

Supporting Information

Role of $\rho(Z)-\pi(\text{Ar}/\text{Nap})$ Conjugation in Structures of 1-(Arylchalcogena)naphthalenes for $Z = \text{Te}$ versus Se , S and O : Experimental and Theoretical Investigations

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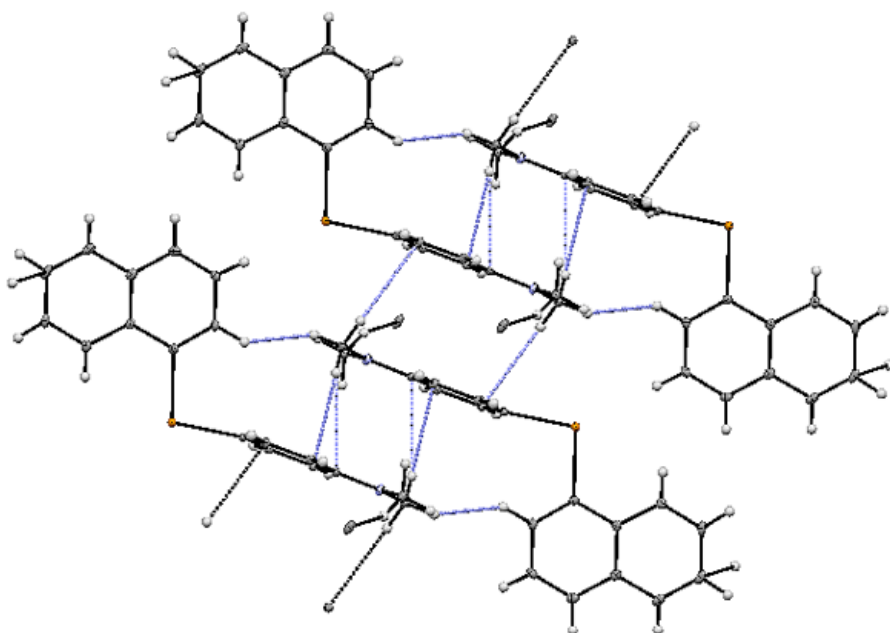


Fig. S1 Intermolecular interactions of **1b** in the solid state.

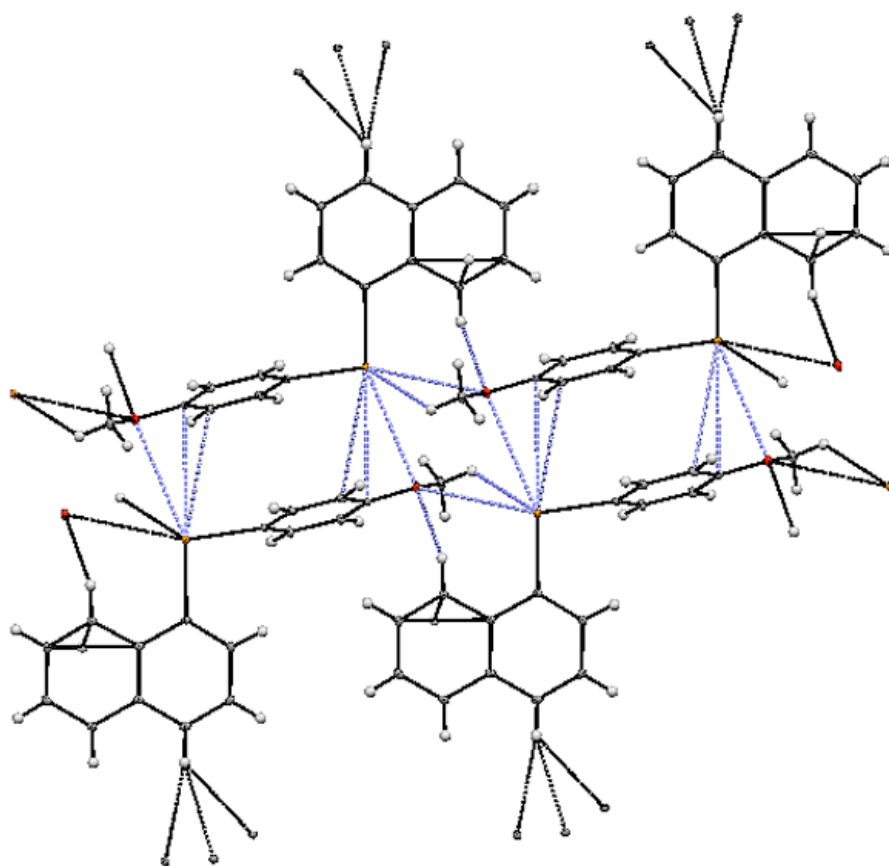


Fig. S2 Intermolecular interactions of **1c** in the solid state.

