Electronic Supporting Information

Symmetric Spirenes: Promising Building Blocks for New Generation Opto-Electronic Materials

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Table S1. Relative values of full electronic energies (E), zero-point energies (ZPE), their sum, enthalpies (H) and Gibbs free energies (G), computed for different multiplicity states of **1** (closed shell singlet (CSS), restricted open shell singlet (ROSS), triplet (T) and quintuplet (Q)) using different levels of theory. All values are computed at T = 298.15 K and p = 1.00 atm and reported in units of kJ · mol^{-1}.

Model chemistry	Basis Set	Spin Multiplicity	E	ZPE	E+ZPE	H	G
DFT B3LYP	6-31+G**	CSS	0.0	23.2	0.0	0.0	0.0
		ROSS	0.0	23.2	0.0	0.0	0.0
		T	212.4	12.3	201.5	203.4	196.9
		Q	446.2	0.0	422.9	427.2	413.2
	6-311++G**	CSS	0.0	23.3	0.0	0.0	0.0
		ROSS	0.0	23.3	0.0	0.0	0.0
		T	214.7	12.4	203.8	205.7	199.2
		Q	451.1	0.0	427.8	432.2	417.5
	Aug-cc-pVTZ	CSS	0.0	23.4	0.0	0.0	0.0
		ROSS	0.0	23.4	0.0	0.0	0.0
		T	216.1	12.5	205.2	207.1	200.6
		Q	454.2	0.0	430.8	435.2	420.3
DFT B3LYP[GD3BJ]	6-31+G**	CSS	0.0	23.4	0.0	0.0	0.0
		ROSS	0.0	23.4	0.0	0.0	0.0
		T	213.2	12.4	202.3	204.2	197.6
		Q	448.6	0.0	425.2	429.6	415.0
	6-311++G**	CSS	0.0	23.5	0.0	0.0	0.0
		ROSS	0.0	23.5	0.0	0.0	0.0
		T	169.7	16.1	162.3	161.7	162.0
		Q	453.4	0.0	430.0	434.5	419.1
	Aug-cc-pVTZ	CSS	0.0	23.6	0.0	0.0	0.0
		ROSS	0.0	23.6	0.0	0.0	0.0
		T	216.9	12.6	206.0	207.9	201.3
		Q	456.5	0.0	433.0	437.5	421.8
DFT BLYP	6-31+G**	CSS	0.0	21.8	0.0	0.0	0.0
		ROSS	0.0	21.8	0.0	0.0	0.0
		T	209.7	11.7	199.6	201.4	195.1
		Q	450.0	0.0	428.2	432.5	418.1
	6-311++G**	CSS	0.0	22.1	0.0	0.0	0.0
		ROSS	0.0	22.1	0.0	0.0	0.0
		T	212.3	11.9	202.2	204.1	197.6
		Q	455.6	0.0	433.5	438.0	422.1
	Aug-cc-pVTZ	CSS	0.0	22.2	0.0	0.0	0.0
		ROSS	0.0	22.2	0.0	0.0	0.0
		T	213.5	12.0	203.3	205.2	198.7
		Q	458.2	0.0	436.0	440.5	424.0

Table S1. (continued)							
DFT BP86	6-31+G**	CSS	0.0	21.7	0.0	0.0	0.0
		ROSS	0.0	21.7	0.0	0.0	0.0
		T	209.2	11.7	199.1	201.0	194.6
		Q	447.8	0.0	426.1	430.5	413.8
	6-311++G**	CSS	0.0	22.0	0.0	0.0	0.0
		ROSS	0.0	22.0	0.0	0.0	0.0
		T	211.3	11.9	201.2	203.1	196.6
		Q	452.4	0.0	430.4	435.1	412.7
	Aug-cc-pVTZ	CSS	0.0	22.0	0.0	0.0	0.0
		ROSS	0.0	22.0	0.0	0.0	0.0
		T	212.1	11.8	202.0	203.9	197.4
		Q	454.1	0.0	432.2	436.7	418.7
DFT CAM-B3LYP	6-31+G**	CSS	0.0	24.4	0.0	0.0	0.0
		ROSS	0.0	24.4	0.0	0.0	0.0
		T	216.8	12.8	205.2	207.2	200.5
		Q	448.6	0.0	424.2	428.6	414.4
	6-311++G**	CSS	0.0	24.3	0.0	0.0	0.0
		ROSS	0.0	24.3	0.0	0.0	0.0
		T	219.3	12.8	207.7	209.7	202.9
		Q	453.7	0.0	429.3	433.8	419.0
	Aug-cc-pVTZ	CSS	0.0	24.4	0.0	0.0	0.0
		ROSS	0.0	24.4	0.0	0.0	0.0
		T	220.9	12.8	209.3	211.3	204.6
		Q	457.2	0.0	432.8	437.2	422.2
DFT CAM-B3LYP[GD3BJ]	6-31+G**	CSS	0.0	24.4	0.0	0.0	0.0
		ROSS	0.0	24.4	0.0	0.0	0.0
		T	217.2	12.8	205.6	207.6	200.8
		Q	449.6	0.0	425.2	429.6	415.1
	6-311++G**	CSS	0.0	24.4	0.0	0.0	0.0
		ROSS	0.0	24.4	0.0	0.0	0.0
		T	219.6	12.8	208.1	210.1	203.3
		Q	454.7	0.0	430.3	434.8	419.7
	Aug-cc-pVTZ	CSS	0.0	24.5	0.0	0.0	0.0
		ROSS	0.0	24.5	0.0	0.0	0.0
		T	221.3	12.9	209.7	211.7	204.9
		Q	458.1	0.0	433.7	438.2	422.9

Table S1. (continued)							
HF	6-31+G**	CSS	17.2	28.6	30.4	29.7	30.8
		ROSS	0.0	15.4	0.0	0.0	0.0
		T	94.8	14.8	94.2	93.3	93.6
		Q	305.0	0.0	289.6	292.4	282.4
	6-311++G**	CSS	670.6	3.2	658.4	658.8	655.0
		ROSS	15.0	28.6	27.8	27.1	28.2
		T	0.0	15.8	0.0	0.0	0.0
		Q	97.9	14.8	96.9	96.1	96.3
	Aug-cc-pVTZ	CSS	305.5	0.0	289.7	292.7	282.3
		ROSS	673.0	3.2	660.4	660.8	656.9
		T	12.1	28.8	24.4	23.7	24.7
		Q	0.0	16.5	0.0	0.0	0.0
DFT M06-2X	6-31+G**	CSS	97.7	15.2	96.4	95.6	95.8
		ROSS	308.4	0.0	291.9	294.9	284.3
		T	677.7	3.1	664.3	664.8	660.8
		Q	0.0	24.0	0.0	0.0	0.0
	6-311++G**	CSS	0.0	24.0	0.0	0.0	0.0
		ROSS	237.2	12.5	225.8	227.9	220.6
		T	486.2	0.0	462.2	466.9	450.8
		Q	0.0	24.1	0.0	0.0	0.0
	Aug-cc-pVTZ	CSS	0.0	24.1	0.0	0.0	0.0
		ROSS	237.0	12.7	225.6	227.7	220.3
		T	486.1	0.0	462.0	466.7	450.0
		Q	0.0	24.3	0.0	0.0	0.0
DFT PBE0	6-31+G**	CSS	0.0	24.3	0.0	0.0	0.0
		ROSS	238.4	12.8	226.9	229.0	221.6
		T	488.7	0.0	464.3	469.2	450.6
		Q	0.0	23.6	0.0	0.0	0.0
	6-311++G**	CSS	0.0	23.6	0.0	0.0	0.0
		ROSS	208.1	12.5	196.9	198.9	192.3
		T	434.2	0.0	410.5	415.0	399.7
		Q	0.0	23.7	0.0	0.0	0.0
	Aug-cc-pVTZ	CSS	0.0	23.7	0.0	0.0	0.0
		ROSS	209.9	12.6	198.8	200.8	194.1
		T	438.2	0.0	414.5	419.0	402.9
		Q	0.0	23.8	0.0	0.0	0.0

Table S1. (continued)							
DFT PBE0[GD3BJ]	6-31+G**	CSS	0.0	23.7	0.0	0.0	0.0
		ROSS	0.0	23.7	0.0	0.0	0.0
		T	208.5	12.5	197.4	199.3	192.6
		Q	435.4	0.0	411.6	416.1	400.4
	6-311++G**	CSS	0.0	23.8	0.0	0.0	0.0
		ROSS	0.0	23.8	0.0	0.0	0.0
		T	210.3	12.6	199.2	201.2	194.4
		Q	439.3	0.0	415.6	420.2	403.4
	Aug-cc-pVTZ	CSS	0.0	23.8	0.0	0.0	0.0
		ROSS	0.0	23.8	0.0	0.0	0.0
		T	211.2	12.7	200.0	202.0	195.3
		Q	441.1	0.0	417.3	421.9	404.6
DFT PBEPBE	6-31+G**	CSS	0.0	22.0	0.0	0.0	0.0
		ROSS	0.0	22.0	0.0	0.0	0.0
		T	209.8	11.9	199.7	201.6	195.1
		Q	449.2	0.0	427.2	431.9	409.9
	6-311++G**	CSS	0.0	21.8	0.0	0.0	0.0
		ROSS	0.0	21.8	0.0	0.0	0.0
		T	211.9	11.7	201.8	203.8	197.1
		Q	453.9	0.0	432.1	436.6	420.2
	Aug-cc-pVTZ	CSS	0.0	21.8	0.0	0.0	0.0
		ROSS	0.0	21.8	0.0	0.0	0.0
		T	212.5	11.7	202.4	204.3	197.8
		Q	455.1	0.0	433.3	437.7	422.3
DFT PW91	6-31+G**	CSS	0.0	22.0	0.0	0.0	0.0
		ROSS	0.0	22.0	0.0	0.0	0.0
		T	209.0	11.9	198.9	200.8	194.3
		Q	447.4	0.0	425.5	430.1	410.6
	6-311++G**	CSS	0.0	21.9	0.0	0.0	0.0
		ROSS	0.0	21.9	0.0	0.0	0.0
		T	211.2	11.8	201.1	203.1	196.5
		Q	452.4	0.0	430.5	435.0	418.1
	Aug-cc-pVTZ	CSS	0.0	22.0	0.0	0.0	0.0
		ROSS	0.0	22.0	0.0	0.0	0.0
		T	212.0	11.8	201.9	203.8	197.3
		Q	454.0	0.0	432.0	436.5	420.5

Table S1. (continued)							
DFT ω-B97X[D]	6-31+G**	CSS	0.0	24.2	0.0	0.0	0.0
		ROSS	0.0	24.2	0.0	0.0	0.0
		T	221.4	12.7	209.9	211.9	205.2
		Q	457.8	0.0	433.6	438.0	423.6
	6-311++G**	CSS	0.0	24.2	0.0	0.0	0.0
		ROSS	0.0	24.2	0.0	0.0	0.0
		T	223.5	12.8	212.0	214.0	207.2
		Q	462.3	0.0	438.1	442.6	427.6
	Aug-cc-pVTZ	CSS	0.0	24.3	0.0	0.0	0.0
		ROSS	0.0	24.3	0.0	0.0	0.0
		T	224.9	12.8	213.4	215.4	208.7
		Q	465.0	0.0	440.8	445.3	430.1

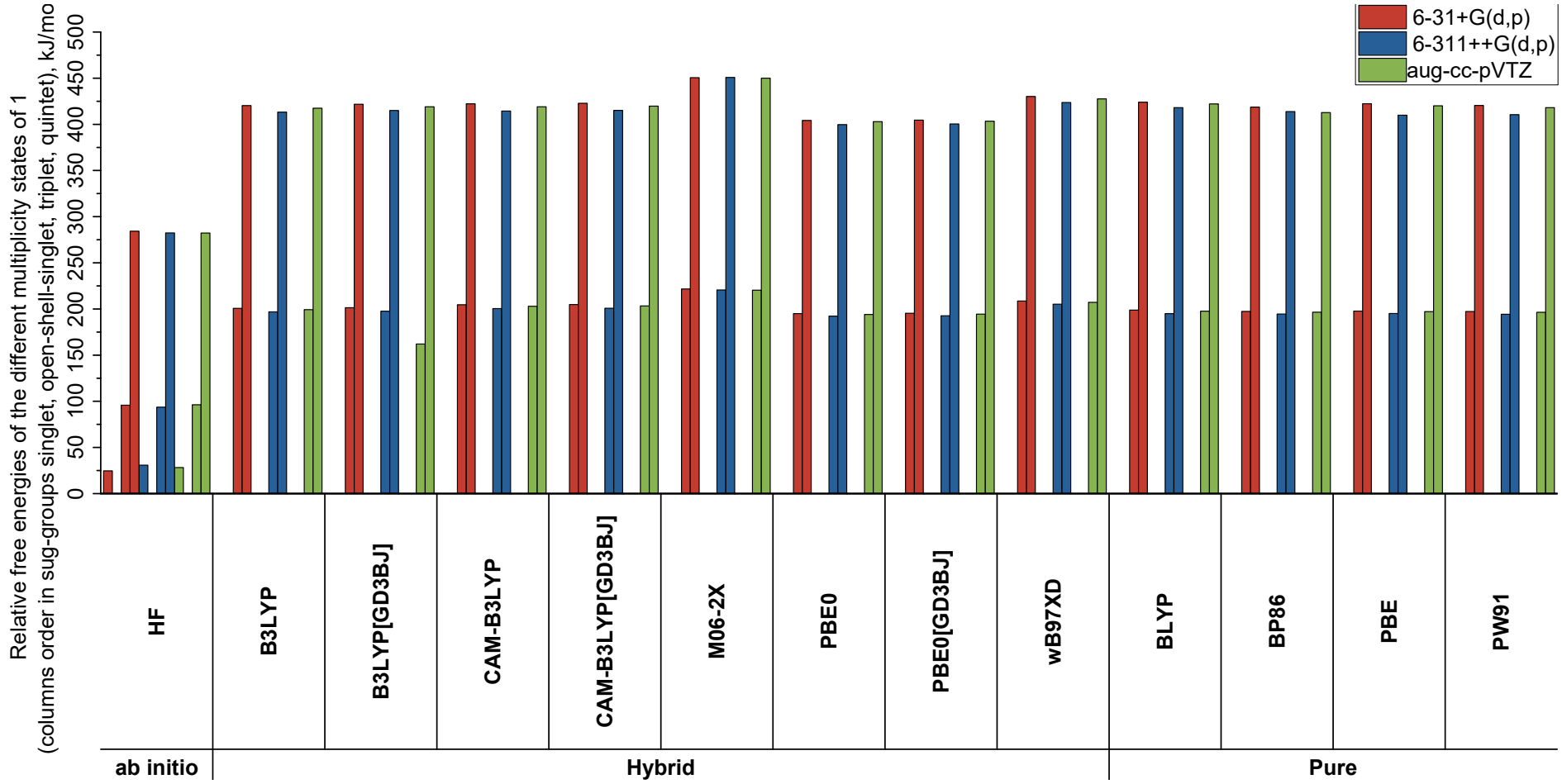

Figure S1. Gibbs free energy differences (ΔG, at T = 298.15 K and p = 1.00 atm, in kJ/mol) between the different spin multiplicity states of **1** (first columns: CS singlet; second columns: OS singlet; third columns: triplet; fourth columns: quintuplet), computed at different levels of theory.

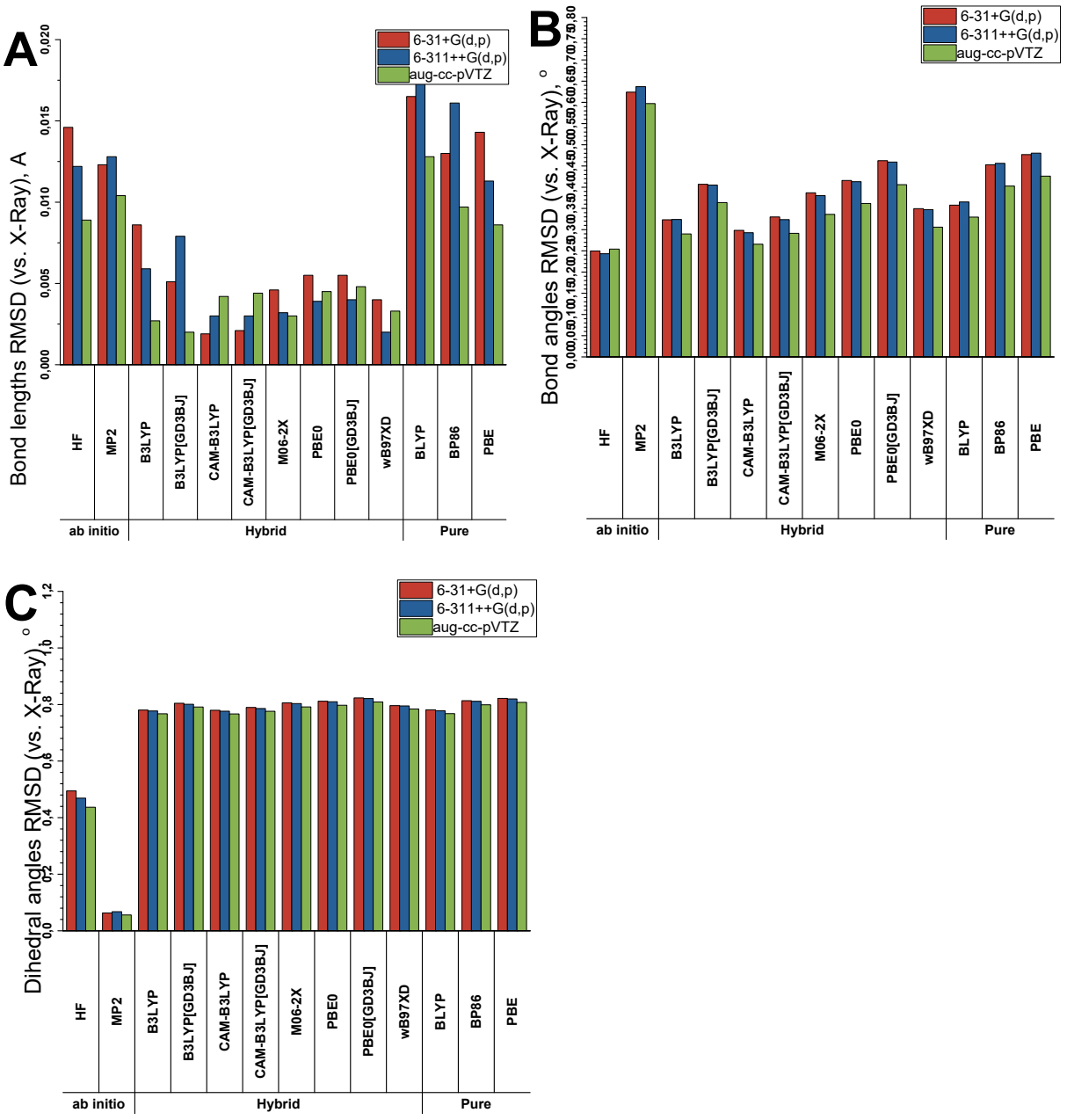

Figure S2. Root mean square deviations (RMSD) of calculated geometrical parameters of **1** vs. X-Ray data: bond lengths (A), bond angles (B); dihedral angles (C).

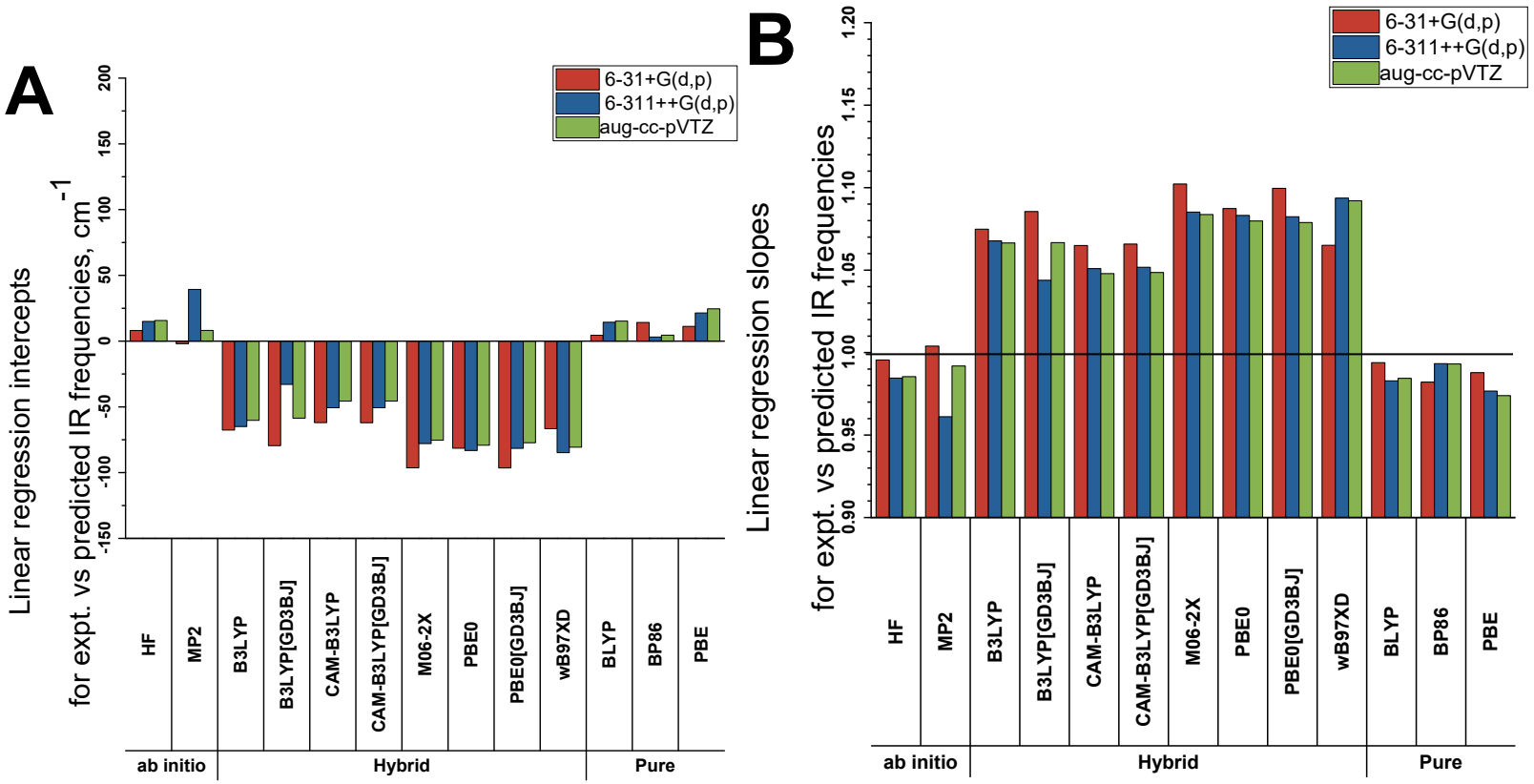

Figure S3. Intercepts (A) and slopes (B) obtained upon least-squares linear regressions between experimental and computed IR wavenumbers for **1**.

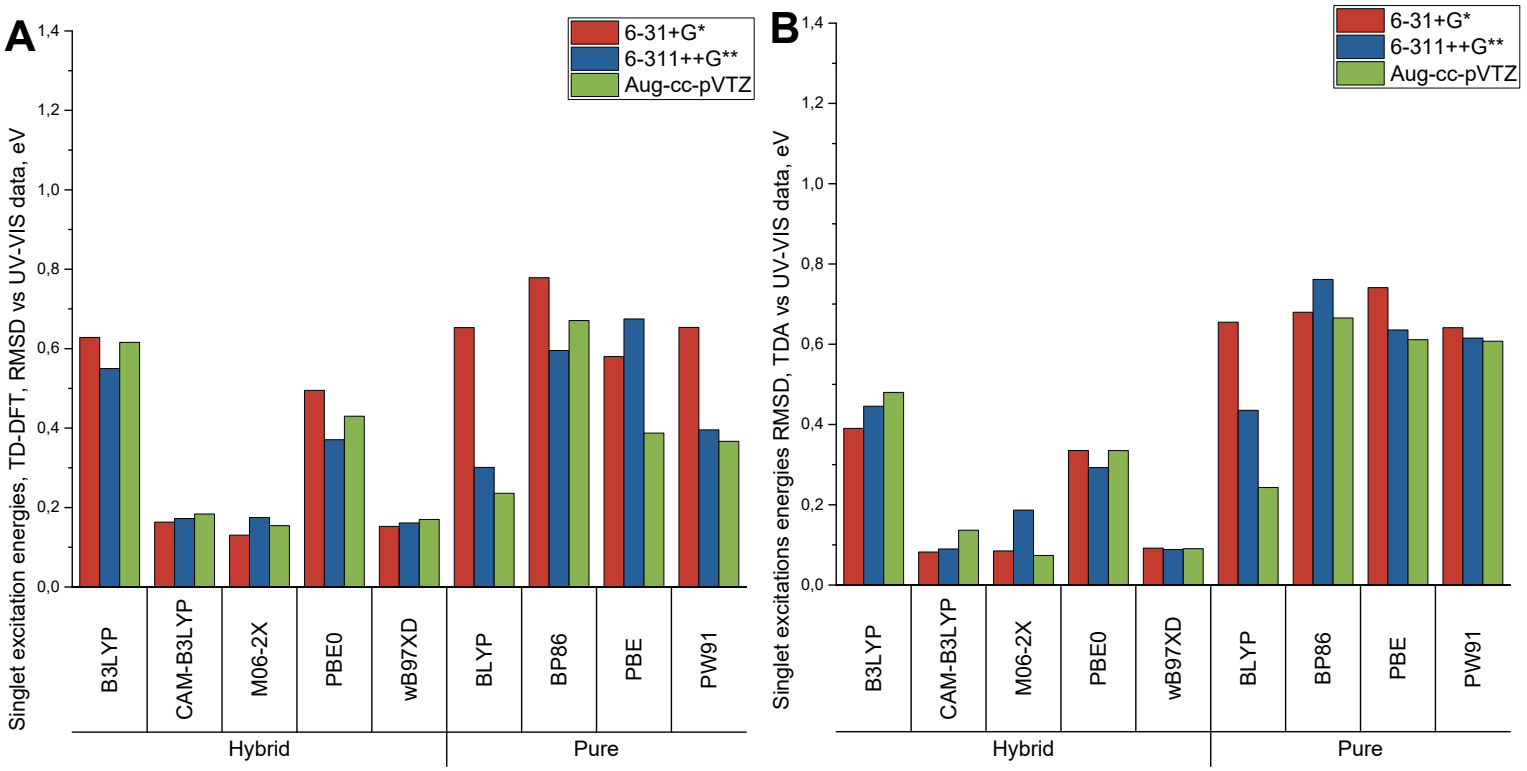

Figure S4. Root mean square deviations (eV) of calculated vertical singlet excitation energies vs experimental UV-Vis data for **1**. TD-DFT without (A) and with the Tamm-Dancoff approximation (B).

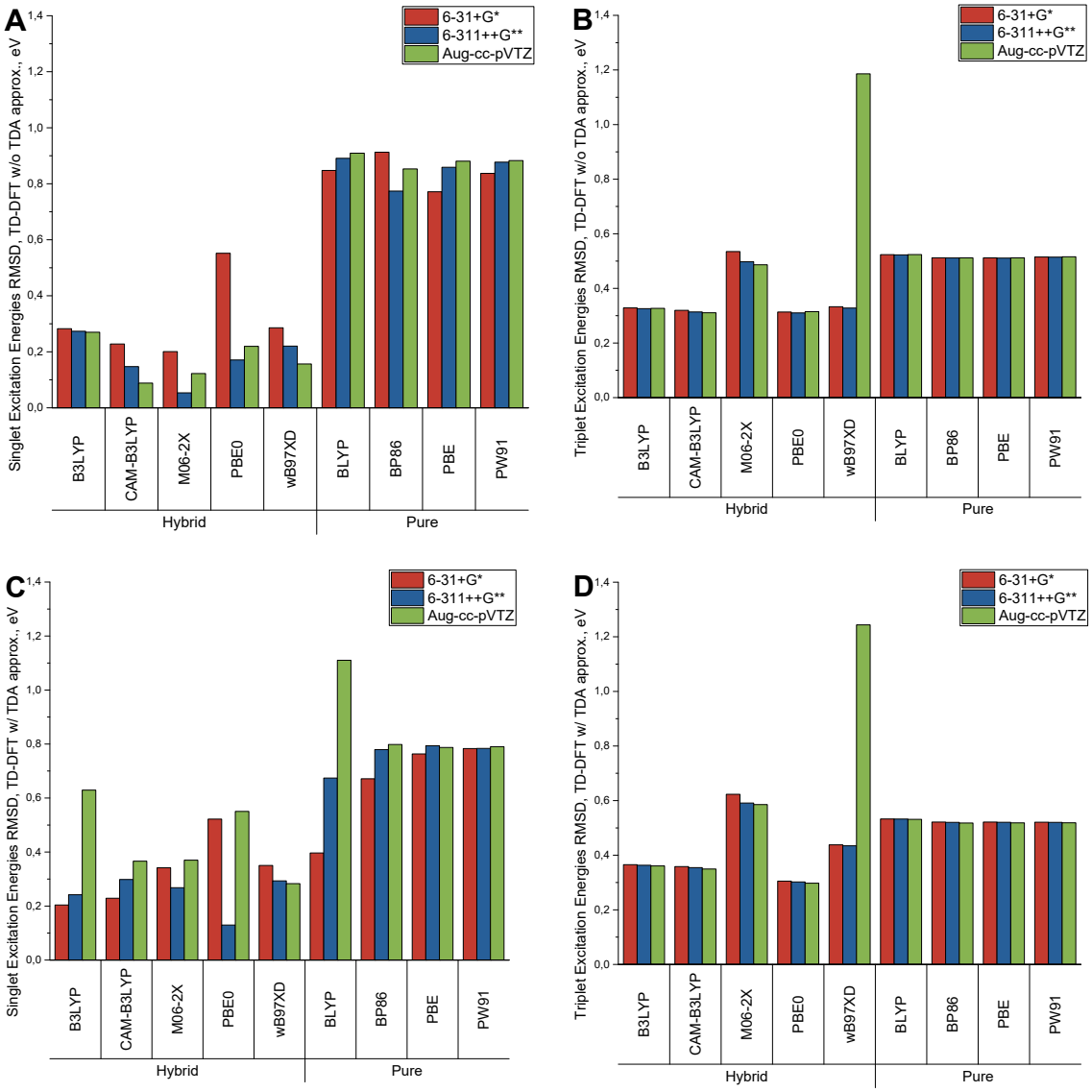

Figure S5. Root mean square deviations (in eV) of calculated vertical excitation energies vs electron energy loss spectroscopy data for **1**: singlet (A,C) and triplet states (B,D) computed at TD-DFT level without (A,B) and with the Tamm-Dancoff approximation (C,D).

Table S2. Interatomic distances (in units of 10^{-10} m) and bond angles (in degrees) of the optimised geometries of neutral, radical cation and radical anion forms of compounds 1-6. For radical spirenes, the values measured for ring A and B are separated by semi-colons. Level of theory: CCSD / 6-31G*.

	parameter	neutral	cation	anion
1	$C^{(sp^3)}$-$C^{(\alpha)}$	1.51888	1.49455 ; 1.50541	1.52226 ; 1.53219
	$C^{(\alpha)}$-$C^{(\beta)}$	1.34722	1.38504 ; 1.36600	1.34905 ; 1.40397
	$C^{(\beta)}$-$C^{(\beta')}$	1.47949	1.42882 ; 1.45237	1.48391 ; 1.41301
	$C^{(\beta')}$-$C^{(\alpha)}$	1.34722	1.38504 ; 1.36600	1.34905 ; 1.40397
	$C^{(\alpha')}$-$C^{(sp^3)}$	1.51888	1.49455 ; 1.50541	1.52778 ; 1.53219
	$C^{(\alpha')}$-$C^{(sp^3)}$-$C^{(\alpha')}$	102.0	103.0 ; 103.5	100.2 ; 101.6
	$C^{(sp^3)}$-$C^{(\alpha)}$-$C^{(\beta)}$	109.9	106.3 ; 108.7	111.4 ; 108.6
	$C^{(\alpha)}$-$C^{(\beta)}$-$C^{(\beta')}$	109.1	109.2 ; 109.5	108.5 ; 110.0
	$C^{(\beta)}$-$C^{(\beta')}$-$C^{(\alpha')}$	109.1	109.2 ; 109.5	108.5 ; 110.0
	$C^{(\beta')}$-$C^{(\alpha')}$-$C^{(sp^3)}$	109.9	106.3 ; 108.7	111.4 ; 108.6
4	$C^{(sp^3)}$-$C^{(\alpha)}$	1.50849	1.49529	1.51931
	$C^{(\alpha)}$-$C^{(\beta)}$	1.34950	1.40136	1.40632
	$C^{(\beta)}$-$C^{(\beta')}$	1.47621	1.40906	1.41404
	$C^{(\beta')}$-$C^{(\alpha)}$	1.34950	1.40136	1.40632
	$C^{(\alpha')}$-$C^{(sp^3)}$	1.50849	1.49529	1.51931
	$C^{(\alpha')}$-$C^{(sp^3)}$-$C^{(\alpha')}$	102.9	102.0	102.6
	$C^{(sp^3)}$-$C^{(\alpha)}$-$C^{(\beta)}$	109.4	109.9	108.2
	$C^{(\alpha)}$-$C^{(\beta)}$-$C^{(\beta')}$	109.1	109.1	109.9
	$C^{(\beta)}$-$C^{(\beta')}$-$C^{(\alpha')}$	109.1	109.1	109.9
	$C^{(\beta')}$-$C^{(\alpha')}$-$C^{(sp^3)}$	109.4	109.9	108.2
2[a]	$C^{(sp^3)}$-$C^{(\alpha)}$	1.48316	1.38080 ; -	1.53089 ; 1.46731
	$C^{(\alpha)}$-$C^{(\alpha')}$	1.32139	1.35635 ; -	1.31955 ; 1.45692
	$C^{(\alpha')}$-$C^{(sp^3)}$	1.48316	1.38080 ; -	1.50653 ; 1.46731
	$C^{(\alpha')}$-$C^{(sp^3)}$-$C^{(\alpha)}$	52.9	58.8 ; -	51.5 ; 59.5
	$C^{(sp^3)}$-$C^{(\alpha)}$-$C^{(\alpha')}$	63.5	60.6 ; -	63.3 ; 60.2
	$C^{(\alpha)}$-$C^{(\alpha')}$-$C^{(sp^3)}$	63.5	60.6 ; -	65.2 ; 60.2
5[a]	$C^{(sp^3)}$-$C^{(\alpha)}$	1.50940	(1.38775)	1.51690
	$C^{(\alpha)}$-$C^{(\alpha')}$	1.30035	(1.36817)	1.42722
	$C^{(\alpha')}$-$C^{(sp^3)}$	1.50940	(2.35385)	1.51690
	$C^{(\alpha')}$-$C^{(sp^3)}$-$C^{(\alpha)}$	51.0	(31.1)	56.1
	$C^{(sp^3)}$-$C^{(\alpha)}$-$C^{(\alpha')}$	64.5	(117.3)	61.9
	$C^{(\alpha)}$-$C^{(\alpha')}$-$C^{(sp^3)}$	64.5	(31.6)	61.9
3	$C^{(sp^3)}$-$C^{(\alpha)}$	1.52512	1.49736 ; 1.54099	1.50805 ; 1.50953
	$C^{(\alpha)}$-$C^{(\beta)}$	1.34807	1.37812 ; 1.34755	1.35777 ; 1.36647
	$C^{(\beta)}$-$C^{(\gamma)}$	1.45666	1.41134 ; 1.45960	1.44704 ; 1.43501
	$C^{(\gamma)}$-$C^{(\gamma')}$	1.35792	1.39715 ; 1.35549	1.35628 ; 1.37357

	$C^{(\gamma')}$-$C^{(\beta')}$	1.45673	1.41812 ; 1.45960	1.45202 ; 1.43501
	$C^{(\beta')}$-$C^{(\alpha')}$	1.34948	1.36882 ; 1.34755	1.35429 ; 1.36647
	$C^{(\alpha')}$-$C^{(sp^3)}$	1.51869	1.50331 ; 1.54100	1.51100 ; 1.50953
	$C^{(\alpha')}$-$C^{(sp^3)}$-$C^{(\alpha)}$	106.1	118.9 ; 109.0	119.0 ; 119.3
	$C^{(sp^3)}$-$C^{(\alpha)}$-$C^{(\beta)}$	123.6	132.7 ; 125.3	132.1 ; 131.7
	$C^{(\alpha)}$-$C^{(\beta)}$-$C^{(\gamma)}$	126.0	128.9 ; 128.1	130.3 ; 130.6
	$C^{(\beta)}$-$C^{(\gamma)}$-$C^{(\gamma')}$	125.5	128.8 ; 125.6	128.0 ; 128.0
	$C^{(\gamma)}$-$C^{(\gamma')}$-$C^{(\beta')}$	125.1	128.8 ; 125.6	128.4 ; 128.0
	$C^{(\gamma')}$-$C^{(\beta')}$-$C^{(\alpha')}$	125.8	128.7 ; 128.1	130.0 ; 130.6
	$C^{(\beta')}$-$C^{(\alpha')}$-$C^{(sp^3)}$	123.9	133.0 ; 125.3	132.2 ; 131.7
6	$C^{(sp^3)}$-$C^{(\alpha)}$	1.50956	1.48919	1.51351
	$C^{(\alpha)}$-$C^{(\beta)}$	1.34829	1.37147	1.38029
	$C^{(\beta)}$-$C^{(\gamma)}$	1.46095	1.41390	1.41861
	$C^{(\gamma)}$-$C^{(\gamma')}$	1.35883	1.39665	1.40596
	$C^{(\gamma')}$-$C^{(\beta')}$	1.46095	1.41390	1.41861
	$C^{(\beta')}$-$C^{(\alpha')}$	1.34829	1.37147	1.38029
	$C^{(\alpha')}$-$C^{(sp^3)}$	1.50956	1.48919	1.51351
	$C^{(\alpha')}$-$C^{(sp^3)}$-$C^{(\alpha)}$	109.1	122.5	118.9
	$C^{(sp^3)}$-$C^{(\alpha)}$-$C^{(\beta)}$	121.6	131.1	127.6
	$C^{(\alpha)}$-$C^{(\beta)}$-$C^{(\gamma)}$	124.6	128.3	130.8
	$C^{(\beta)}$-$C^{(\gamma)}$-$C^{(\gamma')}$	125.8	129.4	127.8
	$C^{(\gamma)}$-$C^{(\gamma')}$-$C^{(\beta')}$	125.8	129.4	127.8
	$C^{(\gamma')}$-$C^{(\beta')}$-$C^{(\alpha')}$	124.6	128.3	130.8
	$C^{(\beta')}$-$C^{(\alpha')}$-$C^{(sp^3)}$	121.6	131.1	127.6

[a] One ring broken upon geometry optimisation of the radical cation geometry.

Table S3. Topological properties for neutral, radical anion and radical cation of molecules **1-6,** computed at the critical points (CPs), *viz.* total electron density ($\rho_{tot}(\mathbf{r})$), spin density ($\sigma(\mathbf{r})$), Lagrangian kinetic energy ($G(\mathbf{r})$), Hamiltonian kinetic energy ($K(\mathbf{r})$), potential energy density ($V(\mathbf{r})$), energy density ($H(\mathbf{r})$), Laplacian of the total electron density ($\Delta\rho(\mathbf{r})$), electron localisation function (ELF($\mathbf{r}$)), source unction (SF($\mathbf{r}$)), electrostatic potential from both electrons and nuclei (ESP$_{tot}$($\mathbf{r}$)), the ellipticity ($\varepsilon(\mathbf{r})$) and eta index ($\eta(\mathbf{r})$). The location and type of CP is also indicated, *viz.* A (atomic CP), B (bond CP), R (ring CP), and C (cage CP). The asterisk indicates one of the two rings when non-equivalent.

	type	location	$\rho_{tot}(\mathbf{r})$	$\sigma(\mathbf{r})$	$G(\mathbf{r})$	$K(\mathbf{r})$	$V(\mathbf{r})$	$H(\mathbf{r})$	$\Delta\rho(\mathbf{r})$	ELF($\mathbf{r}$)	SF($\mathbf{r}$)	ESP($\mathbf{r}$)	$\varepsilon(\mathbf{r})$	$\eta(\mathbf{r})$
2	A	C(sp3)	1.178E+02	0.000000	4.761E+00	1.088E+05	-1.088E+05	-1.088E+05	-4.352E+05	1.000000	1.016E+10	-1.000008	0.000008	9.656E+10
	A	C(α)	1.181E+02	0.000000	4.845E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	1.240E+04	-1.000013	0.000006	5.328E+06
	A	C(α)	1.181E+02	0.000000	4.845E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	1.240E+04	-1.000013	0.000006	5.328E+06
	A	C(α)	1.181E+02	0.000000	4.845E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	1.240E+04	-1.000013	0.000006	5.328E+06
	A	C(α)	1.181E+02	0.000000	4.845E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	1.240E+04	-1.000013	0.000006	5.328E+06
	A	H(α)	4.096E-01	0.000000	4.336E-03	4.473E+00	-4.477E+00	-4.473E+00	-1.788E+01	0.999955	3.057E-01	-1.113901	0.000384	2.532E+01
	A	H(α)	4.096E-01	0.000000	4.336E-03	4.473E+00	-4.477E+00	-4.473E+00	-1.788E+01	0.999955	3.057E-01	-1.113901	0.000384	2.532E+01
	A	H(α)	4.096E-01	0.000000	4.336E-03	4.473E+00	-4.477E+00	-4.473E+00	-1.788E+01	0.999955	3.057E-01	-1.113900	0.000384	2.532E+01
	A	H(α)	4.096E-01	0.000000	4.336E-03	4.473E+00	-4.477E+00	-4.473E+00	-1.788E+01	0.999955	3.057E-01	-1.113901	0.000384	2.532E+01
	B	C(sp3)-C(α)	2.518E-01	0.000000	9.781E-02	2.224E-01	-3.202E-01	-2.224E-01	-4.983E-01	0.896819	2.916E-02	1.483421	0.271706	7.455E-01
	B	C(α)-C(α)	3.426E-01	0.000000	1.647E-01	4.017E-01	-5.664E-01	-4.017E-01	-9.483E-01	0.895306	2.834E-02	3.054533	0.292273	1.024E+00
	B	C(sp3)-C(α)	2.518E-01	0.000000	9.781E-02	2.224E-01	-3.202E-01	-2.224E-01	-4.983E-01	0.896819	2.916E-02	1.483423	0.271705	7.455E-01
	B	C(α)-H(α)	2.764E-01	0.000000	2.748E-02	2.862E-01	-3.137E-01	-2.862E-01	-1.035E+00	0.993382	2.056E-02	1.619138	0.003768	8.857E-01
	B	C(α)-H(α)	2.764E-01	0.000000	2.748E-02	2.862E-01	-3.137E-01	-2.862E-01	-1.035E+00	0.993382	2.056E-02	1.619138	0.003767	8.857E-01
	B	C(sp3)-C(α)	2.518E-01	0.000000	9.781E-02	2.224E-01	-3.202E-01	-2.224E-01	-4.983E-01	0.896819	2.916E-02	1.483421	0.271709	7.455E-01
	B	C(α)-C(α)	3.426E-01	0.000000	1.647E-01	4.017E-01	-5.664E-01	-4.017E-01	-9.483E-01	0.895306	2.834E-02	3.054520	0.292274	1.024E+00
	B	C(sp3)-C(α)	2.518E-01	0.000000	9.781E-02	2.224E-01	-3.202E-01	-2.224E-01	-4.983E-01	0.896819	2.916E-02	1.483421	0.271706	7.455E-01
	B	C(α)-H(α)	2.764E-01	0.000000	2.748E-02	2.862E-01	-3.137E-01	-2.862E-01	-1.035E+00	0.993382	2.056E-02	1.619141	0.003768	8.857E-01
	B	C(α)-H(α)	2.764E-01	0.000000	2.748E-02	2.862E-01	-3.137E-01	-2.862E-01	-1.035E+00	0.993382	2.056E-02	1.619138	0.003768	8.857E-01
	R	O	2.119E-01	0.000000	2.111E-01	1.418E-01	-3.528E-01	-1.418E-01	2.773E-01	0.512204	-1.487E-02	0.928977	-2.152895	7.497E-01
	R	O	2.119E-01	0.000000	2.111E-01	1.418E-01	-3.528E-01	-1.418E-01	2.773E-01	0.512204	-1.487E-02	0.928976	-2.152893	7.497E-01
2(-)	A	C(sp3)	1.179E+02	-0.011632	4.721E+00	1.089E+05	-1.089E+05	-1.089E+05	-4.355E+05	1.000000	2.275E+05	-1.000013	0.000002	1.188E+06
	A	C(α)	1.181E+02	0.073072	4.844E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	1.222E+04	-1.000014	0.000004	4.383E+06
	A	C(α)	1.181E+02	-0.141388	4.854E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	1.286E+04	-1.000013	0.000003	5.190E+06
	A	H(α)	4.142E-01	0.010587	5.075E-03	4.561E+00	-4.566E+00	-4.561E+00	-1.822E+01	0.999941	3.173E-01	-1.100397	0.000447	2.777E+01
	A	H(α)	4.136E-01	-0.013184	5.083E-03	4.550E+00	-4.555E+00	-4.550E+00	-1.818E+01	0.999941	3.037E-01	-1.101544	0.000379	2.749E+01
	A	C(α)*	1.181E+02	0.265547	4.689E+00	1.091E+05	-1.092E+05	-1.091E+05	-4.366E+05	1.000000	1.211E+04	-1.000011	0.000005	9.990E+05
	A	C(α)*	1.181E+02	0.265548	4.689E+00	1.091E+05	-1.092E+05	-1.091E+05	-4.366E+05	1.000000	1.211E+04	-1.000011	0.000005	9.990E+05
	A	H(α)*	4.168E-01	0.010559	6.131E-03	4.606E+00	-4.612E+00	-4.606E+00	-1.840E+01	0.999917	3.397E-01	-1.087135	0.000778	3.092E+01
	A	H(α)*	4.168E-01	0.010559	6.130E-03	4.606E+00	-4.612E+00	-4.606E+00	-1.840E+01	0.999917	3.397E-01	-1.087135	0.000778	3.092E+01
	B	C(sp3)-C(α)	2.359E-01	0.004201	9.390E-02	2.061E-01	-3.000E-01	-2.061E-01	-4.489E-01	0.883920	3.063E-02	1.455506	0.277266	5.470E-01
	B	C(α)-C(α)	3.418E-01	0.000387	1.609E-01	4.018E-01	-5.626E-01	-4.018E-01	-9.636E-01	0.899035	2.913E-02	3.144610	0.245331	8.404E-01
	B	C(sp3)-C(α)	2.240E-01	-0.002440	9.432E-02	1.896E-01	-2.839E-01	-1.896E-01	-3.811E-01	0.863419	2.345E-02	1.396344	0.425218	5.249E-01
	B	C(α)-H(α)	2.671E-01	-0.000868	3.432E-02	2.665E-01	-3.008E-01	-2.665E-01	-9.285E-01	0.988525	1.818E-02	1.535936	0.004286	6.957E-01
	B	C(α)-H(α)	2.661E-01	0.001203	3.436E-02	2.642E-01	-2.986E-01	-2.642E-01	-9.195E-01	0.988346	1.886E-02	1.522362	0.001575	6.942E-01
	B	C(sp3)-C(α)*	2.582E-01	0.001716	1.050E-01	2.398E-01	-3.448E-01	-2.398E-01	-5.391E-01	0.891325	2.731E-02	1.734133	0.393353	5.338E-01
	B	C(α)-C(α)*	2.642E-01	-0.001708	1.074E-01	2.454E-01	-3.528E-01	-2.454E-01	-5.518E-01	0.894229	1.667E-02	1.672979	0.248210	5.031E-01
	B	C(sp3)-C(α)*	2.582E-01	0.001716	1.050E-01	2.398E-01	-3.448E-01	-2.398E-01	-5.391E-01	0.891325	2.731E-02	1.734133	0.393354	5.338E-01
	B	C(α)-H(α)*	2.530E-01	0.001161	4.700E-02	2.423E-01	-2.893E-01	-2.423E-01	-7.812E-01	0.974619	1.681E-02	1.456063	0.049244	5.927E-01
	B	C(α)-H(α)*	2.530E-01	0.001161	4.700E-02	2.423E-01	-2.893E-01	-2.423E-01	-7.812E-01	0.974619	1.681E-02	1.456063	0.049244	5.927E-01
	R	O	1.991E-01	0.000114	1.827E-01	1.292E-01	-3.120E-01	-1.292E-01	2.140E-01	0.532073	-1.244E-02	1.036682	-2.300750	5.111E-01
	R	O*	2.112E-01	-0.000470	1.813E-01	1.417E-01	-3.229E-01	-1.417E-01	1.584E-01	0.584597	-7.388E-03	1.222011	-2.545853	4.232E-01
1	A	C(sp3)	1.181E+02	0.000000	4.875E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.363E+05	1.000000	6.425E+10	-1.000004	0.000000	4.075E+12

