4.47    4.51
Singlet 2:    5.37    5.35
Triplet 1:    2.76    1.80
Triplet 1:    2.76    1.80
Triplet 2:    5.17    4.89

Method LH-PBEhyb molecule 3:
Singlet 1:    2.72    2.76
Singlet 2:    3.01    3.08
Triplet 1:    2.06    1.23
Triplet 2:    2.72    2.21

Method LH-PBEhyb molecule 4:
Singlet 1:    2.86    3.00
Singlet 2:    3.38    3.59
Triplet 1:    2.04    1.22
Triplet 2:    3.15    3.07
```

```
Method LH-PBEhyb molecule 5:
Singlet 1:    3.25    3.33
Singlet 2:    3.43    3.62
Triplet 1:    2.30    1.41
Triplet 2:    3.19    3.07

Method LH-PBEhyb molecule 6:
Singlet 1:    1.85    1.86
Singlet 2:    2.93    3.09
Triplet 1:    1.38    0.31
Triplet 2:    2.67    2.24

Method LH-PBEhyb molecule 7:
Singlet 1:    2.22    2.24
Singlet 2:    2.93    3.06
Triplet 1:    1.68    0.78
Triplet 2:    2.66    2.22

Method LH-PBEhyb molecule 8:
Singlet 1:    2.13    2.02
Singlet 2:    2.98    3.11
Triplet 1:    1.59    0.52
Triplet 2:    2.71    2.22

Method LH-PBEhyb molecule 9:
Singlet 1:    3.02    3.05
Singlet 2:    3.61    3.77
Triplet 1:    2.09    1.07
Triplet 2:    3.36    3.20

Method LH-PBEhyb molecule 10:
Singlet 1:    1.92    2.05
Singlet 2:    2.99    3.12
Triplet 1:    1.50    0.86
Triplet 2:    2.73    2.25

Method LH-PBEhyb molecule 11:
Singlet 1:    2.47    2.34
Singlet 2:    3.05    3.20
Triplet 1:    1.88    1.01
Triplet 2:    2.78    2.29
```