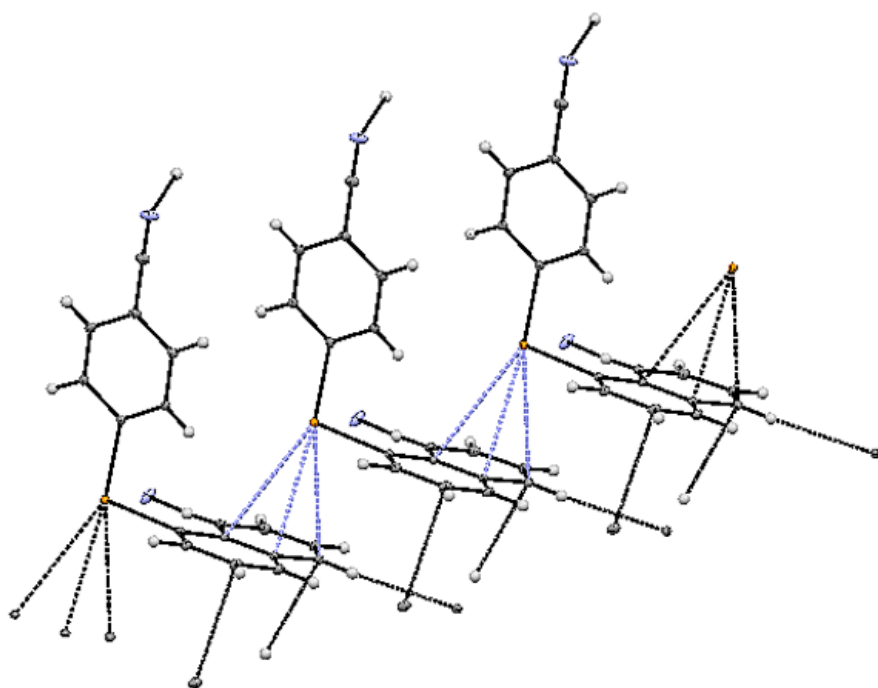


Fig. S3 Intermolecular interactions of **1i** in the solid state.

Table S1 Substituent Induced Chemical Shifts (δ_{SCS}) of ^1H and ^{13}C Nuclei of **3** and **4**

	NMe ₂ (b)	OMe (c)	Me (d)	H (a)	F (e)	Cl (f)	Br (g)	COOEt (h)	CN (i)	NO ₂ (j)
3 (Z = S)										
$\delta(\text{H}_2)_{\text{SCS}}$		-0.288	-0.105	0.000 (7.652) ^a		0.024	0.040	0.200		0.286
$\delta(\text{H}_8)_{\text{SCS}}$		-0.001	0.000	0.000 (8.348) ^a		-0.053	-0.057	-0.074		-0.126
$\delta(\text{C}_i)_{\text{SCS}}$		-11.7	-4.4	0.0 (136.9) ^a		-1.2	-0.3	7.8		11.6
4 (Z = O)										
$\delta(\text{H}_2)_{\text{SCS}}$		-0.063	-0.025	0.000 (7.602) ^a		0.003	0.011	0.118		0.182
$\delta(\text{H}_8)_{\text{SCS}}$		0.091	0.035	0.000 (8.201) ^a		0.021	0.000	-0.174		-0.272
$\delta(\text{C}_i)_{\text{SCS}}$		-7.2	-3.5	0.0 (157.9) ^a		-1.2	-0.6	4.5		6.1

^a $\delta(\text{H})_{\text{SCS}}$ and $\delta(\text{C})_{\text{SCS}}$ are given for **3** and **4**, together with $\delta(\text{H})$ and $\delta(\text{C})$ for **3a** and **4a** in parenthesis, measured in chloroform-*d* (0.050 mol/L) at 24 °C.