Table S3 (continued)

	A	C(α)	1.182E+02	0.000000	4.789E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.368E+05	1.000000	1.211E+04	-1.000009	0.000006	3.358E+06
	A	C(β)	1.182E+02	0.000000	4.806E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	7.830E+03	-1.000010	0.000007	3.208E+06
	A	C(β)	1.182E+02	0.000000	4.806E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	7.830E+03	-1.000010	0.000007	3.208E+06
	A	C(α)	1.182E+02	0.000000	4.789E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.368E+05	1.000000	1.211E+04	-1.000009	0.000006	3.358E+06
	A	H(α)	4.188E-01	0.000000	4.337E-03	4.558E+00	-4.562E+00	-4.558E+00	-1.822E+01	0.999958	3.368E-01	-1.111237	0.001109	2.562E+01
	A	H(β)	4.209E-01	0.000000	4.209E-03	4.591E+00	-4.595E+00	-4.591E+00	-1.835E+01	0.999961	2.281E-01	-1.109652	0.001042	2.590E+01
	A	H(β)	4.209E-01	0.000000	4.209E-03	4.591E+00	-4.595E+00	-4.591E+00	-1.835E+01	0.999961	2.281E-01	-1.109652	0.001042	2.590E+01
	A	H(α)	4.188E-01	0.000000	4.337E-03	4.558E+00	-4.562E+00	-4.558E+00	-1.822E+01	0.999958	3.368E-01	-1.111237	0.001109	2.562E+01
	A	C(α)	1.182E+02	0.000000	4.789E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.368E+05	1.000000	1.211E+04	-1.000009	0.000006	3.358E+06
	A	C(β)	1.182E+02	0.000000	4.806E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	7.830E+03	-1.000010	0.000007	3.208E+06
	A	C(β)	1.182E+02	0.000000	4.806E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	7.830E+03	-1.000010	0.000007	3.208E+06
	A	C(α)	1.182E+02	0.000000	4.789E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.368E+05	1.000000	1.211E+04	-1.000009	0.000006	3.358E+06
	A	H(α)	4.188E-01	0.000000	4.337E-03	4.558E+00	-4.562E+00	-4.558E+00	-1.822E+01	0.999958	3.368E-01	-1.111237	0.001109	2.562E+01
	A	H(β)	4.209E-01	0.000000	4.209E-03	4.591E+00	-4.595E+00	-4.591E+00	-1.835E+01	0.999961	2.281E-01	-1.109652	0.001042	2.590E+01
	A	H(β)	4.209E-01	0.000000	4.209E-03	4.591E+00	-4.595E+00	-4.591E+00	-1.835E+01	0.999961	2.281E-01	-1.109652	0.001042	2.590E+01
	A	H(α)	4.188E-01	0.000000	4.337E-03	4.558E+00	-4.562E+00	-4.558E+00	-1.822E+01	0.999958	3.368E-01	-1.111237	0.001109	2.562E+01
	B	C(sp3)-C(α)	2.592E-01	0.000000	5.562E-02	2.263E-01	-2.819E-01	-2.263E-01	-6.826E-01	0.967316	3.804E-02	1.656178	0.037706	6.545E-01
	B	C(α)-C(β)	3.465E-01	0.000000	1.289E-01	3.951E-01	-5.240E-01	-3.951E-01	-1.065E+00	0.935503	2.399E-02	3.286185	0.436004	9.553E-01
	B	C(β)-C(β)	2.773E-01	0.000000	6.229E-02	2.557E-01	-3.180E-01	-2.557E-01	-7.737E-01	0.967235	1.447E-02	1.869802	0.101512	7.145E-01
	B	C(α)-C(β)	3.465E-01	0.000000	1.289E-01	3.951E-01	-5.240E-01	-3.951E-01	-1.065E+00	0.935503	2.399E-02	3.286185	0.436004	9.553E-01
	B	C(sp3)-C(α)	2.592E-01	0.000000	5.562E-02	2.263E-01	-2.819E-01	-2.263E-01	-6.826E-01	0.967316	3.804E-02	1.656178	0.037706	6.545E-01
	B	C(α)-H(α)	2.796E-01	0.000000	3.070E-02	2.872E-01	-3.179E-01	-2.872E-01	-1.026E+00	0.992061	2.180E-02	1.610912	0.018425	8.571E-01
	B	C(β)-H(β)	2.794E-01	0.000000	3.047E-02	2.860E-01	-3.164E-01	-2.860E-01	-1.022E+00	0.992153	1.424E-02	1.601391	0.014593	8.583E-01
	B	C(β)-H(β)	2.794E-01	0.000000	3.047E-02	2.860E-01	-3.164E-01	-2.860E-01	-1.022E+00	0.992153	1.424E-02	1.601391	0.014593	8.583E-01
	B	C(α)-H(α)	2.796E-01	0.000000	3.070E-02	2.872E-01	-3.179E-01	-2.872E-01	-1.026E+00	0.992061	2.180E-02	1.610912	0.018425	8.571E-01
	B	C(sp3)-C(α)	2.592E-01	0.000000	5.562E-02	2.263E-01	-2.819E-01	-2.263E-01	-6.826E-01	0.967316	3.804E-02	1.656179	0.037706	6.545E-01
	B	C(α)-C(β)	3.465E-01	0.000000	1.289E-01	3.951E-01	-5.240E-01	-3.951E-01	-1.065E+00	0.935503	2.399E-02	3.286185	0.436004	9.553E-01
	B	C(β)-C(β)	2.773E-01	0.000000	6.229E-02	2.557E-01	-3.180E-01	-2.557E-01	-7.737E-01	0.967235	1.447E-02	1.869802	0.101512	7.145E-01
	B	C(α)-C(β)	3.465E-01	0.000000	1.289E-01	3.951E-01	-5.240E-01	-3.951E-01	-1.065E+00	0.935503	2.399E-02	3.286185	0.436004	9.553E-01
	B	C(sp3)-C(α)	2.592E-01	0.000000	5.562E-02	2.263E-01	-2.819E-01	-2.263E-01	-6.826E-01	0.967316	3.804E-02	1.656179	0.037706	6.545E-01
	B	C(α)-H(α)	2.796E-01	0.000000	3.070E-02	2.872E-01	-3.179E-01	-2.872E-01	-1.026E+00	0.992061	2.180E-02	1.610912	0.018425	8.571E-01
	B	C(β)-H(β)	2.794E-01	0.000000	3.047E-02	2.860E-01	-3.164E-01	-2.860E-01	-1.022E+00	0.992153	1.424E-02	1.601391	0.014593	8.583E-01
	B	C(β)-H(β)	2.794E-01	0.000000	3.047E-02	2.860E-01	-3.164E-01	-2.860E-01	-1.022E+00	0.992153	1.424E-02	1.601391	0.014593	8.583E-01
	B	C(α)-H(α)	2.796E-01	0.000000	3.070E-02	2.872E-01	-3.179E-01	-2.872E-01	-1.026E+00	0.992061	2.180E-02	1.610912	0.018425	8.571E-01
	R	O	4.321E-02	0.000000	7.169E-02	-8.594E-03	-6.309E-02	8.594E-03	3.211E-01	0.043444	-1.074E-02	0.219026	-1.229412	2.287E-01
	R	O	4.321E-02	0.000000	7.169E-02	-8.594E-03	-6.309E-02	8.594E-03	3.211E-01	0.043444	-1.074E-02	0.219026	-1.229412	2.287E-01
1(+)	A	C(sp3)	1.181E+02	-0.029987	4.967E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.364E+05	1.000000	4.754E+06	-1.000006	0.000004	2.910E+06
	A	C(α)	1.183E+02	0.093949	4.762E+00	1.093E+05	-1.093E+05	-1.093E+05	-4.371E+05	1.000000	1.234E+04	-1.000021	0.000019	8.942E+06
	A	C(β)	1.182E+02	-0.015609	4.796E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.369E+05	1.000000	7.844E+03	-1.000018	0.000016	6.200E+06
	A	C(β)	1.182E+02	-0.015609	4.796E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.369E+05	1.000000	7.844E+03	-1.000018	0.000016	6.200E+06
	A	C(α)	1.183E+02	0.093949	4.762E+00	1.093E+05	-1.093E+05	-1.093E+05	-4.371E+05	1.000000	1.234E+04	-1.000021	0.000019	8.942E+06
	A	H(α)	4.076E-01	-0.014438	3.602E-03	4.401E+00	-4.404E+00	-4.401E+00	-1.759E+01	0.999969	3.272E-01	-1.126435	0.000682	2.358E+01
	A	H(β)	4.097E-01	-0.000216	3.510E-03	4.428E+00	-4.431E+00	-4.428E+00	-1.770E+01	0.999971	2.207E-01	-1.124740	0.000803	2.378E+01
	A	H(β)	4.097E-01	-0.000216	3.510E-03	4.428E+00	-4.431E+00	-4.428E+00	-1.770E+01	0.999971	2.207E-01	-1.124740	0.000803	2.378E+01
	A	H(α)	4.076E-01	-0.014438	3.602E-03	4.401E+00	-4.404E+00	-4.401E+00	-1.759E+01	0.999969	3.272E-01	-1.126435	0.000682	2.358E+01
	A	C(α)*	1.182E+02	0.011165	4.794E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	1.220E+04	-1.000008	0.000003	2.242E+06
	A	C(β)*	1.182E+02	0.007625	4.792E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	7.864E+03	-1.000014	0.000012	6.887E+06
	A	C(β)*	1.182E+02	0.007624	4.792E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	7.864E+03	-1.000014	0.000012	6.887E+06
	A	C(α)*	1.182E+02	0.011165	4.794E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	1.220E+04	-1.000008	0.000003	2.242E+06
	A	H(α)*	4.117E-01	-0.000183	4.310E-03	4.457E+00	-4.461E+00	-4.457E+00	-1.781E+01	0.999956	3.298E-01	-1.117368	0.001287	2.474E+01
	A	H(β)*	4.140E-01	-0.001480	3.733E-03	4.491E+00	-4.495E+00	-4.491E+00	-1.795E+01	0.999968	2.241E-01	-1.118911	0.000873	2.454E+01
	A	H(β)*	4.140E-01	-0.001480	3.733E-03	4.491E+00	-4.495E+00	-4.491E+00	-1.795E+01	0.999968	2.241E-01	-1.118911	0.000873	2.454E+01
	A	H(α)*	4.117E-01	-0.000183	4.310E-03	4.457E+00	-4.461E+00	-4.457E+00	-1.781E+01	0.999956	3.298E-01	-1.117368	0.001287	2.474E+01
	B	C(sp3)-C(α)	2.740E-01	-0.002428	6.254E-02	2.544E-01	-3.169E-01	-2.544E-01	-7.673E-01	0.965740	4.589E-02	1.804235	0.033246	9.311E-01
	B	C(α)-C(β)	3.330E-01	-0.003662	9.818E-02	3.606E-01	-4.588E-01	-3.606E-01	-1.050E+00	0.956357	2.386E-02	2.603862	0.184666	1.124E+00
	B	C(β)-H(β)	3.076E-01	0.001431	8.082E-02	3.087E-01	-3.895E-01	-3.087E-01	-9.114E-01	0.961227	1.707E-02	2.167691	0.157831	1.035E+00

Table S3 (continued)

	B	C(α)-C(β)	3.330E-01	-0.003662	9.818E-02	3.606E-01	-4.588E-01	-3.606E-01	-1.050E+00	0.956357	2.386E-02	2.603860	0.184666	1.124E+00
	B	C(sp3)-C(α)	2.740E-01	-0.002428	6.254E-02	2.544E-01	-3.169E-01	-2.544E-01	-7.673E-01	0.965740	4.589E-02	1.804233	0.033246	9.311E-01
	B	C(α)-H(α)	2.862E-01	-0.002509	2.237E-02	3.070E-01	-3.293E-01	-3.070E-01	-1.138E+00	0.996108	2.410E-02	1.681024	0.001634	1.090E+00
	B	C(β)-H(β)	2.861E-01	-0.000029	2.230E-02	3.049E-01	-3.272E-01	-3.049E-01	-1.131E+00	0.996102	1.564E-02	1.669114	0.000690	1.084E+00
	B	C(β)-H(β)	2.861E-01	-0.000029	2.230E-02	3.049E-01	-3.272E-01	-3.049E-01	-1.131E+00	0.996102	1.564E-02	1.669114	0.000690	1.084E+00
	B	C(α)-H(α)	2.862E-01	-0.002509	2.237E-02	3.070E-01	-3.293E-01	-3.070E-01	-1.138E+00	0.996108	2.410E-02	1.681024	0.001633	1.090E+00
	B	C(sp3)-C(α)*	2.633E-01	0.001593	5.981E-02	2.356E-01	-2.954E-01	-2.356E-01	-7.032E-01	0.964224	3.794E-02	1.722503	0.041894	8.762E-01
	B	C(α)-C(β)*	3.364E-01	-0.000376	1.181E-01	3.711E-01	-4.892E-01	-3.711E-01	-1.012E+00	0.939912	2.296E-02	2.896941	0.388767	1.087E+00
	B	C(β)-C(β)*	2.944E-01	-0.000204	6.755E-02	2.851E-01	-3.526E-01	-2.851E-01	-8.702E-01	0.968409	1.635E-02	2.025931	0.089609	9.325E-01
	B	C(α)-C(β)*	3.364E-01	-0.000376	1.181E-01	3.711E-01	-4.892E-01	-3.711E-01	-1.012E+00	0.939912	2.296E-02	2.896941	0.388767	1.087E+00
	B	C(sp3)-C(α)*	2.633E-01	0.001593	5.981E-02	2.356E-01	-2.954E-01	-2.356E-01	-7.032E-01	0.964224	3.794E-02	1.722503	0.041894	8.762E-01
	B	C(α)-H(α)*	2.810E-01	0.000015	2.848E-02	2.920E-01	-3.204E-01	-2.920E-01	-1.054E+00	0.993273	2.238E-02	1.641488	0.025968	1.027E+00
	B	C(β)-H(β)*	2.838E-01	-0.000182	2.515E-02	2.973E-01	-3.225E-01	-2.973E-01	-1.089E+00	0.994916	1.514E-02	1.638425	0.005558	1.020E+00
	B	C(β)-H(β)*	2.838E-01	-0.000182	2.515E-02	2.973E-01	-3.225E-01	-2.973E-01	-1.089E+00	0.994916	1.514E-02	1.638425	0.005558	1.020E+00
	B	C(α)-H(α)*	2.810E-01	0.000015	2.848E-02	2.920E-01	-3.204E-01	-2.920E-01	-1.054E+00	0.993273	2.238E-02	1.641488	0.025968	1.027E+00
	R	O	4.497E-02	-0.000063	7.605E-02	-8.596E-03	-6.746E-02	8.596E-03	3.386E-01	0.044047	-1.140E-02	0.222788	-1.234877	4.704E-01
	R	O*	4.397E-02	-0.000054	7.371E-02	-8.521E-03	-6.519E-02	8.521E-03	3.289E-01	0.043520	-1.111E-02	0.220304	-1.224049	4.094E-01
1(-)	A	C(sp3)	1.180E+02	-0.064974	4.779E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.362E+05	1.000000	2.288E+05	-1.000006	0.000005	2.786E+06
	A	C(α)	1.182E+02	0.067056	4.756E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.370E+05	1.000000	1.162E+04	-1.000013	0.000010	3.458E+06
	A	C(β)	1.181E+02	-0.005268	4.805E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	7.664E+03	-1.000007	0.000003	2.209E+06
	A	C(β)	1.181E+02	-0.009547	4.806E+00	1.091E+05	-1.092E+05	-1.091E+05	-4.366E+05	1.000000	7.817E+03	-1.000007	0.000003	2.226E+06
	A	C(α)	1.182E+02	0.085639	4.749E+00	1.093E+05	-1.093E+05	-1.093E+05	-4.370E+05	1.000000	1.256E+04	-1.000013	0.000010	3.287E+06
	A	H(α)	4.238E-01	-0.002554	4.372E-03	4.635E+00	-4.639E+00	-4.635E+00	-1.852E+01	0.999959	3.550E-01	-1.105928	0.000889	2.649E+01
	A	H(β)	4.247E-01	0.002285	4.649E-03	4.657E+00	-4.661E+00	-4.657E+00	-1.861E+01	0.999954	2.312E-01	-1.100854	0.001193	2.750E+01
	A	H(β)	4.250E-01	0.001123	4.637E-03	4.659E+00	-4.663E+00	-4.659E+00	-1.862E+01	0.999955	2.274E-01	-1.101028	0.001177	2.746E+01
	A	H(α)	4.244E-01	-0.001610	4.359E-03	4.643E+00	-4.648E+00	-4.643E+00	-1.856E+01	0.999960	3.329E-01	-1.105766	0.000914	2.653E+01
	A	C(α)*	1.180E+02	0.148378	4.847E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.363E+05	1.000000	1.197E+04	-1.000011	0.000004	2.105E+06
	A	C(β)*	1.181E+02	-0.026182	4.780E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.364E+05	1.000000	7.724E+03	-1.000005	0.000002	2.650E+06
	A	C(β)*	1.181E+02	-0.026182	4.780E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.364E+05	1.000000	7.724E+03	-1.000005	0.000002	2.650E+06
	A	C(α)*	1.180E+02	0.148378	4.847E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.363E+05	1.000000	1.197E+04	-1.000011	0.000004	2.105E+06
	A	H(α)*	4.224E-01	-0.014550	5.818E-03	4.626E+00	-4.632E+00	-4.626E+00	-1.848E+01	0.999928	3.414E-01	-1.096891	0.001941	2.831E+01
	A	H(β)*	4.262E-01	0.000497	4.961E-03	4.682E+00	-4.687E+00	-4.682E+00	-1.871E+01	0.999949	2.305E-01	-1.096434	0.001389	2.845E+01
	A	H(β)*	4.262E-01	0.000497	4.961E-03	4.682E+00	-4.687E+00	-4.682E+00	-1.871E+01	0.999949	2.305E-01	-1.096434	0.001389	2.845E+01
	A	H(α)*	4.224E-01	-0.014550	5.818E-03	4.626E+00	-4.632E+00	-4.626E+00	-1.848E+01	0.999928	3.414E-01	-1.096891	0.001941	2.831E+01
	B	C(sp3)-C(α)	2.600E-01	0.003362	5.765E-02	2.323E-01	-2.900E-01	-2.323E-01	-6.986E-01	0.965435	3.782E-02	1.710511	0.048206	4.774E-01
	B	C(α)-C(β)	3.442E-01	0.000266	1.283E-01	3.911E-01	-5.194E-01	-3.911E-01	-1.051E+00	0.934704	2.298E-02	3.244663	0.426713	7.883E-01
	B	C(β)-C(β)	2.725E-01	0.000221	6.283E-02	2.483E-01	-3.112E-01	-2.483E-01	-7.420E-01	0.964765	1.368E-02	1.845027	0.124786	5.443E-01
	B	C(α)-C(β)	3.439E-01	0.000175	1.284E-01	3.906E-01	-5.190E-01	-3.906E-01	-1.049E+00	0.934401	2.389E-02	3.240985	0.423792	7.882E-01
	B	C(sp3)-C(α)	2.565E-01	0.003641	5.855E-02	2.275E-01	-2.861E-01	-2.275E-01	-6.758E-01	0.962920	4.352E-02	1.668701	0.048805	4.717E-01
	B	C(α)-H(α)	2.775E-01	0.000202	3.254E-02	2.823E-01	-3.149E-01	-2.823E-01	-9.992E-01	0.990864	2.058E-02	1.582605	0.006125	6.933E-01
	B	C(β)-H(β)	2.727E-01	0.000049	3.569E-02	2.737E-01	-3.094E-01	-2.737E-01	-9.521E-01	0.988377	1.308E-02	1.571728	0.024346	7.076E-01
	B	C(β)-H(β)	2.723E-01	0.000075	3.577E-02	2.731E-01	-3.088E-01	-2.731E-01	-9.492E-01	0.988281	1.328E-02	1.569353	0.025160	7.065E-01
	B	C(α)-H(α)	2.773E-01	0.000029	3.246E-02	2.821E-01	-3.145E-01	-2.821E-01	-9.985E-01	0.990892	2.211E-02	1.582095	0.005182	6.929E-01
	B	C(sp3)-C(α)*	2.465E-01	0.000420	5.849E-02	2.107E-01	-2.692E-01	-2.107E-01	-6.089E-01	0.957815	3.191E-02	1.638631	0.094703	4.312E-01
	B	C(α)-C(β)*	3.084E-01	-0.000287	9.808E-02	3.163E-01	-4.143E-01	-3.163E-01	-8.727E-01	0.944478	1.953E-02	2.451946	0.351068	6.123E-01
	B	C(β)-C(β)*	3.054E-01	-0.001174	9.301E-02	3.091E-01	-4.021E-01	-3.091E-01	-8.643E-01	0.948136	1.587E-02	2.333204	0.299596	5.983E-01
	B	C(α)-C(β)*	3.084E-01	-0.000287	9.808E-02	3.163E-01	-4.143E-01	-3.163E-01	-8.727E-01	0.944478	1.953E-02	2.451944	0.351068	6.123E-01
	B	C(sp3)-C(α)*	2.465E-01	0.000420	5.849E-02	2.107E-01	-2.692E-01	-2.107E-01	-6.089E-01	0.957815	3.191E-02	1.638634	0.094703	4.312E-01
	B	C(α)-H(α)*	2.666E-01	0.000285	4.492E-02	2.655E-01	-3.104E-01	-2.655E-01	-8.822E-01	0.980414	1.890E-02	1.587521	0.089416	6.439E-01
	B	C(β)-H(β)*	2.681E-01	-0.000006	3.971E-02	2.671E-01	-3.068E-01	-2.671E-01	-9.097E-01	0.984837	1.265E-02	1.566798	0.038757	6.530E-01
	B	C(β)-H(β)*	2.681E-01	-0.000006	3.971E-02	2.671E-01	-3.068E-01	-2.671E-01	-9.097E-01	0.984837	1.265E-02	1.566799	0.038757	6.530E-01
	B	C(α)-H(α)*	2.666E-01	0.000285	4.492E-02	2.655E-01	-3.104E-01	-2.655E-01	-8.822E-01	0.980414	1.890E-02	1.587521	0.089416	6.439E-01
	R	O	4.255E-02	-0.000063	7.026E-02	-8.615E-03	-6.165E-02	8.615E-03	3.155E-01	0.042981	-1.035E-02	0.209297	-1.242907	5.494E-02
	R	O*	4.075E-02	0.000063	6.576E-02	-8.720E-03	-5.704E-02	8.720E-03	2.979E-01	0.042486	-9.889E-03	0.222872	-1.225920	-2.235E-03
3	A	C(sp3)	1.180E+02	0.000000	4.855E+00	1.090E+05	-1.091E+05	-1.090E+05	-4.362E+05	1.000000	2.714E+04	-1.000001	0.000001	1.852E+07
	A	C(α)	1.182E+02	0.000000	4.738E+00	1.093E+05	-1.093E+05	-1.093E+05	-4.370E+05	1.000000	1.437E+04	-1.000012	0.000009	3.748E+06

Table S3 (continued)

A	C(β)	1.181E+02	0.000000	4.842E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.365E+05	1.000000	8.666E+03	-1.000008	0.000006	3.482E+06
A	C(γ)	1.181E+02	0.000000	4.793E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	6.905E+03	-1.000011	0.000009	4.778E+06
A	C(γ)	1.181E+02	0.000000	4.810E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	6.342E+03	-1.000009	0.000007	4.165E+06
A	C(β)	1.181E+02	0.000000	4.827E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	6.765E+03	-1.000009	0.000007	3.977E+06
A	C(α)	1.182E+02	0.000000	4.756E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.369E+05	1.000000	9.272E+03	-1.000011	0.000008	3.780E+06
A	C(α)	1.182E+02	0.000000	4.738E+00	1.093E+05	-1.093E+05	-1.093E+05	-4.370E+05	1.000000	1.437E+04	-1.000012	0.000009	3.748E+06
A	C(β)	1.181E+02	0.000000	4.842E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.365E+05	1.000000	8.666E+03	-1.000008	0.000006	3.482E+06
A	C(γ)	1.181E+02	0.000000	4.793E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	6.905E+03	-1.000011	0.000009	4.778E+06
A	C(γ)	1.181E+02	0.000000	4.810E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	6.342E+03	-1.000009	0.000007	4.165E+06
A	C(β)	1.181E+02	0.000000	4.827E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	6.765E+03	-1.000009	0.000007	3.977E+06
A	C(α)	1.182E+02	0.000000	4.756E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.369E+05	1.000000	9.272E+03	-1.000011	0.000008	3.780E+06
A	H(α)	4.227E-01	0.000000	4.457E-03	4.604E+00	-4.608E+00	-4.604E+00	-1.840E+01	0.999957	3.667E-01	-1.111116	0.001528	2.577E+01
A	H(β)	4.227E-01	0.000000	4.432E-03	4.618E+00	-4.623E+00	-4.618E+00	-1.846E+01	0.999958	2.529E-01	-1.106645	0.001518	2.653E+01
A	H(γ)	4.243E-01	0.000000	4.421E-03	4.635E+00	-4.639E+00	-4.635E+00	-1.852E+01	0.999959	2.009E-01	-1.107269	0.001550	2.643E+01
A	H(γ)	4.247E-01	0.000000	4.333E-03	4.640E+00	-4.644E+00	-4.640E+00	-1.854E+01	0.999960	2.183E-01	-1.107639	0.001476	2.638E+01
A	H(β)	4.230E-01	0.000000	4.378E-03	4.621E+00	-4.625E+00	-4.621E+00	-1.847E+01	0.999959	2.073E-01	-1.107031	0.001483	2.647E+01
A	H(α)	4.237E-01	0.000000	4.567E-03	4.628E+00	-4.633E+00	-4.628E+00	-1.849E+01	0.999956	2.750E-01	-1.107422	0.001584	2.642E+01
A	H(α)	4.227E-01	0.000000	4.457E-03	4.604E+00	-4.608E+00	-4.604E+00	-1.840E+01	0.999957	3.667E-01	-1.111116	0.001528	2.577E+01
A	H(β)	4.227E-01	0.000000	4.432E-03	4.618E+00	-4.623E+00	-4.618E+00	-1.846E+01	0.999958	2.529E-01	-1.106645	0.001518	2.653E+01
A	H(γ)	4.247E-01	0.000000	4.333E-03	4.640E+00	-4.644E+00	-4.640E+00	-1.854E+01	0.999960	2.183E-01	-1.107639	0.001476	2.638E+01
A	H(γ)	4.243E-01	0.000000	4.421E-03	4.635E+00	-4.639E+00	-4.635E+00	-1.852E+01	0.999959	2.009E-01	-1.107269	0.001550	2.643E+01
A	H(β)	4.230E-01	0.000000	4.378E-03	4.621E+00	-4.625E+00	-4.621E+00	-1.847E+01	0.999959	2.073E-01	-1.107031	0.001483	2.647E+01
A	H(α)	4.237E-01	0.000000	4.567E-03	4.628E+00	-4.633E+00	-4.628E+00	-1.849E+01	0.999956	2.750E-01	-1.107422	0.001584	2.642E+01
B	C(sp3)-C(α)	2.622E-01	0.000000	5.315E-02	2.301E-01	-2.832E-01	-2.301E-01	-7.076E-01	0.971131	2.360E-02	1.701458	0.036371	6.600E-01
B	C(α)-C(β)	3.444E-01	0.000000	1.234E-01	3.900E-01	-5.134E-01	-3.900E-01	-1.066E+00	0.939396	1.972E-02	3.268941	0.418817	9.570E-01
B	C(β)-C(γ)	2.885E-01	0.000000	6.439E-02	2.747E-01	-3.391E-01	-2.747E-01	-8.411E-01	0.969276	1.550E-02	2.023587	0.099611	7.558E-01
B	C(γ)-C(γ)	3.386E-01	0.000000	1.179E-01	3.770E-01	-4.948E-01	-3.770E-01	-1.036E+00	0.941372	1.623E-02	3.060379	0.391425	9.386E-01
B	C(β)-C(γ)	2.883E-01	0.000000	6.457E-02	2.742E-01	-3.388E-01	-2.742E-01	-8.385E-01	0.969032	1.304E-02	2.022332	0.103106	7.581E-01
B	C(α)-C(β)	3.454E-01	0.000000	1.241E-01	3.924E-01	-5.165E-01	-3.924E-01	-1.073E+00	0.939289	2.796E-02	3.312633	0.420164	9.542E-01
B	C(sp3)-C(α)	2.578E-01	0.000000	5.225E-02	2.234E-01	-2.757E-01	-2.234E-01	-6.847E-01	0.970525	4.296E-02	1.655653	0.035034	6.481E-01
B	C(sp3)-C(α)	2.578E-01	0.000000	5.225E-02	2.234E-01	-2.757E-01	-2.234E-01	-6.847E-01	0.970525	4.296E-02	1.655653	0.035034	6.481E-01
B	C(α)-C(β)	3.454E-01	0.000000	1.241E-01	3.924E-01	-5.165E-01	-3.924E-01	-1.073E+00	0.939289	2.796E-02	3.312633	0.420164	9.542E-01
B	C(β)-C(γ)	2.885E-01	0.000000	6.439E-02	2.747E-01	-3.391E-01	-2.747E-01	-8.411E-01	0.969276	1.550E-02	2.023587	0.099611	7.558E-01
B	C(γ)-C(γ)	3.386E-01	0.000000	1.179E-01	3.770E-01	-4.948E-01	-3.770E-01	-1.036E+00	0.941372	1.623E-02	3.060379	0.391425	9.386E-01
B	C(β)-C(γ)	2.883E-01	0.000000	6.457E-02	2.742E-01	-3.388E-01	-2.742E-01	-8.385E-01	0.969032	1.304E-02	2.022332	0.103106	7.581E-01
B	C(α)-C(β)	3.444E-01	0.000000	1.234E-01	3.900E-01	-5.134E-01	-3.900E-01	-1.066E+00	0.939396	1.972E-02	3.268941	0.418817	9.570E-01
B	C(sp3)-C(α)	2.622E-01	0.000000	5.315E-02	2.301E-01	-2.832E-01	-2.301E-01	-7.076E-01	0.971131	2.360E-02	1.701458	0.036371	6.600E-01
B	C(α)-H(α)	2.786E-01	0.000000	3.312E-02	2.833E-01	-3.164E-01	-2.833E-01	-1.001E+00	0.990657	1.677E-02	1.580688	0.023164	8.478E-01
B	C(β)-H(β)	2.776E-01	0.000000	3.325E-02	2.820E-01	-3.152E-01	-2.820E-01	-9.949E-01	0.990479	1.238E-02	1.576943	0.021405	8.435E-01
B	C(γ)-H(γ)	2.787E-01	0.000000	3.326E-02	2.836E-01	-3.169E-01	-2.836E-01	-1.002E+00	0.990590	1.195E-02	1.582881	0.022878	8.432E-01
B	C(γ)-H(γ)	2.792E-01	0.000000	3.259E-02	2.847E-01	-3.173E-01	-2.847E-01	-1.008E+00	0.991021	1.309E-02	1.581775	0.018388	8.430E-01
B	C(β)-H(β)	2.770E-01	0.000000	3.375E-02	2.810E-01	-3.147E-01	-2.810E-01	-9.890E-01	0.990124	1.527E-02	1.575780	0.024303	8.379E-01
B	C(α)-H(α)	2.786E-01	0.000000	3.312E-02	2.833E-01	-3.164E-01	-2.833E-01	-1.001E+00	0.990657	1.677E-02	1.580688	0.023164	8.478E-01
B	C(α)-H(α)	2.817E-01	0.000000	3.125E-02	2.897E-01	-3.210E-01	-2.897E-01	-1.034E+00	0.991977	2.425E-02	1.601940	0.020335	8.412E-01
B	C(β)-H(β)	2.770E-01	0.000000	3.375E-02	2.810E-01	-3.147E-01	-2.810E-01	-9.890E-01	0.990124	1.527E-02	1.575780	0.024303	8.379E-01
B	C(γ)-H(γ)	2.787E-01	0.000000	3.326E-02	2.836E-01	-3.169E-01	-2.836E-01	-1.002E+00	0.990590	1.195E-02	1.582881	0.022878	8.432E-01
B	C(γ)-H(γ)	2.792E-01	0.000000	3.259E-02	2.847E-01	-3.173E-01	-2.847E-01	-1.008E+00	0.991021	1.309E-02	1.581775	0.018388	8.430E-01
B	C(β)-H(β)	2.776E-01	0.000000	3.325E-02	2.820E-01	-3.152E-01	-2.820E-01	-9.949E-01	0.990479	1.238E-02	1.576943	0.021405	8.435E-01
B	C(α)-H(α)	2.817E-01	0.000000	3.125E-02	2.897E-01	-3.210E-01	-2.897E-01	-1.034E+00	0.991977	2.425E-02	1.601940	0.020335	8.412E-01
R	O	8.549E-03	0.000000	7.174E-03	-1.457E-03	-5.716E-03	1.457E-03	3.452E-02	0.020005	-1.050E-03	0.015463	-1.218138	2.836E-02
R	O	8.549E-03	0.000000	7.174E-03	-1.457E-03	-5.716E-03	1.457E-03	3.452E-02	0.020005	-1.050E-03	0.015463	-1.218138	2.836E-02
R	O	8.580E-03	0.000000	6.864E-03	-1.339E-03	-5.525E-03	1.339E-03	3.281E-02	0.022060	-1.067E-03	0.037767	-1.783253	2.177E-02
R	O	8.580E-03	0.000000	6.864E-03	-1.339E-03	-5.525E-03	1.339E-03	3.281E-02	0.022060	-1.067E-03	0.037767	-1.783253	2.177E-02
R	O	1.148E-02	0.000000	1.341E-02	-3.603E-03	-9.805E-03	3.603E-03	6.805E-02	0.015407	-1.680E-03	0.094174	-1.173767	6.556E-02
R	O	1.148E-02	0.000000	1.341E-02	-3.603E-03	-9.805E-03	3.603E-03	6.805E-02	0.015407	-1.680E-03	0.094174	-1.173767	6.556E-02
C	K	8.545E-03	0.000000	7.309E-03	-1.533E-03	-5.776E-03	1.533E-03	3.537E-02	0.019249	-1.128E-03	0.017484	-0.721218	3.239E-02

Table S3 (continued)

	C	K	8.545E-03	0.000000	7.309E-03	-1.533E-03	-5.776E-03	1.533E-03	3.537E-02	0.019249	-1.128E-03	0.017484	-0.721218	3.239E-02
	B	C(α)-[C(γ)-C(γ)]	8.609E-03	0.000000	6.315E-03	-1.109E-03	-5.206E-03	1.109E-03	2.969E-02	0.026242	-8.816E-04	0.060965	1.191818	1.242E-02
	B	C(α)-[C(γ)-C(γ)]	8.609E-03	0.000000	6.315E-03	-1.109E-03	-5.206E-03	1.109E-03	2.969E-02	0.026242	-8.816E-04	0.060965	1.191818	1.242E-02
3(+)	A	C(sp3)	1.180E+02	-0.060898	4.867E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.362E+05	1.000000	4.090E+04	-1.000003	0.000002	4.124E+06
	A	C(α)	1.182E+02	0.128222	4.838E+00	1.093E+05	-1.093E+05	-1.093E+05	-4.370E+05	1.000000	1.004E+04	-1.000013	0.000011	6.275E+06
	A	C(β)	1.181E+02	-0.101810	4.888E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	6.532E+03	-1.000011	0.000008	3.687E+06
	A	C(γ)	1.182E+02	0.081553	4.816E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	5.626E+03	-1.000017	0.000015	5.582E+06
	A	C(γ')	1.182E+02	-0.005162	4.755E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.369E+05	1.000000	5.973E+03	-1.000021	0.000020	7.198E+06
	A	C(β')	1.181E+02	-0.033016	4.863E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	8.056E+03	-1.000012	0.000010	4.059E+06
	A	C(α')	1.183E+02	0.091364	4.744E+00	1.093E+05	-1.093E+05	-1.093E+05	-4.372E+05	1.000000	1.731E+04	-1.000024	0.000022	5.500E+06
	A	H(α)	4.179E-01	-0.018240	4.289E-03	4.535E+00	-4.539E+00	-4.535E+00	-1.812E+01	0.999960	2.972E-01	-1.116512	0.001460	2.503E+01
	A	H(β)	4.178E-01	0.011052	4.102E-03	4.533E+00	-4.537E+00	-4.533E+00	-1.812E+01	0.999963	2.021E-01	-1.117148	0.001671	2.491E+01
	A	H(γ)	4.176E-01	-0.011629	3.883E-03	4.529E+00	-4.533E+00	-4.529E+00	-1.810E+01	0.999967	1.758E-01	-1.120057	0.001451	2.453E+01
	A	H(γ')	4.175E-01	-0.000825	3.686E-03	4.526E+00	-4.529E+00	-4.526E+00	-1.809E+01	0.999970	1.859E-01	-1.121662	0.001329	2.433E+01
	A	H(β')	4.171E-01	0.002589	4.051E-03	4.522E+00	-4.526E+00	-4.522E+00	-1.807E+01	0.999963	2.439E-01	-1.118556	0.001702	2.472E+01
	A	H(α')	4.169E-01	-0.013569	4.313E-03	4.505E+00	-4.509E+00	-4.505E+00	-1.800E+01	0.999959	4.436E-01	-1.125574	0.001110	2.381E+01
	A	C(α)*	1.182E+02	0.070050	4.766E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.368E+05	1.000000	1.091E+04	-1.000009	0.000003	2.006E+06
	A	C(β)*	1.182E+02	-0.011900	4.813E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	7.171E+03	-1.000012	0.000010	4.874E+06
	A	C(γ)*	1.182E+02	0.001119	4.819E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	6.099E+03	-1.000011	0.000009	3.521E+06
	A	C(γ)*	1.182E+02	0.001119	4.819E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	6.099E+03	-1.000011	0.000009	3.521E+06
	A	C(β)*	1.182E+02	-0.011900	4.813E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	7.171E+03	-1.000012	0.000010	4.874E+06
	A	C(α)*	1.182E+02	0.070050	4.766E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.368E+05	1.000000	1.091E+04	-1.000009	0.000003	2.006E+06
	A	H(α)*	4.187E-01	-0.002592	4.567E-03	4.552E+00	-4.557E+00	-4.552E+00	-1.819E+01	0.999954	3.124E-01	-1.112689	0.001774	2.559E+01
	A	H(β)*	4.187E-01	0.002449	4.121E-03	4.557E+00	-4.561E+00	-4.557E+00	-1.821E+01	0.999962	2.171E-01	-1.113497	0.001424	2.545E+01
	A	H(γ)*	4.197E-01	-0.000004	4.200E-03	4.564E+00	-4.568E+00	-4.564E+00	-1.824E+01	0.999961	1.929E-01	-1.113631	0.001524	2.541E+01
	A	H(γ)*	4.197E-01	-0.000004	4.200E-03	4.564E+00	-4.568E+00	-4.564E+00	-1.824E+01	0.999961	1.929E-01	-1.113631	0.001524	2.541E+01
	A	H(β)*	4.187E-01	0.002449	4.121E-03	4.557E+00	-4.561E+00	-4.557E+00	-1.821E+01	0.999962	2.171E-01	-1.113497	0.001424	2.545E+01
	A	H(α)*	4.187E-01	-0.002592	4.567E-03	4.552E+00	-4.557E+00	-4.552E+00	-1.819E+01	0.999954	3.124E-01	-1.112689	0.001774	2.559E+01
	B	C(sp3)-C(α)	2.698E-01	-0.002797	5.504E-02	2.431E-01	-2.982E-01	-2.431E-01	-7.523E-01	0.971935	2.959E-02	1.776263	0.033255	8.713E-01
	B	C(α)-C(β)	3.317E-01	-0.003475	9.883E-02	3.605E-01	-4.593E-01	-3.605E-01	-1.047E+00	0.955230	2.675E-02	2.725426	0.204580	1.119E+00
	B	C(β)-C(γ)	3.096E-01	-0.000067	7.927E-02	3.162E-01	-3.954E-01	-3.162E-01	-9.475E-01	0.963503	1.355E-02	2.327507	0.141616	1.036E+00
	B	C(γ)-C(γ')	3.240E-01	-0.003047	8.686E-02	3.421E-01	-4.290E-01	-3.421E-01	-1.021E+00	0.962329	1.394E-02	2.488990	0.150459	1.089E+00
	B	C(β')-C(γ')	3.145E-01	0.001485	8.223E-02	3.245E-01	-4.067E-01	-3.245E-01	-9.690E-01	0.962658	1.574E-02	2.374630	0.152299	1.059E+00
	B	C(α')-C(β')	3.344E-01	-0.002434	1.048E-01	3.668E-01	-4.716E-01	-3.668E-01	-1.048E+00	0.951352	1.948E-02	2.851641	0.264183	1.114E+00
	B	C(sp3)-C(α')	2.721E-01	-0.002332	5.953E-02	2.534E-01	-3.129E-01	-2.534E-01	-7.753E-01	0.968159	1.143E-01	1.842036	0.021846	9.145E-01
	B	C(α)-H(α)	2.839E-01	-0.002027	2.942E-02	2.953E-01	-3.248E-01	-2.953E-01	-1.064E+00	0.993123	1.955E-02	1.609963	0.012887	1.017E+00
	B	C(β)-H(β)	2.842E-01	0.001249	2.876E-02	2.963E-01	-3.250E-01	-2.963E-01	-1.070E+00	0.993409	1.308E-02	1.625874	0.020970	1.022E+00
	B	C(γ)-H(γ)	2.867E-01	-0.001506	2.637E-02	3.022E-01	-3.286E-01	-3.022E-01	-1.103E+00	0.994619	1.166E-02	1.636442	0.008876	1.044E+00
	B	C(γ')-H(γ')	2.880E-01	-0.000102	2.473E-02	3.055E-01	-3.302E-01	-3.055E-01	-1.123E+00	0.995320	1.257E-02	1.644087	0.001010	1.056E+00
	B	C(β')-H(β')	2.851E-01	0.000310	2.785E-02	2.984E-01	-3.262E-01	-2.984E-01	-1.082E+00	0.993863	1.613E-02	1.632463	0.019085	1.034E+00
	B	C(α')-H(α')	2.913E-01	-0.002174	2.500E-02	3.143E-01	-3.393E-01	-3.143E-01	-1.157E+00	0.995416	3.363E-02	1.675157	0.004465	1.048E+00
	B	C(sp3)-C(α)*	2.479E-01	0.007179	5.111E-02	2.101E-01	-2.612E-01	-2.101E-01	-6.359E-01	0.968088	2.745E-02	1.612335	0.045172	7.969E-01
	B	C(α)-C(β)*	3.447E-01	0.000608	1.244E-01	3.916E-01	-5.160E-01	-3.916E-01	-1.069E+00	0.938634	2.187E-02	3.313591	0.417980	1.107E+00
	B	C(β)-C(γ)*	2.876E-01	0.000287	6.264E-02	2.729E-01	-3.356E-01	-2.729E-01	-8.412E-01	0.970573	1.315E-02	2.001452	0.081703	8.959E-01
	B	C(γ)-C(γ)*	3.406E-01	-0.000117	1.187E-01	3.810E-01	-4.997E-01	-3.810E-01	-1.049E+00	0.941692	1.510E-02	3.101194	0.383923	1.082E+00
	B	C(β)-C(γ)*	2.876E-01	0.000287	6.264E-02	2.729E-01	-3.356E-01	-2.729E-01	-8.412E-01	0.970573	1.315E-02	2.001452	0.081703	8.959E-01
	B	C(α)-C(β)*	3.447E-01	0.000608	1.244E-01	3.916E-01	-5.160E-01	-3.916E-01	-1.069E+00	0.938634	2.187E-02	3.313591	0.417980	1.107E+00
	B	C(sp3)-C(α)*	2.479E-01	0.007179	5.111E-02	2.101E-01	-2.612E-01	-2.101E-01	-6.359E-01	0.968088	2.745E-02	1.612335	0.045172	7.969E-01
	B	C(α)-H(α)*	2.807E-01	0.000057	3.159E-02	2.887E-01	-3.203E-01	-2.887E-01	-1.028E+00	0.991703	2.008E-02	1.611056	0.031083	9.892E-01
	B	C(β)-H(β)*	2.814E-01	0.000313	2.968E-02	2.903E-01	-3.200E-01	-2.903E-01	-1.043E+00	0.992732	1.374E-02	1.599306	0.014496	9.772E-01
	B	C(γ)-H(γ)*	2.822E-01	-0.000026	2.995E-02	2.915E-01	-3.214E-01	-2.915E-01	-1.046E+00	0.992666	1.209E-02	1.609970	0.019749	9.746E-01
	B	C(γ)-H(γ)*	2.822E-01	-0.000026	2.995E-02	2.915E-01	-3.214E-01	-2.915E-01	-1.046E+00	0.992666	1.209E-02	1.609970	0.019749	9.746E-01
	B	C(β)-H(β)*	2.814E-01	0.000313	2.968E-02	2.903E-01	-3.200E-01	-2.903E-01	-1.043E+00	0.992732	1.374E-02	1.599306	0.014496	9.772E-01
	B	C(α)-H(α)*	2.807E-01	0.000057	3.159E-02	2.887E-01	-3.203E-01	-2.887E-01	-1.028E+00	0.991703	2.008E-02	1.611056	0.031083	9.892E-01
	R	O	8.393E-03	0.000034	1.042E-02	-3.155E-03	-7.264E-03	3.155E-03	5.430E-02	0.009026	-1.379E-03	0.136422	-1.151433	2.762E-01
	R	O*	1.051E-02	-0.000071	1.233E-02	-3.380E-03	-8.952E-03	3.380E-03	6.285E-02	0.013588	-1.471E-03	0.095966	-1.168198	2.122E-01