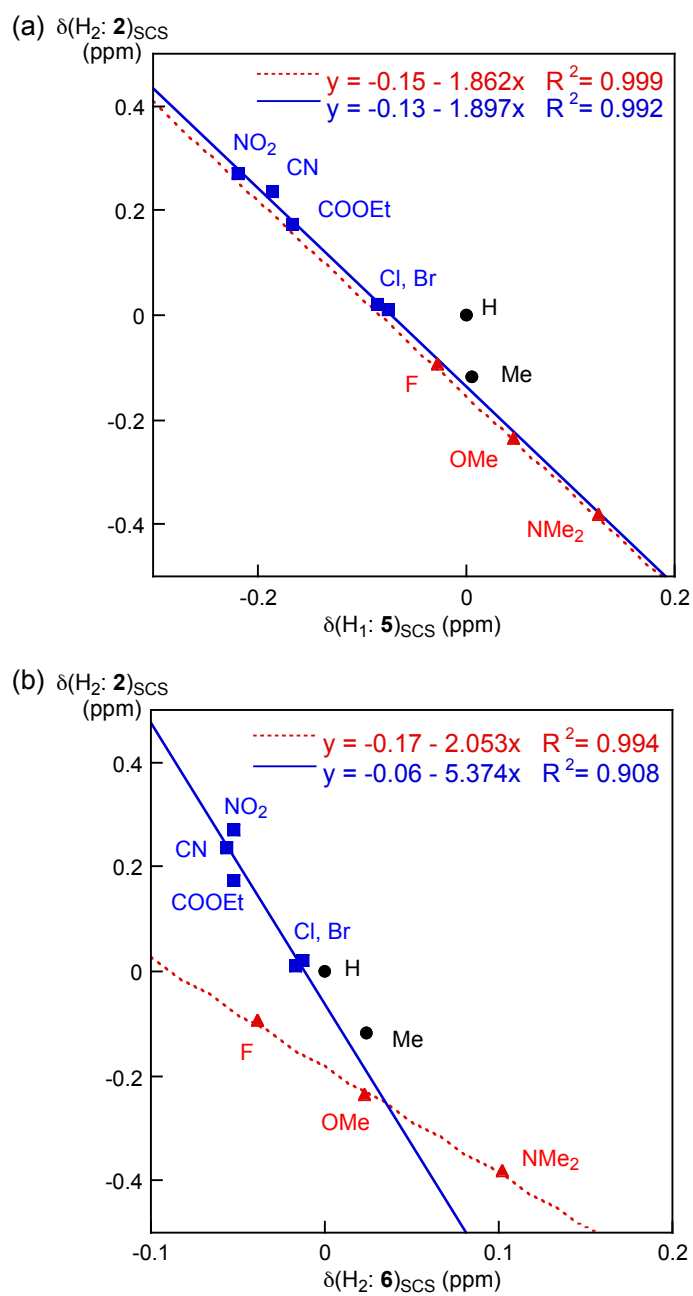


Fig. S4 Plots of $\delta(\text{H}_2: \mathbf{2})_{\text{SCS}}$ versus $\delta(\text{H}_1: \mathbf{5})_{\text{SCS}}$ (a) and $\delta(\text{H}_2: \mathbf{2})_{\text{SCS}}$ versus $\delta(\text{H}_2: \mathbf{6})_{\text{SCS}}$ (b).

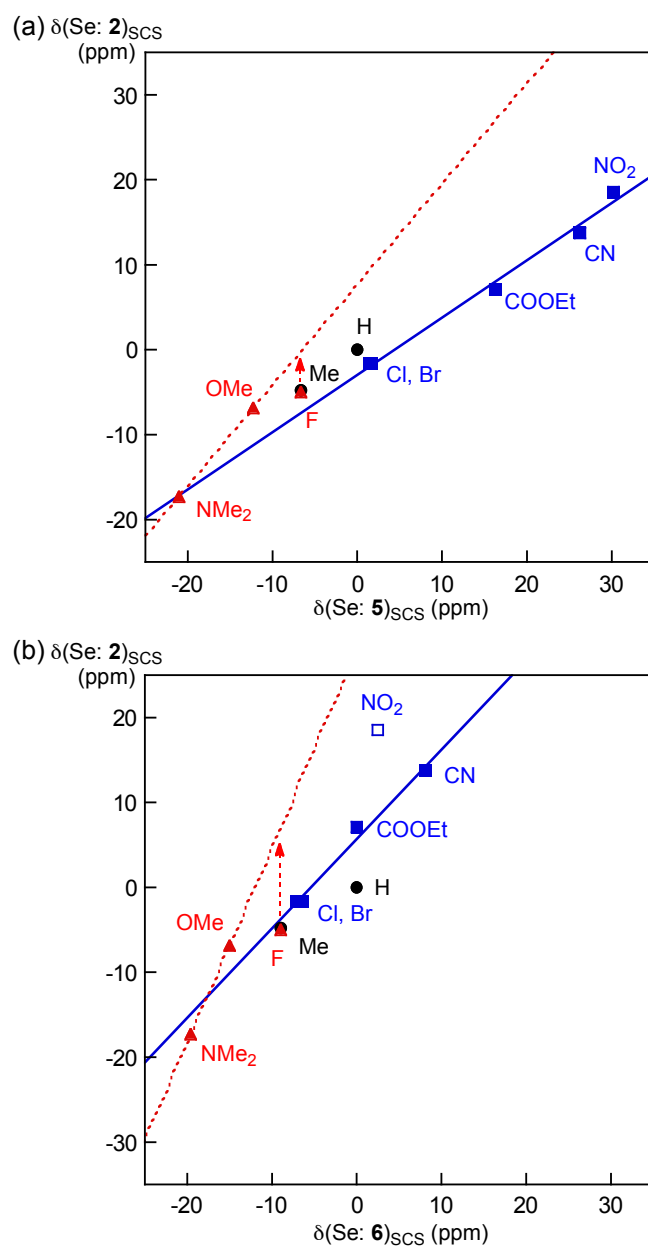


Fig. S5 Plots of $\delta(\text{Se: } \mathbf{2})_{\text{SCS}}$ versus $\delta(\text{Se: } \mathbf{5})_{\text{SCS}}$ (a) and $\delta(\text{Se: } \mathbf{2})_{\text{SCS}}$ versus $\delta(\text{Se: } \mathbf{6})_{\text{SCS}}$ (b). G(l), G(m) and G(n) are drawn in black, red, and blue, respectively.

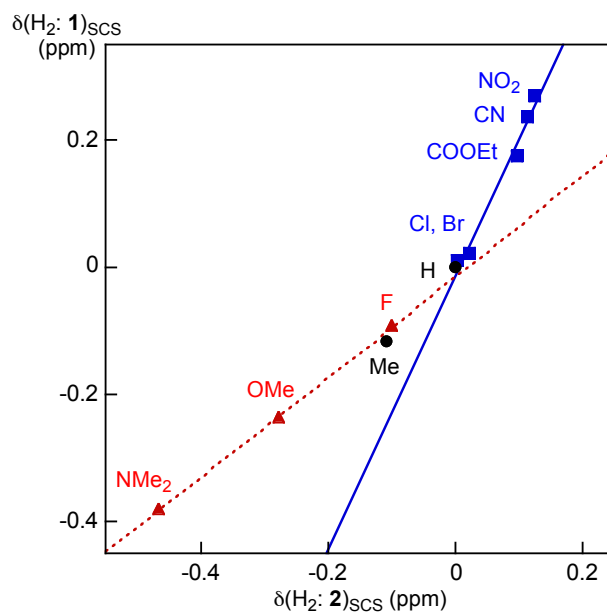


Fig. S6 Plots of $\delta(\text{H}_2: 1)_{\text{SCS}}$ versus $\delta(\text{H}_2: 2)_{\text{SCS}}$. G(I), G(m) and G(n) are drawn in black, red, and blue, respectively.

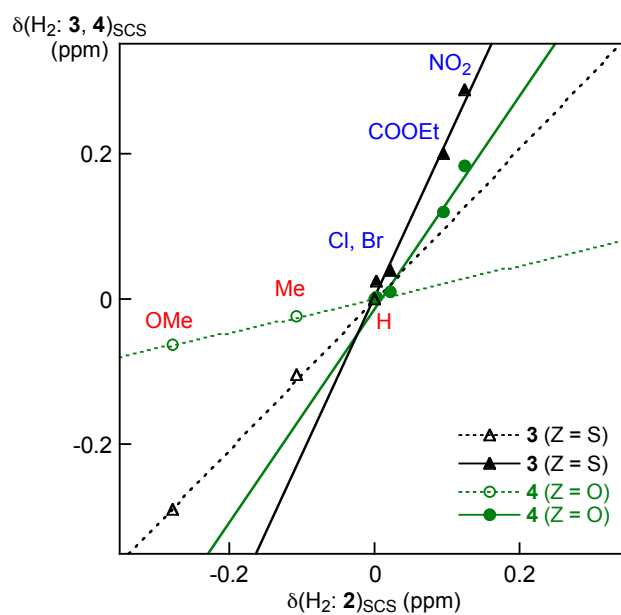


Fig. S7 Plots of $\delta(\text{H}_2)_{\text{SCS}}$ of **3** and **4** versus $\delta(\text{H}_2: 2)_{\text{SCS}}$. G(I) and G(m) are drawn in hollow and G(n) in solid.