Table S3 (continued)

	R	O'*	9.009E-03	-0.000030	8.325E-03	-2.123E-03	-6.202E-03	2.123E-03	4.179E-02	0.017733	-1.121E-03	0.131694	-1.525733	2.034E-01
	R	O'*	9.009E-03	-0.000030	8.325E-03	-2.123E-03	-6.202E-03	2.123E-03	4.179E-02	0.017733	-1.121E-03	0.131694	-1.525733	2.034E-01
	C	K*	7.663E-03	-0.000071	8.118E-03	-1.943E-03	-6.175E-03	1.943E-03	4.024E-02	0.010952	-1.218E-03	0.212055	-0.279564	2.227E-01
	B	H(α')-[C(γ)-C(γ')]*	1.170E-02	-0.000132	8.221E-03	-1.494E-03	-6.727E-03	1.494E-03	3.886E-02	0.042339	-8.468E-04	0.183468	0.945565	1.906E-01
3(-)	A	C(sp3)	1.180E+02	-0.047942	4.847E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.362E+05	1.000000	8.911E+05	-1.000003	0.000003	4.281E+06
	A	C(α)	1.183E+02	0.140162	4.796E+00	1.093E+05	-1.093E+05	-1.093E+05	-4.371E+05	1.000000	1.204E+04	-1.000012	0.000009	1.424E+07
	A	C(β)	1.181E+02	-0.115670	4.867E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.365E+05	1.000000	6.980E+03	-1.000005	0.000002	2.954E+06
	A	C(γ)	1.181E+02	0.144443	4.879E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.365E+05	1.000000	5.559E+03	-1.000007	0.000004	3.554E+06
	A	C(γ)	1.181E+02	-0.142867	4.891E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.365E+05	1.000000	5.569E+03	-1.000006	0.000003	3.864E+06
	A	C(β)	1.181E+02	0.131738	4.866E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.365E+05	1.000000	7.048E+03	-1.000006	0.000003	2.931E+06
	A	C(α)	1.182E+02	-0.087168	4.809E+00	1.093E+05	-1.093E+05	-1.093E+05	-4.370E+05	1.000000	1.235E+04	-1.000009	0.000007	2.468E+07
	A	H(α)	4.258E-01	-0.015585	4.553E-03	4.651E+00	-4.655E+00	-4.651E+00	-1.858E+01	0.999957	3.622E-01	-1.107513	0.001491	2.633E+01
	A	H(β)	4.283E-01	0.011906	4.799E-03	4.698E+00	-4.702E+00	-4.698E+00	-1.877E+01	0.999953	2.234E-01	-1.100291	0.001881	2.776E+01
	A	H(γ)	4.290E-01	-0.017376	4.659E-03	4.707E+00	-4.712E+00	-4.707E+00	-1.881E+01	0.999956	1.818E-01	-1.100951	0.001717	2.764E+01
	A	H(γ)	4.288E-01	0.016465	4.706E-03	4.703E+00	-4.707E+00	-4.703E+00	-1.879E+01	0.999955	1.820E-01	-1.100811	0.001764	2.765E+01
	A	H(β)	4.287E-01	-0.013847	4.743E-03	4.703E+00	-4.708E+00	-4.703E+00	-1.879E+01	0.999954	2.258E-01	-1.100320	0.001826	2.777E+01
	A	H(α)	4.250E-01	0.014265	4.743E-03	4.638E+00	-4.643E+00	-4.638E+00	-1.853E+01	0.999953	3.687E-01	-1.107421	0.001655	2.632E+01
	A	C(α)*	1.181E+02	0.110860	4.858E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	1.218E+04	-1.000004	0.000003	3.221E+06
	A	C(β)*	1.181E+02	-0.063292	4.771E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.365E+05	1.000000	7.006E+03	-1.000008	0.000005	4.188E+06
	A	C(γ)*	1.181E+02	0.037984	4.834E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.363E+05	1.000000	5.562E+03	-1.000003	0.000001	3.266E+06
	A	C(γ)*	1.181E+02	0.037984	4.834E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.363E+05	1.000000	5.562E+03	-1.000003	0.000001	3.266E+06
	A	C(β)*	1.181E+02	-0.063292	4.771E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.365E+05	1.000000	7.006E+03	-1.000008	0.000005	4.188E+06
	A	C(α)*	1.181E+02	0.110860	4.858E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	1.218E+04	-1.000004	0.000003	3.221E+06
	A	H(α)*	4.283E-01	-0.014952	5.500E-03	4.683E+00	-4.689E+00	-4.683E+00	-1.871E+01	0.999939	3.674E-01	-1.099945	0.002097	2.776E+01
	A	H(β)*	4.311E-01	0.005533	4.768E-03	4.739E+00	-4.744E+00	-4.739E+00	-1.894E+01	0.999954	2.264E-01	-1.097524	0.001771	2.841E+01
	A	H(γ)*	4.302E-01	-0.005820	5.120E-03	4.724E+00	-4.729E+00	-4.724E+00	-1.888E+01	0.999947	1.826E-01	-1.096393	0.001999	2.859E+01
	A	H(γ)*	4.302E-01	-0.005820	5.120E-03	4.724E+00	-4.729E+00	-4.724E+00	-1.888E+01	0.999947	1.826E-01	-1.096393	0.001999	2.859E+01
	A	H(β)*	4.311E-01	0.005533	4.768E-03	4.739E+00	-4.744E+00	-4.739E+00	-1.894E+01	0.999954	2.264E-01	-1.097524	0.001771	2.841E+01
	A	H(α)*	4.283E-01	-0.014952	5.500E-03	4.683E+00	-4.689E+00	-4.683E+00	-1.871E+01	0.999939	3.674E-01	-1.099945	0.002097	2.776E+01
	B	C(sp3)-C(α)	2.643E-01	-0.001504	5.626E-02	2.378E-01	-2.941E-01	-2.378E-01	-7.263E-01	0.968747	4.164E-02	1.751492	0.033920	5.291E-01
	B	C(α)-C(β)	3.400E-01	-0.000769	1.172E-01	3.811E-01	-4.983E-01	-3.811E-01	-1.056E+00	0.942820	2.183E-02	3.143260	0.371302	8.110E-01
	B	C(β)-C(γ)	2.903E-01	0.000410	7.093E-02	2.785E-01	-3.494E-01	-2.785E-01	-8.303E-01	0.963888	1.217E-02	2.077554	0.162732	6.390E-01
	B	C(γ)-C(γ)	3.412E-01	-0.000333	1.106E-01	3.830E-01	-4.936E-01	-3.830E-01	-1.090E+00	0.949468	1.423E-02	3.155981	0.312975	8.198E-01
	B	C(β)-C(γ)	2.879E-01	-0.001189	6.891E-02	2.743E-01	-3.432E-01	-2.743E-01	-8.217E-01	0.964897	1.199E-02	2.051172	0.152130	6.328E-01
	B	C(α)-C(β)	3.380E-01	0.000529	1.137E-01	3.772E-01	-4.909E-01	-3.772E-01	-1.054E+00	0.945079	2.222E-02	3.095427	0.343752	8.029E-01
	B	C(sp3)-C(α)	2.654E-01	0.004416	5.700E-02	2.383E-01	-2.953E-01	-2.383E-01	-7.253E-01	0.968251	4.329E-02	1.752576	0.045224	5.235E-01
	B	C(α)-H(α)	2.798E-01	-0.000692	3.367E-02	2.854E-01	-3.191E-01	-2.854E-01	-1.007E+00	0.990547	2.238E-02	1.573940	0.015007	6.941E-01
	B	C(β)-H(β)	2.733E-01	0.000109	3.860E-02	2.740E-01	-3.126E-01	-2.740E-01	-9.415E-01	0.986578	1.240E-02	1.559052	0.038392	7.070E-01
	B	C(γ)-H(γ)	2.745E-01	-0.000251	3.777E-02	2.759E-01	-3.137E-01	-2.759E-01	-9.526E-01	0.987365	1.009E-02	1.560101	0.031635	7.214E-01
	B	C(γ)-H(γ)	2.742E-01	0.000199	3.822E-02	2.755E-01	-3.138E-01	-2.755E-01	-9.493E-01	0.987015	1.008E-02	1.563257	0.035180	7.202E-01
	B	C(β)-H(β)	2.736E-01	-0.000158	3.827E-02	2.743E-01	-3.125E-01	-2.743E-01	-9.440E-01	0.986858	1.255E-02	1.555103	0.034738	7.059E-01
	B	C(α)-H(α)	2.793E-01	0.000816	3.474E-02	2.845E-01	-3.193E-01	-2.845E-01	-9.992E-01	0.989862	2.273E-02	1.578771	0.023715	6.878E-01
	B	C(sp3)-C(α)*	2.628E-01	-0.001472	5.673E-02	2.319E-01	-2.886E-01	-2.319E-01	-7.007E-01	0.967580	3.865E-02	1.725264	0.062358	4.945E-01
	B	C(α)-C(β)*	3.301E-01	-0.000479	1.107E-01	3.605E-01	-4.711E-01	-3.605E-01	-9.992E-01	0.943661	2.083E-02	2.955233	0.380984	7.369E-01
	B	C(β)-C(γ)*	2.940E-01	-0.000878	7.991E-02	2.866E-01	-3.665E-01	-2.866E-01	-8.269E-01	0.956170	1.202E-02	2.180548	0.241908	5.971E-01
	B	C(γ)-C(γ)*	3.278E-01	-0.000115	1.034E-01	3.545E-01	-4.579E-01	-3.545E-01	-1.005E+00	0.949317	1.313E-02	2.873276	0.332837	7.048E-01
	B	C(β)-C(γ)*	2.940E-01	-0.000878	7.991E-02	2.866E-01	-3.665E-01	-2.866E-01	-8.269E-01	0.956170	1.202E-02	2.180548	0.241908	5.971E-01
	B	C(α)-C(β)*	3.301E-01	-0.000479	1.107E-01	3.605E-01	-4.711E-01	-3.605E-01	-9.992E-01	0.943661	2.083E-02	2.955232	0.380984	7.369E-01
	B	C(sp3)-C(α)*	2.628E-01	-0.001472	5.673E-02	2.319E-01	-2.886E-01	-2.319E-01	-7.007E-01	0.967580	3.865E-02	1.725265	0.062358	4.945E-01
	B	C(α)-H(α)*	2.731E-01	-0.000020	4.283E-02	2.749E-01	-3.177E-01	-2.749E-01	-9.282E-01	0.983505	2.098E-02	1.581381	0.058500	6.668E-01
	B	C(β)-H(β)*	2.717E-01	-0.000141	3.938E-02	2.719E-01	-3.112E-01	-2.719E-01	-9.300E-01	0.985723	1.232E-02	1.552327	0.029910	6.661E-01
	B	C(γ)-H(γ)*	2.699E-01	0.000097	4.250E-02	2.698E-01	-3.123E-01	-2.698E-01	-9.094E-01	0.983047	9.670E-03	1.571434	0.053870	6.601E-01
	B	C(γ)-H(γ)*	2.699E-01	0.000097	4.250E-02	2.698E-01	-3.123E-01	-2.698E-01	-9.094E-01	0.983047	9.670E-03	1.571435	0.053870	6.601E-01
	B	C(β)-H(β)*	2.717E-01	-0.000141	3.938E-02	2.719E-01	-3.112E-01	-2.719E-01	-9.300E-01	0.985723	1.232E-02	1.552327	0.029910	6.661E-01
	B	C(α)-H(α)*	2.731E-01	-0.000020	4.283E-02	2.749E-01	-3.177E-01	-2.749E-01	-9.282E-01	0.983505	2.098E-02	1.581381	0.058500	6.668E-01
	R	O	8.216E-03	-0.000010	1.018E-02	-3.091E-03	-7.086E-03	3.091E-03	5.307E-02	0.008812	-1.276E-03	0.126818	-1.147377	-6.803E-02

Table S3 (continued)

	R	O*	7.991E-03	-0.000016	9.952E-03	-3.059E-03	-6.894E-03	3.059E-03	5.204E-02	0.008404	-1.258E-03	0.115806	-1.138723	-1.195E-01
5	A	C(sp3)	1.179E+02	0.000000	4.847E+00	1.089E+05	-1.090E+05	-1.089E+05	-4.358E+05	1.000000	2.130E+04	-1.000007	0.000006	1.221E+06
	A	C(α)	1.181E+02	0.000000	4.841E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.365E+05	1.000000	2.240E+04	-1.000011	0.000004	2.385E+06
	A	C(α)	1.181E+02	0.000000	4.841E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.365E+05	1.000000	2.240E+04	-1.000011	0.000004	2.385E+06
	A	H(α)	4.098E-01	0.000000	4.255E-03	4.466E+00	-4.470E+00	-4.466E+00	-1.785E+01	0.999957	4.005E-01	-1.117409	0.000479	2.479E+01
	A	H(α)	4.098E-01	0.000000	4.255E-03	4.466E+00	-4.470E+00	-4.466E+00	-1.785E+01	0.999957	4.005E-01	-1.117409	0.000479	2.479E+01
	A	H(sp3)	4.298E-01	0.000000	4.784E-03	4.721E+00	-4.726E+00	-4.721E+00	-1.886E+01	0.999953	4.652E-01	-1.102546	0.001316	2.752E+01
	A	H(sp3)	4.298E-01	0.000000	4.784E-03	4.721E+00	-4.726E+00	-4.721E+00	-1.886E+01	0.999953	4.652E-01	-1.102546	0.001316	2.752E+01
	B	C(sp3)-C(α)	2.373E-01	0.000000	9.605E-02	1.998E-01	-2.959E-01	-1.998E-01	-4.151E-01	0.880865	3.977E-02	1.490746	0.533267	7.269E-01
	B	C(α)-C(α')	3.526E-01	0.000000	1.815E-01	4.279E-01	-6.094E-01	-4.279E-01	-9.855E-01	0.885718	7.140E-02	3.552362	0.301626	1.079E+00
	B	C(sp3)-C(α)	2.373E-01	0.000000	9.605E-02	1.998E-01	-2.959E-01	-1.998E-01	-4.151E-01	0.880865	3.977E-02	1.490746	0.533267	7.269E-01
	B	C(α)-H(α)	2.794E-01	0.000000	2.704E-02	2.937E-01	-3.207E-01	-2.937E-01	-1.066E+00	0.993819	2.953E-02	1.656399	0.001303	9.005E-01
	B	C(α)-H(α)	2.794E-01	0.000000	2.704E-02	2.937E-01	-3.207E-01	-2.937E-01	-1.066E+00	0.993819	2.953E-02	1.656399	0.001303	9.005E-01
	B	C(sp3)-H(sp3)	2.772E-01	0.000000	3.530E-02	2.792E-01	-3.145E-01	-2.792E-01	-9.754E-01	0.989220	3.004E-02	1.555031	0.036340	8.169E-01
	B	C(sp3)-H(sp3)	2.772E-01	0.000000	3.530E-02	2.792E-01	-3.145E-01	-2.792E-01	-9.754E-01	0.989220	3.004E-02	1.555031	0.036340	8.169E-01
	R	O	2.120E-01	0.000000	1.838E-01	1.448E-01	-3.286E-01	-1.448E-01	1.560E-01	0.580890	-7.814E-02	1.145341	-2.618769	7.233E-01
5(-)	A	C(sp3)	1.179E+02	-0.020350	4.822E+00	1.089E+05	-1.089E+05	-1.089E+05	-4.357E+05	1.000000	2.224E+04	-1.000012	0.000001	1.042E+07
	A	C(α)	1.182E+02	0.165576	4.605E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	2.092E+04	-1.000011	0.000006	7.507E+05
	A	C(α)	1.182E+02	0.165576	4.605E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	2.092E+04	-1.000011	0.000006	7.507E+05
	A	H(sp3)	4.299E-01	-0.003599	5.417E-03	4.761E+00	-4.767E+00	-4.761E+00	-1.902E+01	0.999941	4.697E-01	-1.087220	0.001442	3.128E+01
	A	H(sp3)	4.299E-01	-0.003599	5.417E-03	4.761E+00	-4.767E+00	-4.761E+00	-1.902E+01	0.999941	4.697E-01	-1.087220	0.001442	3.128E+01
	A	H(α)	4.187E-01	0.017222	6.094E-03	4.631E+00	-4.637E+00	-4.631E+00	-1.850E+01	0.999920	4.341E-01	-1.087765	0.000868	3.085E+01
	A	H(α)	4.187E-01	0.017222	6.094E-03	4.631E+00	-4.637E+00	-4.631E+00	-1.850E+01	0.999920	4.341E-01	-1.087765	0.000868	3.085E+01
	B	C(sp3)-C(α)	2.331E-01	0.000294	9.298E-02	1.968E-01	-2.898E-01	-1.968E-01	-4.154E-01	0.881523	3.927E-02	1.542674	0.506354	4.477E-01
	B	C(α)-C(α')	2.726E-01	0.009099	1.153E-01	2.649E-01	-3.802E-01	-2.649E-01	-5.985E-01	0.890928	4.310E-02	1.698900	0.079878	5.486E-01
	B	C(sp3)-C(α)	2.331E-01	0.000294	9.298E-02	1.968E-01	-2.898E-01	-1.968E-01	-4.154E-01	0.881524	3.927E-02	1.542676	0.506351	4.477E-01
	B	C(α)-H(α)	2.544E-01	0.002213	4.651E-02	2.450E-01	-2.916E-01	-2.450E-01	-7.942E-01	0.975680	2.354E-02	1.467786	0.048943	5.813E-01
	B	C(α)-H(α)	2.544E-01	0.002213	4.651E-02	2.450E-01	-2.916E-01	-2.450E-01	-7.942E-01	0.975680	2.354E-02	1.467792	0.048943	5.813E-01
	B	C(sp3)-H(sp3)	2.591E-01	0.000864	4.407E-02	2.499E-01	-2.940E-01	-2.499E-01	-8.232E-01	0.979183	2.599E-02	1.485811	0.062197	5.807E-01
	B	C(sp3)-H(sp3)	2.591E-01	0.000864	4.407E-02	2.499E-01	-2.940E-01	-2.499E-01	-8.232E-01	0.979183	2.599E-02	1.485811	0.062197	5.807E-01
	R	O	2.017E-01	0.004479	1.607E-01	1.306E-01	-2.913E-01	-1.306E-01	1.202E-01	0.606115	-1.864E-01	1.237649	-2.762696	3.759E-01
4	A	C(sp3)	1.180E+02	0.000000	4.949E+00	1.090E+05	-1.091E+05	-1.090E+05	-4.362E+05	1.000000	1.503E+04	-1.000003	0.000002	4.158E+07
	A	C(α)	1.182E+02	0.000000	4.796E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	1.516E+04	-1.000009	0.000007	3.520E+06
	A	C(β)	1.182E+02	0.000000	4.803E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	1.486E+04	-1.000010	0.000007	3.279E+06
	A	C(β)	1.182E+02	0.000000	4.803E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	1.486E+04	-1.000010	0.000007	3.279E+06
	A	C(α)	1.182E+02	0.000000	4.796E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.367E+05	1.000000	1.516E+04	-1.000009	0.000007	3.520E+06
	A	H(α)	4.204E-01	0.000000	4.397E-03	4.582E+00	-4.587E+00	-4.582E+00	-1.831E+01	0.999958	3.384E-01	-1.109618	0.001115	2.589E+01
	A	H(β)	4.216E-01	0.000000	4.200E-03	4.600E+00	-4.604E+00	-4.600E+00	-1.838E+01	0.999962	3.359E-01	-1.109316	0.001038	2.596E+01
	A	H(β)	4.216E-01	0.000000	4.200E-03	4.600E+00	-4.604E+00	-4.600E+00	-1.838E+01	0.999962	3.359E-01	-1.109316	0.001038	2.596E+01
	A	H(α)	4.204E-01	0.000000	4.397E-03	4.582E+00	-4.587E+00	-4.582E+00	-1.831E+01	0.999958	3.384E-01	-1.109618	0.001115	2.589E+01
	A	H(sp3)	4.148E-01	0.000000	4.750E-03	4.542E+00	-4.547E+00	-4.542E+00	-1.815E+01	0.999948	3.709E-01	-1.100720	0.000289	2.756E+01
	A	H(sp3)	4.148E-01	0.000000	4.750E-03	4.542E+00	-4.547E+00	-4.542E+00	-1.815E+01	0.999948	3.709E-01	-1.100720	0.000289	2.756E+01
	B	C(sp3)-C(α)	2.645E-01	0.000000	5.614E-02	2.342E-01	-2.903E-01	-2.342E-01	-7.122E-01	0.968826	3.092E-02	1.718934	0.049663	6.613E-01
	B	C(α)-C(β)	3.452E-01	0.000000	1.275E-01	3.921E-01	-5.196E-01	-3.921E-01	-1.059E+00	0.936077	4.298E-02	3.249776	0.428544	9.453E-01
	B	C(β)-C(β')	2.789E-01	0.000000	6.354E-02	2.585E-01	-3.220E-01	-2.585E-01	-7.797E-01	0.966583	3.230E-02	1.886245	0.106966	7.153E-01
	B	C(α)-C(β)	3.452E-01	0.000000	1.275E-01	3.921E-01	-5.196E-01	-3.921E-01	-1.059E+00	0.936077	4.298E-02	3.249776	0.428544	9.453E-01
	B	C(sp3)-C(α)	2.645E-01	0.000000	5.614E-02	2.342E-01	-2.903E-01	-2.342E-01	-7.122E-01	0.968826	3.092E-02	1.718934	0.049663	6.613E-01
	B	C(α)-H(α)	2.790E-01	0.000000	3.165E-02	2.857E-01	-3.174E-01	-2.857E-01	-1.016E+00	0.991502	2.245E-02	1.605352	0.018477	8.559E-01
	B	C(β)-H(β)	2.794E-01	0.000000	3.065E-02	2.860E-01	-3.166E-01	-2.860E-01	-1.021E+00	0.992068	2.227E-02	1.601809	0.014334	8.551E-01
	B	C(β)-H(β)	2.794E-01	0.000000	3.065E-02	2.860E-01	-3.166E-01	-2.860E-01	-1.021E+00	0.992068	2.227E-02	1.601809	0.014334	8.551E-01
	B	C(α)-H(α)	2.790E-01	0.000000	3.165E-02	2.857E-01	-3.174E-01	-2.857E-01	-1.016E+00	0.991502	2.245E-02	1.605352	0.018477	8.559E-01
	B	C(sp3)-H(sp3)	2.671E-01	0.000000	3.642E-02	2.632E-01	-2.996E-01	-2.632E-01	-9.072E-01	0.987047	2.206E-02	1.483723	0.013232	8.290E-01
	B	C(sp3)-H(sp3)	2.671E-01	0.000000	3.642E-02	2.632E-01	-2.996E-01	-2.632E-01	-9.072E-01	0.987047	2.206E-02	1.483723	0.013232	8.290E-01
	R	O	4.322E-02	0.000000	7.226E-02	-8.770E-03	-6.349E-02	8.770E-03	3.241E-01	0.042821	-5.547E-01	0.221374	-1.228421	2.286E-01
4(+)	A	C(sp3)	1.180E+02	-0.040121	5.045E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.362E+05	1.000000	1.479E+04	-1.000006	0.000005	2.363E+06
	A	C(α)	1.183E+02	0.110846	4.767E+00	1.093E+05	-1.093E+05	-1.093E+05	-4.370E+05	1.000000	1.533E+04	-1.000021	0.000019	7.447E+06

Table S3 (continued)

	A	C(β)	1.182E+02	-0.023342	4.797E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.369E+05	1.000000	1.481E+04	-1.000019	0.000017	5.849E+06
	A	C(β)	1.182E+02	-0.023342	4.797E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.369E+05	1.000000	1.481E+04	-1.000019	0.000017	5.849E+06
	A	C(α)	1.183E+02	0.110846	4.767E+00	1.093E+05	-1.093E+05	-1.093E+05	-4.370E+05	1.000000	1.533E+04	-1.000021	0.000019	7.447E+06
	A	H(α)	4.079E-01	-0.016975	3.594E-03	4.408E+00	-4.411E+00	-4.408E+00	-1.762E+01	0.999969	3.274E-01	-1.126506	0.000687	2.360E+01
	A	H(β)	4.081E-01	0.000890	3.420E-03	4.406E+00	-4.409E+00	-4.406E+00	-1.761E+01	0.999972	3.214E-01	-1.126607	0.000770	2.355E+01
	A	H(β)	4.081E-01	0.000890	3.420E-03	4.406E+00	-4.409E+00	-4.406E+00	-1.761E+01	0.999972	3.214E-01	-1.126607	0.000770	2.355E+01
	A	H(α)	4.079E-01	-0.016975	3.594E-03	4.408E+00	-4.411E+00	-4.408E+00	-1.762E+01	0.999969	3.274E-01	-1.126506	0.000687	2.360E+01
	A	H(sp3)	3.996E-01	0.007167	4.352E-03	4.345E+00	-4.349E+00	-4.345E+00	-1.736E+01	0.999951	3.512E-01	-1.111193	0.000565	2.569E+01
	A	H(sp3)	3.996E-01	0.007167	4.352E-03	4.345E+00	-4.349E+00	-4.345E+00	-1.736E+01	0.999951	3.512E-01	-1.111193	0.000565	2.569E+01
	B	C(sp3)-C(α)	2.734E-01	-0.003110	6.047E-02	2.533E-01	-3.137E-01	-2.533E-01	-7.712E-01	0.967719	3.329E-02	1.824568	0.037917	9.492E-01
	B	C(α)-C(β)	3.242E-01	-0.003840	9.157E-02	3.416E-01	-4.332E-01	-3.416E-01	-1.000E+00	0.958397	4.158E-02	2.416810	0.168180	1.110E+00
	B	C(β)-C(β')	3.194E-01	0.001807	8.715E-02	3.318E-01	-4.190E-01	-3.318E-01	-9.787E-01	0.960267	3.974E-02	2.338751	0.162384	1.092E+00
	B	C(α)-C(β)	3.242E-01	-0.003840	9.157E-02	3.416E-01	-4.332E-01	-3.416E-01	-1.000E+00	0.958397	4.158E-02	2.416810	0.168180	1.110E+00
	B	C(sp3)-C(α)	2.734E-01	-0.003110	6.047E-02	2.533E-01	-3.137E-01	-2.533E-01	-7.712E-01	0.967719	3.329E-02	1.824568	0.037917	9.492E-01
	B	C(α)-H(α)	2.864E-01	-0.003062	2.229E-02	3.075E-01	-3.297E-01	-3.075E-01	-1.141E+00	0.996154	2.491E-02	1.678456	0.001235	1.106E+00
	B	C(β)-H(β)	2.865E-01	0.000147	2.146E-02	3.073E-01	-3.287E-01	-3.073E-01	-1.143E+00	0.996408	2.446E-02	1.682117	0.000476	1.105E+00
	B	C(β)-H(β)	2.865E-01	0.000147	2.146E-02	3.073E-01	-3.287E-01	-3.073E-01	-1.143E+00	0.996408	2.446E-02	1.682117	0.000476	1.105E+00
	B	C(α)-H(α)	2.864E-01	-0.003062	2.229E-02	3.075E-01	-3.297E-01	-3.075E-01	-1.141E+00	0.996154	2.491E-02	1.678456	0.001235	1.106E+00
	B	C(sp3)-H(sp3)	2.682E-01	0.001307	3.057E-02	2.681E-01	-2.987E-01	-2.681E-01	-9.503E-01	0.990971	2.262E-02	1.517473	0.022260	1.049E+00
	B	C(sp3)-H(sp3)	2.682E-01	0.001307	3.057E-02	2.681E-01	-2.987E-01	-2.681E-01	-9.503E-01	0.990971	2.262E-02	1.517473	0.022260	1.049E+00
	R	O	4.412E-02	0.000035	7.474E-02	-8.866E-03	-6.588E-02	8.866E-03	3.344E-01	0.042860	-6.629E-01	0.218227	-1.245753	4.925E-01
4(-)	A	C(sp3)	1.180E+02	-0.072742	4.772E+00	1.090E+05	-1.090E+05	-1.090E+05	-4.361E+05	1.000000	1.480E+04	-1.000004	0.000003	3.048E+06
	A	C(α)	1.180E+02	0.151224	4.847E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.362E+05	1.000000	1.500E+04	-1.000010	0.000003	2.224E+06
	A	C(β)	1.181E+02	-0.030409	4.773E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.364E+05	1.000000	1.479E+04	-1.000004	0.000001	2.428E+06
	A	C(β)	1.181E+02	-0.030409	4.773E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.364E+05	1.000000	1.479E+04	-1.000004	0.000001	2.428E+06
	A	C(α)	1.180E+02	0.151224	4.847E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.362E+05	1.000000	1.500E+04	-1.000010	0.000003	2.224E+06
	A	H(α)	4.241E-01	-0.014010	5.832E-03	4.658E+00	-4.664E+00	-4.658E+00	-1.861E+01	0.999929	3.433E-01	-1.093409	0.001860	2.916E+01
	A	H(β)	4.269E-01	0.001007	5.014E-03	4.695E+00	-4.700E+00	-4.695E+00	-1.876E+01	0.999948	3.408E-01	-1.094828	0.001411	2.883E+01
	A	H(β)	4.269E-01	0.001007	5.014E-03	4.695E+00	-4.700E+00	-4.695E+00	-1.876E+01	0.999948	3.408E-01	-1.094828	0.001411	2.883E+01
	A	H(α)	4.241E-01	-0.014010	5.832E-03	4.658E+00	-4.664E+00	-4.658E+00	-1.861E+01	0.999929	3.433E-01	-1.093409	0.001860	2.916E+01
	A	H(sp3)	4.212E-01	0.039362	5.181E-03	4.686E+00	-4.691E+00	-4.686E+00	-1.872E+01	0.999947	3.826E-01	-1.081540	0.000118	3.307E+01
	A	H(sp3)	4.270E-01	0.029828	5.011E-03	4.735E+00	-4.740E+00	-4.735E+00	-1.892E+01	0.999950	3.682E-01	-1.085962	0.000180	3.152E+01
	B	C(sp3)-C(α)	2.550E-01	-0.000538	5.847E-02	2.211E-01	-2.796E-01	-2.211E-01	-6.506E-01	0.962177	2.768E-02	1.700316	0.102214	4.120E-01
	B	C(α)-C(β)	3.070E-01	-0.000109	9.750E-02	3.138E-01	-4.113E-01	-3.138E-01	-8.651E-01	0.944283	3.528E-02	2.439856	0.347512	5.874E-01
	B	C(β)-C(β')	3.045E-01	-0.001030	9.303E-02	3.074E-01	-4.004E-01	-3.074E-01	-8.575E-01	0.947615	3.458E-02	2.326000	0.304758	5.765E-01
	B	C(α)-C(β)	3.070E-01	-0.000109	9.750E-02	3.138E-01	-4.113E-01	-3.138E-01	-8.651E-01	0.944283	3.528E-02	2.439855	0.347512	5.874E-01
	B	C(sp3)-C(α)	2.550E-01	-0.000538	5.847E-02	2.211E-01	-2.796E-01	-2.211E-01	-6.506E-01	0.962177	2.768E-02	1.700316	0.102214	4.120E-01
	B	C(α)-H(α)	2.635E-01	0.000684	4.682E-02	2.611E-01	-3.079E-01	-2.611E-01	-8.570E-01	0.977918	1.919E-02	1.577469	0.089038	6.294E-01
	B	C(β)-H(β)	2.666E-01	-0.000033	4.080E-02	2.650E-01	-3.058E-01	-2.650E-01	-8.966E-01	0.983702	1.972E-02	1.564704	0.041114	6.365E-01
	B	C(β)-H(β)	2.666E-01	-0.000033	4.080E-02	2.650E-01	-3.058E-01	-2.650E-01	-8.966E-01	0.983702	1.972E-02	1.564704	0.041114	6.365E-01
	B	C(α)-H(α)	2.635E-01	0.000684	4.682E-02	2.611E-01	-3.079E-01	-2.611E-01	-8.570E-01	0.977918	1.919E-02	1.577469	0.089038	6.294E-01
	B	C(sp3)-H(sp3)	2.482E-01	0.001191	4.128E-02	2.281E-01	-2.694E-01	-2.281E-01	-7.473E-01	0.979329	1.836E-02	1.331832	0.001695	5.648E-01
	B	C(sp3)-H(sp3)	2.565E-01	0.002971	4.107E-02	2.436E-01	-2.847E-01	-2.436E-01	-8.102E-01	0.981448	1.902E-02	1.403386	0.000616	5.873E-01
	R	O	4.074E-02	0.000071	6.634E-02	-8.867E-03	-5.747E-02	8.867E-03	3.008E-01	0.041747	-6.641E-01	0.222914	-1.223164	-2.002E-02
6	A	C(sp3)	1.180E+02	0.000000	4.948E+00	1.090E+05	-1.090E+05	-1.090E+05	-4.361E+05	1.000000	1.192E+04	-1.000003	0.000000	4.142E+06
	A	C(α)	1.182E+02	0.000000	4.749E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.368E+05	1.000000	1.167E+04	-1.000011	0.000009	3.553E+06
	A	C(β)	1.181E+02	0.000000	4.826E+00	1.091E+05	-1.092E+05	-1.091E+05	-4.366E+05	1.000000	1.151E+04	-1.000009	0.000006	3.421E+06
	A	C(γ)	1.181E+02	0.000000	4.792E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	1.154E+04	-1.000010	0.000008	4.595E+06
	A	C(γ)	1.181E+02	0.000000	4.792E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	1.154E+04	-1.000010	0.000008	4.595E+06
	A	C(β)	1.181E+02	0.000000	4.826E+00	1.091E+05	-1.092E+05	-1.091E+05	-4.366E+05	1.000000	1.151E+04	-1.000009	0.000006	3.421E+06
	A	C(α)	1.182E+02	0.000000	4.749E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.368E+05	1.000000	1.167E+04	-1.000011	0.000009	3.553E+06
	A	H(α)	4.236E-01	0.000000	4.437E-03	4.625E+00	-4.629E+00	-4.625E+00	-1.848E+01	0.999958	2.982E-01	-1.108029	0.001456	2.629E+01
	A	H(β)	4.230E-01	0.000000	4.391E-03	4.622E+00	-4.626E+00	-4.622E+00	-1.847E+01	0.999959	2.941E-01	-1.106916	0.001483	2.648E+01
	A	H(γ)	4.247E-01	0.000000	4.397E-03	4.639E+00	-4.644E+00	-4.639E+00	-1.854E+01	0.999959	2.938E-01	-1.107342	0.001525	2.644E+01
	A	H(γ)	4.247E-01	0.000000	4.397E-03	4.639E+00	-4.644E+00	-4.639E+00	-1.854E+01	0.999959	2.938E-01	-1.107342	0.001525	2.644E+01
	A	H(β)	4.230E-01	0.000000	4.391E-03	4.622E+00	-4.626E+00	-4.622E+00	-1.847E+01	0.999959	2.941E-01	-1.106916	0.001483	2.648E+01

Table S3 (continued)

	A	H(α)	4.236E-01	0.000000	4.437E-03	4.625E+00	-4.629E+00	-4.625E+00	-1.848E+01	0.999958	2.982E-01	-1.108029	0.001456	2.629E+01
	A	H(sp3;eq)	4.273E-01	0.000000	4.611E-03	4.669E+00	-4.674E+00	-4.669E+00	-1.866E+01	0.999956	3.028E-01	-1.102106	0.000504	2.727E+01
	A	H(sp3;ax)	4.196E-01	0.000000	4.803E-03	4.581E+00	-4.585E+00	-4.581E+00	-1.830E+01	0.999949	4.154E-01	-1.102633	0.000601	2.725E+01
	B	C(sp3)-C(α)	2.632E-01	0.000000	5.402E-02	2.327E-01	-2.867E-01	-2.327E-01	-7.148E-01	0.970575	2.201E-02	1.724157	0.034233	6.696E-01
	B	C(α)-C(β)	3.455E-01	0.000000	1.242E-01	3.925E-01	-5.167E-01	-3.925E-01	-1.073E+00	0.939254	3.162E-02	3.313793	0.422587	9.543E-01
	B	C(β)-C(γ)	2.865E-01	0.000000	6.329E-02	2.709E-01	-3.342E-01	-2.709E-01	-8.306E-01	0.969593	2.473E-02	1.999780	0.097804	7.490E-01
	B	C(γ)-C(γ')	3.380E-01	0.000000	1.176E-01	3.755E-01	-4.931E-01	-3.755E-01	-1.032E+00	0.941292	3.036E-02	3.042657	0.391929	9.368E-01
	B	C(β)-C(γ)	2.865E-01	0.000000	6.329E-02	2.709E-01	-3.342E-01	-2.709E-01	-8.306E-01	0.969593	2.473E-02	1.999780	0.097804	7.490E-01
	B	C(α)-C(β)	3.455E-01	0.000000	1.242E-01	3.925E-01	-5.167E-01	-3.925E-01	-1.073E+00	0.939254	3.162E-02	3.313793	0.422587	9.543E-01
	B	C(sp3)-C(α)	2.632E-01	0.000000	5.402E-02	2.327E-01	-2.867E-01	-2.327E-01	-7.148E-01	0.970575	2.201E-02	1.724157	0.034233	6.696E-01
	B	C(sp3)-H(sp3;eq)	2.757E-01	0.000000	3.670E-02	2.770E-01	-3.137E-01	-2.770E-01	-9.612E-01	0.988159	1.829E-02	1.536623	0.009868	8.282E-01
	B	C(sp3)-H(sp3;ax)	2.719E-01	0.000000	3.571E-02	2.699E-01	-3.056E-01	-2.699E-01	-9.367E-01	0.988260	2.362E-02	1.493540	0.005828	8.124E-01
	B	C(α)-H(α)	2.791E-01	0.000000	3.244E-02	2.847E-01	-3.171E-01	-2.847E-01	-1.009E+00	0.991089	1.894E-02	1.586520	0.019469	8.466E-01
	B	C(β)-H(β)	2.775E-01	0.000000	3.334E-02	2.819E-01	-3.152E-01	-2.819E-01	-9.941E-01	0.990415	1.842E-02	1.579252	0.022787	8.414E-01
	B	C(γ)-H(γ)	2.789E-01	0.000000	3.299E-02	2.841E-01	-3.170E-01	-2.841E-01	-1.004E+00	0.990765	1.853E-02	1.580682	0.020405	8.424E-01
	B	C(γ)-H(γ)	2.789E-01	0.000000	3.299E-02	2.841E-01	-3.170E-01	-2.841E-01	-1.004E+00	0.990765	1.853E-02	1.580682	0.020405	8.424E-01
	B	C(β)-H(β)	2.775E-01	0.000000	3.334E-02	2.819E-01	-3.152E-01	-2.819E-01	-9.941E-01	0.990415	1.842E-02	1.579252	0.022787	8.414E-01
	B	C(α)-H(α)	2.791E-01	0.000000	3.244E-02	2.847E-01	-3.171E-01	-2.847E-01	-1.009E+00	0.991089	1.894E-02	1.586520	0.019469	8.466E-01
	R	O	1.117E-02	0.000000	1.362E-02	-3.800E-03	-9.824E-03	3.800E-03	6.969E-02	0.013610	-1.475E-02	0.051602	-1.070612	7.237E-02
6(+)	A	C(sp3)	1.180E+02	-0.059795	5.021E+00	1.090E+05	-1.090E+05	-1.090E+05	-4.361E+05	1.000000	1.110E+04	-1.000004	0.000003	2.691E+06
	A	C(α)	1.182E+02	0.112502	4.809E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.368E+05	1.000000	1.144E+04	-1.000016	0.000015	5.528E+06
	A	C(β)	1.181E+02	-0.074695	4.869E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	1.115E+04	-1.000012	0.000010	3.426E+06
	A	C(γ)	1.182E+02	0.040746	4.771E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.368E+05	1.000000	1.112E+04	-1.000020	0.000018	5.556E+06
	A	C(γ)	1.182E+02	0.040746	4.771E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.368E+05	1.000000	1.112E+04	-1.000020	0.000018	5.556E+06
	A	C(β)	1.181E+02	-0.074695	4.869E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.366E+05	1.000000	1.115E+04	-1.000012	0.000010	3.426E+06
	A	C(α)	1.182E+02	0.112502	4.809E+00	1.092E+05	-1.092E+05	-1.092E+05	-4.368E+05	1.000000	1.144E+04	-1.000016	0.000015	5.528E+06
	A	H(α)	4.175E-01	-0.016740	3.994E-03	4.534E+00	-4.538E+00	-4.534E+00	-1.812E+01	0.999965	2.850E-01	-1.118971	0.001347	2.472E+01
	A	H(β)	4.165E-01	0.007853	4.007E-03	4.513E+00	-4.517E+00	-4.513E+00	-1.804E+01	0.999964	2.796E-01	-1.119295	0.001632	2.460E+01
	A	H(γ)	4.167E-01	-0.006541	3.732E-03	4.515E+00	-4.519E+00	-4.515E+00	-1.804E+01	0.999969	2.790E-01	-1.122252	0.001378	2.425E+01
	A	H(γ)	4.167E-01	-0.006541	3.732E-03	4.515E+00	-4.519E+00	-4.515E+00	-1.804E+01	0.999969	2.790E-01	-1.122252	0.001378	2.425E+01
	A	H(β)	4.165E-01	0.007853	4.007E-03	4.513E+00	-4.517E+00	-4.513E+00	-1.804E+01	0.999964	2.796E-01	-1.119295	0.001632	2.460E+01
	A	H(α)	4.175E-01	-0.016740	3.994E-03	4.534E+00	-4.538E+00	-4.534E+00	-1.812E+01	0.999965	2.850E-01	-1.118971	0.001347	2.472E+01
	A	H(sp3)	4.051E-01	0.032686	4.654E-03	4.427E+00	-4.432E+00	-4.427E+00	-1.769E+01	0.999948	2.992E-01	-1.105979	0.001013	2.678E+01
	A	H(sp3)	4.051E-01	0.032686	4.654E-03	4.427E+00	-4.432E+00	-4.427E+00	-1.769E+01	0.999948	2.992E-01	-1.105979	0.001013	2.678E+01
	B	C(sp3)-C(α)	2.731E-01	-0.002563	5.683E-02	2.502E-01	-3.070E-01	-2.502E-01	-7.735E-01	0.971253	2.279E-02	1.843484	0.045908	9.214E-01
	B	C(α)-C(β)	3.350E-01	-0.002835	1.025E-01	3.672E-01	-4.697E-01	-3.672E-01	-1.059E+00	0.953605	3.056E-02	2.827392	0.240333	1.134E+00
	B	C(β)-C(γ)	3.095E-01	0.000789	7.876E-02	3.154E-01	-3.942E-01	-3.154E-01	-9.465E-01	0.963845	2.702E-02	2.307311	0.136079	1.056E+00
	B	C(γ)-C(γ')	3.245E-01	-0.003427	8.707E-02	3.423E-01	-4.293E-01	-3.423E-01	-1.021E+00	0.962302	2.899E-02	2.476063	0.149705	1.106E+00
	B	C(β)-C(γ)	3.095E-01	0.000789	7.876E-02	3.154E-01	-3.942E-01	-3.154E-01	-9.465E-01	0.963845	2.702E-02	2.307311	0.136079	1.056E+00
	B	C(α)-C(β)	3.350E-01	-0.002835	1.025E-01	3.672E-01	-4.697E-01	-3.672E-01	-1.059E+00	0.953605	3.056E-02	2.827392	0.240333	1.134E+00
	B	C(sp3)-C(α)	2.731E-01	-0.002563	5.683E-02	2.502E-01	-3.070E-01	-2.502E-01	-7.735E-01	0.971253	2.279E-02	1.843484	0.045908	9.214E-01
	B	C(α)-H(α)	2.857E-01	-0.002147	2.720E-02	3.002E-01	-3.274E-01	-3.002E-01	-1.092E+00	0.994233	1.979E-02	1.623797	0.007250	1.046E+00
	B	C(β)-H(β)	2.853E-01	0.000976	2.751E-02	2.994E-01	-3.269E-01	-2.994E-01	-1.087E+00	0.994040	1.938E-02	1.637922	0.018413	1.045E+00
	B	C(γ)-H(γ)	2.881E-01	-0.000914	2.486E-02	3.060E-01	-3.308E-01	-3.060E-01	-1.124E+00	0.995277	1.994E-02	1.648151	0.003568	1.067E+00
	B	C(γ)-H(γ)	2.881E-01	-0.000914	2.486E-02	3.060E-01	-3.308E-01	-3.060E-01	-1.124E+00	0.995277	1.994E-02	1.648151	0.003568	1.067E+00
	B	C(β)-H(β)	2.853E-01	0.000976	2.751E-02	2.994E-01	-3.269E-01	-2.994E-01	-1.087E+00	0.994040	1.938E-02	1.637922	0.018413	1.045E+00
	B	C(α)-H(α)	2.857E-01	-0.002147	2.720E-02	3.002E-01	-3.274E-01	-3.002E-01	-1.092E+00	0.994233	1.979E-02	1.623797	0.007250	1.046E+00
	B	C(sp3)-H(sp3)	2.662E-01	0.008272	3.377E-02	2.622E-01	-2.960E-01	-2.622E-01	-9.139E-01	0.988854	1.768E-02	1.479979	0.029165	1.006E+00
	B	C(sp3)-H(sp3)	2.662E-01	0.008272	3.377E-02	2.622E-01	-2.960E-01	-2.622E-01	-9.139E-01	0.988854	1.768E-02	1.479979	0.029165	1.006E+00
	R	O	8.246E-03	0.000023	1.025E-02	-3.166E-03	-7.087E-03	3.166E-03	5.368E-02	0.008787	-6.336E-02	0.142885	-1.145379	2.938E-01
6(-)	A	C(sp3)	1.180E+02	-0.067142	4.841E+00	1.090E+05	-1.090E+05	-1.090E+05	-4.360E+05	1.000000	1.104E+04	-1.000002	0.000000	1.117E+07
	A	C(α)	1.181E+02	0.154239	4.864E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.363E+05	1.000000	1.133E+04	-1.000006	0.000003	2.986E+06
	A	C(β)	1.181E+02	-0.088990	4.770E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.365E+05	1.000000	1.132E+04	-1.000007	0.000004	3.400E+06
	A	C(γ)	1.180E+02	0.048105	4.819E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.362E+05	1.000000	1.102E+04	-1.000003	0.000002	4.325E+06
	A	C(γ)	1.180E+02	0.048105	4.819E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.362E+05	1.000000	1.102E+04	-1.000003	0.000002	4.325E+06
	A	C(β)	1.181E+02	-0.088990	4.770E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.365E+05	1.000000	1.132E+04	-1.000007	0.000004	3.400E+06

Table S3 (continued)

A	C(α)	1.181E+02	0.154248	4.864E+00	1.091E+05	-1.091E+05	-1.091E+05	-4.363E+05	1.000000	1.133E+04	-1.000006	0.000003	2.986E+06
A	H(α)	4.289E-01	-0.018010	5.474E-03	4.713E+00	-4.718E+00	-4.713E+00	-1.883E+01	0.999940	2.939E-01	-1.095128	0.002087	2.890E+01
A	H(β)	4.314E-01	0.008688	4.795E-03	4.753E+00	-4.758E+00	-4.753E+00	-1.899E+01	0.999954	2.959E-01	-1.094736	0.001765	2.909E+01
A	H(γ)	4.299E-01	-0.006898	5.241E-03	4.725E+00	-4.730E+00	-4.725E+00	-1.888E+01	0.999944	2.898E-01	-1.094679	0.002050	2.899E+01
A	H(γ)	4.299E-01	-0.006898	5.241E-03	4.725E+00	-4.730E+00	-4.725E+00	-1.888E+01	0.999944	2.898E-01	-1.094679	0.002050	2.899E+01
A	H(β)	4.314E-01	0.008688	4.795E-03	4.753E+00	-4.758E+00	-4.753E+00	-1.899E+01	0.999954	2.959E-01	-1.094736	0.001765	2.909E+01
A	H(α)	4.292E-01	-0.018008	5.497E-03	4.714E+00	-4.720E+00	-4.714E+00	-1.883E+01	0.999939	2.940E-01	-1.095318	0.002092	2.885E+01
A	H(sp3;eq)	4.317E-01	0.008040	4.910E-03	4.758E+00	-4.763E+00	-4.758E+00	-1.901E+01	0.999952	3.042E-01	-1.091365	0.000422	2.990E+01
A	H(sp3;ax)	4.260E-01	0.021688	5.142E-03	4.704E+00	-4.709E+00	-4.704E+00	-1.880E+01	0.999946	3.446E-01	-1.090163	0.000498	3.031E+01
B	C(sp3)-C(α)	2.586E-01	-0.001081	5.414E-02	2.247E-01	-2.788E-01	-2.247E-01	-6.821E-01	0.968873	1.983E-02	1.721149	0.079909	4.592E-01
B	C(α)-C(β)	3.227E-01	-0.000230	1.046E-01	3.444E-01	-4.490E-01	-3.444E-01	-9.593E-01	0.945758	2.771E-02	2.762982	0.362757	6.823E-01
B	C(β)-C(γ)	3.021E-01	-0.000479	8.664E-02	3.031E-01	-3.898E-01	-3.031E-01	-8.660E-01	0.953118	2.470E-02	2.340925	0.274821	6.049E-01
B	C(γ)-C(γ')	3.078E-01	-0.000284	9.114E-02	3.132E-01	-4.044E-01	-3.132E-01	-8.884E-01	0.951323	2.488E-02	2.441689	0.313101	6.127E-01
B	C(β)-C(γ)	3.021E-01	-0.000479	8.664E-02	3.031E-01	-3.898E-01	-3.031E-01	-8.660E-01	0.953118	2.470E-02	2.340926	0.274821	6.049E-01
B	C(α)-C(β)	3.227E-01	-0.000229	1.046E-01	3.444E-01	-4.490E-01	-3.444E-01	-9.593E-01	0.945753	2.771E-02	2.763016	0.362758	6.822E-01
B	C(sp3)-C(α)	2.586E-01	-0.001081	5.414E-02	2.247E-01	-2.788E-01	-2.247E-01	-6.822E-01	0.968881	1.983E-02	1.721210	0.079924	4.592E-01
B	C(α)-H(α)	2.678E-01	0.000512	4.511E-02	2.666E-01	-3.117E-01	-2.666E-01	-8.859E-01	0.980549	1.626E-02	1.567113	0.070171	6.516E-01
B	C(β)-H(β)	2.685E-01	-0.000256	4.054E-02	2.666E-01	-3.071E-01	-2.666E-01	-9.040E-01	0.984310	1.655E-02	1.535362	0.031404	6.424E-01
B	C(γ)-H(γ)	2.677E-01	0.000257	4.388E-02	2.666E-01	-3.105E-01	-2.666E-01	-8.907E-01	0.981457	1.604E-02	1.569098	0.061823	6.373E-01
B	C(γ)-H(γ)	2.677E-01	0.000257	4.388E-02	2.666E-01	-3.105E-01	-2.666E-01	-8.907E-01	0.981457	1.604E-02	1.569098	0.061823	6.372E-01
B	C(β)-H(β)	2.685E-01	-0.000256	4.054E-02	2.666E-01	-3.071E-01	-2.666E-01	-9.040E-01	0.984310	1.655E-02	1.535362	0.031403	6.424E-01
B	C(α)-H(α)	2.682E-01	0.000519	4.529E-02	2.675E-01	-3.128E-01	-2.675E-01	-8.889E-01	0.980495	1.632E-02	1.571965	0.070208	6.533E-01
B	C(sp3)-H(sp3;eq)	2.656E-01	0.000872	4.153E-02	2.597E-01	-3.013E-01	-2.597E-01	-8.728E-01	0.982924	1.628E-02	1.468231	0.008250	6.371E-01
B	C(sp3)-H(sp3;ax)	2.611E-01	0.001875	4.120E-02	2.511E-01	-2.923E-01	-2.511E-01	-8.395E-01	0.982312	1.754E-02	1.420747	0.005886	6.188E-01
R	O	7.944E-03	-0.000050	9.852E-03	-3.053E-03	-6.799E-03	3.053E-03	5.162E-02	0.008407	-2.763E-02	0.105194	-1.122383	-1.436E-01

Cartesian coordinates of optimised geometry of molecule **1** and its SCF electronic energy in different spin states employing different levels of theory.

B3LYP, closed-shell singlet

6-31+G(d,p)
Electronic energy: -347.7130495
Hartree

C	-1.22639	-0.65433	-7.08778
C	-0.76333	0.43068	-8.05125
C	-0.15472	1.45318	-7.10044
C	-0.26021	1.01466	-5.82969
C	-0.92802	-0.29866	-5.82181
C	-1.88607	0.99641	-8.91111
C	-1.58686	0.83640	-10.21613
C	-0.27827	0.17026	-10.33738
C	0.21385	-0.07256	-9.10568
H	0.20212	-0.07967	-11.27712
H	-2.20244	1.14437	-11.05432
H	0.08704	1.53560	-4.94403
H	-1.14009	-0.87766	-4.92954
H	-1.71818	-1.55958	-7.42209
H	0.28540	2.38062	-7.44576
H	-2.77328	1.45010	-8.48669
H	1.15274	-0.54844	-8.85048

6-311++G(d,p)
Electronic energy: -347.7771241
Hartree

C	-1.22583	-0.65314	-7.08835
C	-0.76333	0.43068	-8.05125
C	-0.15536	1.45202	-7.10100
C	-0.26081	1.01439	-5.83475
C	-0.92819	-0.29806	-5.82687
C	-1.88486	0.99580	-8.91066
C	-1.58604	0.83601	-10.21111
C	-0.27832	0.17032	-10.33228
C	0.21272	-0.07198	-9.10501
H	0.20103	-0.07907	-11.27041
H	-2.20035	1.14335	-11.04791
H	0.08573	1.53421	-4.95058
H	-1.13977	-0.87585	-4.93611
H	-1.71673	-1.55682	-7.42159
H	0.28402	2.37782	-7.44522
H	-2.77055	1.44871	-8.48747
H	1.14993	-0.54701	-8.85074

Aug-cc-pVTZ
Electronic energy: -347.809437 Hartree

C	-1.22441	-0.65014	-7.08944
C	-0.76333	0.43068	-8.05125
C	-0.15695	1.44909	-7.10205
C	-0.26190	1.01310	-5.83943
C	-0.92781	-0.29646	-5.83157
C	-1.88182	0.99426	-8.90985
C	-1.58425	0.83513	-10.20655
C	-0.27939	0.17090	-10.32746
C	0.20985	-0.07051	-9.10367
H	0.19954	-0.07827	-11.26303
H	-2.19777	1.14207	-11.04089
H	0.08414	1.53240	-4.95777
H	-1.13929	-0.87357	-4.94332
H	-1.71428	-1.55215	-7.42083
H	0.28169	2.37310	-7.44441
H	-2.76593	1.44635	-8.48869
H	1.14519	-0.54460	-8.85110

B3LYP, restricted open shell singlet

6-31+G(d,p)
Electronic energy: -347.7130495
Hartree

C	-1.22639	-0.65433	-7.08778
C	-0.76333	0.43068	-8.05125
C	-0.15472	1.45318	-7.10044
C	-0.26021	1.01466	-5.82969
C	-0.92802	-0.29866	-5.82181
C	-1.88607	0.99641	-8.91111
C	-1.58686	0.83640	-10.21613
C	-0.27827	0.17026	-10.33738
C	0.21385	-0.07256	-9.10568
H	0.20212	-0.07967	-11.27712
H	-2.20244	1.14437	-11.05432
H	0.08704	1.53560	-4.94403
H	-1.14009	-0.87766	-4.92954
H	-1.71818	-1.55958	-7.42209
H	0.28540	2.38062	-7.44576
H	-2.77328	1.45010	-8.48669
H	1.15274	-0.54844	-8.85048

6-311++G(d,p)
Electronic energy: -347.7771241
Hartree

C	-1.22583	-0.65314	-7.08835
C	-0.76333	0.43068	-8.05125
C	-0.15536	1.45202	-7.10100
C	-0.26081	1.01439	-5.83475
C	-0.92819	-0.29806	-5.82687
C	-1.88486	0.99580	-8.91066
C	-1.58604	0.83602	-10.21111
C	-0.27832	0.17032	-10.33228
C	0.21272	-0.07198	-9.10501
H	0.20103	-0.07907	-11.27041
H	-2.20035	1.14335	-11.04791
H	0.08573	1.53421	-4.95058
H	-1.13977	-0.87585	-4.93611
H	-1.71673	-1.55682	-7.42159
H	0.28402	2.37782	-7.44522
H	-2.77055	1.44871	-8.48747
H	1.14993	-0.54701	-8.85074

Aug-cc-pVTZ
Electronic energy: -347.809437 Hartree

C	-1.22441	-0.65014	-7.08944
C	-0.76333	0.43068	-8.05125
C	-0.15695	1.44909	-7.10205
C	-0.26190	1.01310	-5.83943
C	-0.92781	-0.29646	-5.83157
C	-1.88182	0.99426	-8.90985
C	-1.58425	0.83513	-10.20655
C	-0.27939	0.17090	-10.32746
C	0.20985	-0.07051	-9.10367
H	0.19954	-0.07827	-11.26303
H	-2.19777	1.14207	-11.04089
H	0.08414	1.53240	-4.95777
H	-1.13929	-0.87357	-4.94332
H	-1.71428	-1.55215	-7.42083
H	0.28169	2.37310	-7.44441
H	-2.76593	1.44635	-8.48869
H	1.14519	-0.54460	-8.85110

B3LYP, triplet

6-31+G(d,p)
Electronic energy: -347.6321618
Hartree

C	-1.22214	-0.64316	-7.10314
C	-0.76541	0.43155	-8.07825
C	-0.16133	1.44299	-7.11569
C	-0.27808	0.96435	-5.74644
C	-0.89750	-0.25378	-5.73911
C	-1.88593	0.99615	-8.94073
C	-1.58672	0.83614	-10.25078
C	-0.28362	0.17279	-10.37152
C	0.20921	-0.07039	-9.13485
H	0.19351	-0.07547	-11.31367
H	-2.19943	1.14265	-11.09196
H	0.07760	1.50478	-4.87707
H	-1.12042	-0.85122	-4.86289
H	-1.71548	-1.55601	-7.41227
H	0.28413	2.37640	-7.43594
H	-2.77359	1.45006	-8.51682
H	1.14847	-0.54646	-8.88021

Aug-cc-pVTZ
Electronic energy: -347.7447937
Hartree

C	-1.22042	-0.63924	-7.10614
C	-0.76543	0.43156	-8.07856
C	-0.16351	1.43927	-7.11864
C	-0.28058	0.96111	-5.75566
C	-0.89639	-0.24993	-5.74837
C	-1.88161	0.99396	-8.93942
C	-1.58398	0.83480	-10.24127
C	-0.28488	0.17350	-10.36163
C	0.20514	-0.06831	-9.13276
H	0.19078	-0.07400	-11.29959
H	-2.19461	1.14028	-11.07858
H	0.07298	1.49782	-4.88874
H	-1.11757	-0.84350	-4.87464
H	-1.71175	-1.54862	-7.41257
H	0.28035	2.36903	-7.43615
H	-2.76597	1.44618	-8.51832
H	1.14072	-0.54253	-8.88027

6-311++G(d,p)
Electronic energy: -347.6953524
Hartree

C	-1.22189	-0.64234	-7.10491
C	-0.76542	0.43155	-8.07834
C	-0.16186	1.44230	-7.11746
C	-0.27933	0.96272	-5.75092
C	-0.89693	-0.25185	-5.74361
C	-1.88472	0.99553	-8.94021
C	-1.58582	0.83571	-10.24574
C	-0.28374	0.17289	-10.36638
C	0.20809	-0.06982	-9.13411
H	0.19238	-0.07485	-11.30688
H	-2.19728	1.14160	-11.08548
H	0.07518	1.50095	-4.88224
H	-1.11877	-0.84704	-4.86810
H	-1.71433	-1.55361	-7.41297
H	0.28286	2.37405	-7.43662
H	-2.77074	1.44861	-8.51723
H	1.14559	-0.54500	-8.88008

B3LYP, quintuplet

6-31+G(d,p)
Electronic energy: -347.5431128
Hartree

C	-1.21542	-0.64009	-7.04805
C	-0.76334	0.43063	-8.05126
C	-0.15960	1.43628	-7.06059
C	-0.27413	0.96180	-5.68932
C	-0.89282	-0.25489	-5.68197
C	-1.87361	0.98976	-8.95232
C	-1.54935	0.81653	-10.36068
C	-0.33705	0.19941	-10.47303
C	0.19528	-0.06341	-9.14405
H	0.16385	-0.06078	-11.39831
H	-2.18293	1.13383	-11.18082
H	0.08168	1.50262	-4.82005
H	-1.11595	-0.85263	-4.80583
H	-1.71007	-1.55734	-7.34762
H	0.28871	2.37340	-7.37136
H	-2.77428	1.45000	-8.56154
H	1.14230	-0.54373	-8.92451

Aug-cc-pVTZ
Electronic energy: -347.6367283
Hartree

C	-1.21373	-0.63622	-7.05089
C	-0.76335	0.43062	-8.05125
C	-0.16174	1.43260	-7.06341
C	-0.27664	0.95856	-5.69858
C	-0.89170	-0.25103	-5.69126
C	-1.86964	0.98773	-8.94984
C	-1.54510	0.81445	-10.35174
C	-0.33986	0.20093	-10.46343
C	0.19173	-0.06161	-9.14087
H	0.15749	-0.05741	-11.38583
H	-2.17471	1.12979	-11.16970
H	0.07709	1.49571	-4.83182
H	-1.11311	-0.84493	-4.81766
H	-1.70634	-1.54997	-7.34770
H	0.28494	2.36604	-7.37141
H	-2.76698	1.44620	-8.56216
H	1.13494	-0.54006	-8.92375

6-311++G(d,p)
Electronic energy: -347.6053226
Hartree

C	-1.21525	-0.63941	-7.04990
C	-0.76334	0.43062	-8.05125
C	-0.16006	1.43571	-7.06245
C	-0.27539	0.96018	-5.69402
C	-0.89226	-0.25295	-5.68668
C	-1.87285	0.98936	-8.95053
C	-1.54721	0.81549	-10.35614
C	-0.33845	0.20017	-10.46816
C	0.19480	-0.06317	-9.14215
H	0.16029	-0.05889	-11.39251
H	-2.17850	1.13166	-11.17577
H	0.07924	1.49880	-4.82546
H	-1.11432	-0.84844	-4.81126
H	-1.70897	-1.55504	-7.34844
H	0.28748	2.37114	-7.37220
H	-2.77197	1.44877	-8.56092
H	1.14007	-0.54265	-8.92347

B3LYP[GD3BJ], closed-shell singlet

6-31+G(d,p)
Electronic energy: -347.8438239
Hartree

C	-1.22676	-0.65442	-7.09131
C	-0.76333	0.43068	-8.05125
C	-0.15489	1.45349	-7.10397
C	-0.26043	1.01491	-5.83352
C	-0.92838	-0.29866	-5.82563
C	-1.88600	0.99640	-8.90756
C	-1.58669	0.83634	-10.21229
C	-0.27785	0.17007	-10.33357
C	0.21431	-0.07277	-9.10218
H	0.20172	-0.07945	-11.27342
H	-2.20149	1.14391	-11.05074
H	0.08642	1.53503	-4.94767
H	-1.14002	-0.87686	-4.93318
H	-1.71799	-1.55790	-7.42932
H	0.28411	2.37941	-7.45296
H	-2.77129	1.44914	-8.47961
H	1.15185	-0.54794	-8.84313

Aug-cc-pVTZ
Electronic energy: -347.8114733
Hartree

C	-1.22483	-0.65035	-7.09287
C	-0.76333	0.43068	-8.05125
C	-0.15705	1.44952	-7.10548
C	-0.26209	1.01341	-5.84313
C	-0.92819	-0.29654	-5.83526
C	-1.88188	0.99431	-8.90639
C	-1.58416	0.83511	-10.20284
C	-0.27892	0.17068	-10.32378
C	0.21043	-0.07078	-9.10027
H	0.19915	-0.07805	-11.25949
H	-2.19685	1.14162	-11.03748
H	0.08354	1.53186	-4.96124
H	-1.13921	-0.87279	-4.94680
H	-1.71414	-1.55058	-7.42800
H	0.28047	2.37200	-7.45156
H	-2.76405	1.44544	-8.48165
H	1.14440	-0.54415	-8.84381

6-311++G(d,p)
Electronic energy: -347.7453257
Hartree

C	-1.22622	-0.65326	-7.09183
C	-0.76333	0.43068	-8.05125
C	-0.15551	1.45236	-7.10447
C	-0.26102	1.01466	-5.83851
C	-0.92855	-0.29809	-5.83063
C	-1.88483	0.99580	-8.90715
C	-1.58590	0.83597	-10.20734
C	-0.27788	0.17012	-10.32854
C	0.21321	-0.07221	-9.10156
H	0.20064	-0.07886	-11.26678
H	-2.19942	1.14289	-11.04439
H	0.08512	1.53367	-4.95416
H	-1.13971	-0.87507	-4.93969
H	-1.71655	-1.55515	-7.42881
H	0.28275	2.37663	-7.45242
H	-2.76857	1.44775	-8.48039
H	1.14905	-0.54652	-8.84339

B3LYP[GD3BJ], restricted open shell singlet

6-31+G(d,p)
Electronic energy: -347.8438239
Hartree

C	-1.22676	-0.65442	-7.09131
C	-0.76333	0.43068	-8.05125
C	-0.15489	1.45349	-7.10397
C	-0.26043	1.01491	-5.83352
C	-0.92838	-0.29866	-5.82563
C	-1.88600	0.99640	-8.90756
C	-1.58669	0.83634	-10.21229
C	-0.27785	0.17007	-10.33357
C	0.21431	-0.07277	-9.10218
H	0.20172	-0.07945	-11.27342
H	-2.20149	1.14391	-11.05074
H	0.08642	1.53503	-4.94767
H	-1.14002	-0.87686	-4.93318
H	-1.71799	-1.55790	-7.42932
H	0.28411	2.37941	-7.45296
H	-2.77129	1.44914	-8.47961
H	1.15185	-0.54794	-8.84313

Aug-cc-pVTZ
Electronic energy: -347.8114733
Hartree

C	-1.22483	-0.65035	-7.09287
C	-0.76333	0.43068	-8.05125
C	-0.15705	1.44952	-7.10548
C	-0.26209	1.01341	-5.84313
C	-0.92819	-0.29654	-5.83526
C	-1.88188	0.99431	-8.90639
C	-1.58416	0.83511	-10.20284
C	-0.27892	0.17068	-10.32378
C	0.21043	-0.07078	-9.10027
H	0.19915	-0.07805	-11.25949
H	-2.19685	1.14162	-11.03748
H	0.08354	1.53186	-4.96124
H	-1.13921	-0.87279	-4.94680
H	-1.71414	-1.55058	-7.42800
H	0.28047	2.37200	-7.45156
H	-2.76405	1.44544	-8.48165
H	1.14440	-0.54415	-8.84381

6-311++G(d,p)
Electronic energy: -347.7453257
Hartree

C	-1.22622	-0.65326	-7.09183
C	-0.76333	0.43068	-8.05125
C	-0.15551	1.45236	-7.10447
C	-0.26102	1.01466	-5.83851
C	-0.92855	-0.29809	-5.83063
C	-1.88483	0.99580	-8.90715
C	-1.58590	0.83597	-10.20734
C	-0.27788	0.17012	-10.32854
C	0.21321	-0.07221	-9.10156
H	0.20064	-0.07886	-11.26678
H	-2.19942	1.14289	-11.04439
H	0.08512	1.53367	-4.95416
H	-1.13971	-0.87507	-4.93969
H	-1.71655	-1.55515	-7.42881
H	0.28275	2.37663	-7.45242
H	-2.76857	1.44775	-8.48039
H	1.14905	-0.54652	-8.84339

B3LYP[GD3BJ], triplet

6-31+G(d,p)

Electronic energy: -347.761192 Hartree

C	-1.22273	-0.64367	-7.10667
C	-0.76540	0.43155	-8.07811
C	-0.16129	1.44374	-7.11923
C	-0.27836	0.96459	-5.75081
C	-0.89787	-0.25373	-5.74347
C	-1.88576	0.99608	-8.93694
C	-1.58647	0.83604	-10.24682
C	-0.28327	0.17264	-10.36756
C	0.20961	-0.07057	-9.13107
H	0.19307	-0.07522	-11.30980
H	-2.19840	1.14215	-11.08823
H	0.07686	1.50404	-4.88109
H	-1.12027	-0.85022	-4.86692
H	-1.71554	-1.55483	-7.41940
H	0.28310	2.37569	-7.44306
H	-2.77150	1.44904	-8.50951
H	1.14750	-0.54593	-8.87260

Aug-cc-pVTZ

Electronic energy: -347.729165 Hartree

C	-1.22108	-0.63988	-7.10959
C	-0.76543	0.43155	-8.07840
C	-0.16339	1.44014	-7.12211
C	-0.28084	0.96137	-5.75991
C	-0.89678	-0.24992	-5.75262
C	-1.88157	0.99396	-8.93570
C	-1.58380	0.83474	-10.23741
C	-0.28447	0.17331	-10.35779
C	0.20567	-0.06856	-9.12908
H	0.19035	-0.07375	-11.29587
H	-2.19361	1.13980	-11.07500
H	0.07226	1.49708	-4.89263
H	-1.11741	-0.84250	-4.87854
H	-1.71187	-1.54756	-7.41967
H	0.27938	2.36843	-7.44324
H	-2.76400	1.44522	-8.51104
H	1.13987	-0.54205	-8.87272

6-311++G(d,p)

Electronic energy: -347.6641108 Hartree

C	-1.60934	-0.56747	-6.84338
C	-1.29416	0.25676	-8.01658
C	-0.13266	1.18709	-7.54756
C	0.14570	0.74706	-6.15869
C	-0.72402	-0.26935	-5.79832
C	-2.16977	0.69088	-9.11200
C	-1.40930	0.93194	-10.26456
C	-0.07274	0.63834	-10.04830
C	0.12739	0.17269	-8.65433
H	0.72912	0.76251	-10.76315
H	-1.81018	1.32637	-11.18953
H	0.94377	1.14704	-5.54835
H	-0.70321	-0.78828	-4.84852
H	-2.39710	-1.30754	-6.82028
H	-0.13683	2.23625	-7.82334
H	-3.23830	0.82281	-9.01385
H	0.77490	-0.66571	-8.42056

B3LYP[GD3BJ], quintuplet

6-31+G(d,p)
Electronic energy: -347.6699399
Hartree

C	-1.21591	-0.64041	-7.05154
C	-0.76334	0.43062	-8.05125
C	-0.15965	1.43682	-7.06409
C	-0.27442	0.96200	-5.69353
C	-0.89316	-0.25480	-5.68618
C	-1.87377	0.98985	-8.94879
C	-1.54909	0.81643	-10.35647
C	-0.33666	0.19925	-10.46883
C	0.19598	-0.06375	-9.14061
H	0.16337	-0.06049	-11.39427
H	-2.18182	1.13332	-11.17693
H	0.08098	1.50196	-4.82401
H	-1.11585	-0.85170	-4.80979
H	-1.71006	-1.55607	-7.35448
H	0.28765	2.37257	-7.37823
H	-2.77273	1.44922	-8.55477
H	1.14178	-0.54344	-8.91755

Aug-cc-pVTZ
Electronic energy: -347.6384952
Hartree

C	-1.21428	-0.63669	-7.05434
C	-0.76335	0.43060	-8.05125
C	-0.16172	1.43328	-7.06689
C	-0.27690	0.95880	-5.70274
C	-0.89206	-0.25097	-5.69540
C	-1.86996	0.98789	-8.94632
C	-1.54486	0.81438	-10.34758
C	-0.33945	0.20077	-10.45929
C	0.19255	-0.06203	-9.13746
H	0.15701	-0.05708	-11.38188
H	-2.17359	1.12930	-11.16590
H	0.07639	1.49505	-4.83570
H	-1.11299	-0.84398	-4.82153
H	-1.70640	-1.54884	-7.35456
H	0.28394	2.36533	-7.37830
H	-2.76557	1.44545	-8.55536
H	1.13451	-0.53987	-8.91679

6-311++G(d,p)
Electronic energy: -347.5744754
Hartree

C	-1.21575	-0.63977	-7.05337
C	-0.76335	0.43060	-8.05125
C	-0.16009	1.43629	-7.06594
C	-0.27568	0.96040	-5.69822
C	-0.89262	-0.25287	-5.69086
C	-1.87306	0.98947	-8.94700
C	-1.54695	0.81541	-10.35195
C	-0.33805	0.20002	-10.46398
C	0.19552	-0.06354	-9.13871
H	0.15983	-0.05858	-11.38849
H	-2.17739	1.13118	-11.17189
H	0.07854	1.49817	-4.82941
H	-1.11422	-0.84750	-4.81520
H	-1.70897	-1.55380	-7.35532
H	0.28643	2.37033	-7.37911
H	-2.77045	1.44797	-8.55412
H	1.13955	-0.54240	-8.91648

BLYP, closed-shell singlet

6-31+G(d,p)
Electronic energy: -347.5476871 Hartree

C	-1.22999	-0.66275	-7.08041
C	-0.76333	0.43068	-8.05125
C	-0.15001	1.46112	-7.09316
C	-0.25734	1.01702	-5.81178
C	-0.92816	-0.30219	-5.80386
C	-1.89478	1.00080	-8.91768
C	-1.59115	0.83848	-10.23379
C	-0.27670	0.16935	-10.35558
C	0.22144	-0.07647	-9.11376
H	0.20624	-0.08192	-11.30178
H	-2.21023	1.14818	-11.07788
H	0.09191	1.54078	-4.91996
H	-1.14129	-0.88442	-4.90540
H	-1.72473	-1.57325	-7.41770
H	0.29260	2.39401	-7.44153
H	-2.78709	1.45711	-8.48976
H	1.16589	-0.55515	-8.85603

Aug-cc-pVTZ
Electronic energy: -347.6503823 Hartree

C	-1.22788	-0.65826	-7.08233
C	-0.76333	0.43068	-8.05125
C	-0.15240	1.45675	-7.09503
C	-0.25924	1.01526	-5.82254
C	-0.92790	-0.29973	-5.81464
C	-1.89023	0.99850	-8.91619
C	-1.58823	0.83706	-10.22322
C	-0.27798	0.17007	-10.34462
C	0.21718	-0.07428	-9.11146
H	0.20295	-0.08015	-11.28615
H	-2.20463	1.14542	-11.06307
H	0.08849	1.53681	-4.93515
H	-1.14018	-0.87946	-4.92064
H	-1.72039	-1.56495	-7.41638
H	0.28847	2.38562	-7.44010
H	-2.77888	1.45292	-8.49190
H	1.15748	-0.55088	-8.85664

6-311++G(d,p)
Electronic energy: -347.616685 Hartree

C	-1.22938	-0.66143	-7.08105
C	-0.76333	0.43068	-8.05125
C	-0.15072	1.45984	-7.09379
C	-0.25807	1.01661	-5.81743
C	-0.92829	-0.30142	-5.80952
C	-1.89344	1.00012	-8.91716
C	-1.59014	0.83800	-10.22819
C	-0.27685	0.16947	-10.34988
C	0.22019	-0.07583	-9.11301
H	0.20462	-0.08104	-11.29407
H	-2.20746	1.14682	-11.07057
H	0.09023	1.53882	-4.92745
H	-1.14074	-0.88198	-4.91291
H	-1.72296	-1.56990	-7.41698
H	0.29094	2.39061	-7.44076
H	-2.78379	1.45542	-8.49081
H	1.16247	-0.55342	-8.85646

BLYP, restricted open shell singlet

6-31+G(d,p)
Electronic energy: -347.5476871
Hartree

C	-1.22999	-0.66275	-7.08041
C	-0.76333	0.43068	-8.05125
C	-0.15001	1.46112	-7.09316
C	-0.25734	1.01702	-5.81178
C	-0.92816	-0.30219	-5.80386
C	-1.89478	1.00080	-8.91768
C	-1.59115	0.83848	-10.23379
C	-0.27670	0.16935	-10.35558
C	0.22144	-0.07647	-9.11376
H	0.20624	-0.08192	-11.30178
H	-2.21023	1.14818	-11.07788
H	0.09191	1.54078	-4.91996
H	-1.14129	-0.88442	-4.90540
H	-1.72473	-1.57325	-7.41770
H	0.29260	2.39401	-7.44153
H	-2.78709	1.45711	-8.48976
H	1.16589	-0.55515	-8.85603

Aug-cc-pVTZ
Electronic energy: -347.6503823
Hartree

C	-1.22788	-0.65826	-7.08233
C	-0.76333	0.43068	-8.05125
C	-0.15240	1.45675	-7.09503
C	-0.25924	1.01526	-5.82254
C	-0.92790	-0.29973	-5.81464
C	-1.89023	0.99850	-8.91619
C	-1.58823	0.83706	-10.22322
C	-0.27798	0.17007	-10.34462
C	0.21718	-0.07428	-9.11146
H	0.20295	-0.08015	-11.28615
H	-2.20463	1.14542	-11.06307
H	0.08849	1.53681	-4.93515
H	-1.14018	-0.87946	-4.92064
H	-1.72039	-1.56495	-7.41638
H	0.28847	2.38562	-7.44010
H	-2.77888	1.45292	-8.49190
H	1.15748	-0.55088	-8.85664

6-311++G(d,p)
Electronic energy: -347.616685 Hartree

C	-1.22938	-0.66143	-7.08105
C	-0.76333	0.43068	-8.05125
C	-0.15072	1.45984	-7.09379
C	-0.25807	1.01661	-5.81743
C	-0.92829	-0.30142	-5.80952
C	-1.89344	1.00012	-8.91716
C	-1.59014	0.83800	-10.22819
C	-0.27685	0.16947	-10.34988
C	0.22019	-0.07583	-9.11301
H	0.20462	-0.08104	-11.29407
H	-2.20746	1.14682	-11.07057
H	0.09023	1.53882	-4.92745
H	-1.14074	-0.88198	-4.91291
H	-1.72296	-1.56990	-7.41698
H	0.29094	2.39061	-7.44076
H	-2.78379	1.45542	-8.49081
H	1.16247	-0.55342	-8.85646

BLYP, triplet

6-31+G(d,p)
Electronic energy: -347.4678201
Hartree

C	-1.22567	-0.65168	-7.09449
C	-0.76519	0.43145	-8.07537
C	-0.15649	1.45095	-7.10714
C	-0.27334	0.97123	-5.73302
C	-0.90020	-0.26153	-5.72560
C	-1.89290	0.99967	-8.94394
C	-1.58989	0.83765	-10.26772
C	-0.28305	0.17240	-10.38880
C	0.21560	-0.07366	-9.13930
H	0.19653	-0.07715	-11.33754
H	-2.20601	1.14586	-11.11493
H	0.08470	1.51533	-4.85828
H	-1.12466	-0.86298	-4.84397
H	-1.72188	-1.56923	-7.40889
H	0.29105	2.38939	-7.43272
H	-2.78587	1.45631	-8.51697
H	1.16056	-0.55262	-8.88262

Aug-cc-pVTZ
Electronic energy: -347.5690666
Hartree

C	-1.22387	-0.64751	-7.09791
C	-0.76522	0.43147	-8.07580
C	-0.15881	1.44701	-7.11052
C	-0.27609	0.96768	-5.74326
C	-0.89900	-0.25732	-5.73588
C	-1.88828	0.99733	-8.94229
C	-1.58678	0.83613	-10.25714
C	-0.28452	0.17321	-10.37780
C	0.21130	-0.07146	-9.13682
H	0.19307	-0.07530	-11.32181
H	-2.20022	1.14301	-11.10006
H	0.07959	1.50770	-4.87159
H	-1.12157	-0.85449	-4.85737
H	-1.71774	-1.56100	-7.40927
H	0.28684	2.38119	-7.43300
H	-2.77735	1.45196	-8.51837
H	1.15193	-0.54824	-8.88242

6-311++G(d,p)
Electronic energy: -347.5358206
Hartree

C	-1.22540	-0.65077	-7.09645
C	-0.76520	0.43145	-8.07549
C	-0.15707	1.45017	-7.10909
C	-0.27472	0.96944	-5.73815
C	-0.89959	-0.25942	-5.73075
C	-1.89158	0.99900	-8.94327
C	-1.58874	0.83710	-10.26205
C	-0.28332	0.17258	-10.38300
C	0.21439	-0.07305	-9.13839
H	0.19485	-0.07624	-11.32967
H	-2.20316	1.14446	-11.10749
H	0.08191	1.51096	-4.86450
H	-1.12281	-0.85821	-4.85024
H	-1.72043	-1.56626	-7.40949
H	0.28950	2.38646	-7.43328
H	-2.78245	1.45456	-8.51750
H	1.15709	-0.55086	-8.88251

BLYP, quintuplet

6-31+G(d,p)
Electronic energy: -347.3762842
Hartree

C	-1.21828	-0.64755	-7.03815
C	-0.76333	0.43061	-8.05126
C	-0.15521	1.44306	-7.05080
C	-0.26946	0.96792	-5.67214
C	-0.89491	-0.26209	-5.66470
C	-1.88146	0.99367	-8.96150
C	-1.55730	0.82049	-10.37728
C	-0.33172	0.19662	-10.49088
C	0.20163	-0.06672	-9.15457
H	0.17284	-0.06544	-11.42176
H	-2.19533	1.14007	-11.20226
H	0.08880	1.51267	-4.79767
H	-1.11976	-0.86406	-4.78330
H	-1.71605	-1.57048	-7.34089
H	0.29583	2.38603	-7.36484
H	-2.78765	1.45669	-8.56695
H	1.15462	-0.55010	-8.93235

Aug-cc-pVTZ
Electronic energy: -347.4758644
Hartree

C	-1.21649	-0.64351	-7.04146
C	-0.76333	0.43055	-8.05126
C	-0.15745	1.43920	-7.05415
C	-0.27225	0.96443	-5.68256
C	-0.89374	-0.25780	-5.67511
C	-1.87731	0.99147	-8.95852
C	-1.55259	0.81828	-10.36721
C	-0.33477	0.19836	-10.48011
C	0.19790	-0.06490	-9.15090
H	0.16592	-0.06159	-11.40749
H	-2.18619	1.13575	-11.18944
H	0.08363	1.50516	-4.81121
H	-1.11672	-0.85545	-4.79683
H	-1.71180	-1.56237	-7.34111
H	0.29173	2.37778	-7.36514
H	-2.77959	1.45226	-8.56742
H	1.14635	-0.54622	-8.93138

6-311++G(d,p)
Electronic energy: -347.4431739
Hartree

C	-1.21809	-0.64685	-7.04021
C	-0.76333	0.43056	-8.05126
C	-0.15568	1.44247	-7.05291
C	-0.27088	0.96618	-5.67760
C	-0.89434	-0.25991	-5.67014
C	-1.88068	0.99321	-8.95946
C	-1.55491	0.81939	-10.37200
C	-0.33323	0.19750	-10.48525
C	0.20112	-0.06651	-9.15245
H	0.16882	-0.06318	-11.41479
H	-2.19020	1.13767	-11.19611
H	0.08593	1.50837	-4.80424
H	-1.11794	-0.85918	-4.78984
H	-1.71461	-1.56770	-7.34163
H	0.29440	2.38319	-7.36568
H	-2.78487	1.45505	-8.56640
H	1.15179	-0.54888	-8.93134

BP86, closed-shell singlet

6-31+G(d,p)
Electronic energy: -347.7021473
Hartree

C	-1.22898	-0.65932	-7.08831
C	-0.76333	0.43069	-8.05125
C	-0.15222	1.45820	-7.10102
C	-0.25906	1.01511	-5.81983
C	-0.92767	-0.29976	-5.81194
C	-1.89102	0.99894	-8.91009
C	-1.58838	0.83711	-10.22592
C	-0.27825	0.17019	-10.34732
C	0.21888	-0.07511	-9.10559
H	0.20695	-0.08224	-11.29411
H	-2.20978	1.14799	-11.07018
H	0.09140	1.54116	-4.92764
H	-1.14194	-0.88430	-4.91308
H	-1.72435	-1.57046	-7.42891
H	0.29052	2.39195	-7.45269
H	-2.78383	1.45551	-8.47880
H	1.16432	-0.55429	-8.84462

6-311++G(d,p)
Electronic energy: -347.7680425
Hartree

C	-1.22835	-0.65791	-7.08923
C	-0.76333	0.43068	-8.05125
C	-0.15299	1.45685	-7.10193
C	-0.25981	1.01463	-5.82523
C	-0.92775	-0.29892	-5.81735
C	-1.88957	0.99821	-8.90930
C	-1.58731	0.83661	-10.22058
C	-0.27849	0.17035	-10.34185
C	0.21757	-0.07444	-9.10455
H	0.20579	-0.08160	-11.28709
H	-2.20757	1.14691	-11.06347
H	0.09001	1.53969	-4.93450
H	-1.14160	-0.88239	-4.91995
H	-1.72288	-1.56761	-7.42865
H	0.28909	2.38909	-7.45240
H	-2.78100	1.45407	-8.47934
H	1.16146	-0.55283	-8.84464

Aug-cc-pVTZ
Electronic energy: -347.799883 Hartree

C	-1.22690	-0.65494	-7.08999
C	-0.76333	0.43068	-8.05125
C	-0.15454	1.45394	-7.10265
C	-0.26081	1.01346	-5.82961
C	-0.92741	-0.29746	-5.82174
C	-1.88659	0.99669	-8.90884
C	-1.58567	0.83579	-10.21631
C	-0.27947	0.17087	-10.33735
C	0.21471	-0.07297	-9.10354
H	0.20447	-0.08089	-11.28017
H	-2.20523	1.14576	-11.05689
H	0.08856	1.53808	-4.94123
H	-1.14119	-0.88033	-4.92672
H	-1.72051	-1.56316	-7.42760
H	0.28690	2.38456	-7.45129
H	-2.77661	1.45183	-8.48083
H	1.15691	-0.55052	-8.84531

BP86, restricted open shell singlet

6-31+G(d,p)
Electronic energy: -347.7021473
Hartree

C	-1.22898	-0.65932	-7.08831
C	-0.76333	0.43069	-8.05125
C	-0.15222	1.45820	-7.10102
C	-0.25906	1.01511	-5.81983
C	-0.92767	-0.29976	-5.81194
C	-1.89102	0.99894	-8.91009
C	-1.58838	0.83711	-10.22592
C	-0.27825	0.17019	-10.34732
C	0.21888	-0.07511	-9.10559
H	0.20695	-0.08224	-11.29411
H	-2.20978	1.14799	-11.07018
H	0.09140	1.54116	-4.92764
H	-1.14194	-0.88430	-4.91308
H	-1.72435	-1.57046	-7.42891
H	0.29052	2.39195	-7.45269
H	-2.78383	1.45551	-8.47880
H	1.16432	-0.55429	-8.84462

6-311++G(d,p)
Electronic energy: -347.7680425
Hartree

C	-1.22835	-0.65791	-7.08923
C	-0.76333	0.43068	-8.05125
C	-0.15299	1.45685	-7.10193
C	-0.25981	1.01463	-5.82523
C	-0.92775	-0.29892	-5.81735
C	-1.88957	0.99821	-8.90930
C	-1.58731	0.83661	-10.22058
C	-0.27849	0.17035	-10.34185
C	0.21757	-0.07444	-9.10455
H	0.20579	-0.08160	-11.28709
H	-2.20757	1.14691	-11.06347
H	0.09001	1.53969	-4.93450
H	-1.14160	-0.88239	-4.91995
H	-1.72288	-1.56761	-7.42865
H	0.28909	2.38909	-7.45240
H	-2.78100	1.45407	-8.47934
H	1.16146	-0.55283	-8.84464

Aug-cc-pVTZ
Electronic energy: -347.799883 Hartree

C	-1.22690	-0.65494	-7.08999
C	-0.76333	0.43068	-8.05125
C	-0.15454	1.45394	-7.10265
C	-0.26081	1.01346	-5.82961
C	-0.92741	-0.29746	-5.82174
C	-1.88659	0.99669	-8.90884
C	-1.58567	0.83579	-10.21631
C	-0.27947	0.17087	-10.33735
C	0.21471	-0.07297	-9.10354
H	0.20447	-0.08089	-11.28017
H	-2.20523	1.14576	-11.05689
H	0.08856	1.53808	-4.94123
H	-1.14119	-0.88033	-4.92672
H	-1.72051	-1.56316	-7.42760
H	0.28690	2.38456	-7.45129
H	-2.77661	1.45183	-8.48083
H	1.15691	-0.55051	-8.84531

BP86, triplet

6-31+G(d,p)
Electronic energy: -347.6224684
Hartree

C	-1.22445	-0.64811	-7.10077
C	-0.76530	0.43150	-8.07666
C	-0.15869	1.44779	-7.11339
C	-0.27449	0.97044	-5.74124
C	-0.90027	-0.26021	-5.73383
C	-1.88920	0.99783	-8.93708
C	-1.58743	0.83645	-10.26042
C	-0.28436	0.17312	-10.38114
C	0.21298	-0.07229	-9.13184
H	0.19711	-0.07740	-11.33076
H	-2.20554	1.14567	-11.10817
H	0.08429	1.51575	-4.86539
H	-1.12528	-0.86297	-4.85107
H	-1.72130	-1.56623	-7.41881
H	0.28892	2.38706	-7.44261
H	-2.78267	1.45474	-8.50649
H	1.15896	-0.55175	-8.87166

Aug-cc-pVTZ
Electronic energy: -347.7190844
Hartree

C	-1.22271	-0.64410	-7.10394
C	-0.76534	0.43151	-8.07720
C	-0.16091	1.44399	-7.11651
C	-0.27705	0.96711	-5.75058
C	-0.89914	-0.25628	-5.74321
C	-1.88471	0.99555	-8.93565
C	-1.58457	0.83505	-10.25080
C	-0.28573	0.17388	-10.37113
C	0.20876	-0.07013	-9.12960
H	0.19443	-0.07595	-11.31677
H	-2.20078	1.14333	-11.09487
H	0.07975	1.50893	-4.87698
H	-1.12250	-0.85539	-4.86275
H	-1.71772	-1.55909	-7.41923
H	0.28527	2.37995	-7.44295
H	-2.77510	1.45088	-8.50768
H	1.15132	-0.54786	-8.87144

6-311++G(d,p)
Electronic energy: -347.6875774
Hartree

C	-1.22419	-0.64719	-7.10292
C	-0.76531	0.43150	-8.07681
C	-0.15928	1.44702	-7.11552
C	-0.27579	0.96883	-5.74638
C	-0.89976	-0.25827	-5.73899
C	-1.88773	0.99709	-8.93604
C	-1.58624	0.83588	-10.25495
C	-0.28471	0.17333	-10.37553
C	0.21168	-0.07162	-9.13055
H	0.19588	-0.07673	-11.32356
H	-2.20323	1.14454	-11.10129
H	0.08184	1.51198	-4.87109
H	-1.12370	-0.85882	-4.85682
H	-1.72019	-1.56385	-7.41990
H	0.28764	2.38475	-7.44368
H	-2.77963	1.45319	-8.50633
H	1.15599	-0.55024	-8.87095

BP86, quintuplet

6-31+G(d,p)
Electronic energy: -347.5315875
Hartree

C	-1.21672	-0.64358	-7.04360
C	-0.76333	0.43055	-8.05126
C	-0.15754	1.43939	-7.05629
C	-0.27056	0.96720	-5.67954
C	-0.89497	-0.26076	-5.67205
C	-1.87727	0.99147	-8.95636
C	-1.55568	0.81984	-10.36999
C	-0.33215	0.19700	-10.48342
C	0.19820	-0.06504	-9.14878
H	0.17364	-0.06556	-11.41553
H	-2.19503	1.14020	-11.19594
H	0.08840	1.51324	-4.80399
H	-1.12041	-0.86400	-4.78951
H	-1.71507	-1.56727	-7.34952
H	0.29373	2.38321	-7.37362
H	-2.78410	1.45461	-8.55850
H	1.15215	-0.54911	-8.92342

Aug-cc-pVTZ
Electronic energy: -347.6269142
Hartree

C	-1.18489	-0.65946	-7.03151
C	-0.75390	0.40068	-8.05294
C	-0.13253	1.41572	-7.08026
C	-0.30214	0.99715	-5.69851
C	-0.92146	-0.22413	-5.66995
C	-1.88270	0.95604	-8.93605
C	-1.54618	0.86151	-10.34708
C	-0.33199	0.24200	-10.48068
C	0.18041	-0.09658	-9.16328
H	0.17763	0.02585	-11.41760
H	-2.17260	1.22546	-11.15929
H	0.02165	1.57174	-4.83274
H	-1.17688	-0.79254	-4.77781
H	-1.61469	-1.61712	-7.32143
H	0.37953	2.31622	-7.41571
H	-2.81297	1.34703	-8.52694
H	1.09698	-0.64819	-8.95949

6-311++G(d,p)
Electronic energy: -347.5957408
Hartree

C	-1.20567	-0.65049	-7.03959
C	-0.76024	0.41866	-8.05187
C	-0.14830	1.43132	-7.06693
C	-0.28216	0.97820	-5.68835
C	-0.90416	-0.24644	-5.67230
C	-1.88056	0.97743	-8.94771
C	-1.55094	0.83605	-10.36018
C	-0.33163	0.21508	-10.48094
C	0.19216	-0.07813	-9.15305
H	0.17544	-0.02839	-11.41526
H	-2.18405	1.17330	-11.18170
H	0.06383	1.53424	-4.81624
H	-1.13977	-0.83560	-4.78533
H	-1.67972	-1.58661	-7.33944
H	0.32444	2.35956	-7.39210
H	-2.79704	1.41202	-8.54517
H	1.13166	-0.58881	-8.93513