Table S2 Optimized structures and energies for 1-PhSC₁₀H₇ (**3a**) at the MP2 level^a

Structure	A	TS- AB' ^b	B' ^c	B₀ ^d
<i>E</i> (au)	-1012.6770	-1012.6744	-1012.6745	-1012.6744
ΔE (kJ mol ⁻¹)	0.0 ^e	7.0	6.8	6.9
<i>r</i> (S, C ₁) (Å)	1.7731	1.7806	1.7802	1.7800
<i>r</i> (S, C ₁₁) (Å)	1.7779	1.7745	1.7721	1.7717
\angle C ₁ SC ₁₁ (°)	101.43	100.67	101.85	102.30
\angle C ₁₀ C ₁ SC ₁₁ (°)	67.48	136.38	163.18	180.00
\angle C ₁ SC ₁₁ C ₁₂ (°)	38.14	-66.09	-77.69	-90.34
ν_1^f (sym) (cm ⁻¹)	27.3 (A)	-11.7 (A)	7.6 (A)	-313.2 (A")
ν_2^g (sym) (cm ⁻¹)	33.2 (A)	23.4 (A)	29.5 (A)	-7.0 (A")
ZC ^h (au)	0.2295	0.2297	0.2293	0.2279
GF ⁱ (au)	0.1876	0.1886	0.1859	0.1877
<i>E</i> _{GF} ^j (au)	-1012.4895	-1012.4858	-1012.4886	-1012.4867
ΔE_{GF} (kJ mol ⁻¹)	0.0 ^e	9.8	2.5	7.4

^a The 6-311+G(3d) basis sets being employed for S with the 6-31G(d,p) basis sets for C and H. ^b Between **A** and **B'**. ^c Closer to **B**. ^d Corresponding to higher TS with two imaginary frequencies. ^e Taken as the standards for the energies. ^f Lowest frequency obtained by the frequency analysis. ^g Second-lowest frequency obtained by the frequency analysis. ^h Zero-point correction. ⁱ Thermal correction to Gibbs free energy at 298.15 K. ^j Sum of electronic and thermal Gibbs free energies at 298.15 K.

Table S3 Optimized structures and energies for 1-PhOC₁₀H₇ (**4a**) at the MP2 level^a

Structure	A	TS- AB ^b	B'	TS- B'B' ^c	B₀ ^d
<i>E</i> (au)	-690.0841	-690.0833	-690.0835	-690.0831	-690.0831
ΔE (kJ mol ⁻¹)	0.0 ^e	1.9	1.4	2.4	2.6
<i>r</i> (O, C ₁) (Å)	1.3854	1.3842	1.3809	1.3805	1.3805
<i>r</i> (O, C ₁₁) (Å)	1.3838	1.3833	1.3846	1.3868	1.3868
\angle C ₁ OC ₁₁ (°)	117.15	117.64	118.05	117.23	117.23
\angle C ₁₀ C ₁ OC ₁₁ (°)	77.82	115.92	149.70	-179.43	180.00
\angle C ₁ OC ₁₁ C ₁₂ (°)	12.64	-22.07	-50.90	-90.30	-91.70
ν_1^f (sym) (cm ⁻¹)	27.4 (A)	-13.7 (A)	15.0 (A)	-22.5 (A)	-335.3 (A")
ν_2^g (sym) (cm ⁻¹)	35.3 (A)	30.9 (A)	34.3 (A)	27.5 (A)	-22.8 (A")
ZC ^h (au)	0.2326	0.2316	0.2322	0.2322	0.2307
GF ⁱ (au)	0.1917	0.1924	0.1908	0.1929	0.1915
<i>E</i> _{GF} ^j (au)	-689.8923	-689.8909	-689.8927	-689.8902	-689.8916
ΔE_{GF} (kJ mol ⁻¹)	0.0 ^f	3.8	-1.0	5.6	2.0

^a The 6-311+G(3d) basis sets being employed for O with the 6-31G(d,p) basis sets for C and H. ^b Between **A** and **B'**, where the **B'** is very close to **C'**. ^c Between **B'** and another **B'**. ^d Corresponding to higher TS with two imaginary frequencies. ^e Taken as the standards for the energies. ^f Lowest frequency obtained by the frequency analysis. ^g Second-lowest frequency obtained by the frequency analysis. ^h Zero-point correction. ⁱ Thermal correction to Gibbs free energy at 298.15 K. ^j Sum of electronic and thermal Gibbs free energies at 298.15 K.