CAM-B3LYP, closed-shell singlet

6-31+G(d,p)
Electronic energy: -347.5043701
Hartree

C	-1.22431	-0.64950	-7.09198
C	-0.76333	0.43067	-8.05125
C	-0.15743	1.44861	-7.10459
C	-0.26126	1.01445	-5.83988
C	-0.92852	-0.29778	-5.83200
C	-1.88107	0.99389	-8.90737
C	-1.58553	0.83579	-10.20599
C	-0.27804	0.17021	-10.32714
C	0.20948	-0.07031	-9.10108
H	0.20292	-0.08000	-11.26554
H	-2.20147	1.14396	-11.04275
H	0.08612	1.53589	-4.95561
H	-1.14092	-0.87719	-4.94111
H	-1.71596	-1.55456	-7.42572
H	0.28263	2.37583	-7.44934
H	-2.76812	1.44750	-8.48354
H	1.14812	-0.54607	-8.84642

6-311++G(d,p)
Electronic energy: -347.5695501
Hartree

C	-1.22376	-0.64831	-7.09251
C	-0.76334	0.43067	-8.05125
C	-0.15807	1.44746	-7.10511
C	-0.26183	1.01424	-5.84495
C	-0.92871	-0.29724	-5.83707
C	-1.87987	0.99328	-8.90695
C	-1.58478	0.83544	-10.20095
C	-0.27802	0.17023	-10.32203
C	0.20835	-0.06974	-9.10044
H	0.20209	-0.07953	-11.25878
H	-2.19963	1.14306	-11.03624
H	0.08493	1.53476	-4.96224
H	-1.14074	-0.87563	-4.94776
H	-1.71454	-1.55186	-7.42523
H	0.28128	2.37309	-7.44881
H	-2.76545	1.44613	-8.48430
H	1.14537	-0.54467	-8.84667

Aug-cc-pVTZ
Electronic energy: -347.584476 Hartree

C	-1.22236	-0.64537	-7.09365
C	-0.76333	0.43067	-8.05125
C	-0.15963	1.44459	-7.10621
C	-0.26288	1.01302	-5.84958
C	-0.92837	-0.29572	-5.84171
C	-1.87688	0.99177	-8.90610
C	-1.58306	0.83459	-10.19645
C	-0.27903	0.17078	-10.31728
C	0.20554	-0.06829	-9.09905
H	0.20070	-0.07878	-11.25148
H	-2.19716	1.14184	-11.02929
H	0.08341	1.53306	-4.96935
H	-1.14030	-0.87346	-4.95489
H	-1.71213	-1.54724	-7.42454
H	0.27898	2.36843	-7.44807
H	-2.76088	1.44380	-8.48544
H	1.14069	-0.54229	-8.84696

CAM-B3LYP, restricted open shell singlet

6-31+G(d,p)
Electronic energy: -347.5043701
Hartree

C	-1.22431	-0.64950	-7.09198
C	-0.76333	0.43067	-8.05125
C	-0.15743	1.44861	-7.10459
C	-0.26126	1.01445	-5.83988
C	-0.92852	-0.29778	-5.83200
C	-1.88107	0.99389	-8.90737
C	-1.58553	0.83579	-10.20599
C	-0.27804	0.17021	-10.32714
C	0.20948	-0.07031	-9.10108
H	0.20292	-0.08000	-11.26554
H	-2.20147	1.14396	-11.04275
H	0.08612	1.53589	-4.95561
H	-1.14092	-0.87719	-4.94111
H	-1.71596	-1.55456	-7.42572
H	0.28263	2.37583	-7.44934
H	-2.76812	1.44750	-8.48354
H	1.14812	-0.54607	-8.84642

6-311++G(d,p)
Electronic energy: -347.5695501
Hartree

C	-1.22376	-0.64831	-7.09251
C	-0.76334	0.43067	-8.05125
C	-0.15807	1.44746	-7.10511
C	-0.26183	1.01424	-5.84495
C	-0.92871	-0.29724	-5.83707
C	-1.87987	0.99328	-8.90695
C	-1.58478	0.83544	-10.20095
C	-0.27802	0.17023	-10.32203
C	0.20835	-0.06974	-9.10044
H	0.20209	-0.07953	-11.25878
H	-2.19963	1.14306	-11.03624
H	0.08493	1.53476	-4.96224
H	-1.14074	-0.87563	-4.94776
H	-1.71454	-1.55186	-7.42523
H	0.28128	2.37309	-7.44881
H	-2.76545	1.44613	-8.48430
H	1.14537	-0.54467	-8.84667

Aug-cc-pVTZ
Electronic energy: -347.584476 Hartree

C	-1.22236	-0.64537	-7.09365
C	-0.76333	0.43067	-8.05125
C	-0.15963	1.44459	-7.10621
C	-0.26288	1.01302	-5.84958
C	-0.92837	-0.29572	-5.84171
C	-1.87688	0.99177	-8.90610
C	-1.58306	0.83459	-10.19645
C	-0.27903	0.17078	-10.31728
C	0.20554	-0.06829	-9.09905
H	0.20070	-0.07878	-11.25148
H	-2.19716	1.14184	-11.02929
H	0.08341	1.53306	-4.96935
H	-1.14030	-0.87346	-4.95489
H	-1.71213	-1.54724	-7.42454
H	0.27898	2.36843	-7.44807
H	-2.76088	1.44380	-8.48544
H	1.14069	-0.54229	-8.84696

CAM-B3LYP, triplet

6-31+G(d,p)
Electronic energy: -347.4217817
Hartree

C	-1.22018	-0.63838	-7.10829
C	-0.76553	0.43161	-8.07994
C	-0.16407	1.43855	-7.12078
C	-0.28095	0.95976	-5.75216
C	-0.89550	-0.24881	-5.74489
C	-1.88224	0.99428	-8.94019
C	-1.58636	0.83601	-10.24176
C	-0.28261	0.17233	-10.36256
C	0.20565	-0.06857	-9.13364
H	0.19532	-0.07634	-11.30317
H	-2.19963	1.14281	-11.08128
H	0.07452	1.49988	-4.88341
H	-1.11830	-0.84591	-4.86929
H	-1.71342	-1.55142	-7.41524
H	0.28162	2.37201	-7.43885
H	-2.76959	1.44804	-8.51660
H	1.14456	-0.54447	-8.87925

Aug-cc-pVTZ
Electronic energy: -347.5008189
Hartree

C	-1.21843	-0.63440	-7.11125
C	-0.76556	0.43162	-8.08024
C	-0.16627	1.43477	-7.12370
C	-0.28342	0.95656	-5.76121
C	-0.89441	-0.24502	-5.75398
C	-1.87799	0.99212	-8.93901
C	-1.58378	0.83476	-10.23237
C	-0.28373	0.17296	-10.35282
C	0.20164	-0.06652	-9.13169
H	0.19294	-0.07504	-11.28925
H	-2.19518	1.14063	-11.06799
H	0.06988	1.49280	-4.89466
H	-1.11537	-0.83809	-4.88064
H	-1.70968	-1.54399	-7.41562
H	0.27782	2.36461	-7.43914
H	-2.76214	1.44423	-8.51825
H	1.13695	-0.54060	-8.87950

6-311++G(d,p)
Electronic energy: -347.4860394
Hartree

C	-1.21992	-0.63754	-7.11005
C	-0.76554	0.43161	-8.08002
C	-0.16460	1.43783	-7.12254
C	-0.28221	0.95809	-5.75660
C	-0.89492	-0.24685	-5.74935
C	-1.88102	0.99366	-8.93976
C	-1.58554	0.83562	-10.23673
C	-0.28265	0.17239	-10.35744
C	0.20452	-0.06799	-9.13299
H	0.19444	-0.07585	-11.29638
H	-2.19773	1.14189	-11.07475
H	0.07206	1.49595	-4.88840
H	-1.11660	-0.84165	-4.87433
H	-1.71228	-1.54902	-7.41607
H	0.28034	2.36966	-7.43965
H	-2.76679	1.44661	-8.51707
H	1.14172	-0.54303	-8.87919

CAM-B3LYP, quintuplet

6-31+G(d,p)
Electronic energy: -347.3335111
Hartree

C	-1.21404	-0.63618	-7.05440
C	-0.76334	0.43065	-8.05125
C	-0.16197	1.43280	-7.06687
C	-0.27698	0.95774	-5.69799
C	-0.89126	-0.25029	-5.69071
C	-1.86944	0.98770	-8.94636
C	-1.54438	0.81403	-10.35238
C	-0.34070	0.20129	-10.46392
C	0.19209	-0.06172	-9.13739
H	0.15976	-0.05870	-11.38861
H	-2.17745	1.13105	-11.17203
H	0.07857	1.49809	-4.82925
H	-1.11419	-0.84757	-4.81511
H	-1.70836	-1.55281	-7.35355
H	0.28602	2.36931	-7.37719
H	-2.76952	1.44767	-8.55607
H	1.13848	-0.54169	-8.91821

Aug-cc-pVTZ
Electronic energy: -347.4113027
Hartree

C	-1.21230	-0.63224	-7.05710
C	-0.76335	0.43064	-8.05125
C	-0.16414	1.42905	-7.06954
C	-0.27944	0.95454	-5.70699
C	-0.89016	-0.24650	-5.69974
C	-1.86541	0.98565	-8.94403
C	-1.54020	0.81197	-10.34370
C	-0.34349	0.20279	-10.45459
C	0.18846	-0.05987	-9.13434
H	0.15325	-0.05529	-11.37664
H	-2.16918	1.12695	-11.16144
H	0.07396	1.49105	-4.84050
H	-1.11125	-0.83979	-4.82644
H	-1.70462	-1.54541	-7.35353
H	0.28225	2.36193	-7.37712
H	-2.76219	1.44389	-8.55681
H	1.13109	-0.53797	-8.91756

6-311++G(d,p)
Electronic energy: -347.3967511
Hartree

C	-1.21384	-0.63544	-7.05621
C	-0.76335	0.43064	-8.05125
C	-0.16246	1.43219	-7.06868
C	-0.27825	0.95608	-5.70261
C	-0.89068	-0.24833	-5.69534
C	-1.86864	0.98729	-8.94461
C	-1.54222	0.81297	-10.34793
C	-0.34215	0.20207	-10.45913
C	0.19155	-0.06145	-9.13551
H	0.15610	-0.05678	-11.38303
H	-2.17296	1.12883	-11.16721
H	0.07611	1.49417	-4.83444
H	-1.11249	-0.84330	-4.82034
H	-1.70726	-1.55046	-7.35447
H	0.28476	2.36703	-7.37811
H	-2.76716	1.44644	-8.55537
H	1.13622	-0.54057	-8.91707

CAM-B3LYP[GD3BJ], closed-shell singlet

6-31+G(d,p)
Electronic energy: -347.6195223
Hartree

C	-1.22456	-0.64977	-7.09320
C	-0.76333	0.43067	-8.05125
C	-0.15737	1.44896	-7.10581
C	-0.26130	1.01462	-5.84124
C	-0.92869	-0.29786	-5.83336
C	-1.88129	0.99401	-8.90611
C	-1.58556	0.83581	-10.20462
C	-0.27781	0.17010	-10.32580
C	0.20988	-0.07051	-9.09988
H	0.20281	-0.07994	-11.26426
H	-2.20117	1.14381	-11.04151
H	0.08592	1.53573	-4.95687
H	-1.14091	-0.87695	-4.94237
H	-1.71602	-1.55421	-7.42835
H	0.28229	2.37565	-7.45196
H	-2.76765	1.44727	-8.48094
H	1.14805	-0.54602	-8.84377

Aug-cc-pVTZ
Electronic energy: -347.6045906
Hartree

C	-1.22264	-0.64570	-7.09482
C	-0.76333	0.43067	-8.05125
C	-0.15953	1.44499	-7.10738
C	-0.26290	1.01322	-5.85087
C	-0.92855	-0.29584	-5.84300
C	-1.87716	0.99192	-8.90489
C	-1.58312	0.83463	-10.19514
C	-0.27878	0.17066	-10.31600
C	0.20600	-0.06852	-9.09792
H	0.20059	-0.07873	-11.25029
H	-2.19688	1.14171	-11.02814
H	0.08322	1.53291	-4.97052
H	-1.14029	-0.87323	-4.95606
H	-1.71222	-1.54695	-7.42713
H	0.27867	2.36830	-7.45065
H	-2.76047	1.44361	-8.48288
H	1.14068	-0.54227	-8.84436

6-311++G(d,p)
Electronic energy: -347.5192864
Hartree

C	-1.22402	-0.64860	-7.09371
C	-0.76333	0.43067	-8.05125
C	-0.15799	1.44782	-7.10631
C	-0.26187	1.01442	-5.84628
C	-0.92889	-0.29734	-5.83840
C	-1.88010	0.99341	-8.90572
C	-1.58481	0.83547	-10.19961
C	-0.27778	0.17012	-10.32072
C	0.20877	-0.06994	-9.09927
H	0.20199	-0.07948	-11.25754
H	-2.19934	1.14292	-11.03503
H	0.08474	1.53461	-4.96346
H	-1.14074	-0.87540	-4.94898
H	-1.71461	-1.55151	-7.42785
H	0.28095	2.37292	-7.45143
H	-2.76499	1.44592	-8.48171
H	1.14531	-0.54463	-8.84403

CAM-B3LYP[GD3BJ], restricted open shell singlet

6-31+G(d,p)
Electronic energy: -347.6195223
Hartree

C	-1.22456	-0.64977	-7.09320
C	-0.76333	0.43067	-8.05125
C	-0.15737	1.44896	-7.10581
C	-0.26130	1.01462	-5.84124
C	-0.92869	-0.29786	-5.83336
C	-1.88129	0.99401	-8.90611
C	-1.58556	0.83581	-10.20462
C	-0.27781	0.17010	-10.32580
C	0.20988	-0.07051	-9.09988
H	0.20281	-0.07994	-11.26426
H	-2.20117	1.14381	-11.04151
H	0.08592	1.53573	-4.95687
H	-1.14091	-0.87695	-4.94237
H	-1.71602	-1.55421	-7.42835
H	0.28229	2.37565	-7.45196
H	-2.76765	1.44727	-8.48094
H	1.14805	-0.54602	-8.84377

Aug-cc-pVTZ
Electronic energy: -347.6045906
Hartree

C	-1.22264	-0.64570	-7.09482
C	-0.76333	0.43067	-8.05125
C	-0.15953	1.44499	-7.10738
C	-0.26290	1.01322	-5.85087
C	-0.92855	-0.29584	-5.84300
C	-1.87716	0.99192	-8.90489
C	-1.58312	0.83463	-10.19514
C	-0.27878	0.17066	-10.31600
C	0.20600	-0.06852	-9.09792
H	0.20059	-0.07873	-11.25029
H	-2.19688	1.14171	-11.02814
H	0.08322	1.53291	-4.97052
H	-1.14029	-0.87323	-4.95606
H	-1.71222	-1.54695	-7.42713
H	0.27867	2.36830	-7.45065
H	-2.76047	1.44361	-8.48288
H	1.14068	-0.54227	-8.84436

6-311++G(d,p)
Electronic energy: -347.5192864
Hartree

C	-1.22402	-0.64860	-7.09371
C	-0.76333	0.43067	-8.05125
C	-0.15799	1.44782	-7.10631
C	-0.26187	1.01442	-5.84628
C	-0.92889	-0.29734	-5.83840
C	-1.88010	0.99341	-8.90572
C	-1.58481	0.83547	-10.19961
C	-0.27778	0.17012	-10.32072
C	0.20877	-0.06994	-9.09927
H	0.20199	-0.07948	-11.25754
H	-2.19934	1.14292	-11.03503
H	0.08474	1.53461	-4.96346
H	-1.14074	-0.87540	-4.94898
H	-1.71461	-1.55151	-7.42785
H	0.28095	2.37292	-7.45143
H	-2.76499	1.44592	-8.48171
H	1.14531	-0.54463	-8.84403

CAM-B3LYP[GD3BJ], triplet

6-31+G(d,p)
Electronic energy: -347.5352505
Hartree

C	-1.22053	-0.63883	-7.10958
C	-0.76553	0.43160	-8.07986
C	-0.16392	1.43908	-7.12208
C	-0.28104	0.95988	-5.75379
C	-0.89566	-0.24883	-5.74652
C	-1.88240	0.99437	-8.93879
C	-1.58635	0.83601	-10.24028
C	-0.28240	0.17223	-10.36110
C	0.20603	-0.06875	-9.13229
H	0.19520	-0.07627	-11.30178
H	-2.19930	1.14265	-11.07993
H	0.07424	1.49959	-4.88486
H	-1.11824	-0.84552	-4.87075
H	-1.71359	-1.55126	-7.41793
H	0.28138	2.37203	-7.44154
H	-2.76906	1.44778	-8.51383
H	1.14445	-0.54440	-8.87642

Aug-cc-pVTZ
Electronic energy: -347.5204649
Hartree

C	-1.21881	-0.63492	-7.11250
C	-0.76555	0.43161	-8.08015
C	-0.16608	1.43537	-7.12495
C	-0.28349	0.95669	-5.76278
C	-0.89457	-0.24505	-5.75555
C	-1.87822	0.99225	-8.93765
C	-1.58381	0.83478	-10.23095
C	-0.28349	0.17285	-10.35142
C	0.20207	-0.06673	-9.13039
H	0.19283	-0.07498	-11.28793
H	-2.19487	1.14048	-11.06671
H	0.06960	1.49250	-4.89604
H	-1.11530	-0.83770	-4.88202
H	-1.70988	-1.54390	-7.41827
H	0.27761	2.36469	-7.44179
H	-2.76167	1.44401	-8.51551
H	1.13691	-0.54056	-8.87671

6-311++G(d,p)
Electronic energy: -347.4365504
Hartree

C	-1.22028	-0.63800	-7.11132
C	-0.76554	0.43161	-8.07993
C	-0.16444	1.43838	-7.12382
C	-0.28229	0.95821	-5.75819
C	-0.89507	-0.24687	-5.75094
C	-1.88121	0.99376	-8.93838
C	-1.58554	0.83563	-10.23528
C	-0.28243	0.17228	-10.35601
C	0.20491	-0.06818	-9.13166
H	0.19433	-0.07578	-11.29502
H	-2.19742	1.14174	-11.07343
H	0.07179	1.49566	-4.88982
H	-1.11653	-0.84127	-4.87576
H	-1.71245	-1.54887	-7.41875
H	0.28011	2.36969	-7.44233
H	-2.76627	1.44636	-8.51430
H	1.14163	-0.54296	-8.87637

CAM-B3LYP[GD3BJ], quintuplet

6-31+G(d,p)
Electronic energy: -347.4450227
Hartree

C	-1.21436	-0.63656	-7.05575
C	-0.76334	0.43065	-8.05125
C	-0.16186	1.43327	-7.06823
C	-0.27708	0.95786	-5.69965
C	-0.89142	-0.25030	-5.69236
C	-1.86976	0.98787	-8.94496
C	-1.54432	0.81401	-10.35073
C	-0.34051	0.20121	-10.46228
C	0.19262	-0.06198	-9.13608
H	0.15956	-0.05858	-11.38708
H	-2.17701	1.13085	-11.17056
H	0.07829	1.49782	-4.83076
H	-1.11414	-0.84720	-4.81662
H	-1.70851	-1.55260	-7.35626
H	0.28576	2.36928	-7.37991
H	-2.76920	1.44752	-8.55336
H	1.13856	-0.54172	-8.91548

Aug-cc-pVTZ
Electronic energy: -347.4304649
Hartree

C	-1.21265	-0.63270	-7.05843
C	-0.76335	0.43064	-8.05125
C	-0.16399	1.42959	-7.07088
C	-0.27952	0.95467	-5.70860
C	-0.89031	-0.24652	-5.70135
C	-1.86581	0.98586	-8.94265
C	-1.54015	0.81196	-10.34208
C	-0.34329	0.20270	-10.45298
C	0.18905	-0.06017	-9.13306
H	0.15305	-0.05516	-11.37516
H	-2.16874	1.12675	-11.16002
H	0.07369	1.49077	-4.84195
H	-1.11119	-0.83941	-4.82789
H	-1.70481	-1.54527	-7.35624
H	0.28201	2.36197	-7.37983
H	-2.76193	1.44377	-8.55410
H	1.13124	-0.53804	-8.91484

6-311++G(d,p)
Electronic energy: -347.3480497
Hartree

C	-1.21417	-0.63584	-7.05754
C	-0.76335	0.43064	-8.05125
C	-0.16234	1.43267	-7.07003
C	-0.27834	0.95620	-5.70424
C	-0.89084	-0.24834	-5.69697
C	-1.86898	0.98747	-8.94323
C	-1.54216	0.81295	-10.34629
C	-0.34196	0.20199	-10.45751
C	0.19209	-0.06172	-9.13421
H	0.15590	-0.05666	-11.38151
H	-2.17253	1.12863	-11.16575
H	0.07583	1.49391	-4.83593
H	-1.11244	-0.84294	-4.82182
H	-1.70742	-1.55027	-7.35719
H	0.28450	2.36701	-7.38084
H	-2.76685	1.44629	-8.55265
H	1.13632	-0.54061	-8.91433

HF, closed-shell singlet

6-31+G(d,p)
Electronic energy: -345.4142858
Hartree

C	-1.22331	-0.64861	-7.08603
C	-0.76334	0.43067	-8.05125
C	-0.15754	1.44733	-7.09863
C	-0.26001	1.01787	-5.84515
C	-0.93057	-0.30086	-5.83722
C	-1.88045	0.99353	-8.91342
C	-1.58837	0.83727	-10.20045
C	-0.27440	0.16839	-10.32220
C	0.20794	-0.06957	-9.10693
H	0.20048	-0.07868	-11.25352
H	-2.19724	1.14189	-11.03135
H	0.08353	1.53293	-4.96731
H	-1.14011	-0.87346	-4.95284
H	-1.71115	-1.54766	-7.41176
H	0.27994	2.36801	-7.43530
H	-2.76185	1.44422	-8.49822
H	1.13972	-0.54188	-8.85974

Aug-cc-pVTZ
Electronic energy: -345.5058384
Hartree

C	-1.22191	-0.64577	-7.08659
C	-0.76334	0.43067	-8.05125
C	-0.15901	1.44452	-7.09915
C	-0.26083	1.01738	-5.85140
C	-0.93069	-0.29996	-5.84348
C	-1.87759	0.99208	-8.91314
C	-1.58721	0.83672	-10.19426
C	-0.27461	0.16854	-10.31588
C	0.20517	-0.06815	-9.10613
H	0.19986	-0.07831	-11.24469
H	-2.19530	1.14095	-11.02276
H	0.08221	1.53192	-4.97600
H	-1.14011	-0.87189	-4.96155
H	-1.70872	-1.54312	-7.41041
H	0.27771	2.36338	-7.43390
H	-2.75738	1.44194	-8.50002
H	1.13504	-0.53951	-8.86069

6-311++G(d,p)
Electronic energy: -345.4689102
Hartree

C	-1.22311	-0.64821	-7.08611
C	-0.76334	0.43067	-8.05125
C	-0.15775	1.44693	-7.09871
C	-0.25999	1.01832	-5.84753
C	-0.93094	-0.30116	-5.83960
C	-1.88004	0.99332	-8.91338
C	-1.58857	0.83739	-10.19803
C	-0.27384	0.16812	-10.31985
C	0.20755	-0.06937	-9.10681
H	0.20116	-0.07901	-11.25104
H	-2.19754	1.14205	-11.02878
H	0.08359	1.53350	-4.96983
H	-1.14055	-0.87387	-4.95536
H	-1.71095	-1.54730	-7.41152
H	0.27977	2.36763	-7.43505
H	-2.76150	1.44404	-8.49850
H	1.13933	-0.54169	-8.85995

HF, restricted open shell singlet

6-31+G(d,p)
Electronic energy: -345.4208425
Hartree

C	-1.22995	-0.64569	-7.08286
C	-0.76334	0.43067	-8.05125
C	-0.15051	1.44424	-7.09670
C	-0.25496	1.00192	-5.81715
C	-0.93125	-0.28679	-5.80781
C	-1.88440	0.98714	-8.91590
C	-1.58408	0.82439	-10.23010
C	-0.28305	0.18316	-10.34996
C	0.21151	-0.06301	-9.10955
H	0.20051	-0.05399	-11.27927
H	-2.20129	1.11892	-11.05835
H	0.10113	1.51402	-4.94271
H	-1.15370	-0.85627	-4.92469
H	-1.72999	-1.54043	-7.40190
H	0.30001	2.36025	-7.42888
H	-2.77380	1.42691	-8.50607
H	1.15043	-0.52404	-8.86816

Aug-cc-pVTZ
Electronic energy: -345.5104399
Hartree

C	-1.22776	-0.64318	-7.08404
C	-0.76334	0.43067	-8.05125
C	-0.15286	1.44180	-7.09769
C	-0.25669	1.00303	-5.82731
C	-0.93108	-0.28723	-5.81816
C	-1.88103	0.98645	-8.91508
C	-1.58299	0.82524	-10.21982
C	-0.28258	0.18163	-10.33972
C	0.20831	-0.06239	-9.10820
H	0.19905	-0.05623	-11.26703
H	-2.19798	1.12037	-11.04635
H	0.09720	1.51449	-4.95459
H	-1.15161	-0.85595	-4.93704
H	-1.72505	-1.53675	-7.40212
H	0.29508	2.35656	-7.42859
H	-2.76766	1.42685	-8.50657
H	1.14429	-0.52398	-8.86773

6-311++G(d,p)
Electronic energy: -345.4746208
Hartree

C	-1.22934	-0.64548	-7.08327
C	-0.76334	0.43067	-8.05125
C	-0.15117	1.44406	-7.09702
C	-0.25542	1.00292	-5.82092
C	-0.93137	-0.28753	-5.81166
C	-1.88375	0.98735	-8.91557
C	-1.58416	0.82507	-10.22623
C	-0.28239	0.18223	-10.34621
C	0.21092	-0.06324	-9.10915
H	0.20062	-0.05541	-11.27561
H	-2.20084	1.12010	-11.05462
H	0.09995	1.51509	-4.94630
H	-1.15308	-0.85710	-4.92848
H	-1.72863	-1.54055	-7.40231
H	0.29861	2.36038	-7.42908
H	-2.77274	1.42781	-8.50581
H	1.14942	-0.52497	-8.86781

HF, triplet

6-31+G(d,p)
Electronic energy: -345.3847523
Hartree

C	-1.30897	-0.35735	-7.52020
C	-0.25986	0.59553	-8.08415
C	0.25751	1.35589	-6.91876
C	-0.44875	0.98047	-5.76841
C	-1.37582	-0.01722	-6.06524
C	-1.72626	0.72471	-8.48373
C	-1.75036	0.35479	-9.93275
C	-0.45633	0.08441	-10.37472
C	0.46470	0.24186	-9.33070
H	-0.20365	-0.23247	-11.36983
H	-2.64449	0.28556	-10.52325
H	-0.31646	1.42341	-4.79845
H	-2.06193	-0.46544	-5.37148
H	-1.36060	-1.38454	-7.84025
H	1.02385	2.10582	-6.97540
H	-2.33513	1.53562	-8.12052
H	1.52582	0.09033	-9.39348

6-311++G(d,p)
Electronic energy: -345.4373234
Hartree

C	-1.30753	-0.36002	-7.52332
C	-0.25845	0.59600	-8.08424
C	0.25916	1.34958	-6.91567
C	-0.44637	0.96958	-5.76802
C	-1.37173	-0.02629	-6.06728
C	-1.72631	0.72783	-8.48070
C	-1.75220	0.36461	-9.93085
C	-0.46090	0.09459	-10.37497
C	0.46193	0.24780	-9.33372
H	-0.21023	-0.21944	-11.37142
H	-2.64709	0.29730	-10.52030
H	-0.31386	1.40908	-4.79660
H	-2.05743	-0.47656	-5.37455
H	-1.35940	-1.38478	-7.84897
H	1.02448	2.10069	-6.96859
H	-2.33329	1.53685	-8.11200
H	1.52250	0.09459	-9.40011

Aug-cc-pVTZ
Electronic energy: -345.4732388
Hartree

C	-1.60532	-0.56289	-6.83891
C	-1.26744	0.26560	-8.01831
C	-0.14226	1.18493	-7.56152
C	0.13885	0.75588	-6.16041
C	-0.73404	-0.25801	-5.79182
C	-2.16436	0.68975	-9.11703
C	-1.41136	0.91674	-10.27026
C	-0.07286	0.62698	-10.04617
C	0.11997	0.16902	-8.63929
H	0.72088	0.73934	-10.75676
H	-1.80785	1.29400	-11.19205
H	0.92310	1.16024	-5.55294
H	-0.72031	-0.76060	-4.84502
H	-2.37313	-1.30970	-6.82373
H	-0.13277	2.22710	-7.82099
H	-3.21995	0.83949	-9.01306
H	0.77213	-0.65648	-8.42305

HF, quintuplet

6-31+G(d,p)
Electronic energy: -345.304672 Hartree

C	-1.14203	-0.63040	-7.00551
C	-0.75627	0.40911	-8.05248
C	-0.07453	1.45646	-7.16043
C	-0.38420	1.11024	-5.72520
C	-0.95488	-0.13562	-5.69876
C	-1.95436	0.93668	-8.85480
C	-1.54851	0.98955	-10.30674
C	-0.35369	0.33172	-10.44165
C	0.13328	-0.08799	-9.18700
H	0.15748	0.16596	-11.37275
H	-2.11938	1.45087	-11.08887
H	-0.16985	1.73635	-4.88112
H	-1.23794	-0.66561	-4.80730
H	-1.53197	-1.59997	-7.25730
H	0.88787	1.85483	-7.43708
H	-2.95636	0.65909	-8.57127
H	1.02860	-0.65987	-9.02304

6-311++G(d,p)
Electronic energy: -345.358243 Hartree

C	-1.14704	-0.62781	-7.00735
C	-0.75704	0.41133	-8.05236
C	-0.07537	1.45615	-7.15847
C	-0.38101	1.10439	-5.72370
C	-0.95565	-0.13672	-5.70046
C	-1.95148	0.94255	-8.85639
C	-1.54581	0.98682	-10.30869
C	-0.35348	0.32941	-10.44017
C	0.13321	-0.08712	-9.18502
H	0.15732	0.15974	-11.37071
H	-2.11714	1.44274	-11.09356
H	-0.15996	1.72512	-4.87745
H	-1.23828	-0.66836	-4.80990
H	-1.54057	-1.59562	-7.26007
H	0.88382	1.86154	-7.43656
H	-2.95612	0.67685	-8.57033
H	1.02788	-0.65962	-9.02011

Aug-cc-pVTZ
Electronic energy: -345.3929722 Hartree

C	-1.39199	-0.64036	-6.99770
C	-0.94254	0.37364	-8.03987
C	-0.38297	1.46907	-7.12650
C	-0.28852	0.90633	-5.73390
C	-0.93285	-0.29433	-5.71431
C	-2.02226	0.87201	-8.98968
C	-1.58947	0.82675	-10.32695
C	-0.35367	0.26006	-10.42091
C	0.06191	-0.19439	-9.04771
H	0.22666	0.13434	-11.31108
H	-2.15842	1.20154	-11.15540
H	0.19027	1.38918	-4.90770
H	-1.06652	-0.90605	-4.84342
H	-0.64422	2.49857	-7.29269
H	-1.96673	-1.51280	-7.23949
H	-2.97673	1.22881	-8.65553
H	0.49488	-1.16599	-8.89188

M06-2X, closed-shell singlet

6-31+G(d,p)
Electronic energy: -347.5534581
Hartree

C	-1.22534	-0.65093	-7.09480
C	-0.76339	0.43067	-8.05125
C	-0.15692	1.45023	-7.10747
C	-0.26069	1.01563	-5.84053
C	-0.92913	-0.29894	-5.83260
C	-1.88241	0.99457	-8.90440
C	-1.58663	0.83640	-10.20527
C	-0.27681	0.16961	-10.32661
C	0.21118	-0.07119	-9.09834
H	0.20414	-0.08056	-11.26506
H	-2.20249	1.14457	-11.04213
H	0.08672	1.53704	-4.95621
H	-1.14143	-0.87833	-4.94163
H	-1.71677	-1.55468	-7.43408
H	0.28211	2.37648	-7.45775
H	-2.76790	1.44741	-8.47519
H	1.14905	-0.54660	-8.83802

6-311++G(d,p)
Electronic energy: -347.6232343
Hartree

C	-1.22495	-0.65004	-7.09516
C	-0.76343	0.43071	-8.05124
C	-0.15741	1.44940	-7.10780
C	-0.26102	1.01561	-5.84443
C	-0.92933	-0.29871	-5.83651
C	-1.88155	0.99414	-8.90415
C	-1.58621	0.83621	-10.20140
C	-0.27663	0.16954	-10.32268
C	0.21033	-0.07075	-9.09787
H	0.20353	-0.08026	-11.25946
H	-2.20102	1.14384	-11.03679
H	0.08586	1.53612	-4.96168
H	-1.14125	-0.87714	-4.94712
H	-1.71551	-1.55219	-7.43371
H	0.28084	2.37404	-7.45730
H	-2.76551	1.44619	-8.47588
H	1.14653	-0.54532	-8.83812

Aug-cc-pVTZ
Electronic energy: -347.659787 Hartree

C	-1.22365	-0.64738	-7.09574
C	-0.76344	0.43070	-8.05124
C	-0.15880	1.44678	-7.10835
C	-0.26191	1.01458	-5.84845
C	-0.92904	-0.29742	-5.84055
C	-1.87887	0.99278	-8.90383
C	-1.58474	0.83549	-10.19748
C	-0.27748	0.17000	-10.31854
C	0.20774	-0.06943	-9.09706
H	0.20223	-0.07955	-11.25326
H	-2.19880	1.14275	-11.03092
H	0.08450	1.53455	-4.96770
H	-1.14080	-0.87518	-4.95317
H	-1.71334	-1.54804	-7.43285
H	0.27877	2.36982	-7.45642
H	-2.76140	1.44410	-8.47713
H	1.14230	-0.54316	-8.83859

M06-2X, restricted open shell singlet

6-31+G(d,p)
Electronic energy: -347.5534581
Hartree

C	-1.22534	-0.65093	-7.09480
C	-0.76339	0.43067	-8.05125
C	-0.15692	1.45023	-7.10747
C	-0.26069	1.01563	-5.84053
C	-0.92913	-0.29894	-5.83260
C	-1.88241	0.99457	-8.90440
C	-1.58663	0.83640	-10.20527
C	-0.27681	0.16961	-10.32661
C	0.21118	-0.07119	-9.09834
H	0.20414	-0.08056	-11.26506
H	-2.20249	1.14457	-11.04213
H	0.08672	1.53704	-4.95621
H	-1.14143	-0.87833	-4.94163
H	-1.71677	-1.55468	-7.43408
H	0.28211	2.37648	-7.45775
H	-2.76790	1.44741	-8.47519
H	1.14905	-0.54660	-8.83802

6-311++G(d,p)
Electronic energy: -347.6232343
Hartree

C	-1.22495	-0.65004	-7.09516
C	-0.76343	0.43071	-8.05124
C	-0.15741	1.44940	-7.10780
C	-0.26102	1.01561	-5.84443
C	-0.92933	-0.29871	-5.83651
C	-1.88155	0.99414	-8.90415
C	-1.58621	0.83621	-10.20140
C	-0.27663	0.16954	-10.32268
C	0.21033	-0.07075	-9.09787
H	0.20353	-0.08026	-11.25946
H	-2.20102	1.14384	-11.03679
H	0.08586	1.53612	-4.96168
H	-1.14125	-0.87714	-4.94712
H	-1.71551	-1.55219	-7.43371
H	0.28084	2.37404	-7.45730
H	-2.76551	1.44619	-8.47588
H	1.14653	-0.54532	-8.83812

Aug-cc-pVTZ
Electronic energy: -347.659787 Hartree

C	-1.22365	-0.64738	-7.09574
C	-0.76344	0.43070	-8.05124
C	-0.15880	1.44678	-7.10835
C	-0.26192	1.01458	-5.84845
C	-0.92904	-0.29742	-5.84055
C	-1.87887	0.99278	-8.90383
C	-1.58474	0.83549	-10.19748
C	-0.27748	0.17000	-10.31854
C	0.20774	-0.06943	-9.09706
H	0.20223	-0.07955	-11.25326
H	-2.19880	1.14274	-11.03092
H	0.08450	1.53455	-4.96770
H	-1.14080	-0.87518	-4.95317
H	-1.71333	-1.54804	-7.43285
H	0.27877	2.36982	-7.45642
H	-2.76140	1.44410	-8.47713
H	1.14230	-0.54316	-8.83860

M06-2X, triplet

6-31+G(d,p)
Electronic energy: -347.4630957
Hartree

C	-1.22080	-0.63907	-7.11008
C	-0.76566	0.43164	-8.08062
C	-0.16392	1.43944	-7.12260
C	-0.28049	0.96003	-5.75063
C	-0.89542	-0.24934	-5.74335
C	-1.88387	0.99511	-8.93899
C	-1.58799	0.83688	-10.24242
C	-0.28097	0.17150	-10.36344
C	0.20742	-0.06949	-9.13262
H	0.19648	-0.07692	-11.30442
H	-2.20071	1.14346	-11.08247
H	0.07541	1.50086	-4.88266
H	-1.11849	-0.84718	-4.86850
H	-1.71373	-1.54994	-7.42166
H	0.28007	2.37136	-7.44531
H	-2.76968	1.44814	-8.50953
H	1.14563	-0.54508	-8.87203

6-311++G(d,p)
Electronic energy: -347.5329538
Hartree

C	-1.22089	-0.63868	-7.11165
C	-0.76580	0.43166	-8.08098
C	-0.16432	1.43921	-7.12422
C	-0.28140	0.95860	-5.75386
C	-0.89481	-0.24777	-5.74655
C	-1.88302	0.99465	-8.93879
C	-1.58746	0.83668	-10.23863
C	-0.28081	0.17149	-10.35953
C	0.20652	-0.06906	-9.13212
H	0.19592	-0.07653	-11.29878
H	-2.19911	1.14277	-11.07719
H	0.07360	1.49747	-4.88666
H	-1.11684	-0.84369	-4.87246
H	-1.71307	-1.54823	-7.42229
H	0.27900	2.36978	-7.44602
H	-2.76712	1.44677	-8.50994
H	1.14289	-0.54375	-8.87166

Aug-cc-pVTZ
Electronic energy: -347.569001 Hartree

C	-1.21948	-0.63570	-7.11233
C	-0.76586	0.43169	-8.08137
C	-0.16589	1.43631	-7.12486
C	-0.28247	0.95707	-5.75749
C	-0.89423	-0.24603	-5.75021
C	-1.88032	0.99327	-8.93882
C	-1.58603	0.83596	-10.23503
C	-0.28166	0.17195	-10.35569
C	0.20384	-0.06769	-9.13161
H	0.19459	-0.07581	-11.29288
H	-2.19687	1.14164	-11.07167
H	0.07172	1.49451	-4.89164
H	-1.11558	-0.84047	-4.87749
H	-1.71074	-1.54358	-7.42149
H	0.27666	2.36515	-7.44516
H	-2.76296	1.44465	-8.51136
H	1.13857	-0.54152	-8.87221

M06-2X, quintuplet

6-31+G(d,p)
Electronic energy: -347.3682796
Hartree

C	-1.21582	-0.63635	-7.05604
C	-0.76417	0.43110	-8.05117
C	-0.16305	1.43437	-7.06844
C	-0.27527	0.95754	-5.69668
C	-0.89005	-0.25169	-5.68944
C	-1.87038	0.98824	-8.94526
C	-1.54459	0.81398	-10.35423
C	-0.33969	0.20065	-10.46502
C	0.19293	-0.06204	-9.13499
H	0.16159	-0.05989	-11.38896
H	-2.17753	1.13087	-11.17386
H	0.08190	1.49746	-4.82850
H	-1.11162	-0.85008	-4.81443
H	-1.71176	-1.54957	-7.36106
H	0.28110	2.37020	-7.38455
H	-2.76790	1.44763	-8.54980
H	1.13760	-0.54103	-8.90888

Aug-cc-pVTZ
Electronic energy: -347.4736683
Hartree

C	-1.21561	-0.63236	-7.05788
C	-0.76502	0.43154	-8.05110
C	-0.16612	1.43182	-7.07021
C	-0.27595	0.95393	-5.70346
C	-0.88760	-0.24908	-5.69627
C	-1.86725	0.98669	-8.94435
C	-1.54048	0.81191	-10.34833
C	-0.34169	0.20169	-10.45768
C	0.18968	-0.06035	-9.13201
H	0.15694	-0.05751	-11.37878
H	-2.16947	1.12676	-11.16652
H	0.08087	1.48980	-4.83759
H	-1.10615	-0.84483	-4.82362
H	-1.71206	-1.54128	-7.36080
H	0.27422	2.36557	-7.38417
H	-2.76196	1.44462	-8.55174
H	1.13092	-0.53753	-8.90680

6-311++G(d,p)
Electronic energy: -347.4380936
Hartree

C	-1.21602	-0.63593	-7.05755
C	-0.76431	0.43122	-8.05116
C	-0.16350	1.43428	-7.06986
C	-0.27604	0.95599	-5.69983
C	-0.88931	-0.25024	-5.69265
C	-1.87003	0.98817	-8.94393
C	-1.54281	0.81301	-10.35130
C	-0.34087	0.20118	-10.46166
C	0.19279	-0.06188	-9.13334
H	0.15865	-0.05857	-11.38453
H	-2.17378	1.12879	-11.17034
H	0.08036	1.49391	-4.83248
H	-1.10976	-0.84689	-4.81853
H	-1.71151	-1.54754	-7.36193
H	0.27954	2.36886	-7.38525
H	-2.76612	1.44702	-8.54935
H	1.13600	-0.53999	-8.90762

PBE0, closed-shell singlet

6-31+G(d,p)
Electronic energy: -347.2944869
Hartree

C	-1.22480	-0.64961	-7.09664
C	-0.76333	0.43068	-8.05125
C	-0.15764	1.44903	-7.10924
C	-0.26236	1.01240	-5.84047
C	-0.92752	-0.29569	-5.83262
C	-1.88098	0.99388	-8.90269
C	-1.58343	0.83472	-10.20558
C	-0.28005	0.17123	-10.32635
C	0.21010	-0.07059	-9.09645
H	0.20188	-0.07949	-11.26534
H	-2.20044	1.14340	-11.04274
H	0.08558	1.53484	-4.95570
H	-1.14041	-0.87614	-4.94123
H	-1.71655	-1.55423	-7.43387
H	0.28198	2.37604	-7.45746
H	-2.76744	1.44720	-8.47541
H	1.14868	-0.54629	-8.83828

Aug-cc-pVTZ
Electronic energy: -347.3694059
Hartree

C	-1.22296	-0.64576	-7.09789
C	-0.76333	0.43068	-8.05125
C	-0.15967	1.44526	-7.11044
C	-0.26375	1.01113	-5.84856
C	-0.92736	-0.29389	-5.84072
C	-1.87709	0.99191	-8.90181
C	-1.58129	0.83368	-10.19762
C	-0.28097	0.17175	-10.31811
C	0.20641	-0.06870	-9.09487
H	0.20046	-0.07870	-11.25400
H	-2.19733	1.14189	-11.03182
H	0.08358	1.53294	-4.96682
H	-1.14010	-0.87351	-4.95237
H	-1.71344	-1.54835	-7.43258
H	0.27908	2.37007	-7.45610
H	-2.76164	1.44424	-8.47728
H	1.14268	-0.54324	-8.83906

6-311++G(d,p)
Electronic energy: -347.3529092
Hartree

C	-1.22422	-0.64830	-7.09750
C	-0.76333	0.43068	-8.05125
C	-0.15836	1.44777	-7.11009
C	-0.26296	1.01206	-5.84510
C	-0.92762	-0.29506	-5.83725
C	-1.87964	0.99320	-8.90195
C	-1.58259	0.83432	-10.20099
C	-0.28018	0.17133	-10.32167
C	0.20889	-0.06997	-9.09547
H	0.20137	-0.07919	-11.25958
H	-2.19906	1.14274	-11.03716
H	0.08467	1.53408	-4.96137
H	-1.14036	-0.87502	-4.94690
H	-1.71544	-1.55204	-7.43393
H	0.28087	2.37385	-7.45749
H	-2.76526	1.44609	-8.47557
H	1.14651	-0.54519	-8.83803

PBE0, restricted open shell singlet

PBE0/6-31+G(d,p)
Electronic energy: -347.2944869
Hartree

C	-1.22480	-0.64961	-7.09664
C	-0.76333	0.43068	-8.05125
C	-0.15764	1.44903	-7.10924
C	-0.26236	1.01240	-5.84047
C	-0.92752	-0.29569	-5.83262
C	-1.88098	0.99388	-8.90269
C	-1.58343	0.83472	-10.20558
C	-0.28005	0.17123	-10.32635
C	0.21010	-0.07059	-9.09645
H	0.20188	-0.07949	-11.26534
H	-2.20044	1.14340	-11.04274
H	0.08558	1.53484	-4.95570
H	-1.14041	-0.87614	-4.94123
H	-1.71655	-1.55423	-7.43387
H	0.28198	2.37604	-7.45746
H	-2.76744	1.44720	-8.47541
H	1.14868	-0.54629	-8.83828

Aug-cc-pVTZ
Electronic energy: -347.3694059
Hartree

C	-1.22296	-0.64576	-7.09789
C	-0.76333	0.43068	-8.05125
C	-0.15967	1.44526	-7.11044
C	-0.26375	1.01113	-5.84856
C	-0.92736	-0.29389	-5.84072
C	-1.87709	0.99191	-8.90181
C	-1.58129	0.83368	-10.19762
C	-0.28097	0.17175	-10.31811
C	0.20641	-0.06870	-9.09487
H	0.20046	-0.07870	-11.25400
H	-2.19733	1.14189	-11.03182
H	0.08358	1.53294	-4.96682
H	-1.14010	-0.87351	-4.95237
H	-1.71344	-1.54835	-7.43258
H	0.27908	2.37007	-7.45610
H	-2.76164	1.44424	-8.47728
H	1.14268	-0.54324	-8.83906

6-311++G(d,p)
Electronic energy: -347.3529092
Hartree

C	-1.22422	-0.64830	-7.09750
C	-0.76333	0.43068	-8.05125
C	-0.15836	1.44777	-7.11009
C	-0.26296	1.01206	-5.84510
C	-0.92762	-0.29506	-5.83725
C	-1.87964	0.99320	-8.90195
C	-1.58259	0.83432	-10.20099
C	-0.28018	0.17133	-10.32167
C	0.20889	-0.06997	-9.09547
H	0.20137	-0.07919	-11.25958
H	-2.19906	1.14274	-11.03716
H	0.08467	1.53408	-4.96137
H	-1.14036	-0.87502	-4.94690
H	-1.71544	-1.55204	-7.43393
H	0.28087	2.37385	-7.45749
H	-2.76526	1.44609	-8.47557
H	1.14651	-0.54519	-8.83803

PBE0, triplet

6-31+G(d,p)
Electronic energy: -347.2152273
Hartree

C	-1.22042	-0.63843	-7.11041
C	-0.76555	0.43162	-8.08002
C	-0.16417	1.43876	-7.12290
C	-0.28003	0.96225	-5.75611
C	-0.89700	-0.25106	-5.74881
C	-1.88129	0.99383	-8.93398
C	-1.58386	0.83474	-10.24113
C	-0.28497	0.17354	-10.36147
C	0.20565	-0.06852	-9.12732
H	0.19344	-0.07539	-11.30304
H	-2.19775	1.14184	-11.08150
H	0.07584	1.50303	-4.88675
H	-1.12009	-0.84886	-4.87261
H	-1.71373	-1.55072	-7.42223
H	0.28085	2.37178	-7.44581
H	-2.76829	1.44743	-8.50736
H	1.14467	-0.54445	-8.86987