Table S4 Various structures and the energies for **1–4** having *p*-Y of NH₂ (**b'**), Me (**c**), H (**a**), Cl (**f**) and NO₂ (**j**) calculated at the MP2 level.^{a,b}

Compound / Y =	NH ₂ (b')	Me (c)	H (a)	Cl (f)	NO ₂ (j)
1: Z = Te					
∠C ₁₀ C ₁ TeC ₁₁ (A) (°)	63.26	62.51	62.92	63.10	64.83
∠C ₁ TeC ₁₁ C ₁₂ (A) (°)	53.71	40.40	38.15	36.84	26.87
∠C ₁₀ C ₁ TeC ₁₁ (B') (°)	178.25	176.61	174.68	171.31	64.83 ^c
∠C ₁ TeC ₁₁ C ₁₂ (B') (°)	-90.08	-88.91	-88.08	-86.01	26.88 ^c
∠C ₁₀ C ₁ TeC ₁₁ (A₀) (°)	72.91	72.97	73.13	73.03	73.13
∠C ₁ TeC ₁₁ C ₁₂ (A₀) (°)	0.00	0.00	0.00	0.00	0.00
∠C ₁₀ C ₁ TeC ₁₁ (B₀) (°)	180.00	180.00	180.00	180.00	180.00
∠C ₁ TeC ₁₁ C ₁₂ (B₀) (°)	-90.09	-89.62	-89.92	-89.99	-90.11
<i>E</i> (A) ^d (au)	-7282.0654	-7266.0487	-7226.8627	-7685.8835	-7430.8558
Δ <i>E</i> (A) ^e (kJ mol ⁻¹)	as 0.0	as 0.0	as 0.0	as 0.0	as 0.0
Δ <i>E</i> (B') ^e (kJ mol ⁻¹)	0.5	2.9	3.5	4.3	0.0 ^c
Δ <i>E</i> (A₀) ^e (kJ mol ⁻¹)	as 0.0	as 0.0	as 0.0	as 0.0	as 0.0
Δ <i>E</i> (B₀) ^e (kJ mol ⁻¹)	-4.1	0.0	0.9	1.9	6.5
2: Z = Se					
∠C ₁₀ C ₁ SeC ₁₁ (A) (°)	65.99	66.23	66.59	66.88	68.28
∠C ₁ SeC ₁₁ C ₁₂ (A) (°)	50.41	42.40	40.31	39.09	29.05
∠C ₁₀ C ₁ SeC ₁₁ (B') (°)	173.37	155.90	150.24	93.99 ^c	68.28 ^c
∠C ₁ SeC ₁₁ C ₁₂ (B') (°)	-88.34	-77.59	-73.16	47.39 ^c	29.05 ^c
∠C ₁₀ C ₁ SeC ₁₁ (A₀) (°)	75.28	75.51	75.69	75.64	75.77
∠C ₁ SeC ₁₁ C ₁₂ (A₀) (°)	0.00	0.00	0.00	0.00	0.00
∠C ₁₀ C ₁ SeC ₁₁ (B₀) (°)	180.00	180.00	180.00	180.00	180.00
∠C ₁ SeC ₁₁ C ₁₂ (B₀) (°)	-90.92	-90.47	-90.71	-90.77	-90.86
<i>E</i> (A) ^d (au)	-3070.2797	-3054.2633	-3015.0774	-3474.0982	-3219.0709
Δ <i>E</i> (A) ^e (kJ mol ⁻¹)	as 0.0	as 0.0	as 0.0	as 0.0	as 0.00
Δ <i>E</i> (B') ^e (kJ mol ⁻¹)	3.1	5.5	5.9	4.1 ^f	0.0 ^c
Δ <i>E</i> (A₀) ^e (kJ mol ⁻¹)	as 0.0	as 0.0	as 0.0	as 0.0	as 0.0
Δ <i>E</i> (B₀) ^e (kJ mol ⁻¹)	-1.9	2.4	3.4	4.5	9.4
3: Z = S					
∠C ₁₀ C ₁ SC ₁₁ (A) (°)	66.99	67.15	67.48	67.78	69.31
∠C ₁ SC ₁₁ C ₁₂ (A) (°)	47.17	40.03	38.14	36.96	26.33
∠C ₁₀ C ₁ SC ₁₁ (B') (°)	179.89	171.18	163.18	67.78 ^c	69.31 ^c
∠C ₁ SC ₁₁ C ₁₂ (B') (°)	-90.65	-83.60	-77.67	37.00 ^c	26.33 ^c