6-311++G(d,p)
Electronic energy: -347.2729566
Hartree

C	-1.22012	-0.63750	-7.11228
C	-0.76556	0.43162	-8.08016
C	-0.16476	1.43794	-7.12476
C	-0.28114	0.96087	-5.76042
C	-0.89655	-0.24939	-5.75314
C	-1.87990	0.99313	-8.93313
C	-1.58295	0.83430	-10.23651
C	-0.28518	0.17367	-10.35674
C	0.20441	-0.06789	-9.12623
H	0.19287	-0.07506	-11.29722
H	-2.19631	1.14115	-11.07587
H	0.07389	1.50000	-4.89118
H	-1.11881	-0.84554	-4.87707
H	-1.71291	-1.54890	-7.42341
H	0.27984	2.37004	-7.44698
H	-2.76593	1.44623	-8.50706
H	1.14238	-0.54329	-8.86914

Aug-cc-pVTZ
Electronic energy: -347.2892894
Hartree

C	-1.21879	-0.63478	-7.11285
C	-0.76558	0.43163	-8.08049
C	-0.16617	1.43526	-7.12531
C	-0.28217	0.95943	-5.76365
C	-0.89602	-0.24775	-5.75639
C	-1.87732	0.99182	-8.93313
C	-1.58162	0.83365	-10.23332
C	-0.28600	0.17411	-10.35336
C	0.20187	-0.06660	-9.12576
H	0.19185	-0.07450	-11.29185
H	-2.19449	1.14026	-11.07076
H	0.07216	1.49743	-4.89572
H	-1.11778	-0.84267	-4.88164
H	-1.71077	-1.54489	-7.42231
H	0.27787	2.36595	-7.44583
H	-2.76221	1.44433	-8.50879
H	1.13845	-0.54130	-8.87017

PBE0, quintuplet

6-31+G(d,p)
Electronic energy: -347.1291115
Hartree

C	-1.21363	-0.63524	-7.05525
C	-0.76333	0.43065	-8.05125
C	-0.16249	1.43191	-7.06770
C	-0.27604	0.95986	-5.69923
C	-0.89243	-0.25232	-5.69193
C	-1.86846	0.98721	-8.94560
C	-1.54637	0.81504	-10.35095
C	-0.33855	0.20020	-10.46289
C	0.19125	-0.06127	-9.13648
H	0.16262	-0.06018	-11.38819
H	-2.18024	1.13245	-11.17107
H	0.07993	1.50096	-4.82996
H	-1.11572	-0.85037	-4.81579
H	-1.70819	-1.55188	-7.35729
H	0.28537	2.36859	-7.38091
H	-2.76841	1.44715	-8.55240
H	1.13796	-0.54136	-8.91442

Aug-cc-pVTZ
Electronic energy: -347.2020709
Hartree

C	-1.21196	-0.63157	-7.05739
C	-0.76335	0.43062	-8.05125
C	-0.16449	1.42837	-7.06985
C	-0.27815	0.95706	-5.70664
C	-0.89142	-0.24900	-5.69935
C	-1.86472	0.98527	-8.94379
C	-1.54273	0.81329	-10.34383
C	-0.34101	0.20155	-10.45519
C	0.18780	-0.05956	-9.13400
H	0.15755	-0.05742	-11.37873
H	-2.17372	1.12931	-11.16268
H	0.07631	1.49547	-4.83887
H	-1.11342	-0.84423	-4.82472
H	-1.70519	-1.54607	-7.35692
H	0.28242	2.36273	-7.38056
H	-2.76268	1.44408	-8.55330
H	1.13205	-0.53851	-8.91423

6-311++G(d,p)
Electronic energy: -347.1860142
Hartree

C	-1.21335	-0.63435	-7.05709
C	-0.76334	0.43063	-8.05125
C	-0.16306	1.43113	-7.06958
C	-0.27714	0.95849	-5.70363
C	-0.89197	-0.25064	-5.69632
C	-1.86750	0.98669	-8.94381
C	-1.54449	0.81415	-10.34671
C	-0.33971	0.20087	-10.45836
C	0.19054	-0.06095	-9.13453
H	0.15988	-0.05865	-11.38334
H	-2.17673	1.13079	-11.16681
H	0.07801	1.49800	-4.83452
H	-1.11444	-0.84706	-4.82034
H	-1.70740	-1.55010	-7.35847
H	0.28437	2.36687	-7.38215
H	-2.76662	1.44612	-8.55136
H	1.13625	-0.54062	-8.91305

PBE0[GD3BJ], closed-shell singlet

6-31+G(d,p)
Electronic energy: -347.4017529
Hartree

C	-1.22506	-0.64984	-7.09813
C	-0.76333	0.43068	-8.05125
C	-0.15762	1.44936	-7.11074
C	-0.26243	1.01256	-5.84213
C	-0.92770	-0.29575	-5.83427
C	-1.88114	0.99397	-8.90117
C	-1.58342	0.83472	-10.20391
C	-0.27982	0.17112	-10.32470
C	0.21049	-0.07078	-9.09498
H	0.20170	-0.07938	-11.26377
H	-2.20002	1.14320	-11.04123
H	0.08531	1.53459	-4.95724
H	-1.14037	-0.87580	-4.94277
H	-1.71655	-1.55364	-7.43714
H	0.28149	2.37566	-7.46073
H	-2.76671	1.44685	-8.47218
H	1.14845	-0.54615	-8.83496

Aug-cc-pVTZ
Electronic energy: -347.3852495
Hartree

C	-1.22324	-0.64605	-7.09934
C	-0.76333	0.43068	-8.05125
C	-0.15961	1.44565	-7.11190
C	-0.26380	1.01132	-5.85015
C	-0.92755	-0.29398	-5.84232
C	-1.87732	0.99203	-8.90033
C	-1.58131	0.83369	-10.19601
C	-0.28070	0.17162	-10.31653
C	0.20685	-0.06892	-9.09345
H	0.20028	-0.07860	-11.25252
H	-2.19693	1.14169	-11.03039
H	0.08332	1.53269	-4.96828
H	-1.14007	-0.87317	-4.95383
H	-1.71347	-1.54781	-7.43583
H	0.27861	2.36975	-7.45934
H	-2.76096	1.44392	-8.47407
H	1.14250	-0.54313	-8.83577

6-311++G(d,p)
Electronic energy: -347.3109719
Hartree

C	-1.22448	-0.64855	-7.09897
C	-0.76333	0.43068	-8.05125
C	-0.15832	1.44812	-7.11156
C	-0.26302	1.01223	-5.84672
C	-0.92781	-0.29512	-5.83887
C	-1.87982	0.99330	-8.90045
C	-1.58259	0.83433	-10.19936
C	-0.27994	0.17122	-10.32006
C	0.20930	-0.07017	-9.09403
H	0.20119	-0.07909	-11.25805
H	-2.19866	1.14254	-11.03568
H	0.08440	1.53384	-4.96287
H	-1.14032	-0.87468	-4.94841
H	-1.71545	-1.55146	-7.43719
H	0.28038	2.37349	-7.46075
H	-2.76454	1.44574	-8.47235
H	1.14628	-0.54505	-8.83472

PBE0[GD3BJ], restricted open shell singlet

6-31+G(d,p)
Electronic energy: -347.4017529
Hartree

C	-1.22506	-0.64984	-7.09813
C	-0.76333	0.43068	-8.05125
C	-0.15762	1.44936	-7.11074
C	-0.26243	1.01256	-5.84213
C	-0.92770	-0.29575	-5.83427
C	-1.88114	0.99397	-8.90117
C	-1.58342	0.83472	-10.20391
C	-0.27982	0.17112	-10.32470
C	0.21049	-0.07078	-9.09498
H	0.20170	-0.07938	-11.26377
H	-2.20002	1.14320	-11.04123
H	0.08531	1.53459	-4.95724
H	-1.14037	-0.87580	-4.94277
H	-1.71655	-1.55364	-7.43714
H	0.28149	2.37566	-7.46073
H	-2.76671	1.44685	-8.47218
H	1.14845	-0.54615	-8.83496

Aug-cc-pVTZ
Electronic energy: -347.3852495
Hartree

C	-1.22324	-0.64605	-7.09934
C	-0.76333	0.43068	-8.05125
C	-0.15961	1.44565	-7.11190
C	-0.26380	1.01132	-5.85015
C	-0.92755	-0.29398	-5.84232
C	-1.87732	0.99203	-8.90033
C	-1.58131	0.83369	-10.19601
C	-0.28070	0.17162	-10.31653
C	0.20685	-0.06892	-9.09345
H	0.20028	-0.07860	-11.25252
H	-2.19693	1.14169	-11.03039
H	0.08332	1.53269	-4.96828
H	-1.14007	-0.87317	-4.95383
H	-1.71347	-1.54781	-7.43583
H	0.27861	2.36975	-7.45934
H	-2.76096	1.44392	-8.47407
H	1.14250	-0.54313	-8.83577

6-311++G(d,p)
Electronic energy: -347.3109719
Hartree

C	-1.22448	-0.64855	-7.09897
C	-0.76333	0.43068	-8.05125
C	-0.15832	1.44812	-7.11156
C	-0.26302	1.01223	-5.84672
C	-0.92781	-0.29512	-5.83887
C	-1.87982	0.99330	-8.90045
C	-1.58259	0.83433	-10.19936
C	-0.27994	0.17122	-10.32006
C	0.20930	-0.07017	-9.09403
H	0.20119	-0.07909	-11.25805
H	-2.19866	1.14254	-11.03568
H	0.08440	1.53384	-4.96287
H	-1.14032	-0.87468	-4.94841
H	-1.71545	-1.55146	-7.43719
H	0.28038	2.37349	-7.46075
H	-2.76454	1.44574	-8.47235
H	1.14628	-0.54505	-8.83472

PBE0[GD3BJ], triplet

6-31+G(d,p)
Electronic energy: -347.3213069
Hartree

C	-1.22080	-0.63887	-7.11196
C	-0.76554	0.43162	-8.07993
C	-0.16404	1.43930	-7.12446
C	-0.28014	0.96239	-5.75806
C	-0.89718	-0.25107	-5.75077
C	-1.88139	0.99390	-8.93229
C	-1.58380	0.83472	-10.23936
C	-0.28476	0.17344	-10.35971
C	0.20601	-0.06870	-9.12568
H	0.19325	-0.07528	-11.30135
H	-2.19730	1.14162	-11.07988
H	0.07550	1.50266	-4.88851
H	-1.12000	-0.84838	-4.87437
H	-1.71386	-1.55037	-7.42553
H	0.28047	2.37165	-7.44912
H	-2.76750	1.44705	-8.50396
H	1.14439	-0.54429	-8.86637

Aug-cc-pVTZ
Electronic energy: -347.3049675
Hartree

C	-1.21920	-0.63529	-7.11438
C	-0.76558	0.43162	-8.08038
C	-0.16601	1.43587	-7.12684
C	-0.28227	0.95958	-5.76556
C	-0.89620	-0.24777	-5.75829
C	-1.87749	0.99192	-8.93148
C	-1.58160	0.83365	-10.23160
C	-0.28576	0.17401	-10.35165
C	0.20229	-0.06680	-9.12416
H	0.19166	-0.07439	-11.29023
H	-2.19405	1.14004	-11.06921
H	0.07182	1.49705	-4.89741
H	-1.11768	-0.84218	-4.88333
H	-1.71093	-1.54460	-7.42560
H	0.27753	2.36588	-7.44913
H	-2.76147	1.44397	-8.50540
H	1.13823	-0.54117	-8.86668

6-311++G(d,p)
Electronic energy: -347.2315468
Hartree

C	-1.22050	-0.63796	-7.11381
C	-0.76555	0.43162	-8.08006
C	-0.16462	1.43850	-7.12630
C	-0.28124	0.96100	-5.76235
C	-0.89673	-0.24940	-5.75507
C	-1.88003	0.99321	-8.93147
C	-1.58290	0.83429	-10.23477
C	-0.28496	0.17357	-10.35501
C	0.20479	-0.06807	-9.12461
H	0.19268	-0.07495	-11.29556
H	-2.19587	1.14094	-11.07428
H	0.07355	1.49963	-4.89291
H	-1.11872	-0.84506	-4.87881
H	-1.71305	-1.54856	-7.42671
H	0.27947	2.36992	-7.45029
H	-2.76515	1.44585	-8.50366
H	1.14211	-0.54314	-8.86563

PBE0[GD3BJ], quintuplet

6-31+G(d,p)
Electronic energy: -347.2337374
Hartree

C	-1.21396	-0.63559	-7.05684
C	-0.76333	0.43065	-8.05125
C	-0.16241	1.43237	-7.06930
C	-0.27616	0.95998	-5.70119
C	-0.89260	-0.25231	-5.69388
C	-1.86874	0.98737	-8.94396
C	-1.54627	0.81500	-10.34900
C	-0.33834	0.20011	-10.46094
C	0.19177	-0.06153	-9.13491
H	0.16236	-0.06003	-11.38636
H	-2.17971	1.13220	-11.16932
H	0.07959	1.50062	-4.83174
H	-1.11565	-0.84991	-4.81758
H	-1.70829	-1.55148	-7.36057
H	0.28497	2.36841	-7.38419
H	-2.76787	1.44689	-8.54915
H	1.13791	-0.54133	-8.91111

Aug-cc-pVTZ
Electronic energy: -347.2176743
Hartree

C	-1.21233	-0.63200	-7.05897
C	-0.76335	0.43061	-8.05125
C	-0.16437	1.42890	-7.07145
C	-0.27825	0.95720	-5.70857
C	-0.89160	-0.24900	-5.70127
C	-1.86509	0.98545	-8.94215
C	-1.54264	0.81328	-10.34190
C	-0.34079	0.20147	-10.45327
C	0.18839	-0.05987	-9.13245
H	0.15730	-0.05723	-11.37694
H	-2.17316	1.12908	-11.16098
H	0.07598	1.49513	-4.84063
H	-1.11333	-0.84376	-4.82646
H	-1.70533	-1.54574	-7.36020
H	0.28204	2.36260	-7.38388
H	-2.76223	1.44380	-8.55003
H	1.13204	-0.53856	-8.91092

6-311++G(d,p)
Electronic energy: -347.1451531
Hartree

C	-1.21369	-0.63473	-7.05868
C	-0.76335	0.43062	-8.05125
C	-0.16297	1.43161	-7.07118
C	-0.27725	0.95862	-5.70557
C	-0.89214	-0.25063	-5.69825
C	-1.86782	0.98685	-8.94218
C	-1.54439	0.81414	-10.34477
C	-0.33950	0.20079	-10.45642
C	0.19108	-0.06123	-9.13298
H	0.15964	-0.05848	-11.38152
H	-2.17618	1.13056	-11.16507
H	0.07768	1.49767	-4.83630
H	-1.11437	-0.84660	-4.82212
H	-1.70751	-1.54971	-7.36175
H	0.28397	2.36670	-7.38545
H	-2.76611	1.44584	-8.54810
H	1.13620	-0.54062	-8.90972

PBEPBE, closed-shell singlet

6-31+G(d,p)
Electronic energy: -347.2564637
Hartree

C	-1.22822	-0.65731	-7.09125
C	-0.76332	0.43069	-8.05125
C	-0.15341	1.45638	-7.10394
C	-0.26000	1.01397	-5.82367
C	-0.92732	-0.29837	-5.81579
C	-1.88888	0.99787	-8.90734
C	-1.58683	0.83634	-10.22220
C	-0.27922	0.17070	-10.34336
C	0.21720	-0.07423	-9.10249
H	0.20608	-0.08177	-11.28934
H	-2.20821	1.14721	-11.06563
H	0.09041	1.54008	-4.93229
H	-1.14168	-0.88292	-4.91775
H	-1.72324	-1.56757	-7.43278
H	0.28883	2.38932	-7.45653
H	-2.78078	1.45399	-8.47519
H	1.16187	-0.55300	-8.84052

Aug-cc-pVTZ
Electronic energy: -347.3496508
Hartree

C	-1.22625	-0.65314	-7.09288
C	-0.76332	0.43069	-8.05125
C	-0.15562	1.45232	-7.10552
C	-0.26162	1.01246	-5.83289
C	-0.92710	-0.29625	-5.82504
C	-1.88466	0.99573	-8.90611
C	-1.58432	0.83512	-10.21313
C	-0.28032	0.17132	-10.33396
C	0.21322	-0.07220	-9.10050
H	0.20397	-0.08063	-11.27640
H	-2.20418	1.14524	-11.05325
H	0.08789	1.53742	-4.94494
H	-1.14108	-0.87943	-4.93043
H	-1.71972	-1.56086	-7.43165
H	0.28549	2.38253	-7.45531
H	-2.77414	1.45060	-8.47699
H	1.15506	-0.54954	-8.84107

6-311++G(d,p)
Electronic energy: -347.317919 Hartree

C	-1.22757	-0.65582	-7.09232
C	-0.76333	0.43069	-8.05125
C	-0.15423	1.45496	-7.10498
C	-0.26077	1.01345	-5.82912
C	-0.92738	-0.29749	-5.82126
C	-1.88735	0.99710	-8.90642
C	-1.58572	0.83581	-10.21680
C	-0.27949	0.17088	-10.33783
C	0.21583	-0.07353	-9.10130
H	0.20500	-0.08118	-11.28233
H	-2.20608	1.14617	-11.05892
H	0.08908	1.53870	-4.93915
H	-1.14139	-0.88109	-4.92462
H	-1.72179	-1.56472	-7.43280
H	0.28738	2.38647	-7.45652
H	-2.77794	1.45254	-8.47545
H	1.15903	-0.55156	-8.84025

PBEPBE, restricted open shell singlet

6-31+G(d,p)
Electronic energy: -347.2564637
Hartree

C	-1.22822	-0.65731	-7.09125
C	-0.76332	0.43069	-8.05125
C	-0.15341	1.45638	-7.10394
C	-0.26000	1.01397	-5.82367
C	-0.92732	-0.29837	-5.81579
C	-1.88888	0.99787	-8.90734
C	-1.58683	0.83634	-10.22220
C	-0.27922	0.17070	-10.34336
C	0.21720	-0.07423	-9.10249
H	0.20608	-0.08177	-11.28934
H	-2.20821	1.14721	-11.06563
H	0.09041	1.54008	-4.93229
H	-1.14168	-0.88292	-4.91775
H	-1.72324	-1.56757	-7.43278
H	0.28883	2.38932	-7.45653
H	-2.78078	1.45399	-8.47519
H	1.16187	-0.55300	-8.84052

Aug-cc-pVTZ
Electronic energy: -347.3496508
Hartree

C	-1.22625	-0.65314	-7.09288
C	-0.76332	0.43069	-8.05125
C	-0.15562	1.45232	-7.10552
C	-0.26162	1.01246	-5.83289
C	-0.92710	-0.29625	-5.82504
C	-1.88466	0.99573	-8.90611
C	-1.58432	0.83512	-10.21313
C	-0.28032	0.17132	-10.33396
C	0.21322	-0.07220	-9.10050
H	0.20397	-0.08063	-11.27640
H	-2.20418	1.14524	-11.05325
H	0.08789	1.53742	-4.94494
H	-1.14108	-0.87943	-4.93043
H	-1.71972	-1.56086	-7.43165
H	0.28549	2.38253	-7.45531
H	-2.77414	1.45060	-8.47699
H	1.15506	-0.54954	-8.84107

6-311++G(d,p)
Electronic energy: -347.317919 Hartree

C	-1.22757	-0.65582	-7.09232
C	-0.76333	0.43069	-8.05125
C	-0.15423	1.45496	-7.10498
C	-0.26077	1.01345	-5.82912
C	-0.92738	-0.29749	-5.82126
C	-1.88736	0.99710	-8.90642
C	-1.58572	0.83581	-10.21680
C	-0.27949	0.17088	-10.33783
C	0.21583	-0.07353	-9.10130
H	0.20500	-0.08118	-11.28233
H	-2.20608	1.14617	-11.05892
H	0.08908	1.53870	-4.93915
H	-1.14138	-0.88109	-4.92462
H	-1.72179	-1.56472	-7.43280
H	0.28738	2.38647	-7.45652
H	-2.77794	1.45254	-8.47545
H	1.15903	-0.55156	-8.84025

PBEPBE, triplet

6-31+G(d,p)
Electronic energy: -347.176554 Hartree

C	-1.22366	-0.64612	-7.10311
C	-0.76529	0.43151	-8.07673
C	-0.15983	1.44597	-7.11570
C	-0.27514	0.96995	-5.74557
C	-0.90029	-0.25945	-5.73817
C	-1.88711	0.99679	-8.93440
C	-1.58592	0.83569	-10.25673
C	-0.28530	0.17361	-10.37723
C	0.21133	-0.07142	-9.12881
H	0.19618	-0.07692	-11.32608
H	-2.20394	1.14485	-11.10372
H	0.08348	1.51505	-4.87033
H	-1.12523	-0.86196	-4.85604
H	-1.72014	-1.56334	-7.42222
H	0.28726	2.38440	-7.44596
H	-2.77961	1.45321	-8.50293
H	1.15649	-0.55045	-8.86759

Aug-cc-pVTZ
Electronic energy: -347.268695 Hartree

C	-1.22197	-0.64226	-7.10613
C	-0.76534	0.43152	-8.07730
C	-0.16198	1.44230	-7.11867
C	-0.27755	0.96681	-5.75430
C	-0.89921	-0.25573	-5.74694
C	-1.88280	0.99461	-8.93303
C	-1.58325	0.83439	-10.24772
C	-0.28657	0.17432	-10.36785
C	0.20729	-0.06936	-9.12667
H	0.19387	-0.07566	-11.31315
H	-2.19970	1.14278	-11.09140
H	0.07931	1.50880	-4.88102
H	-1.12268	-0.85500	-4.86680
H	-1.71683	-1.55674	-7.42266
H	0.28388	2.37782	-7.44634
H	-2.77261	1.44964	-8.50398
H	1.14943	-0.54687	-8.86734

6-311++G(d,p)
Electronic energy: -347.2372093
Hartree

C	-1.22334	-0.64509	-7.10531
C	-0.76531	0.43151	-8.07688
C	-0.16049	1.44508	-7.11789
C	-0.27643	0.96836	-5.75079
C	-0.89979	-0.25752	-5.74341
C	-1.88555	0.99600	-8.93325
C	-1.58468	0.83510	-10.25124
C	-0.28569	0.17385	-10.37158
C	0.20996	-0.07072	-9.12739
H	0.19503	-0.07628	-11.31892
H	-2.20171	1.14377	-11.09687
H	0.08109	1.51139	-4.87605
H	-1.12370	-0.85792	-4.86179
H	-1.71903	-1.56089	-7.42354
H	0.28593	2.38204	-7.44726
H	-2.77655	1.45165	-8.50252
H	1.15353	-0.54895	-8.86662

PBEPBE, quintuplet

6-31+G(d,p)
Electronic energy: -347.0853666
Hartree

C	-1.21524	-0.64185	-7.04572
C	-0.76306	0.43010	-8.05129
C	-0.15817	1.43707	-7.05883
C	-0.27184	0.96725	-5.68380
C	-0.89557	-0.25945	-5.67607
C	-1.87516	0.98991	-8.95393
C	-1.55478	0.81997	-10.36561
C	-0.33255	0.19779	-10.47934
C	0.19620	-0.06451	-9.14668
H	0.17310	-0.06409	-11.41094
H	-2.19386	1.14081	-11.19069
H	0.08628	1.51367	-4.80898
H	-1.12165	-0.86193	-4.79400
H	-1.71194	-1.56540	-7.35235
H	0.29387	2.37937	-7.37728
H	-2.78139	1.45173	-8.55500
H	1.14903	-0.54904	-8.92080

6-311++G(d,p)
Electronic energy: -347.1450386
Hartree

C	-1.25617	-0.61070	-7.07069
C	-0.77769	0.47442	-8.04874
C	-0.20264	1.46531	-7.03024
C	-0.23309	0.91844	-5.68269
C	-0.85410	-0.30535	-5.70641
C	-1.85906	1.03690	-8.97832
C	-1.55820	0.75540	-10.37334
C	-0.33627	0.13567	-10.45515
C	0.21387	-0.01440	-9.11688
H	0.15839	-0.19052	-11.37022
H	-2.20687	1.01003	-11.21144
H	0.17019	1.41733	-4.80151
H	-1.03132	-0.95234	-4.84710
H	-1.84126	-1.47452	-7.38862
H	0.15384	2.45787	-7.30893
H	-2.72131	1.59492	-8.61080
H	1.20497	-0.39708	-8.87023

Aug-cc-pVTZ
Electronic energy: -347.1762981
Hartree

C	-1.16162	-0.67119	-7.02284
C	-0.74688	0.37928	-8.05418
C	-0.11486	1.39906	-7.09728
C	-0.32423	1.02099	-5.71155
C	-0.94159	-0.20008	-5.66785
C	-1.88623	0.93147	-8.92137
C	-1.54164	0.89232	-10.33089
C	-0.33013	0.27251	-10.47967
C	0.16783	-0.11929	-9.17396
H	0.18432	0.08706	-11.42029
H	-2.16173	1.28863	-11.13260
H	-0.02472	1.61900	-4.85306
H	-1.21945	-0.74659	-4.76900
H	-1.54091	-1.65307	-7.30154
H	0.44035	2.26822	-7.44590
H	-2.83225	1.27188	-8.50377
H	1.05704	-0.71883	-8.98556

PW91, closed-shell singlet

6-31+G(d,p)
Electronic energy: -347.5673203
Hartree

C	-1.22793	-0.65672	-7.09133
C	-0.76333	0.43069	-8.05125
C	-0.15371	1.45580	-7.10400
C	-0.26027	1.01367	-5.82496
C	-0.92724	-0.29798	-5.81709
C	-1.88830	0.99758	-8.90733
C	-1.58639	0.83613	-10.22093
C	-0.27946	0.17083	-10.34203
C	0.21662	-0.07394	-9.10236
H	0.20492	-0.08117	-11.28660
H	-2.20665	1.14643	-11.06314
H	0.08953	1.53880	-4.93490
H	-1.14118	-0.88148	-4.92038
H	-1.72222	-1.56571	-7.43200
H	0.28793	2.38741	-7.45571
H	-2.77896	1.45306	-8.47617
H	1.15993	-0.55202	-8.84114

Aug-cc-pVTZ
Electronic energy: -347.6638474
Hartree

C	-1.22588	-0.65240	-7.09298
C	-0.76332	0.43068	-8.05125
C	-0.15600	1.45158	-7.10560
C	-0.26199	1.01206	-5.83460
C	-0.92701	-0.29574	-5.82675
C	-1.88392	0.99535	-8.90608
C	-1.58374	0.83484	-10.21146
C	-0.28064	0.17150	-10.33221
C	0.21249	-0.07183	-9.10035
H	0.20261	-0.07991	-11.27318
H	-2.20236	1.14432	-11.05033
H	0.08683	1.53592	-4.94799
H	-1.14051	-0.87773	-4.93351
H	-1.71854	-1.55870	-7.43084
H	0.28445	2.38031	-7.45448
H	-2.77202	1.44952	-8.47800
H	1.15282	-0.54841	-8.84170

6-311++G(d,p)
Electronic energy: -347.6309368
Hartree

C	-1.22727	-0.65522	-7.09238
C	-0.76333	0.43069	-8.05125
C	-0.15454	1.45437	-7.10504
C	-0.26106	1.01314	-5.83065
C	-0.92732	-0.29708	-5.82278
C	-1.88676	0.99679	-8.90641
C	-1.58525	0.83558	-10.21531
C	-0.27973	0.17101	-10.33627
C	0.21524	-0.07323	-9.10118
H	0.20372	-0.08051	-11.27937
H	-2.20437	1.14532	-11.05624
H	0.08810	1.53729	-4.94195
H	-1.14083	-0.87950	-4.92745
H	-1.72072	-1.56272	-7.43215
H	0.28641	2.38443	-7.45584
H	-2.77598	1.45154	-8.47630
H	1.15697	-0.55052	-8.84073

PW91, restricted open shell singlet

6-31+G(d,p)
Electronic energy: -347.5673203
Hartree

C	-1.22793	-0.65672	-7.09133
C	-0.76333	0.43069	-8.05125
C	-0.15371	1.45580	-7.10400
C	-0.26027	1.01367	-5.82496
C	-0.92724	-0.29798	-5.81709
C	-1.88830	0.99758	-8.90733
C	-1.58639	0.83613	-10.22093
C	-0.27946	0.17083	-10.34203
C	0.21662	-0.07394	-9.10236
H	0.20492	-0.08117	-11.28660
H	-2.20665	1.14643	-11.06314
H	0.08953	1.53880	-4.93490
H	-1.14118	-0.88148	-4.92038
H	-1.72222	-1.56571	-7.43200
H	0.28793	2.38741	-7.45571
H	-2.77896	1.45306	-8.47617
H	1.15993	-0.55202	-8.84114

Aug-cc-pVTZ
Electronic energy: -347.6638474
Hartree

C	-1.22588	-0.65240	-7.09298
C	-0.76332	0.43068	-8.05125
C	-0.15600	1.45158	-7.10560
C	-0.26199	1.01206	-5.83460
C	-0.92701	-0.29574	-5.82675
C	-1.88392	0.99535	-8.90608
C	-1.58374	0.83484	-10.21146
C	-0.28064	0.17150	-10.33221
C	0.21249	-0.07183	-9.10035
H	0.20261	-0.07991	-11.27318
H	-2.20236	1.14432	-11.05033
H	0.08683	1.53592	-4.94799
H	-1.14051	-0.87773	-4.93351
H	-1.71854	-1.55870	-7.43084
H	0.28445	2.38031	-7.45448
H	-2.77202	1.44952	-8.47800
H	1.15282	-0.54841	-8.84170

6-311++G(d,p)
Electronic energy: -347.6309368
Hartree

C	-1.22727	-0.65522	-7.09238
C	-0.76333	0.43069	-8.05125
C	-0.15454	1.45437	-7.10504
C	-0.26106	1.01314	-5.83065
C	-0.92732	-0.29708	-5.82278
C	-1.88676	0.99679	-8.90641
C	-1.58525	0.83558	-10.21531
C	-0.27973	0.17101	-10.33627
C	0.21524	-0.07323	-9.10118
H	0.20372	-0.08051	-11.27937
H	-2.20437	1.14532	-11.05624
H	0.08810	1.53729	-4.94195
H	-1.14083	-0.87950	-4.92745
H	-1.72072	-1.56272	-7.43215
H	0.28641	2.38443	-7.45584
H	-2.77598	1.45154	-8.47630
H	1.15697	-0.55052	-8.84073

PW91, triplet

6-31+G(d,p)
Electronic energy: -347.4877247
Hartree

C	-1.22347	-0.64568	-7.10347
C	-0.76530	0.43151	-8.07673
C	-0.16008	1.44555	-7.11605
C	-0.27551	0.96945	-5.74687
C	-0.90011	-0.25886	-5.73947
C	-1.88653	0.99650	-8.93430
C	-1.58545	0.83546	-10.25534
C	-0.28555	0.17375	-10.37577
C	0.21077	-0.07114	-9.12860
H	0.19509	-0.07634	-11.32315
H	-2.20241	1.14410	-11.10103
H	0.08248	1.51354	-4.87287
H	-1.12460	-0.86028	-4.85858
H	-1.71925	-1.56165	-7.42174
H	0.28643	2.38268	-7.44547
H	-2.77778	1.45227	-8.50379
H	1.15455	-0.54947	-8.86809

Aug-cc-pVTZ
Electronic energy: -347.5830868
Hartree

C	-1.22169	-0.64165	-7.10654
C	-0.76533	0.43152	-8.07728
C	-0.16230	1.44171	-7.11907
C	-0.27804	0.96616	-5.75594
C	-0.89898	-0.25497	-5.74859
C	-1.88208	0.99424	-8.93295
C	-1.58266	0.83410	-10.24593
C	-0.28690	0.17449	-10.36599
C	0.20660	-0.06900	-9.12647
H	0.19256	-0.07498	-11.30977
H	-2.19792	1.14189	-11.08829
H	0.07810	1.50701	-4.88394
H	-1.12197	-0.85301	-4.86975
H	-1.71576	-1.55475	-7.42221
H	0.28290	2.37579	-7.44585
H	-2.77048	1.44856	-8.50489
H	1.14721	-0.54573	-8.86787

6-311++G(d,p)
Electronic energy: -347.550482 Hartree

C	-1.22314	-0.64463	-7.10570
C	-0.76531	0.43151	-8.07687
C	-0.16074	1.44464	-7.11827
C	-0.27686	0.96779	-5.75227
C	-0.89959	-0.25685	-5.74489
C	-1.88496	0.99570	-8.93318
C	-1.58418	0.83486	-10.24964
C	-0.28594	0.17399	-10.36991
C	0.20939	-0.07043	-9.12721
H	0.19381	-0.07564	-11.31578
H	-2.20004	1.14294	-11.09400
H	0.07998	1.50972	-4.87876
H	-1.12302	-0.85606	-4.86453
H	-1.71807	-1.55909	-7.42319
H	0.28504	2.38021	-7.44689
H	-2.77457	1.45064	-8.50325
H	1.15147	-0.54791	-8.86697

PW91, quintuplet

6-31+G(d,p)
Electronic energy: -347.3969013
Hartree

C	-1.21532	-0.64131	-7.04644
C	-0.76311	0.43035	-8.05128
C	-0.15859	1.43688	-7.05922
C	-0.27203	0.96648	-5.68528
C	-0.89523	-0.25912	-5.67774
C	-1.87465	0.99002	-8.95351
C	-1.55418	0.81926	-10.36419
C	-0.33302	0.19763	-10.47767
C	0.19601	-0.06405	-9.14594
H	0.17155	-0.06414	-11.40788
H	-2.19219	1.13912	-11.18823
H	0.08568	1.51160	-4.81161
H	-1.12062	-0.86073	-4.79702
H	-1.71178	-1.56326	-7.35249
H	0.29236	2.37812	-7.37676
H	-2.77935	1.45181	-8.55554
H	1.14775	-0.54727	-8.92051

Aug-cc-pVTZ
Electronic energy: -347.4909274
Hartree

C	-1.16715	-0.66701	-7.02623
C	-0.74866	0.38503	-8.05386
C	-0.12009	1.40279	-7.09403
C	-0.31858	1.01409	-5.71079
C	-0.93549	-0.20546	-5.67101
C	-1.88440	0.93739	-8.92402
C	-1.54249	0.88298	-10.33256
C	-0.33180	0.26433	-10.47732
C	0.17038	-0.11251	-9.17000
H	0.17998	0.07095	-11.41569
H	-2.16345	1.26947	-11.13589
H	-0.01308	1.60472	-4.85165
H	-1.20658	-0.75665	-4.77516
H	-1.55938	-1.64102	-7.30760
H	0.42261	2.27904	-7.43902
H	-2.82458	1.29099	-8.50882
H	1.06604	-0.69776	-8.97768

6-311++G(d,p)
Electronic energy: -347.4586232
Hartree

C	-1.17603	-0.66605	-7.02918
C	-0.75076	0.39161	-8.05348
C	-0.12528	1.41048	-7.08850
C	-0.30983	1.00707	-5.70409
C	-0.92866	-0.21592	-5.66926
C	-1.88532	0.94639	-8.92842
C	-1.54616	0.87268	-10.34014
C	-0.33119	0.25297	-10.48042
C	0.17760	-0.10579	-9.16679
H	0.17968	0.04857	-11.41925
H	-2.17106	1.24834	-11.14816
H	0.00482	1.59090	-4.84115
H	-1.19209	-0.77592	-4.77417
H	-1.58876	-1.63214	-7.31643
H	0.40036	2.30043	-7.43142
H	-2.82003	1.32031	-8.51319
H	1.08599	-0.67254	-8.96726

ωB97X[D], closed-shell singlet

6-31+G(d,p)
Electronic energy: -347.5915652
Hartree

C	-1.22485	-0.65040	-7.09350
C	-0.76316	0.43071	-8.05125
C	-0.15693	1.44961	-7.10603
C	-0.26125	1.01457	-5.83963
C	-0.92867	-0.29789	-5.83178
C	-1.88186	0.99436	-8.90573
C	-1.58571	0.83578	-10.20614
C	-0.27798	0.17012	-10.32742
C	0.21064	-0.07081	-9.09979
H	0.20307	-0.08020	-11.26573
H	-2.20190	1.14393	-11.04271
H	0.08607	1.53620	-4.95546
H	-1.14132	-0.87743	-4.94105
H	-1.71638	-1.55480	-7.42952
H	0.28274	2.37634	-7.45293
H	-2.76816	1.44759	-8.47968
H	1.14894	-0.54630	-8.84295

Aug-cc-pVTZ
Electronic energy: -347.6852192
Hartree

C	-1.22288	-0.64625	-7.09511
C	-0.76310	0.43076	-8.05126
C	-0.15908	1.44562	-7.10751
C	-0.26286	1.01309	-5.84875
C	-0.92850	-0.29581	-5.84099
C	-1.87765	0.99226	-8.90455
C	-1.58328	0.83455	-10.19713
C	-0.27907	0.17069	-10.31810
C	0.20675	-0.06877	-9.09789
H	0.20074	-0.07906	-11.25265
H	-2.19776	1.14177	-11.03020
H	0.08341	1.53336	-4.96818
H	-1.14071	-0.87376	-4.95391
H	-1.71266	-1.54766	-7.42873
H	0.27921	2.36920	-7.45190
H	-2.76107	1.44402	-8.48121
H	1.14181	-0.54261	-8.84323

6-311++G(d,p)
Electronic energy: -347.6525889
Hartree

C	-1.22424	-0.64912	-7.09437
C	-0.76307	0.43073	-8.05126
C	-0.15757	1.44840	-7.10682
C	-0.26189	1.01429	-5.84444
C	-0.92886	-0.29726	-5.83664
C	-1.88052	0.99371	-8.90498
C	-1.58492	0.83537	-10.20132
C	-0.27809	0.17016	-10.32256
C	0.20952	-0.07019	-9.09889
H	0.20235	-0.07990	-11.25980
H	-2.20045	1.14312	-11.03690
H	0.08497	1.53533	-4.96128
H	-1.14134	-0.87613	-4.94695
H	-1.71518	-1.55254	-7.42959
H	0.28166	2.37409	-7.45285
H	-2.76585	1.44646	-8.47982
H	1.14676	-0.54513	-8.84283

ωB97X[D], restricted open shell singlet

6-31+G(d,p)
Electronic energy: -347.5915652
Hartree

C	-1.22485	-0.65040	-7.09350
C	-0.76316	0.43071	-8.05125
C	-0.15693	1.44961	-7.10603
C	-0.26125	1.01457	-5.83963
C	-0.92867	-0.29789	-5.83178
C	-1.88186	0.99436	-8.90573
C	-1.58571	0.83578	-10.20614
C	-0.27798	0.17012	-10.32742
C	0.21064	-0.07081	-9.09979
H	0.20307	-0.08020	-11.26573
H	-2.20190	1.14393	-11.04271
H	0.08607	1.53620	-4.95546
H	-1.14132	-0.87743	-4.94105
H	-1.71638	-1.55480	-7.42952
H	0.28274	2.37634	-7.45293
H	-2.76816	1.44759	-8.47968
H	1.14894	-0.54630	-8.84295

Aug-cc-pVTZ
Electronic energy: -347.6852192
Hartree

C	-1.22288	-0.64625	-7.09511
C	-0.76310	0.43076	-8.05126
C	-0.15908	1.44562	-7.10751
C	-0.26286	1.01309	-5.84875
C	-0.92850	-0.29581	-5.84099
C	-1.87765	0.99226	-8.90455
C	-1.58328	0.83455	-10.19713
C	-0.27907	0.17069	-10.31810
C	0.20675	-0.06877	-9.09789
H	0.20074	-0.07906	-11.25265
H	-2.19776	1.14177	-11.03020
H	0.08341	1.53336	-4.96818
H	-1.14072	-0.87376	-4.95391
H	-1.71266	-1.54766	-7.42873
H	0.27921	2.36920	-7.45190
H	-2.76107	1.44402	-8.48121
H	1.14181	-0.54261	-8.84324

6-311++G(d,p)
Electronic energy: -347.6525889
Hartree

C	-1.22424	-0.64912	-7.09437
C	-0.76307	0.43073	-8.05126
C	-0.15757	1.44840	-7.10682
C	-0.26189	1.01429	-5.84444
C	-0.92886	-0.29726	-5.83664
C	-1.88052	0.99371	-8.90498
C	-1.58492	0.83537	-10.20132
C	-0.27809	0.17016	-10.32256
C	0.20952	-0.07019	-9.09889
H	0.20235	-0.07990	-11.25980
H	-2.20045	1.14312	-11.03690
H	0.08497	1.53533	-4.96128
H	-1.14134	-0.87613	-4.94695
H	-1.71518	-1.55254	-7.42959
H	0.28166	2.37409	-7.45285
H	-2.76585	1.44646	-8.47982
H	1.14676	-0.54513	-8.84283

ωB97X[D], triplet

6-31+G(d,p)
Electronic energy: -347.5072496
Hartree

C	-1.21996	-0.63913	-7.10938
C	-0.76493	0.43162	-8.07984
C	-0.16322	1.43905	-7.12154
C	-0.28093	0.96099	-5.75216
C	-0.89653	-0.24964	-5.74505
C	-1.88289	0.99481	-8.93804
C	-1.58666	0.83595	-10.24165
C	-0.28280	0.17222	-10.36290
C	0.20707	-0.06908	-9.13239
H	0.19464	-0.07653	-11.30376
H	-2.20017	1.14255	-11.08109
H	0.07391	1.50135	-4.88331
H	-1.12001	-0.84656	-4.86953
H	-1.71287	-1.55172	-7.41923
H	0.28241	2.37199	-7.44219
H	-2.76968	1.44838	-8.51255
H	1.14590	-0.54486	-8.87669

Aug-cc-pVTZ
Electronic energy: -347.5995741
Hartree

C	-1.21801	-0.63508	-7.11208
C	-0.76482	0.43163	-8.08016
C	-0.16535	1.43512	-7.12413
C	-0.28341	0.95797	-5.76068
C	-0.89559	-0.24598	-5.75366
C	-1.87860	0.99269	-8.93695
C	-1.58418	0.83472	-10.23278
C	-0.28402	0.17284	-10.35379
C	0.20314	-0.06704	-9.13071
H	0.19209	-0.07530	-11.29093
H	-2.19597	1.14043	-11.06869
H	0.06934	1.49499	-4.89392
H	-1.11760	-0.83931	-4.88030
H	-1.70894	-1.54452	-7.41955
H	0.27890	2.36465	-7.44231
H	-2.76232	1.44471	-8.51376
H	1.13864	-0.54115	-8.87687

6-311++G(d,p)
Electronic energy: -347.5674751
Hartree

C	-1.21941	-0.63819	-7.11128
C	-0.76472	0.43159	-8.07995
C	-0.16365	1.43809	-7.12335
C	-0.28227	0.95963	-5.75648
C	-0.89625	-0.24783	-5.74944
C	-1.88145	0.99414	-8.93715
C	-1.58585	0.83552	-10.23678
C	-0.28304	0.17231	-10.35811
C	0.20596	-0.06846	-9.13155
H	0.19373	-0.07617	-11.29793
H	-2.19876	1.14177	-11.07516
H	0.07144	1.49840	-4.88782
H	-1.11911	-0.84296	-4.87416
H	-1.71156	-1.54982	-7.42041
H	0.28167	2.36988	-7.44320
H	-2.76710	1.44715	-8.51216
H	1.14366	-0.54367	-8.87639

ωB97X[D], quintuplet

6-31+G(d,p)
Electronic energy: -347.4171856
Hartree

C	-1.21397	-0.63671	-7.05471
C	-0.76286	0.43109	-8.05126
C	-0.16130	1.43334	-7.06626
C	-0.27682	0.95853	-5.69666
C	-0.89214	-0.25151	-5.68988
C	-1.86953	0.98876	-8.94635
C	-1.54597	0.81385	-10.35323
C	-0.34031	0.20007	-10.46514
C	0.19307	-0.06125	-9.13778
H	0.15962	-0.06086	-11.38984
H	-2.17967	1.13002	-11.17271
H	0.07830	1.49883	-4.82771
H	-1.11560	-0.84898	-4.81456
H	-1.70794	-1.55330	-7.35586
H	0.28701	2.36973	-7.37773
H	-2.76876	1.44982	-8.55440
H	1.14014	-0.54004	-8.91723

Aug-cc-pVTZ
Electronic energy: -347.5080931
Hartree

C	-1.21379	-0.63176	-7.05707
C	-0.76396	0.43181	-8.05117
C	-0.16518	1.43032	-7.06836
C	-0.27738	0.95444	-5.70525
C	-0.88929	-0.24891	-5.69865
C	-1.86565	0.98703	-8.94528
C	-1.54140	0.81131	-10.34570
C	-0.34232	0.20089	-10.45582
C	0.18909	-0.05898	-9.13401
H	0.15499	-0.05899	-11.37751
H	-2.17107	1.12513	-11.16386
H	0.07783	1.49031	-4.83863
H	-1.10920	-0.84401	-4.82580
H	-1.70889	-1.54361	-7.35544
H	0.27870	2.36491	-7.37682
H	-2.76195	1.44708	-8.55715
H	1.13273	-0.53557	-8.91480

6-311++G(d,p)
Electronic energy: -347.4764895
Hartree

C	-1.21403	-0.63548	-7.05654
C	-0.76310	0.43134	-8.05124
C	-0.16231	1.43269	-7.06792
C	-0.27755	0.95680	-5.70102
C	-0.89126	-0.25006	-5.69436
C	-1.86848	0.98841	-8.94489
C	-1.54396	0.81266	-10.34917
C	-0.34145	0.20049	-10.46049
C	0.19226	-0.06066	-9.13566
H	0.15697	-0.05988	-11.38462
H	-2.17595	1.12775	-11.16865
H	0.07718	1.49516	-4.83236
H	-1.11343	-0.84619	-4.81942
H	-1.70809	-1.55066	-7.35692
H	0.28485	2.36838	-7.37846
H	-2.76667	1.44927	-8.55404
H	1.13830	-0.53862	-8.91556

MP2, closed-shell singlet

6-31+G(d,p)
Electronic energy: -345.41027331
Hartree

C	-1.226212	-0.651117	-7.103591
C	-0.763337	0.430669	-8.051253
C	-0.157306	1.450979	-7.116227
C	-0.261893	1.012642	-5.836820
C	-0.927421	-0.296178	-5.828953
C	-1.882177	0.994518	-8.895559
C	-1.584068	0.835036	-10.209201
C	-0.279963	0.171180	-10.330039
C	0.212348	-0.071702	-9.089637
H	0.203328	-0.080186	-11.264404
H	-2.201696	1.144093	-11.041555
H	0.086194	1.536245	-4.956782
H	-1.141170	-0.877471	-4.942272
H	-1.716902	-1.553744	-7.440364
H	0.281334	2.375959	-7.463986
H	-2.766664	1.446838	-8.468925
H	1.148886	-0.546375	-8.831739

Aug-cc-pVTZ
Electronic energy: -345.50130945
Hartree

C	-1.224939	-0.648381	-7.104979
C	-0.763320	0.430673	-8.051255
C	-0.158769	1.448335	-7.117574
C	-0.263121	1.011322	-5.842692
C	-0.927107	-0.294465	-5.834848
C	-1.879383	0.993110	-8.894434
C	-1.582115	0.834067	-10.203453
C	-0.281031	0.171748	-10.324020
C	0.209782	-0.070380	-9.088031
H	0.202870	-0.079933	-11.256828
H	-2.200129	1.143320	-11.034150
H	0.085085	1.535483	-4.964258
H	-1.141245	-0.876204	-4.949771
H	-1.715227	-1.550301	-7.441318
H	0.279541	2.372581	-7.464879
H	-2.763182	1.445083	-8.468303
H	1.145570	-0.544672	-8.830516

6-311++G(d,p)
Electronic energy: -345.46373335
Hartree

C	-1.226954	-0.652728	-7.102725
C	-0.763340	0.430674	-8.051254
C	-0.156437	1.452541	-7.115379
C	-0.260937	1.014146	-5.834780
C	-0.928061	-0.297814	-5.826894
C	-1.883825	0.995352	-8.896272
C	-1.585789	0.835895	-10.211107
C	-0.278554	0.170445	-10.332232
C	0.213863	-0.072478	-9.090637
H	0.206792	-0.081988	-11.269350
H	-2.205857	1.146178	-11.045800
H	0.088494	1.539921	-4.952210
H	-1.142760	-0.881450	-4.937655
H	-1.719099	-1.557753	-7.442029
H	0.283270	2.380085	-7.465698
H	-2.770590	1.448851	-8.466866
H	1.153065	-0.548492	-8.830419

CASSCF (8,8) / 6-31G*

C	-0.96387	-0.61978	1.00025
C	0.00000	-0.00000	0.00000
C	-0.96387	0.61978	-1.00025
C	-2.23729	0.38958	-0.62874
C	-2.23729	-0.38958	0.62874
C	0.96387	-1.00025	-0.61978
C	2.23729	-0.62873	-0.38958
C	2.23729	0.62874	0.38958
C	0.96386	1.00025	0.61978
H	3.12010	1.14815	0.71142
H	3.12010	-1.14814	-0.71142
H	-3.12010	0.71142	-1.14815
H	-3.12010	-0.71142	1.14815
H	-0.63093	-1.15720	1.86758
H	-0.63093	1.15720	-1.86757
H	0.63093	-1.86758	-1.15720
H	0.63092	1.86757	1.15720

Cartesian coordinates of optimised geometries of molecules **1-6** and their corresponding monoanions and monocations at CCSD / 6-31G* level.