$\angle C_{10}C_1SC_{11}$ (A₀) (°)	75.57	75.82	76.06	76.04	76.28
$\angle C_1SC_{11}C_{12}$ (A₀) (°)	0.00	0.00	0.00	0.00	0.00
$\angle C_{10}C_1SC_{11}$ (B₀) (°)	180.00	180.00	180.00	180.00	180.00
$\angle C_1SC_{11}C_{12}$ (B₀) (°)	-91.12	-90.74	-90.94	-90.99	-91.07
$E(\mathbf{A})^d$ (au)	-1067.8791	-1051.8630	-1012.6770	-1471.6978	-1216.6708
$\Delta E(\mathbf{A})^e$ (kJ mol ⁻¹)	as 0.0	as 0.0	as 0.0	as 0.0	as 0.0
$\Delta E(\mathbf{B}')^e$ (kJ mol ⁻¹)	3.1	6.2	6.8	0.0 ^c	0.0 ^c
$\Delta E(\mathbf{A}_0)^e$ (kJ mol ⁻¹)	as 0.0	as 0.0	as 0.0	as 0.0	as 0.0
$\Delta E(\mathbf{B}_0)^e$ (kJ mol ⁻¹)	-1.8	3.2	4.2	5.4	11.0
4: Z = O					
$\angle C_{10}C_1OC_{11}$ (A) (°)	75.82	77.27	77.82	78.35	80.34
$\angle C_1OC_{11}C_{12}$ (A) (°)	17.16	13.36	12.64	11.27	7.14
$\angle C_{10}C_1OC_{11}$ (B') (°)	166.06	154.02	149.70	141.01	80.36 ^c
$\angle C_1OC_{11}C_{12}$ (B') (°)	-72.21	-55.61	-50.90	-42.51	7.11 ^c
$\angle C_{10}C_1OC_{11}$ (A₀) (°)	83.86	83.93	84.23	83.99	84.11
$\angle C_1OC_{11}C_{12}$ (A₀) (°)	0.00	0.00	0.00	0.00	0.00
$\angle C_{10}C_1OC_{11}$ (B₀) (°)	180.00	180.00	180.00	180.00	180.00
$\angle C_1OC_{11}C_{12}$ (B₀) (°)	-92.11	-91.50	-91.70	-91.80	-91.74
$E(\mathbf{A})^d$ (au)	-745.2841	-729.2694	-690.0841	-1149.1045	-894.2207
$\Delta E(\mathbf{A})^e$ (kJ mol ⁻¹)	as 0.0	as 0.0	as 0.0	as 0.0	as 0.0
$\Delta E(\mathbf{B}')^e$ (kJ mol ⁻¹)	-1.4	1.1	1.4	2.0	0.0 ^c
$\Delta E(\mathbf{A}_0)^e$ (kJ mol ⁻¹)	as 0.0	as 0.0	as 0.0	as 0.0	as 0.0
$\Delta E(\mathbf{B}_0)^e$ (kJ mol ⁻¹)	-1.7	1.5	2.2	3.3	8.7

^a The basis sets of the (7433111/743111/7411/2 + 1s1p1d1f) type being employed for Te with the 6-31G(d,p) basis sets for C and H. ^b A stationary point being not obtained for typical **B**. ^c The value is almost the same if the thermal effect is considered, but it becomes -8.4 kJ mol⁻¹ if solvent effect is calculated by the IPCM method. ^d $\Delta E = E(\mathbf{A}) - E(\mathbf{B})$. ^e **A**. ^f **A'**.

Optimized structures given by Cartesian coordinates

Optimized structures given by Cartesian coordinates for **1a–4a**, **1b'–4b'**, **1c–4c**, **1f–4f** and **1j–4j**, together with the total energies using the Gaussian 03 program.²⁴ The Møller-Plesset second-order energy correlation (MP2) level is applied to the calculations²³ with the 6-311+G(3d) basis sets²⁷ for O, S and Se, the (7433111/743111/7411/2 + 1s1p1d1f) basis sets³² for Te and with the 6-31G(d,p) basis sets for C and H.

1a (A): MP2 = -7226.8626611 a.u.

6	0	-1.641229	0.236844	-0.284560
6	0	-2.912843	0.573475	0.296573
6	0	-1.050541	1.153197	-1.194320
6	0	-1.706717	2.314530	-1.556870
6	0	-2.959413	2.639685	-0.990369
6	0	-3.560914	1.771334	-0.102215
1	0	-0.094296	0.908253	-1.640498
1	0	-1.241808	2.994294	-2.261206
1	0	-3.462216	3.554599	-1.280465
1	0	-4.525949	2.010312	0.332465
6	0	-0.998752	-0.966106	0.152023
6	0	-1.631929	-1.816761	1.052064
6	0	-2.907258	-1.498877	1.571553
6	0	-3.538251	-0.332129	1.192905
1	0	-1.127394	-2.718460	1.379899
1	0	-3.385844	-2.180043	2.265470
1	0	-4.509016	-0.073824	1.603341
52	0	0.891063	-1.554363	-0.578265
6	0	1.936505	0.115123	0.183841
6	0	1.607358	0.645292	1.440737
6	0	2.970204	0.688156	-0.572696
6	0	2.303926	1.754338	1.926734
6	0	3.677616	1.781937	-0.064854
6	0	3.343004	2.319370	1.180662
1	0	0.810613	0.200083	2.026560
1	0	3.211656	0.291260	-1.552856
1	0	2.041876	2.168713	2.893375
1	0	4.477773	2.220629	-0.649582
1	0	3.884746	3.174617	1.566014

1a (TS-AB'): MP2 = -7226.860425 a.u.