Molecule 1

1 neutral close-shell singlet			$1^{\bullet+}$ monocation doublet			$1^{\bullet-}$ monoanion doublet		
C	-0.95577	0.83472 -0.83471	C	2.22320	-0.72618 0.00000	C	-2.30752	-0.65576 0.00007
C	0.00000	-0.00000 0.00000	C	0.93564	1.18239 -0.00000	C	-0.89588	1.15974 -0.00012
C	-0.95577	-0.83472 0.83471	C	0.00387	-0.00000 0.00000	C	-0.00334	-0.08022 0.00001
C	-2.22886	-0.52308 0.52307	C	0.93564	-1.18239 0.00000	C	-1.06202	-1.17407 0.00012
C	-2.22886	0.52308 -0.52307	C	-0.92602	0.00000 1.17004	C	0.96403	-0.12688 -1.18727
C	0.95577	0.83471 0.83472	C	-0.92602	-0.00000 -1.17004	C	0.96403	-0.12664 1.18730
C	2.22886	0.52307 0.52308	C	-2.23397	-0.00000 -0.71441	C	2.27142	0.04855 0.70650
C	2.22886	-0.52307 -0.52308	H	3.11567	-1.34570 0.00000	H	-3.24856	-1.20712 0.00012
C	0.95577	-0.83471 -0.83472	H	0.59394	2.21318 -0.00000	H	-0.47108	2.16169 -0.00022
H	3.12387	-0.95946 -0.95947	H	-0.59157	0.00001 2.20406	H	0.61941	0.03753 -2.20856
H	3.12386	0.95946 0.95947	H	-3.12274	-0.00000 -1.33946	H	3.16482	0.09488 1.33277
H	-3.12387	-0.95947 0.95945	H	-0.59157	-0.00001 -2.20407	H	0.61940	0.03798 2.20855
H	-3.12386	0.95947 -0.95945	H	0.59394	-2.21318 0.00001	H	-0.78855	-2.22721 0.00022
H	-0.61121	1.56327 -1.56325	C	2.22320	0.72618 -0.00000	C	-2.20259	0.82444 -0.00008
H	-0.61121	-1.56327 1.56325	H	3.11567	1.34570 -0.00001	H	-3.05743	1.50234 -0.00015
H	0.61121	1.56325 1.56327	C	-2.23397	0.00000 0.71441	C	2.27142	0.04840 -0.70651
H	0.61121	-1.56325 -1.56327	H	-3.12274	0.00000 1.33946	H	3.16482	0.09461 -1.33278

Molecule 2

2 neutral close-singlet			$2^{\bullet+}$ monocation doublet			$2^{\bullet-}$ monoanion doublet		
C	1.32788	0.65715 -0.06838	C	-1.63086	0.48893 0.00004	C	1.32520	0.13609 -0.72847
C	1.32788	-0.65715 0.06838	C	-1.27392	-0.81961 -0.00002	C	1.32520	0.13613 0.72846
C	-0.00000	0.00000 0.00000	C	-0.29196	0.15138 -0.00003	C	0.05377	0.06004 -0.00000
H	1.92452	-1.55746 0.16208	H	-1.55628	-1.86626 -0.00004	H	1.69934	-0.66400 1.39101
H	1.92452	1.55747 -0.16205	H	-2.40789	1.24476 0.00011	H	1.69934	-0.66407 -1.39097
C	-1.32788	0.06838 0.65715	C	2.02282	-0.42823 0.00004	C	-1.37172	0.61826 -0.00002
C	-1.32788	-0.06838 -0.65715	C	1.09367	0.52728 -0.00004	C	-1.24954	-0.69562 0.00002
H	-1.92452	-0.16207 -1.55746	H	1.33988	1.59159 -0.00008	H	-1.80307	-1.63759 0.00004
H	-1.92452	0.16207 1.55746	H	3.10583	-0.48859 0.00009	H	-2.09312	1.43634 -0.00003

Molecule 3

3 neutral close-singlet			$3^{\bullet+}$ monocation doublet			$3^{\bullet-}$ monoanion doublet		
C	0.00000	2.32136 1.30424	C	-2.79928	1.28436 -0.00000	C	3.23158	-0.68678 -0.01492
C	1.13255	1.43376 1.07759	C	-1.46653	1.74875 -0.00000	C	2.10150	-1.57095 0.00558
C	1.19056	0.43975 0.16882	C	-0.29585	1.02161 -0.00000	C	0.76180	-1.30270 0.02766
C	-0.86845	2.74347 0.34948	C	-3.26882	-0.03152 -0.00000	C	3.23158	0.68679 -0.01482
C	-0.81457	2.36756 -1.05688	C	-2.52688	-1.24007 0.00000	C	2.10150	1.57095 0.00581
C	-0.36326	1.19275 -1.54394	C	-1.16879	-1.41117 0.00000	C	0.76180	1.30270 0.02785
C	0.00000	-0.00000 -0.67686	C	-0.01379	-0.44893 0.00000	C	-0.00082	-0.00000 0.02060
C	0.36326	-1.19275 -1.54394	C	0.82066	-0.77092 -1.25487	C	-0.74701	0.00010 -1.28991
C	-1.19056	-0.43975 0.16882	C	0.82066	-0.77092 1.25487	C	-0.78641	-0.00010 1.31132
C	0.81457	-2.36756 -1.05688	C	2.04182	-0.27062 -1.52757	C	-2.07287	0.00012 -1.58255
C	-1.13255	-1.43376 1.07759	C	2.04182	-0.27062 1.52757	C	-2.11640	-0.00012 1.56672
C	0.86845	-2.74347 0.34948	C	2.88265	0.56676 -0.67774	C	-3.22443	0.00005 -0.70628
C	-0.00000	-2.32136 1.30424	C	2.88265	0.56676 0.67774	C	-3.24236	-0.00005 0.64989
H	0.27588	-1.07181 -2.62521	H	0.34530	-1.42664 -1.98438	H	-0.04999	0.00016 -2.13041
H	1.14014	-3.12694 -1.77045	H	2.46805	-0.53503 -2.49616	H	-2.31853	0.00020 -2.64960
H	1.60654	-3.49790 0.62604	H	3.63681	1.16305 -1.19032	H	-4.19380	0.00009 -1.21283
H	0.08548	-2.75985 2.29979	H	3.63680	1.16305 1.19032	H	-4.22551	-0.00008 1.13004
H	-2.01736	-1.62047 1.68923	H	2.46805	-0.53503 2.49616	H	-2.39585	-0.00020 2.62506
H	-2.12781	0.09385 0.01522	H	0.34530	-1.42664 1.98438	H	-0.11369	-0.00016 2.17217
H	-0.27588	1.07181 -2.62521	H	-0.82605	-2.44820 0.00000	H	0.08152	2.15678 0.04151
H	-1.14014	3.12694 -1.77045	H	-3.12381	-2.15121 0.00000	H	2.36010	2.63545 0.00222
H	-1.60654	3.49790 0.62604	H	-4.35275	-0.14482 -0.00000	H	4.20871	1.17810 -0.03134
H	-0.08548	2.75985 2.29979	H	-3.56779	2.05728 -0.00000	H	4.20871	-1.17809 -0.03151
H	2.01736	1.62047 1.68923	H	-1.35110	2.83210 -0.00000	H	2.36010	-2.63545 0.00182
H	2.12781	-0.09385 0.01522	H	0.61929	1.61119 -0.00000	H	0.08152	-2.15678 0.04118

Molecule 4

4 neutral close-shell			4 monocation doublet			4 monoanion doublet		
C	-1.279857	0.026239 -0.286704	C	-1.295559	0.040745 -0.246256	C	-0.210529	-0.680517 1.057034
C	-0.715307	0.392995 1.027055	C	-0.756666	0.390810 1.007733	C	0.242050	0.659119 1.064414
C	0.626595	0.256334 0.985077	C	0.636712	0.248302 0.962901	C	0.263760	1.164442 -0.247806
C	1.039805	-0.218461 -0.385826	C	1.057770	-0.222410 -0.392471	C	-0.041940	0.021253 -1.200688
C	-0.275928	-0.329985 -1.115180	C	-0.252194	-0.329132 -1.105560	C	-0.495332	-1.082471 -0.260185
H	-2.339302	0.046358 -0.529030	H	-2.349971	0.054519 -0.507477	H	-0.393550	-1.281758 1.951329
H	-1.303729	0.719112 1.880846	H	-1.327424	0.718767 1.871961	H	0.458156	1.239292 1.965219
H	1.325257	0.449915 1.794034	H	1.318181	0.448075 1.786487	H	0.770372	2.079427 -0.563817
H	1.722821	0.491510 -0.877531	H	1.745794	0.483478 -0.885201	H	-0.797103	0.280681 -1.982070
H	1.568966	-1.183126 -0.343916	H	1.592227	-1.185354 -0.353333	H	0.860708	-0.280348 -1.808168
H	-0.369068	-0.650794 -2.148824	H	-0.368675	-0.647708 -2.138780	H	-0.646342	-2.114050 -0.586922

Molecule 5

2 neutral close-shell			2 monocation doublet			2 monoanion doublet		
C	-0.599571	0.650176 0.040971	C	-0.218348	-0.433790 0.150288	C	0.112352	0.701040 -0.406050
C	-0.599571	-0.650176 0.040969	C	-1.137754	0.531551 -0.157453	C	-0.113098	-0.708116 -0.385923
C	0.759442	-0.000000 -0.051991	C	1.122638	-0.088494 0.058811	C	0.013715	0.013324 0.942394
H	-1.139068	1.585372 0.077875	H	-0.533837	-1.431267 0.454180	H	1.022370	1.212565 -0.764354
H	-1.139069	-1.585372 0.077872	H	-1.131138	1.572636 -0.478223	H	-1.030318	-1.228262 -0.711994
H	1.296537	0.000001 -1.004981	H	1.907432	-0.809655 0.289805	H	0.885363	-0.246886 1.574472
H	1.421302	-0.000001 0.818988	H	1.436684	0.910144 -0.245455	H	-0.844504	0.289604 1.585925

Molecule 6

6 neutral close-shell			6 monocation doublet			6 monoanion doublet		
C	0.692411	1.171988 -0.917403	C	0.982887	1.226007 -0.739931	C	1.509330	0.702978 -0.069542
C	1.048398	-0.093941 -1.259616	C	1.348789	-0.075158 -1.091676	C	1.509330	-0.702978 -0.069542
C	0.881405	-1.282483 -0.426632	C	0.779829	-1.311278 -0.686201	C	0.397344	-1.572013 0.074398
C	-0.135754	-1.476096 0.436952	C	-0.279167	-1.522885 0.159184	C	-0.955626	-1.303731 0.126284
C	-1.288512	-0.506077 0.531760	C	-1.146404	-0.565819 0.900552	C	-1.650878	-0.000000 -0.201790
C	-0.780006	0.814937 1.056278	C	-0.963234	0.909692 0.816784	C	-0.955626	1.303731 0.126284
C	0.078084	1.574217 0.345608	C	-0.057870	1.667626 0.119088	C	0.397344	1.572013 0.074398
H	0.971925	1.976956 -1.599292	H	1.583171	2.016512 -1.190026	H	2.487401	1.190567 -0.138978
H	1.592501	-0.229880 -2.195857	H	2.193157	-0.152632 -1.776412	H	2.487401	-1.190567 -0.138978
H	1.654279	-2.047889 -0.514616	H	1.249558	-2.200448 -1.103847	H	0.661036	-2.632729 0.185283
H	-0.141258	-2.359937 1.075462	H	-0.548594	-2.565982 0.331326	H	-1.627072	-2.159223 0.254842
H	-1.722491	-0.357535 -0.469180	H	-2.198596	-0.789852 0.634747	H	-1.920736	-0.000000 -1.281496
H	-2.078652	-0.903199 1.178867	H	-1.119609	-0.847888 1.971845	H	-2.629303	-0.000000 0.316249
H	-1.131937	1.163029 2.027811	H	-1.682144	1.464979 1.421019	H	-1.627072	2.159223 0.254842
H	0.359632	2.556022 0.729940	H	-0.141780	2.747222 0.233660	H	0.661036	2.632729 0.185283

Comparison of the geometrical parameters of molecule **1**, computed at different levels of theory, and corresponding linear regression parameters and RMSDs, compared to experimental data.

Bond length

		B3LYP			B3LYP[GD3BJ]			BLYP			BP86			CAMB3LYP			CAMB3LYP[GD3BJ]		
Atom I	Atom J	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ
1	2	1.5231	1.5218	1.5185	1.5211	1.5198	1.5166	1.5349	1.5334	1.5298	1.5272	1.5254	1.5223	1.5164	1.5151	1.5118	1.5159	1.5146	1.5114
1	5	1.3484	1.3439	1.3399	1.3482	1.3436	1.3397	1.3604	1.3554	1.3511	1.3599	1.3553	1.3513	1.3412	1.3366	1.3327	1.3411	1.3365	1.3326
2	3	1.5231	1.5218	1.5185	1.5211	1.5198	1.5166	1.5349	1.5334	1.5298	1.5271	1.5254	1.5223	1.5164	1.5151	1.5118	1.5159	1.5146	1.5114
2	6	1.5231	1.5218	1.5185	1.5211	1.5198	1.5166	1.5349	1.5334	1.5298	1.5272	1.5254	1.5223	1.5164	1.5151	1.5118	1.5159	1.5146	1.5114
2	9	1.5231	1.5218	1.5185	1.5211	1.5198	1.5166	1.5349	1.5334	1.5298	1.5272	1.5254	1.5223	1.5164	1.5151	1.5118	1.5159	1.5146	1.5114
3	4	1.3484	1.3439	1.3399	1.3482	1.3436	1.3397	1.3604	1.3554	1.3511	1.3599	1.3553	1.3513	1.3412	1.3366	1.3327	1.3411	1.3365	1.3326
4	5	1.4734	1.4724	1.4692	1.4737	1.4727	1.4696	1.4800	1.4787	1.4753	1.4751	1.4736	1.4707	1.4722	1.4713	1.4682	1.4724	1.4716	1.4686
6	7	1.3484	1.3439	1.3399	1.3482	1.3436	1.3397	1.3604	1.3554	1.3511	1.3599	1.3553	1.3513	1.3412	1.3366	1.3327	1.3411	1.3365	1.3326
7	8	1.4734	1.4724	1.4692	1.4737	1.4727	1.4696	1.4800	1.4787	1.4753	1.4751	1.4736	1.4707	1.4722	1.4713	1.4682	1.4724	1.4716	1.4686
8	9	1.3484	1.3439	1.3399	1.3482	1.3436	1.3397	1.3604	1.3554	1.3511	1.3599	1.3553	1.3513	1.3412	1.3366	1.3327	1.3411	1.3365	1.3326
INTERCEPT		0,0385	0,0084	-0,0012	0,0192	0,0493	0,0089	0,0260	0,0586	0,0159	0,0846	0,1110	0,0723	-0,0107	0,0204	-0,0196	-0,0083	0,0226	-0,0179
SLOPE		0,9789	0,9981	1,0023	0,9900	0,9708	0,9948	0,9931	0,9724	0,9975	0,9493	0,9329	0,9555	1,0073	0,9875	1,0111	1,0056	0,9858	1,0098
CORREL		0,9997	0,9998	0,9998	0,9998	0,9998	0,9999	0,9991	0,9988	0,9992	0,9992	0,9990	0,9993	0,9997	0,9998	0,9997	0,9997	0,9998	0,9997
RMSD		0,0086	0,0059	0,0027	0,0051	0,0079	0,0020	0,0165	0,0195	0,0128	0,0130	0,0161	0,0097	0,0019	0,0030	0,0042	0,0021	0,0030	0,0044

Bond length (continuation)

		M06-2X			PBE0			PBE0[GD3BJ]			PBE			PW91			wB97		
Atom I	Atom J	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ
1	2	1.5159	1.5150	1.5123	1.5137	1.5120	1.5096	1.5130	1.5114	1.5090	1.5236	1.5217	1.5190	1.5231	1.5211	1.5183	1.5163	1.5147	1.5118
1	5	1.3434	1.3398	1.3360	1.3459	1.3420	1.3385	1.3458	1.3419	1.3385	1.3587	1.3543	1.3507	1.3575	1.3528	1.3490	1.3431	1.3390	1.3350
2	3	1.5159	1.5150	1.5123	1.5137	1.5120	1.5096	1.5130	1.5114	1.5090	1.5236	1.5217	1.5190	1.5231	1.5211	1.5183	1.5163	1.5147	1.5118
2	6	1.5159	1.5150	1.5123	1.5137	1.5120	1.5096	1.5130	1.5114	1.5090	1.5236	1.5217	1.5190	1.5231	1.5211	1.5183	1.5164	1.5148	1.5118
2	9	1.5159	1.5150	1.5123	1.5137	1.5120	1.5096	1.5130	1.5114	1.5090	1.5236	1.5217	1.5190	1.5231	1.5211	1.5183	1.5163	1.5147	1.5118
3	4	1.3434	1.3398	1.3360	1.3459	1.3420	1.3385	1.3458	1.3419	1.3385	1.3587	1.3543	1.3507	1.3575	1.3528	1.3490	1.3431	1.3390	1.3350
4	5	1.4748	1.4745	1.4719	1.4675	1.4664	1.4641	1.4678	1.4667	1.4644	1.4723	1.4707	1.4682	1.4715	1.4699	1.4672	1.4724	1.4714	1.4684
6	7	1.3434	1.3398	1.3360	1.3459	1.3420	1.3385	1.3458	1.3419	1.3385	1.3587	1.3543	1.3507	1.3575	1.3528	1.3490	1.3431	1.3390	1.3350
7	8	1.4748	1.4745	1.4719	1.4675	1.4664	1.4641	1.4678	1.4667	1.4644	1.4723	1.4707	1.4682	1.4715	1.4699	1.4672	1.4724	1.4714	1.4684
8	9	1.3434	1.3398	1.3360	1.3459	1.3420	1.3385	1.3458	1.3419	1.3385	1.3587	1.3543	1.3507	1.3575	1.3528	1.3490	1.3431	1.3390	1.3350
INTERCEPT		0.0398	0.0143	0.0017	0.0857	0.0638	0.0515	0.0891	0.0665	0.0551	0.1278	0.1034	0.0925	0.1215	0.0951	0.0833	0.0374	0.0129	0.0006
SLOPE		0.9747	0.9913	0.9978	0.9418	0.9554	0.9620	0.9393	0.9534	0.9594	0.9195	0.9345	0.9401	0.9233	0.9396	0.9456	0.9761	0.9915	0.9977
CORREL		0.9996	0.9995	0.9995	0.9998	0.9998	0.9999	0.9998	0.9999	0.9999	0.9990	0.9992	0.9993	0.9990	0.9992	0.9993	0.9998	0.9998	0.9997
RMSD		0.0046	0.0032	0.0030	0.0055	0.0039	0.0045	0.0055	0.0040	0.0048	0.0143	0.0113	0.0086	0.0135	0.0102	0.0075	0.0040	0.0020	0.0033

Bond length (continuation)

		HF			MP2			CCSD	CASSCF (8,8)	
Atom I	Atom J	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31G(d)	6-31G(d)	X-Ray [from Haselbach et al]
1	2	1.5212	1.5206	1.5180	1.5108	1.5127	1.5076	1.5189	1.5211	1.5137
1	5	1.3579	1.3542	1.3480	1.3565	1.3576	1.3517	1.3472	1.3463	1.3391
2	3	1.5212	1.5206	1.5180	1.5108	1.5127	1.5076	1.5189	1.5211	1.5157
2	6	1.5212	1.5206	1.5180	1.5108	1.5127	1.5076	1.5189	1.5211	1.5150
2	9	1.5212	1.5206	1.5180	1.5108	1.5127	1.5076	1.5189	1.5211	1.5176
3	4	1.3579	1.3542	1.3480	1.3565	1.3576	1.3517	1.3472	1.3463	1.3355
4	5	1.4554	1.4568	1.4559	1.4683	1.4719	1.4649	1.4795	1.4793	1.4693
6	7	1.3579	1.3542	1.3480	1.3565	1.3576	1.3517	1.3472	1.3463	1.3396
7	8	1.4554	1.4568	1.4559	1.4683	1.4719	1.4649	1.4795	1.4793	1.4684
8	9	1.3579	1.3542	1.3480	1.3565	1.3576	1.3517	1.3472	1.3463	1.3370
INTERCEPT		0.1580	0.1274	0.0907	0.1978	0.1904	0.1806	0.0478	0.0256	
SLOPE		0.8952	0.9156	0.9385	0.8660	0.8725	0.8753	0.9718	0.9876	
CORREL		0.9923	0.9943	0.9959	0.9998	0.9999	0.9998	0.9995	0.9997	
RMSD		0.0146	0.0122	0.0089	0.0123	0.0128	0.0104	0.0080	0.0081	

Bond angles

			B3LYP			B3LYP[GD3BJ]			BLYP			BP86			CAMB3LYP			CAMB3LYP[GD3BJ]		
Atom I	Atom J	Atom K	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ
1	2	3	101.819	101.789	101.694	102.036	102.006	101.913	101.825	101.793	101.701	102.117	102.097	101.985	101.813	101.781	101.691	101.902	101.87	101.78
1	2	6	113.427	113.443	113.494	113.311	113.328	113.377	113.424	113.441	113.49	113.268	113.279	113.338	113.431	113.448	113.495	113.383	113.4	113.448
1	2	9	113.428	113.443	113.494	113.312	113.328	113.377	113.424	113.441	113.49	113.268	113.279	113.339	113.431	113.448	113.496	113.383	113.401	113.448
2	3	4	109.799	109.783	109.849	109.682	109.667	109.73	109.71	109.687	109.751	109.606	109.585	109.663	109.904	109.892	109.957	109.85	109.837	109.901
2	6	7	109.799	109.783	109.849	109.682	109.667	109.73	109.71	109.687	109.751	109.606	109.585	109.663	109.904	109.892	109.957	109.85	109.837	109.901
3	4	5	109.292	109.322	109.305	109.3	109.33	109.314	109.377	109.416	109.399	109.335	109.366	109.345	109.189	109.218	109.197	109.2	109.228	109.209
6	7	8	109.292	109.322	109.305	109.3	109.33	109.314	109.377	109.416	109.399	109.335	109.366	109.345	109.189	109.218	109.197	109.2	109.228	109.209
7	8	9	109.292	109.322	109.305	109.3	109.33	109.314	109.377	109.416	109.399	109.335	109.366	109.345	109.189	109.218	109.197	109.2	109.228	109.209
INTERCEPT			6.0765	5.7403	4.3760	9.1100	8.7641	7.4391	6.3748	6.0285	4.7097	10.3242	10.1208	8.5159	5.7350	5.3632	4.0671	7.0013	6.6233	5.3321
SLOPE			0.9435	0.9466	0.9592	0.9156	0.9188	0.9310	0.9409	0.9441	0.9562	0.9044	0.9063	0.9211	0.9465	0.9500	0.9619	0.9348	0.9384	0.9502
CORREL			0.9978	0.9975	0.9977	0.9975	0.9971	0.9975	0.9968	0.9963	0.9967	0.9968	0.9964	0.9970	0.9984	0.9983	0.9983	0.9984	0.9983	0.9983
RMSD			0.3232	0.3240	0.2898	0.4069	0.4052	0.3639	0.3577	0.3652	0.3295	0.4528	0.4563	0.4027	0.2984	0.2928	0.2657	0.3299	0.3237	0.2913

Bond angles (continuation)

			M06-2X			PBE0			PBE0[GD3BJ]			PBE			PW91			wB97		
Atom I	Atom J	Atom K	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ
1	2	3	102.062	102.037	101.929	102.102	102.084	101.971	102.205	102.187	102.075	102.187	102.172	102.063	102.16	102.144	102.029	101.952	101.935	101.825
1	2	6	113.3	113.314	113.373	113.276	113.286	113.346	113.221	113.231	113.291	113.231	113.239	113.296	113.245	113.254	113.314	113.348	113.354	113.412
1	2	9	113.297	113.308	113.366	113.277	113.286	113.347	113.222	113.232	113.291	113.231	113.239	113.297	113.245	113.254	113.316	113.359	113.369	113.426
2	3	4	109.795	109.791	109.863	109.712	109.703	109.783	109.65	109.642	109.72	109.587	109.567	109.645	109.594	109.571	109.652	109.82	109.808	109.88
2	6	7	109.795	109.791	109.863	109.712	109.703	109.783	109.65	109.642	109.72	109.587	109.567	109.645	109.594	109.571	109.652	109.818	109.806	109.879
3	4	5	109.174	109.191	109.173	109.238	109.255	109.232	109.247	109.265	109.243	109.319	109.347	109.323	109.326	109.357	109.333	109.205	109.226	109.208
6	7	8	109.174	109.191	109.172	109.238	109.255	109.232	109.247	109.265	109.243	109.319	109.347	109.323	109.326	109.357	109.333	109.206	109.226	109.208
7	8	9	109.174	109.19	109.172	109.238	109.255	109.232	109.247	109.265	109.243	109.319	109.347	109.323	109.326	109.357	109.333	109.204	109.225	109.208
INTERCEPT			9.1503	8.8533	7.3015	9.8690	9.6633	8.0356	11.3220	11.1128	9.5065	11.2526	11.1139	9.5476	10.8988	10.7497	9.0971	7.7307	7.5549	5.9957
SLOPE			0.9150	0.9178	0.9320	0.9085	0.9104	0.9254	0.8951	0.8971	0.9118	0.8959	0.8972	0.9116	0.8991	0.9005	0.9157	0.9281	0.9298	0.9441
CORREL			0.9985	0.9984	0.9985	0.9981	0.9979	0.9982	0.9978	0.9976	0.9980	0.9969	0.9965	0.9971	0.9968	0.9964	0.9970	0.9984	0.9983	0.9984
RMSD			0.3868	0.3801	0.3360	0.4159	0.4131	0.3617	0.4626	0.4593	0.4061	0.4769	0.4804	0.4261	0.4677	0.4723	0.4157	0.3494	0.3472	0.3058

Bond angles (continuation)

			HF			MP2			CCSD	CASSCF(8,8)	
Atom I	Atom J	Atom K	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31G*	6-31G*	X-Ray [from Haselbach et al]
1	2	3	101.277	101.277	101.185	102.607	102.64	102.545	102.009	101.356	101.714
1	2	6	113.242	113.273	113.348	113.009	112.991	113.041	113.326	113.675	113.693
1	2	9	114.194	114.164	114.186	113.009	112.991	113.042	113.326	113.675	114.175
2	3	4	110.077	110.075	110.134	109.547	109.546	109.567	109.901	110.379	110.108
2	6	7	110.077	110.075	110.134	109.547	109.546	109.567	109.901	110.379	109.920
3	4	5	109.282	109.285	109.272	109.15	109.134	109.161	109.095	108.943	109.008
6	7	8	109.282	109.285	109.272	109.15	109.134	109.161	109.095	108.943	109.243
7	8	9	109.282	109.285	109.272	109.15	109.134	109.161	109.095	108.943	109.241
INTERCEPT			-1.7291	-1.7108	-3.0006	16.6407	17.0627	15.8128	8.2242	-1.2208	
SLOPE			1.0153	1.0152	1.0270	0.8460	0.8421	0.8537	0.9234	1.0102	
CORREL			0.9978	0.9979	0.9980	0.9982	0.9983	0.9982	0.9987	0.9964	
RMSD			0.2497	0.2432	0.2542	0.6241	0.6371	0.5972	0.3600	0.3251	

Dihedral angles

				B3LYP			B3LYP[GD3BJ]			BLYP			BP86			CAMB3LYP			CAMB3LYP[GD3BJ]		
Atom I	Atom J	Atom K	Atom L	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ
1	2	3	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	2	6	7	122.233	122.241	122.267	122.172	122.181	122.206	122.231	122.24	122.265	122.149	122.155	122.186	122.235	122.243	122.268	122,21	122,219	122,244
2	3	4	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	6	7	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	7	8	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
INTERCEPT				-0,3887	-0,3887	-0,3888	-0.3885	-0.3885	-0.3886	-0.3887	-0.3887	-0.3888	-0.3884	-0.3885	-0.3886	-0.3887	-0.3887	-0.3888	-0.3886	-0.3887	-0.3887
SLOPE				0,9907	0,9908	0,9910	0.9902	0.9903	0.9905	0.9907	0.9908	0.9910	0.9901	0.9901	0.9904	0.9908	0.9908	0.9910	0.9906	0.9906	0.9908
CORREL				1,0000	1,0000	1,0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
RMSD				0,7805	0,7774	0,7672	0.8046	0.8010	0.7912	0.7813	0.7778	0.7680	0.8137	0.8114	0.7991	0.7797	0.7766	0.7668	0.7896	0.7860	0.7762

Dihedral angles (continuation)

				M06-2X			PBE0			PBE0[GD3BJ]			PBE			PW91			wB97		
Atom I	Atom J	Atom K	Atom L	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ
1	2	3	4	0.002	0.004	0.004	0	0	0	0	0	0	0	0	0	0	0	0	0.005	0,006	0,004
1	2	6	7	122.168	122.173	122.203	122.154	122.159	122.19	122.125	122.13	122.161	122.129	122.134	122.164	122.137	122.141	122.173	122.19	122,192	122,221
2	3	4	5	0.001	0.002	0.002	0	0	0	0	0	0	0	0	0	0	0	0	0.003	0,004	0,002
2	6	7	8	0.001	0.002	0.001	0	0	0.001	0	0	0	0.001	0.001	0.001	0.001	0.001	0.001	0.004	0,005	0,005
6	7	8	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.002	0,002	0,001
INTERCEPT				-0,3875	-0,3865	-0,3869	-0.3885	-0.3885	-0.3883	-0.3884	-0.3884	-0.3885	-0.3881	-0.3881	-0.3882	-0.3882	-0.3882	-0.3883	-0.3851	-0.3843	-0.3857
SLOPE				0,9902	0,9902	0,9905	0.9901	0.9901	0.9904	0.9899	0.9899	0.9902	0.9899	0.9899	0.9902	0.9900	0.9900	0.9903	0.9904	0.9904	0.9906
CORREL				1,0000	1,0000	1,0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
RMSD				0,8058	0,8034	0,7916	0.8118	0.8098	0.7974	0.8233	0.8213	0.8090	0.8217	0.8197	0.8077	0.8185	0.8169	0.8042	0.7962	0.7951	0.7842

Dihedral angles (continuation)

				HF			MP2			CCSD	CASSCF (8,8)	X-Ray [from Haselbach et al]
Atom I	Atom J	Atom K	Atom L	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31G*	6-31G*	
1	2	3	4	0.214	0.203	0.186	0	0	0.001	0	0	0.408
1	2	6	7	122.5	122.49	122.514	122.014	122.004	122.03	122,18	122,361	123.767
2	3	4	5	0.541	0.511	0.467	0	0	0	0	0	0.584
2	6	7	8	0.541	0.511	0.467	0	0	0	0	0	0.193
6	7	8	9	0.688	0.651	0.596	0	0	0	0	0	0.385
INTERCEPT				0,4960	0,4690	0,4290	0.0000	0.0000	0.0003	0.0000	0.0000	
SLOPE				0,9988	0,9989	0,9994	0.9988	0.9988	0.9990	1.0002	1.0017	
CORREL				1,0000	1,0000	1,0000	1.0000	1.0000	1.0000	1.0000	1.0000	
RMSD				0,4947	0,4689	0,4370	0.0631	0.0675	0.0559	0.0112	0.0921	

Comparison of the vibrational frequencies of molecule **1**, computed at different levels of theory, and corresponding linear regression parameters, compared to experimental data.

	B3LYP			B3LYP[GD3BJ]			BLYP			BP86			CAM-B3LYP		
	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ
	1557.1	1545.88	1547.77	1558.61	1547.35	1549.21	1508.83	1500.05	1503.81	1498.97	1511.42	1513.27	1418.12	1594.12	1595.8
	1197.44	1195.53	1196.5	1203.32	1201.58	1202.59	1153.83	1152.35	1153.57	1161.36	1160.1	1159.89	1170.12	1163.35	1163.57
	1303.6	1296.68	1303.41	1303.9	1296.89	1303.58	1261.33	1255.44	1262.07	1253.02	1246.06	1250.54	1222.15	1220.02	1221.08
	1056.72	1052.6	1052.14	1058.73	1054.5	1054.15	1082.05	1077.89	1080.24	1073.7	1068.2	1068.75	1070.71	1065.67	1065.58
	NOT FOUND	NOT FOUND	NOT FOUND	NOT FOUND	NOT FOUND	NOT FOUND	1039.13	1034.55	1033.38	1026.33	1042.58	1040.94	1016.21	1010.17	1009.73
	955.77	957.36	965.85	954.54	956.12	964.57	956.5	970.33	969.87	966.93	961.36	960.04	975.87	978.58	984.4
	813.49	818.76	820.08	819.16	824.67	826.37	NOT FOUND	NOT FOUND	NOT FOUND	NOT FOUND	NOT FOUND	NOT FOUND	823.47	828.72	829.88
	813.48	NOT FOUND	NOT FOUND	NOT FOUND	NOT FOUND	NOT FOUND	798.51	800.94	801.52	800.38	803.31	803.38	796.9	792.78	796.57
	723.17	721.66	725.97	722.15	751.36	724.9	742.4	735.61	742.65	739.03	734.13	739.91	743.81	742.15	745.27
INTERCEPT	-67.6071	-64.9399	-60.2411	-79.5106	-32.9460	-58.5629	4.4688	14.3293	15.2257	14.1954	3.1624	4.5827	102.205	-50.6364	-45.6539
SLOPE	1.0748	1.0677	1.0664	1.0855	1.0438	1.0667	0.9939	0.9829	0.9844	0.9821	0.9933	0.9931	0.8873	1.0509	1.0479
CORREL	0.9991	0.9992	0.9991	0.9992	0.9985	0.9990	0.9989	0.9991	0.9991	0.9996	0.9993	0.9993	0.9969	0.9913	0.9909

	CAM-B3LYP[GD3BJ]			M06-2X			PBE0			PBE0[GD3BJ]			PBE		
	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ
	1418.06	1594.56	1596.22	1601.47	1588.09	1588.84	1584.43	1574.44	1572.91	1585	1574.98	1573.45	1506.67	1497.33	1496.36
	1170.67	1163.87	1164	1163.23	1157.83	1155.9	1162.07	1155.95	1154.34	1162.91	1156.75	1155.06	1166.41	1165.36	1164.19
	1224.59	1222.53	1223.62	1304.2	1298.72	1301.6	1305.02	1297.15	1300.52	1305.19	1297.3	1300.63	1253.49	1246.41	1249.68
	1071.15	1066.07	1066	1060.23	1056.88	1054.7	1065.78	1060.48	1058.27	1066.35	1060.99	1058.81	1073.01	1067.21	1066.88
	1017.63	1011.71	1011.35	1013.84	NOT FOUND	NOT FOUND	1024.02	1019.54	1017.73	1025.83	1021.48	1019.77	1030.01	1046.15	1044.13
	975.52	978.23	984.03	969.12	971.32	975.23	960.78	962.39	966.97	960.16	961.77	966.54	973.19	967.85	965.93
	826.25	831.62	832.97	814.01	818.65	818.03	814.74	819.13	819.11	817.89	822.41	822.57	NOT FOUND	NOT FOUND	NOT FOUND
	796.56	792.44	796.22	796.04	792.91	795.17	814.74	NOT FOUND	NOT FOUND	NOT FOUND	NOT FOUND	NOT FOUND	801.71	804.68	804.23
	743.49	741.83	744.95	742.59	740.81	743.24	727.94	727.1	729.66	727.5	726.65	729.2	740.19	735.82	740.88
INTERCEPT	102.5720	-50.6435	-45.5271	-96.3762	-77.8880	-75.3580	-81.4760	-83.1673	-79.1681	-96.4563	-81.5384	-77.2871	11.1844	21.4507	24.6065
SLOPE	0.8876	1.0517	1.0485	1.1022	1.0852	1.0837	1.0873	1.0832	1.0798	1.0996	1.0823	1.0788	0.9879	0.9767	0.9739
CORREL	0.9969	0.9915	0.9911	0.9959	0.9969	0.9965	0.9971	0.9971	0.9967	0.9973	0.9970	0.9967	0.9996	0.9995	0.9997

	PW91			wB97			HF			MP2			Experimental
	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	6-31+G(d,p)	6-311++G(d,p)	aug-cc-pVTZ	
	1507.01	1497.37	1497.48	1600.32	1589.69	1590.75	1527.4	1517.68	1523	1553.16	1523.46	1517.37	1508
	1167.5	1166.32	1165.56	1167.03	1160.75	1160.31	1170.82	1166.44	1167.12	1173.32	1157.82	1147.63	1177
	1257.51	1250.14	1254.12	1217.48	1307.3	1313.18	1235.39	1229.82	1229.75	1221.44	1209.38	1291.44	1266
	1076.42	1070.33	1070.48	1068.05	1062.91	1062.4	1065.32	1054.82	NOT FOUND	1081.37	1061.99	1054.42	1065
	1031.71	1026.95	1045.45	1013.51	NOT FOUND	NOT FOUND	1040.76	1029.69	1048.6	1033.26	1020.6	1018.61	1036
	973.4	967.83	966.2	967.92	970.96	976.69	957.85	963.4	976.67	926.62	1000.7	941.99	966
	NOT FOUND	NOT FOUND	NOT FOUND	819.12	822.86	823.42	NOT FOUND	NOT FOUND	NOT FOUND	832.98	826.78	825.04	815
	803.36	806.38	806.32	791.33	788.07	791.94	789.27	790.65	800.44	821.78	816.25	815.72	805
	731.08	737.98	731.98	739.55	738.29	741.72	732.68	735.36	745.12	748.99	746.31	758.77	736
INTERCEPT	2.8456	19.7314	15.8466	-66.6162	-84.7824	-80.6563	-24.0839	-10.2734	11.7375	-1.9677	39.3162	8.1185	
SLOPE	0.9961	0.9774	0.9827	1.0651	1.0937	1.0921	1.0179	1.0013	0.9886	1.0039	0.9611	0.9919	
CORREL	0.9996	0.9997	0.9996	0.9915	0.9972	0.9969	0.9985	0.9986	0.9977	0.9934	0.9947	0.9966	

Vibrational Spectra

Level of theory: DFT B3LYP[GD3BJ] / 6-311++G** (harmonic approximation).

1$^{\cdot -}$

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	104.9916	0.0233	0.4910	512659.2065
2	A	108.4074	0.0272	911.0605	625420.4927
3	A	199.7079	0.0601	6.0412	6799953.6005
4	A	395.6048	0.5229	0.9202	**********
5	A	480.2545	0.3389	169.8778	**********
6	A	510.0115	0.5213	28.6860	**********
7	A	522.9184	0.4525	1353.5216	570935.7932
8	A	589.7404	0.4848	106.2395	4900879.8238
9	A	625.7780	0.3071	4989.8839	2020782.4769
10	A	656.5956	0.2974	144.2716	541739.9428
11	A	690.3315	0.4359	0.1913	2633686.0925
12	A	697.0260	0.4113	8780.4704	5775606.4489
13	A	760.5893	0.7578	38628.6549	**********
14	A	806.8459	1.8637	1598.5060	**********
15	A	812.9131	1.2652	72.3823	**********
16	A	818.3722	1.5491	5120.3070	2275714.3410
17	A	842.9643	0.6496	4.3836	5037907.6568
18	A	857.4211	1.2911	30.2633	1684852.1022
19	A	869.4377	0.6772	45.2117	7091754.0616
20	A	869.6524	0.6613	7638.0517	3644327.9285
21	A	880.6157	0.7891	8166.6549	4465808.2701
22	A	1000.8842	1.0886	12708.9626	**********
23	A	1015.8497	1.3119	14.9930	**********
24	A	1051.2499	1.4114	117.0804	**********
25	A	1061.9395	0.9977	15.5844	**********
26	A	1064.0458	0.9525	88.3801	**********
27	A	1076.5138	1.5838	13270.8179	**********
28	A	1111.1970	1.0093	910.3376	3235732.4065
29	A	1123.8595	1.5513	7.4512	4404160.0252
30	A	1199.4809	1.7325	7773.4537	3880275.9407
31	A	1279.0418	1.3866	4.3594	**********
32	A	1280.8435	1.3877	88.0989	**********
33	A	1334.6419	2.7720	312.4143	**********
34	A	1389.2265	2.5325	1651.6158	**********
35	A	1422.9913	3.2438	4.6697	**********
36	A	1545.7825	6.5018	4.1448	**********
37	A	1564.0452	7.0768	331.3215	**********
38	A	3136.9936	6.3080	13502.2837	**********
39	A	3144.4097	6.3391	471.1656	**********
40	A	3177.7270	6.4742	2992.3239	899879.4207
41	A	3179.3109	6.4826	0.3746	5876382.5283
42	A	3203.0786	6.6251	1317.0729	1977828.0885
43	A	3204.2865	6.6317	1.8997	**********
44	A	3205.0720	6.6254	609.3946	**********
45	A	3209.5771	6.6641	141.3085	**********

1$^{\cdot +}$

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	90.8622	0.0176	1.0530	3.2594
2	A	90.8626	0.0176	1.0530	3.2594
3	A	237.5889	0.1043	0.0000	8.3303
4	A	443.6205	0.6449	0.0000	160.8292
5	A	487.5110	0.3552	0.0000	0.0000
6	A	491.7830	0.4023	1.9149	0.6933

7	A	491.7833	0.4023	1.9149	0.6933
8	A	596.1657	0.4600	0.0000	1.2072
9	A	774.2235	0.4266	73.2991	1.6836
10	A	774.2239	0.4266	73.2991	1.6836
11	A	799.9747	0.4778	0.0000	0.0000
12	A	803.8013	2.3467	100.7140	0.2065
13	A	820.1315	0.5611	0.0000	0.1523
14	A	830.6412	2.2650	0.1136	3.4137
15	A	830.6415	2.2650	0.1136	3.4137
16	A	894.4698	1.5365	0.0000	45.3017
17	A	974.6290	0.7724	0.0094	0.8210
18	A	974.6292	0.7724	0.0094	0.8210
19	A	999.0758	0.8769	0.0000	0.1822
20	A	1004.2636	0.8762	0.0000	0.0000
21	A	1029.6170	1.0787	92.2506	0.0042
22	A	1063.8875	1.5287	0.0000	67.3102
23	A	1071.0589	0.8447	22.4313	0.3187
24	A	1085.6350	1.1065	2.5879	4.9724
25	A	1085.6355	1.1065	2.5879	4.9723
26	A	1117.8179	0.8083	0.0000	0.8260
27	A	1169.2349	1.7123	0.6054	3.3724
28	A	1169.2369	1.7123	0.6054	3.3725
29	A	1215.2080	4.3204	151.1911	8.5798
30	A	1315.7039	1.5724	0.9236	0.0632
31	A	1315.7043	1.5724	0.9236	0.0632
32	A	1403.2844	5.0624	259.8610	22.5643
33	A	1424.0549	2.5122	0.0000	16.9463
34	A	1426.7096	2.6770	4.0541	0.0176
35	A	1494.1138	7.5539	0.0000	85.1128
36	A	1526.4511	5.7101	42.7213	97.1589
37	A	1526.4515	5.7101	42.7212	97.1593
38	A	3215.2899	6.6400	0.5599	89.8339
39	A	3215.2900	6.6400	0.5597	89.8368
40	A	3223.5132	6.6865	9.7029	7.7200
41	A	3224.5184	6.6972	0.0000	262.2930
42	A	3237.2506	6.7806	9.5423	17.3915
43	A	3237.2520	6.7806	9.5424	17.3887
44	A	3241.9178	6.8531	0.9552	102.1151
45	A	3242.7136	6.8516	0.0000	434.6747

1

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	118.2916	0.0300	0.8895	2.3551
2	A	118.2916	0.0300	0.8895	2.3551
3	A	223.0457	0.0781	0.0000	5.7093
4	A	442.4684	0.6362	0.0000	6.8495
5	A	516.8042	0.4509	2.7688	0.1324
6	A	516.8042	0.4509	2.7688	0.1324
7	A	525.9862	0.4406	0.0000	0.0000
8	A	620.2567	0.5918	0.0000	0.9528
9	A	720.6414	0.3963	0.0000	0.0000
10	A	751.3584	0.4118	88.6750	0.0013
11	A	751.3584	0.4118	88.6751	0.0013
12	A	770.7977	0.5117	0.0000	0.0016
13	A	824.6880	2.2540	0.9564	1.7849
14	A	824.6880	2.2540	0.9564	1.7849
15	A	833.2668	1.9541	11.0519	2.0977
16	A	872.5291	1.4345	0.0000	9.2845
17	A	950.8626	0.7384	0.0000	0.0000
18	A	955.5142	0.7589	0.0000	2.3759
19	A	956.1211	0.7048	0.0014	1.9869
20	A	956.1211	0.7048	0.0014	1.9869

21	A	981.2530	1.1781	21.9413	1.4600
22	A	1003.0227	1.5893	0.0000	18.3018
23	A	1054.4868	0.9088	10.0676	1.5257
24	A	1081.6062	1.3707	14.7563	0.3726
25	A	1081.6062	1.3707	14.7563	0.3726
26	A	1107.0128	0.7764	0.0000	47.7401
27	A	1142.0415	1.2800	0.0003	7.9802
28	A	1142.0415	1.2800	0.0003	7.9802
29	A	1201.5795	2.3770	5.3946	0.1889
30	A	1296.8948	1.4320	0.5559	0.7592
31	A	1296.8948	1.4320	0.5559	0.7592
32	A	1384.8665	2.2349	0.2944	4.3113
33	A	1385.0642	2.1158	0.0000	8.3210
34	A	1547.3501	9.9503	12.3843	17.4279
35	A	1569.4994	9.7424	0.0000	166.5514
36	A	1630.6031	8.7127	0.1462	0.1264
37	A	1630.6031	8.7127	0.1462	0.1264
38	A	3190.5356	6.5211	5.7127	105.5349
39	A	3190.5356	6.5211	5.7127	105.5349
40	A	3201.3335	6.5780	16.4481	1.8995
41	A	3202.0100	6.5845	0.0000	277.3453
42	A	3224.7317	6.7350	8.1088	1.2807
43	A	3224.7317	6.7350	8.1088	1.2807
44	A	3228.5994	6.7922	10.9348	139.0652
45	A	3230.5915	6.7970	0.0000	321.6543

2$^{\cdot-}$

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	263.0799	0.0539	46.1842	2330.2538
2	A	345.1527	0.1739	7.3989	132.1945
3	A	385.3743	0.2058	10.7621	41.8978
4	A	465.1976	0.3855	16.4422	375.6310
5	A	515.7766	0.2445	295.9968	7505.6941
6	A	636.7913	0.4482	93.0651	3791.8671
7	A	673.4508	0.4762	157.4315	1570.1727
8	A	677.8829	0.8182	25.8861	413.0320
9	A	791.7904	0.5138	2.5346	756.3107
10	A	831.1098	0.6005	32.1463	5610.9182
11	A	882.3818	0.8967	0.3743	2760.1392
12	A	978.4789	0.8134	28.7880	1666.1192
13	A	1024.5932	1.0534	21.4931	229.0195
14	A	1059.7410	1.2884	9.2653	741.5375
15	A	1150.6086	2.7228	11.5264	1876.6610
16	A	1461.6312	9.6211	110.1877	438.7255
17	A	1592.7581	8.6333	274.0796	675.5147
18	A	2932.9244	5.4945	255.9619	43222.7313
19	A	2992.6462	5.8035	366.4617	3743.3313
20	A	3097.6593	6.1567	136.3865	900.5111
21	A	3165.3541	6.6275	25.1235	632.6333

2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	377.9427	0.1842	26.8940	7.0325
2	A	377.9427	0.1842	26.8940	7.0325
3	A	404.0199	0.2648	0.0000	10.1451
4	A	566.1637	0.2669	32.5827	2.9855
5	A	566.1637	0.2669	32.5827	2.9855
6	A	699.0307	0.8701	0.0000	22.5762
7	A	802.2120	1.3168	25.4145	15.2687

8	A	802.2120	1.3168	25.4145	15.2687
9	A	895.8326	0.6638	0.0000	0.6849
10	A	896.0709	0.6744	0.0000	0.0000
11	A	904.5517	0.5245	2.3689	3.3070
12	A	997.1515	0.7664	0.0000	13.6462
13	A	1074.5790	1.2281	18.8743	0.7892
14	A	1074.5790	1.2281	18.8743	0.7892
15	A	1466.0886	10.7556	160.0363	4.5491
16	A	1646.2260	9.0886	0.0000	96.9949
17	A	1661.2166	9.0705	101.6751	13.3432
18	A	3193.7956	6.5146	5.8784	166.1075
19	A	3193.7956	6.5146	5.8784	166.1075
20	A	3233.5814	6.9991	0.0000	387.7864
21	A	3237.5724	7.0356	3.2543	112.5739

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	55.2311	0.0070	0.0875	4.7174
2	A	55.2316	0.0070	0.0875	4.7174
3	A	124.0855	0.0354	0.0000	11.3426
4	A	239.8815	0.2183	0.0000	133.3404
5	A	269.5643	0.1491	0.0000	0.0000
6	A	270.3216	0.1269	0.6716	2.4691
7	A	270.3218	0.1269	0.6716	2.4691
8	A	427.9048	0.7350	0.6143	7.5597
9	A	427.9048	0.7350	0.6143	7.5597
10	A	433.3324	0.7969	0.4259	4.2966
11	A	453.9114	0.3284	0.0000	0.0312
12	A	521.0264	0.4250	13.2124	0.9787
13	A	521.0264	0.4250	13.2124	0.9787
14	A	587.0358	0.7094	0.0000	0.0000
15	A	600.6605	1.2439	0.0000	85.8593
16	A	634.4966	1.1106	0.0000	0.1344
17	A	660.8023	0.3337	86.6775	28.9459
18	A	660.8023	0.3337	86.6774	28.9459
19	A	728.3487	0.4152	0.0000	0.0000
20	A	742.8538	0.4383	0.0000	1.2853
21	A	761.0328	0.4764	0.9069	0.5485
22	A	761.0329	0.4764	0.9069	0.5485
23	A	804.5308	2.2244	15.2689	9.6626
24	A	843.1932	2.5040	0.0000	87.1457
25	A	878.1873	0.5684	0.0000	1.0443
26	A	879.1710	0.5650	0.0000	0.0000
27	A	893.3782	2.2270	0.2718	5.8451
28	A	893.3783	2.2270	0.2718	5.8451
29	A	920.4119	1.7522	19.9856	0.5155
30	A	920.8430	0.6324	0.1039	0.0112
31	A	920.8431	0.6324	0.1039	0.0112
32	A	929.7184	0.6021	0.0000	3.0832
33	A	934.3889	1.5163	0.0000	82.0682
34	A	934.7510	0.6141	0.0000	0.0000
35	A	996.0253	2.6104	1.5165	5.5028
36	A	1004.1609	1.6253	23.3224	3.6287
37	A	1004.1610	1.6253	23.3225	3.6287
38	A	1165.5214	1.8423	5.2892	3.7275
39	A	1165.5217	1.8423	5.2893	3.7275
40	A	1230.3651	1.0761	40.0384	11.3640
41	A	1231.1155	1.0671	0.0000	150.4840
42	A	1272.2358	0.9893	0.0000	37.9772
43	A	1279.5642	1.0459	33.0717	1.6034
44	A	1310.1965	1.3004	1.5184	0.9024
45	A	1310.1968	1.3004	1.5184	0.9024

46	A	1398.0926	1.5324	0.5885	0.7353
47	A	1398.0927	1.5324	0.5885	0.7353
48	A	1442.1497	1.8369	64.1618	3.2424
49	A	1451.5287	1.7437	0.0000	31.8368
50	A	1476.0088	2.2768	0.0651	30.4529
51	A	1476.0088	2.2768	0.0652	30.4529
52	A	1514.7416	9.3554	1092.7800	29.1640
53	A	1582.5666	9.5790	15.3326	0.3065
54	A	1582.5666	9.5790	15.3326	0.3065
55	A	1602.7801	11.2986	0.0000	88.6788
56	A	1626.3590	6.2487	0.0599	1.6386
57	A	1633.6140	7.2333	0.0000	1312.4368
58	A	3079.4937	6.0366	34.1638	7.1230
59	A	3079.4937	6.0366	34.1637	7.1229
60	A	3082.9424	6.0654	13.2250	119.9913
61	A	3083.3486	6.0681	0.0000	123.7230
62	A	3103.9725	6.1611	60.3410	234.8716
63	A	3103.9725	6.1611	60.3411	234.8715
64	A	3126.2403	6.2836	265.3863	16.3638
65	A	3127.0524	6.2865	0.0000	466.6217
66	A	3137.5122	6.3136	54.4899	0.0008
67	A	3137.5124	6.3136	54.4895	0.0008
68	A	3142.2411	6.3429	5.8736	171.4669
69	A	3144.3634	6.3515	0.0000	397.3104

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	51.6707	0.0053	16.3901	3.2173
2	A	73.1165	0.0117	0.0008	3.0991
3	A	142.6577	0.0458	0.3073	175.0390
4	A	225.0043	0.1006	25.0813	2.2761
5	A	228.6634	0.1095	0.2626	290.2489
6	A	290.2979	0.1491	0.2521	523.4794
7	A	298.0529	0.1490	14.6109	1.5132
8	A	310.0532	0.2431	0.1204	226.0529
9	A	393.3404	0.5566	7.8251	17.2283
10	A	419.8740	0.4735	7.7426	5.7321
11	A	433.9768	0.3570	7.0939	537.7759
12	A	460.9003	0.5016	2.0171	8.8830
13	A	470.2707	0.3149	7.1838	0.2212
14	A	567.6043	0.4945	10.5371	0.2778
15	A	588.2412	0.6510	0.0134	705.9767
16	A	610.7368	1.0130	0.1856	27.5809
17	A	673.0328	0.5902	79.7251	3.8511
18	A	698.7059	0.3709	20.2142	149.0715
19	A	764.0657	0.5429	10.5371	9.8822
20	A	784.6680	1.2157	87.6796	3.4079
21	A	786.3997	0.6185	2.1847	33.5251
22	A	822.3592	1.1780	4.1202	152.7279
23	A	828.2337	0.6304	265.5591	0.6096
24	A	880.8034	0.6464	0.1331	2.9420
25	A	900.6601	1.8877	1.4138	23.1422
26	A	900.7916	2.0337	0.2646	56.2987
27	A	940.2156	1.7600	30.3072	4.7685
28	A	943.3178	1.1578	26.9770	0.7804
29	A	949.5288	1.5068	1.6577	84.6648
30	A	1001.0390	0.8631	13.5662	2.3816
31	A	1002.2237	0.7981	0.0108	143.5585
32	A	1013.1989	0.8308	2.1631	32.2881
33	A	1013.4661	0.9266	36.0507	3.1616
34	A	1026.5495	0.8837	0.1422	23.4372
35	A	1029.7693	0.9161	6.3807	8.1293

36	A	1035.3558	1.4464	3.0487	1.5948
37	A	1045.2780	1.6063	1.2342	144.4124
38	A	1129.4207	2.0263	60.1488	26.6107
39	A	1179.1426	2.1370	1.4411	880.5462
40	A	1253.3358	1.1362	19.6239	1.7179
41	A	1253.6191	1.1208	4.5101	158.0551
42	A	1269.1380	1.1152	381.3374	22.0441
43	A	1283.6203	1.0250	0.4886	42.9234
44	A	1296.3024	1.1066	33.2067	14.0877
45	A	1337.1615	1.4000	1.3316	72.7404
46	A	1387.8056	1.4892	72.2342	13.7063
47	A	1398.6260	1.5564	3.1096	19.8942
48	A	1448.6972	1.7869	10.6737	14.6586
49	A	1459.9847	1.7559	10.8296	22.6170
50	A	1470.7328	3.9948	874.2158	24.5146
51	A	1493.0152	2.1710	6.7024	149.5686
52	A	1497.1442	2.5507	279.4157	33.6376
53	A	1565.5011	7.9456	0.2837	533.3652
54	A	1595.2107	7.7361	13.9597	858.9246
55	A	1600.4404	6.9253	17.1266	95.6883
56	A	1652.4237	7.2751	2.6833	183.2093
57	A	1662.3943	7.7836	10.7988	55.7034
58	A	3153.5120	6.3586	0.1993	52.8216
59	A	3155.1418	6.3684	0.9316	53.3429
60	A	3155.2083	6.3683	0.0555	69.7471
61	A	3157.2612	6.3817	0.1354	42.7858
62	A	3167.7531	6.4432	0.0309	35.5367
63	A	3170.8754	6.4418	0.4112	194.4211
64	A	3174.1406	6.4749	0.0655	189.4364
65	A	3177.2326	6.4962	0.1884	132.7484
66	A	3179.7610	6.5045	0.2506	16.8562
67	A	3180.0726	6.5066	0.4419	69.8258
68	A	3187.0935	6.5503	0.0031	885.7825
69	A	3187.1583	6.5506	0.6460	101.1433

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	93.2556	0.0220	0.0006	5.1442
2	A	133.4488	0.0397	0.2705	1.3981
3	A	151.8978	0.0504	0.0273	3.6272
4	A	257.9699	0.1383	0.5335	2.9555
5	A	262.8659	0.1226	0.1375	2.2214
6	A	296.5912	0.2163	0.2463	2.7511
7	A	346.9537	0.2178	3.6248	1.5033
8	A	372.9775	0.2375	0.1766	7.8682
9	A	378.5575	0.2726	1.9748	2.5268
10	A	412.3789	0.4305	4.5251	1.3917
11	A	441.0490	0.3685	4.6402	7.7519
12	A	465.5691	0.3918	5.3321	1.7789
13	A	485.8066	0.4754	0.9853	1.7706
14	A	619.0940	1.0406	0.0005	15.2047
15	A	625.5120	0.6800	0.4547	0.1403
16	A	662.4941	0.7744	0.0065	6.7210
17	A	701.4853	0.4241	135.9632	0.0085
18	A	704.2406	0.4150	12.7844	2.0994
19	A	760.6200	0.6466	40.4658	0.5357
20	A	762.2242	0.6284	29.4340	0.3342
21	A	765.2468	0.4970	18.4448	0.2759
22	A	800.5142	1.0129	2.3092	8.7164
23	A	833.2851	0.7828	0.0965	5.3760
24	A	834.1401	0.7808	0.2575	0.2002
25	A	904.4905	2.1279	0.0501	0.1141

26	A	926.0902	2.3311	0.4517	5.1701
27	A	951.3363	1.4652	2.0204	0.8334
28	A	955.9754	1.1927	0.1627	2.6911
29	A	966.3244	0.8265	1.5982	3.5516
30	A	974.3934	0.9126	0.2632	35.0739
31	A	982.6246	0.7547	0.1681	6.2440
32	A	983.4034	0.7578	1.9100	1.0975
33	A	1001.3421	0.7652	0.0193	6.2850
34	A	1001.4764	0.7664	0.8446	4.8730
35	A	1021.8779	1.4780	5.8833	0.2601
36	A	1038.6955	1.4496	3.2931	1.9079
37	A	1106.6033	2.5807	11.2382	1.9335
38	A	1115.5610	1.7476	0.6638	1.0729
39	A	1127.0292	1.8012	0.0065	1.6208
40	A	1223.9917	0.9933	0.8215	11.0414
41	A	1228.5708	0.9996	0.2402	10.9485
42	A	1240.1490	1.0044	2.0547	12.7658
43	A	1241.6863	0.9905	0.9490	5.4831
44	A	1258.9842	1.1925	2.7905	0.3098
45	A	1272.4428	1.2423	4.1355	13.9780
46	A	1377.5363	1.4779	0.2720	0.2231
47	A	1382.9259	1.4790	0.0974	0.8160
48	A	1419.8151	1.8537	0.7965	0.1304
49	A	1434.6361	1.7705	2.1662	0.5981
50	A	1475.1033	2.2712	0.7817	5.4695
51	A	1476.8833	2.2710	0.9194	17.4582
52	A	1561.1378	11.5834	0.3915	265.5368
53	A	1563.4346	11.7989	0.4793	8.3650
54	A	1650.4673	11.5264	2.1341	5.8906
55	A	1659.7853	10.2229	2.2421	29.4558
56	A	1659.9395	7.8328	0.4489	2.1880
57	A	1666.5804	8.6293	0.1916	17.7555
58	A	3127.8233	6.2420	4.0034	44.2489
59	A	3128.5153	6.2452	1.0578	32.2041
60	A	3131.1389	6.2648	4.7032	127.4615
61	A	3131.9398	6.2713	0.0124	58.7801
62	A	3141.6878	6.3189	10.7243	47.2510
63	A	3142.5315	6.3203	3.2783	210.5026
64	A	3151.1173	6.3997	1.2387	112.0616
65	A	3154.6045	6.4088	65.9859	49.4707
66	A	3160.9642	6.4418	56.0382	26.0275
67	A	3161.8205	6.4457	0.9498	615.9352
68	A	3175.3529	6.4937	13.2862	8.4036
69	A	3176.9507	6.5020	0.5372	206.5884

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	297.7736	0.0808	122.0281	104418.4284
2	A	522.0787	0.3832	0.0000	24979.6930
3	A	668.8617	0.3141	331.6978	29129.2367
4	A	716.6664	0.3844	0.0001	348019.4554
5	A	813.6166	1.9382	39.9924	45397.5923
6	A	816.8731	2.1532	79.1791	93076.4276
7	A	919.3227	0.7544	210.5560	143720.7286
8	A	920.5587	1.0195	377.0686	39586.3660
9	A	955.8127	0.7124	0.0000	2186.0883
10	A	962.2968	0.8469	484.5110	544.9389
11	A	966.3820	0.8260	61.0958	67418.9686
12	A	1013.5906	1.4487	28.5092	57359.0688
13	A	1094.2743	0.7965	44.7447	77748.1619
14	A	1116.9090	0.9704	1.6318	165656.9127
15	A	1135.2000	0.8678	0.0000	2179.1984

16	A	1263.1286	1.5761	70.6962	4065.0932
17	A	1308.7990	1.7432	48.1393	18780.6717
18	A	1385.0019	1.4919	1101.5684	18595.2370
19	A	1399.4048	1.7980	111.2277	76962.9584
20	A	1541.4238	8.0713	38.2400	35093.3586
21	A	1625.9268	8.2042	1.9016	107.1145
22	A	2825.7304	5.2067	2741.5704	651.7841
23	A	2972.1766	5.5245	14.0844	263070.3164
24	A	3149.5443	6.3637	1.7240	4889.0778
25	A	3159.9325	6.4346	13.2725	608469.5886
26	A	3181.6318	6.5673	8.1156	538176.5024
27	A	3186.2949	6.5640	4.1307	12012.2378

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	273.6523	0.0677	1.5064	0.1675
2	A	426.3326	0.2418	0.0000	0.1669
3	A	632.1426	0.2660	63.0475	0.0347
4	A	802.0286	0.4483	0.0000	0.4205
5	A	811.5202	2.4813	1.7441	2.8243
6	A	819.8192	2.0549	0.4855	3.9261
7	A	890.1410	0.6413	19.0023	0.7403
8	A	935.0726	0.8725	6.8796	3.8230
9	A	954.6812	1.2122	22.2670	6.3926
10	A	990.5140	1.0614	0.0413	1.1505
11	A	1012.3613	0.8713	0.0000	0.1789
12	A	1085.5264	0.8707	11.1465	5.1977
13	A	1109.1465	1.4356	0.0986	49.6500
14	A	1128.3341	0.9881	3.2423	23.0562
15	A	1151.7454	0.9193	0.0000	4.4761
16	A	1303.1762	1.3881	12.2756	0.0408
17	A	1339.1658	2.3376	6.5632	0.3347
18	A	1370.2605	1.3451	71.8260	20.6954
19	A	1448.9173	3.4154	142.8763	0.7656
20	A	1455.4270	3.0160	2.3825	6.9454
21	A	1478.4524	4.1629	23.7025	8.5372
22	A	3016.4559	5.6994	31.4304	174.8854
23	A	3034.3500	5.9449	11.8297	86.5047
24	A	3213.1316	6.6327	5.6253	64.1749
25	A	3218.3576	6.6814	10.3140	88.2467
26	A	3227.3819	6.7350	16.6018	15.3998
27	A	3236.7959	6.8267	7.9761	186.2615

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	346.0129	0.1069	7.5573	0.3961
2	A	523.2015	0.3786	0.0000	0.0656
3	A	677.9304	0.3172	85.6699	0.0036
4	A	711.2078	0.3814	0.0000	0.0297
5	A	819.1097	1.9830	0.0038	1.3877
6	A	823.1060	2.2296	5.9511	0.5068
7	A	915.7893	0.9092	33.3363	1.3795
8	A	926.0980	1.0660	11.9053	7.1843
9	A	953.7668	0.7159	0.0000	1.8561
10	A	954.5471	0.7167	0.2808	2.0451
11	A	971.2010	0.8969	16.4307	2.2472
12	A	1016.3692	1.5761	0.1943	4.9883
13	A	1111.8577	0.8174	2.5451	9.9137
14	A	1125.1910	0.8466	0.0000	8.2360

15	A	1130.3713	0.9504	0.2708	26.1396
16	A	1265.4707	1.5963	2.1614	1.5321
17	A	1314.3604	1.6794	0.9241	0.0176
18	A	1396.0234	1.9603	17.5217	11.2743
19	A	1412.9588	1.4266	9.5080	19.8640
20	A	1545.5837	7.9872	1.1402	102.1873
21	A	1631.2683	8.1810	0.0136	1.0936
22	A	3012.7764	5.6711	9.4901	190.4702
23	A	3034.9951	5.9600	7.1936	102.5668
24	A	3189.5996	6.5143	3.4696	107.1879
25	A	3199.6505	6.5678	11.6967	59.0444
26	A	3218.0206	6.7093	17.4882	0.7657
27	A	3224.3816	6.7762	2.0174	279.4971

5$^{\cdot-}$

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	566.5438	0.2788	393.0598	143.3573
2	A	670.7852	0.3225	68.1891	27398.6742
3	A	808.5585	0.6645	3.6630	60.7206
4	A	898.0564	0.6621	16.6555	70.7167
5	A	918.7915	0.9302	7.0941	1718.3054
6	A	973.8196	0.7464	13.7758	600.3960
7	A	980.5222	0.8950	0.0218	1584.1918
8	A	1039.3170	0.8947	4.7902	404.3439
9	A	1089.3304	0.9600	0.5233	14.6631
10	A	1320.0475	3.7038	0.5720	4208.1426
11	A	1492.8158	1.5415	26.1866	292.5450
12	A	2915.2649	5.2262	259.6061	2714.1958
13	A	2929.3210	5.6217	65.0803	476.6114
14	A	2977.7121	5.6794	395.8363	364.2171
15	A	2981.8088	5.7559	3.7699	30532.4592

5

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	603.7453	0.2413	92.2686	0.1780
2	A	782.5728	0.9463	16.8304	15.8710
3	A	868.1285	0.6315	0.0000	0.0693
4	A	921.0511	0.5688	4.9464	4.5139
5	A	1012.5989	0.6589	0.0000	6.2317
6	A	1026.3150	0.9694	39.7698	0.0322
7	A	1065.9821	0.9081	25.9075	1.5406
8	A	1107.9555	0.9291	1.4070	0.2641
9	A	1146.6491	3.4664	0.2002	15.8447
10	A	1519.0829	1.5167	1.8177	15.4164
11	A	1726.6433	8.0686	17.5075	60.9053
12	A	3035.2345	5.6813	72.0758	152.8319
13	A	3099.4187	6.3253	47.4036	119.3004
14	A	3249.1644	6.7428	0.2134	83.1500
15	A	3296.2113	7.3384	0.0343	142.1508

6$^{\cdot-}$

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	56.8169	0.0037	1.3649	30.1205
2	A	219.0896	0.1013	0.1435	300.0481
3	A	379.6259	0.2862	12.6504	13.8223
4	A	413.4195	0.6047	0.0908	46.0843

5	A	456.9097	0.4376	4.9117	10.8724
6	A	500.4881	0.2555	0.0413	62.2052
7	A	550.4030	0.2124	159.7269	141.7454
8	A	601.8723	0.4737	0.5929	18.3261
9	A	637.2268	0.2961	31.8850	7.0105
10	A	734.0136	0.3799	1.2373	37.0851
11	A	777.4739	1.3000	0.6012	8.7596
12	A	836.1484	1.5317	12.3284	7.8557
13	A	860.1375	0.5983	4.1871	21.1623
14	A	861.5113	0.6011	2.9120	17.6157
15	A	896.8479	1.3874	1.1184	3.6495
16	A	917.5529	1.3838	34.4934	19.6195
17	A	938.6031	1.3933	47.3804	90.8476
18	A	974.4923	1.1794	13.3709	3.8681
19	A	1107.1531	1.1357	8.8400	12.3152
20	A	1185.3598	0.9613	13.9843	73.8419
21	A	1187.7468	1.0726	10.8307	41.6474
22	A	1240.9203	0.9853	3.5572	23.0630
23	A	1253.7731	0.9777	0.2863	0.2509
24	A	1324.8009	1.9447	5.2661	94.6026
25	A	1383.4431	1.4441	0.1753	27.4475
26	A	1431.1296	1.7483	2.8557	4.4680
27	A	1467.3733	1.4140	2.6693	37.6320
28	A	1469.8763	2.3161	0.4500	108.2090
29	A	1525.4630	5.2695	55.0005	242.2902
30	A	1536.9025	6.4708	1.8679	248.3042
31	A	1575.8019	6.5024	66.8137	137.8516
32	A	2822.6271	5.0587	157.6468	355.0061
33	A	2955.1047	5.5453	88.3324	91.1763
34	A	3047.1613	5.9089	48.8040	545.2713
35	A	3049.5340	5.9267	16.0227	123.1382
36	A	3082.1036	6.0598	4.3822	295.9385
37	A	3096.3826	6.1450	133.3289	168.0421
38	A	3097.2164	6.1586	210.9276	22.4847
39	A	3115.9863	6.2453	48.7095	302.9104

6$^{\cdot+}$

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	86.6615	0.0084	2.0813	0.0764
2	A	216.6233	0.0779	0.0000	0.0046
3	A	359.0629	0.1528	0.6257	0.0000
4	A	412.1169	0.6308	0.0426	6.0108
5	A	424.9265	0.7207	0.9800	7.9255
6	A	508.0547	0.3751	0.0000	0.0158
7	A	625.8519	0.2609	81.2046	0.1358
8	A	797.5018	1.9767	5.3816	55.2951
9	A	801.3579	0.5663	9.0592	1.6523
10	A	806.4003	0.4597	0.0000	0.1630
11	A	876.6746	2.6043	0.0008	4.6949
12	A	889.2143	2.5169	0.1341	0.8225
13	A	937.7140	1.4998	0.0141	26.5630
14	A	941.8116	1.1371	2.6420	0.4624
15	A	960.1747	0.8303	1.5020	1.1874
16	A	1012.9805	0.7599	0.0000	0.0339
17	A	1041.7878	0.9445	0.0000	0.0896
18	A	1046.4997	0.9222	0.8071	0.8770
19	A	1134.5910	1.1898	0.4813	7.2420
20	A	1220.6620	0.9856	0.0000	4.6316
21	A	1250.7215	1.1782	18.4614	15.0331
22	A	1274.8942	1.1146	25.9145	2.3918
23	A	1315.4035	1.0719	0.0168	0.0241
24	A	1358.4596	1.1573	78.2967	31.5811

25	A	1417.7509	1.5648	13.4069	1.5735
26	A	1453.9453	2.1618	8.9795	0.6308
27	A	1484.9456	1.8514	23.3876	0.7367
28	A	1523.6679	2.7090	31.8011	0.3393
29	A	1571.1571	6.6198	94.3114	39.9898
30	A	1596.4011	6.5136	6.0444	8.5405
31	A	1655.8933	8.2404	47.4628	22.2807
32	A	2919.0533	5.4606	6.0554	122.9528
33	A	2932.3701	5.3876	16.3490	238.6548
34	A	3158.1715	6.3846	0.8651	52.8974
35	A	3159.3003	6.4004	1.5705	64.1587
36	A	3167.8421	6.4338	0.3528	78.2169
37	A	3176.9418	6.4875	0.1608	120.2997
38	A	3183.5126	6.5234	2.0461	18.6159
39	A	3188.5295	6.5551	1.1220	325.7772

6

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	223.0715	0.0639	0.3528	3.2992
2	A	293.7621	0.1525	0.7494	2.1344
3	A	357.6109	0.2390	2.3800	2.2108
4	A	417.8744	0.5320	0.5743	4.2375
5	A	431.7936	0.2402	7.4039	7.6365
6	A	609.6695	0.5604	4.4131	2.9823
7	A	668.3919	0.5020	19.1340	1.4450
8	A	724.6652	0.4709	80.8890	0.5965
9	A	758.6422	0.4926	33.7529	0.1910
10	A	812.5716	0.6252	2.0514	2.7233
11	A	890.8468	1.8117	0.0687	0.1268
12	A	924.7551	1.5056	3.2104	33.3127
13	A	942.1515	1.2316	0.5593	6.0279
14	A	963.1399	1.4016	1.5342	0.8823
15	A	978.1776	0.8390	0.3309	8.1704
16	A	982.4191	0.7571	0.8074	5.0068
17	A	1000.6328	0.7593	0.0446	4.1559
18	A	1043.3358	1.4580	2.0735	3.1224
19	A	1069.7183	1.2079	1.5872	1.7773
20	A	1209.3182	0.9560	0.0435	0.1556
21	A	1220.3627	1.0153	0.7503	16.8548
22	A	1247.2755	1.0037	0.3481	11.8382
23	A	1269.8123	1.0595	0.5392	3.3412
24	A	1325.8545	1.5146	2.1378	1.6072
25	A	1384.9618	1.4928	0.9905	0.5451
26	A	1424.0744	1.7705	4.0083	2.0312
27	A	1475.8508	2.2680	0.0254	12.9989
28	A	1480.4855	1.4227	7.6468	8.2552
29	A	1569.9408	11.4327	0.1025	185.7126
30	A	1659.2388	10.0474	1.9016	33.8804
31	A	1666.1704	7.8021	0.3433	8.2688
32	A	2994.6744	5.6507	29.0494	111.3139
33	A	3092.6901	6.1556	21.1880	77.8906
34	A	3127.9390	6.2412	0.4289	21.2650
35	A	3134.2306	6.2807	2.1416	113.6725
36	A	3140.6701	6.3109	7.2737	141.8785
37	A	3154.7731	6.4057	47.0739	59.8538
38	A	3161.7211	6.4501	36.7002	76.8092
39	A	3165.9212	6.4716	5.5993	420.0422

Comparison of the diabatic electronic excitations of molecule **1**, computed at different levels off theory, corresponding linear regression parameters and RMSDs, compared to experimental data.

Reference data:
(1) Data from Haselbach *et al* [10.1002/1522-2675(20010613)84:6<1670::AID-HLCA1670>3.0.CO;2-K], obtained with eletron-energy loss spectroscopy with residual electron energy 1.1 eV, and their symmetry description as in the cited paper.

Exper. EELS (eV)	Exper. UV-vis (eV)	Transition symmetry	Type of transition (valence/Rydberg)	Main orbitals involved		
4.46	4.53	1^1E	V	$1a_2 \rightarrow 8e$		
5.78	6.05	2^1E	V	$1b_1 \rightarrow 8e$		
5.90		3^1E	R	$1a_2 \rightarrow 9e(R)$		
6.40		4^1E	R	$1a_2 \rightarrow 10e(R)$		
7.13		5^1E	R	$1b_1 \rightarrow 9e(R)$	$+1a_2 \rightarrow 11e(R)$	$+1b_1 \rightarrow 10e(R)$
7.40		3^1B_2	V	$1a_2 \rightarrow 2b_1$	$+7e \rightarrow 8e$	

(2) Data from Batich *et al*. [10.1021/ja00832a011], obtained from UV-Vis spectrum, i.e. transitions with energies 4.53 and 6.05 eV.

Data obtained in the present work at different levels of theory, and corresponding RMSDs with respect to both reference data sets are reported as follows. The considered electronic transitions were correlated with those of Haselbach *et al.* and Batich *et al*. by means of symmetry. For the sake of clarity, the numbers of transitions in the left column are those indicated in the work of Haselbach *et al.*.

Singlet excitations (TD-DFT) for molecule 1

	Hybrid functionals														
	B3LYP			CAM-B3LYP			M06-2X			PBE0			wB97XD		
Transition	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ
S_1	3.97	3.97	3.95	4.46	4.45	4.43	4.49	4.47	4.47	4.11	4.10	4.09	4.48	4.47	4.46
S_4	5.36	5.51	5.40	5.83	5.82	5.81	5.87	5.81	5.84	5.49	5.75	5.63	5.84	5.83	5.82
S_6	5.73	6.11	5.91	6.22	5.99	5.87	6.12	5.86	5.73	5.99	5.75	6.16	6.52	6.21	6.04
S_{11}	6.27	6.11	6.56	6.22	6.61	6.43	6.64	6.44	6.30	6.53	6.37	6.16	6.52	6.21	6.58
S_{19}	7.25	7.12	7.12	6.75	7.33	7.17	7.42	7.14	7.03	7.23	6.98	7.10	7.03	6.82	7.32
S_{20}	7.42	7.40	7.31	7.58	7.58	7.61	7.60	7.51	7.60	6.14	7.39	7.46	7.67	7.65	7.64
RMSD vs EELS	0.2826	0.2734	0.2700	0.2278	0.1471	0.0883	0.2008	0.0536	0.1224	0.5518	0.1709	0.2197	0.2858	0.2203	0.1566
RMSD vs UV-Vis	0.6284	0.5501	0.6160	0.1632	0.1722	0.1838	0.1304	0.1749	0.1544	0.4950	0.3707	0.4301	0.1526	0.1612	0.1700

	Pure functionals											
Transition	BLYP			BP86			PBE			PW91		
	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ
S_1	5.04	4.95	4.86	5.12	5.10	5.07	5.11	5.08	5.04	5.07	5.04	5.02
S_4	5.28	6.12	6.00	5.12	5.43	5.27	5.47	5.27	6.25	5.30	6.28	6.22
S_6	5.79	5.62	6.32	5.72	6.01	5.75	5.98	5.85	5.67	5.83	5.78	5.67
S_{11}	6.73	6.64	6.32	6.22	6.01	6.66	5.98	6.88	6.58	6.72	6.82	6.59
S_{19}	5.28	5.11	5.06	5.12	5.43	5.27	5.47	5.27	5.18	5.30	5.21	5.17
S_{20}	6.99	6.97	6.87	7.28	7.29	6.97	7.08	7.07	6.94	7.00	6.98	6.92
RMSD vs EELS	0.8477	0.8908	0.9091	0.9127	0.7739	0.8531	0.7715	0.8588	0.8808	0.8370	0.8772	0.8828
RMSD vs UV-Vis	0.6531	0.3011	0.2360	0.7788	0.5955	0.6708	0.5800	0.6749	0.3874	0.6535	0.3956	0.3667

Singlet excitations (TDA-DFT) for molecule 1

	Hybrid functionals														
	B3LYP			CAM-B3LYP			M06-2X			PBE0			wB97XD		
Transition	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ
S_1	4.06	4.06	4.04	4.63	4.62	4.60	4.65	4.64	4.63	4.21	4.20	4.19	4.65	4.64	4.63
S_4	5.76	5.63	5.58	5.99	5.96	5.87	6.04	5.81	6.02	5.70	5.80	5.72	6.00	5.99	5.97
S_6	5.76	6.12	5.91	5.99	5.96	5.87	6.04	5.81	5.74	6.01	5.80	5.72	6.53	6.22	5.97
S_{11}	6.27	6.12	6.57	6.23	6.62	6.44	6.64	6.45	6.31	6.54	6.37	6.17	6.53	6.22	6.59
S_{19}	7.25	7.12	7.12	6.76	7.34	7.17	7.43	7.15	7.04	7.23	6.98	7.10	7.04	6.83	7.32
S_{20}	7.20	7.21	5.94	7.66	8.02	6.52	8.05	8.02	6.57	6.16	7.44	6.11	7.87	7.86	7.98
RMSD vs EELS	0.2039	0.2418	0.6295	0.2291	0.2985	0.3661	0.3416	0.2679	0.3700	0.5220	0.1298	0.5505	0.3503	0.2934	0.2832
RMSD vs UV-Vis	0.4801	0.0825	0.0900	0.1366	0.0851	0.1867	0.0738	0.3353	0.2927	0.3350	0.0919	0.0886	0.0906	0.4801	0.0825

	Pure functionals											
Transition	BLYP			BP86			PBE			PW91		
	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ
S_1	5.19	4.98	4.87	3.62	3.61	5.22	3.62	5.19	5.10	5.21	5.12	5.08
S_4	5.40	5.63	6.00	5.74	5.49	5.41	5.53	5.44	5.40	5.45	5.41	5.39
S_6	5.79	5.63	6.33	5.74	6.02	5.75	5.99	5.86	5.67	5.84	5.79	5.67
S_{11}	6.73	6.65	6.33	6.23	6.02	6.66	6.77	6.88	6.59	6.76	6.74	6.60
S_{19}	6.82	5.63	5.42	5.74	5.49	5.41	5.53	5.44	5.40	5.45	5.41	5.39
S_{20}	7.17	7.15	5.39	7.36	7.36	7.18	7.25	7.23	7.15	7.20	7.19	7.13
RMSD vs EELS	0.3966	0.6740	1.1101	0.6713	0.7796	0.7984	0.7634	0.7937	0.7873	0.7832	0.7839	0.7904
RMSD vs UV-Vis	0.6550	0.4353	0.2430	0.6798	0.7616	0.6655	0.7411	0.6355	0.6113	0.6412	0.6155	0.6075

Triplet excitations (TD-DFT) for molecule 1

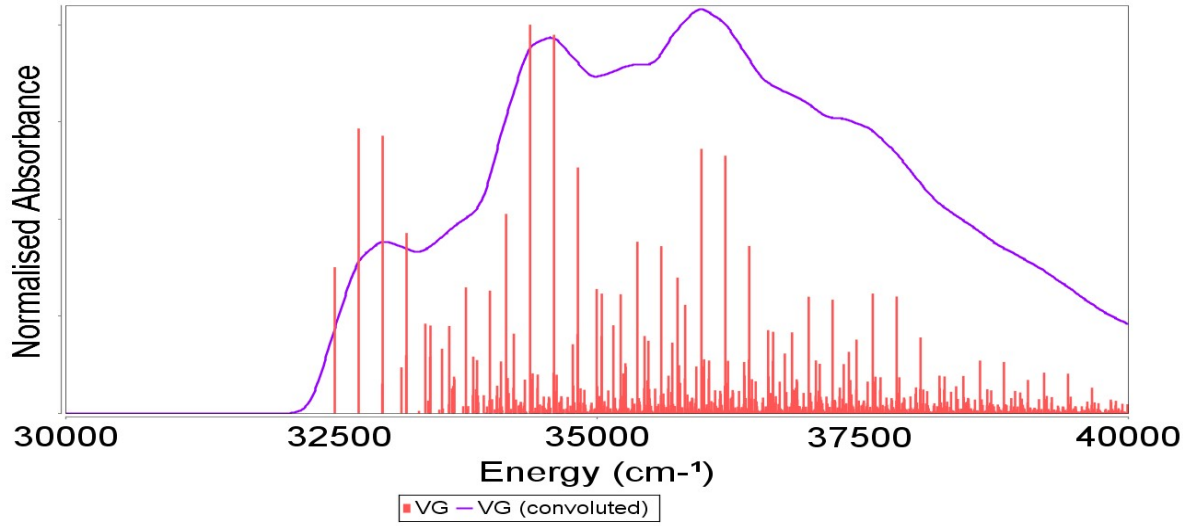
	Hybrid functionals														
	B3LYP			CAM-B3LYP			M06-2X			PBE0			wB97XD		
Transition	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ
T_1	2.57	2.58	2.57	2.50	2.51	2.51	3.10	3.06	3.05	2.44	2.44	2.43	2.65	2.66	5.29
T_2	4.58	4.57	4.55	4.53	4.53	4.51	5.08	5.02	5.00	4.48	4.47	4.44	4.70	4.69	4.67
T_3	4.84	4.84	4.83	4.73	4.73	4.73	5.29	5.25	5.23	4.71	4.71	4.69	4.89	4.89	4.87
T_4	4.51	4.51	4.50	5.26	5.25	5.24	5.32	5.30	5.31	4.65	4.65	4.64	5.29	5.29	5.29
RMSD vs EELS	0.3285	0.3258	0.3269	0.3196	0.3137	0.3108	0.5350	0.4976	0.4865	0.3136	0.3103	0.3148	0.3329	0.3281	1.1857

	Pure functionals											
Transition	BLYP			BP86			PBE			PW91		
	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ
T_1	2.66	2.67	2.66	2.64	2.65	2.64	2.65	2.65	2.64	2.63	2.63	2.62
T_2	4.60	4.59	4.57	4.59	4.57	4.55	4.59	4.58	4.55	4.57	4.56	4.53
T_3	4.96	4.96	4.95	4.94	4.94	4.92	4.94	4.94	4.92	4.91	4.92	4.90
T_4	4.01	4.01	4.00	4.04	4.03	4.02	4.03	4.03	4.02	4.02	4.02	4.01
RMSD vs EELS	0.5235	0.5228	0.5239	0.5120	0.5115	0.5119	0.5117	0.5110	0.5117	0.5151	0.5144	0.5157

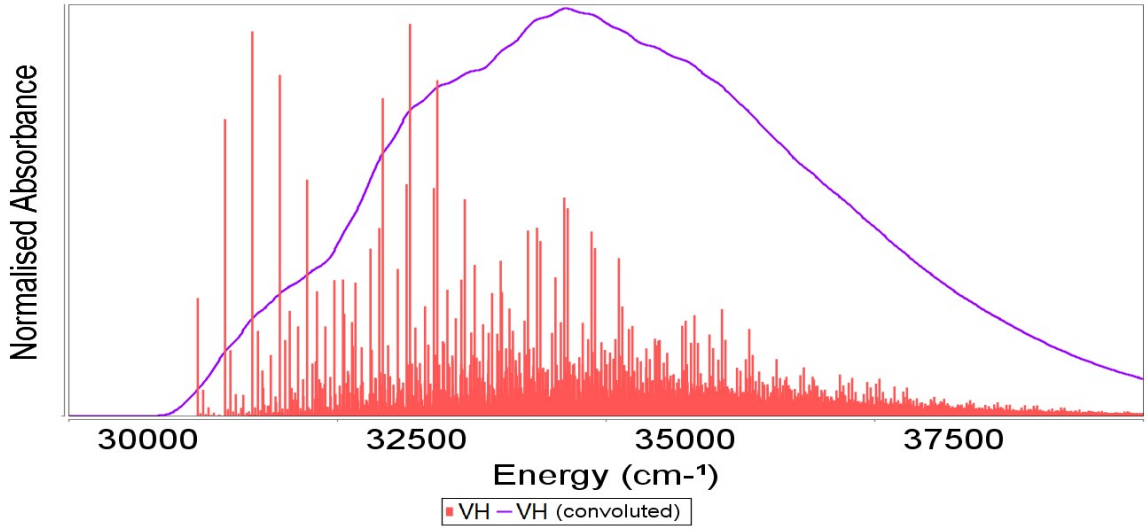
Triplet excitations (TDA-DFT) for molecule 1

	Hybrid functionals														
	B3LYP			CAM-B3LYP			M06-2X			PBE0			wB97XD		
Transition	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ
T_1	2.86	2.86	2.86	2.92	2.92	2.92	3.25	3.23	3.23	2.83	2.83	2.83	3.00	3.01	5.32
T_2	4.78	4.77	4.76	4.80	4.79	4.78	5.18	5.13	5.12	4.74	4.73	4.72	4.93	4.92	4.91
T_3	5.07	5.07	5.07	5.02	5.02	5.02	5.41	5.37	5.37	5.01	5.01	5.00	5.14	5.14	5.13
T_4	4.55	4.55	4.54	5.29	5.29	5.28	5.34	5.33	5.33	4.70	4.69	4.69	5.32	5.32	5.32
RMSD vs EELS	0.3655	0.3633	0.3607	0.3585	0.3546	0.3496	0.6233	0.5912	0.5856	0.3052	0.3021	0.2977	0.4380	0.4346	1.2437

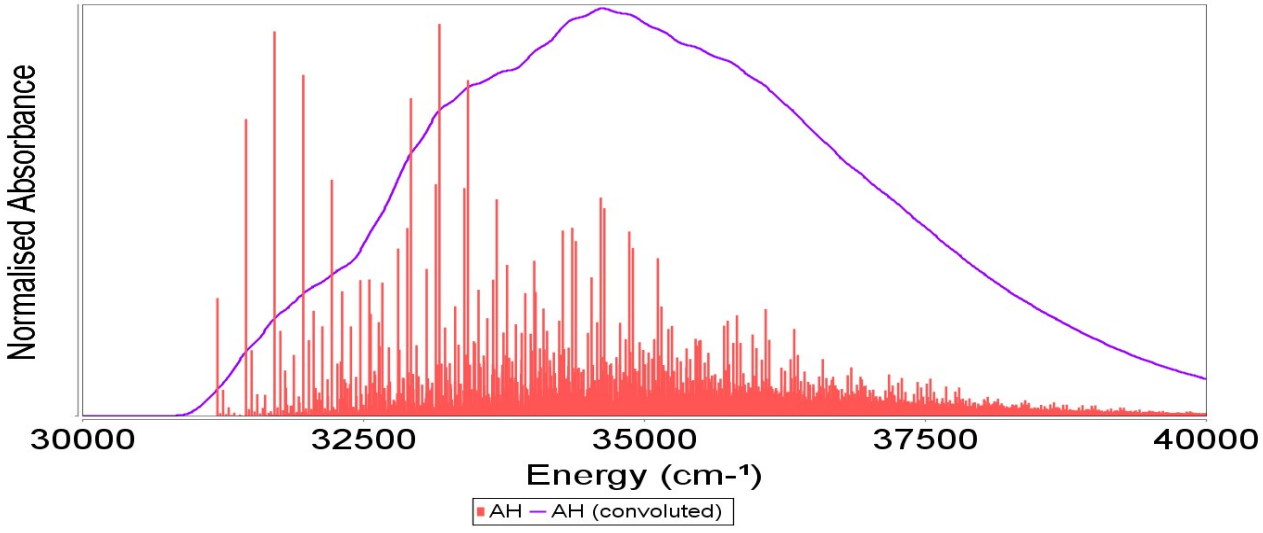
	Pure functionals											
Transition	BLYP			BP86			PBE			PW91		
	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ	6-31+G*	6-311++G**	Aug-cc-pVTZ
T_1	2.79	2.80	2.80	2.79	2.80	2.79	2.80	2.80	2.80	2.78	2.79	2.78
T_2	4.70	4.69	4.68	4.70	4.69	4.67	4.71	4.69	4.68	4.69	4.68	4.66
T_3	5.10	5.10	5.09	5.09	5.09	5.08	5.09	5.09	5.08	5.07	5.07	5.06
T_4	4.05	4.05	4.04	4.08	4.07	4.07	4.07	4.07	4.07	4.06	4.06	4.06
RMSD vs EELS	0.5329	0.5325	0.5315	0.5215	0.5205	0.5181	0.5215	0.5206	0.5186	0.5208	0.5204	0.5189



(a)



(b)



(c)

Figure S6. Vibronic progressions of the first UV-Vis absorption band computed at TD-DFT CAM-B3LYP / 6-311++G** ((a) VG, (b) VH and (c) AH; red sticks) and their Gaussian convolution (HWHM = 150 cm^{-1}; purple line) in gas phase. No shift along the energy axis was applied.