6	0	-2.007284	-0.014494	-0.001907
6	0	-2.953057	1.047888	-0.225719
6	0	-2.341749	-1.025543	0.939497
6	0	-3.566063	-1.023601	1.579979
6	0	-4.502819	0.006456	1.338192
6	0	-4.204787	1.012917	0.442846
1	0	-1.626114	-1.814389	1.138259
1	0	-3.799563	-1.807680	2.290626
1	0	-5.460569	-0.004382	1.844760
1	0	-4.915447	1.811545	0.256909
6	0	-0.760437	0.037437	-0.701208
6	0	-0.496673	1.065214	-1.599770
6	0	-1.430183	2.104984	-1.799985
6	0	-2.644817	2.082989	-1.144604
1	0	0.446332	1.079819	-2.135100
1	0	-1.200645	2.900149	-2.499860
1	0	-3.371445	2.872729	-1.305116
52	0	0.744932	-1.426407	-0.425769
6	0	2.185985	-0.041735	0.250226
6	0	1.894869	0.801500	1.335372
6	0	3.439158	0.026875	-0.377768
6	0	2.849956	1.722651	1.770444
6	0	4.397159	0.935530	0.083524
6	0	4.103352	1.785420	1.152425
1	0	0.928996	0.741287	1.824681
1	0	3.656231	-0.613322	-1.225244

1	0	2.620951	2.379283	2.601729
1	0	5.365150	0.985916	-0.401204
1	0	4.844025	2.495275	1.500292

1a (B'): MP2 = -7226.8613271 a.u.

6	0	-2.144279	0.125853	0.020223
6	0	-3.012238	1.270726	-0.019910
6	0	-2.732715	-1.166263	0.054830
6	0	-4.104417	-1.324666	0.111547
6	0	-4.954723	-0.196653	0.089328
6	0	-4.415807	1.073477	0.048557
1	0	-2.096438	-2.045194	0.081877
1	0	-4.529538	-2.320751	0.146033
1	0	-6.029003	-0.330026	0.134246
1	0	-5.063827	1.943688	0.032095
6	0	-0.733384	0.339248	-0.053748
6	0	-0.217705	1.626392	-0.099244
6	0	-1.083833	2.743228	-0.110161
6	0	-2.451649	2.573366	-0.052116
1	0	0.852943	1.784272	-0.152075
1	0	-0.658994	3.740069	-0.143158
1	0	-3.115861	3.431007	-0.066473
52	0	0.552719	-1.346912	-0.052403
6	0	2.345657	-0.247782	0.017596
6	0	2.889049	0.129369	1.257576
6	0	2.997576	0.111208	-1.174322
6	0	4.072398	0.871538	1.298769
6	0	4.181790	0.852070	-1.121004
6	0	4.718834	1.231472	0.112467
1	0	2.384569	-0.152582	2.174303
1	0	2.576191	-0.183899	-2.128137
1	0	4.490153	1.163401	2.255121
1	0	4.683702	1.129262	-2.040545
1	0	5.637379	1.804701	0.149348

1a (B₀): MP2 = -7226.8612967 a.u.

6	0	-1.243574	-1.753104	0.000000
6	0	-2.675226	-1.880522	0.000000
6	0	-0.459760	-2.937495	0.000000
6	0	-1.052620	-4.185883	0.000000
6	0	-2.460148	-4.308014	0.000000
6	0	-3.251696	-3.177171	0.000000
1	0	0.623272	-2.865103	0.000000
1	0	-0.433475	-5.075146	0.000000
1	0	-2.916276	-5.290788	0.000000
1	0	-4.333297	-3.264700	0.000000
6	0	-0.677388	-0.441187	0.000000
6	0	-1.495707	0.679119	0.000000
6	0	-2.901951	0.536814	0.000000
6	0	-3.482945	-0.714406	0.000000
1	0	-1.062485	1.672240	0.000000
1	0	-3.522166	1.425982	0.000000
1	0	-4.562411	-0.822683	0.000000
52	0	1.434194	-0.245660	0.000000
6	0	1.454388	1.858407	0.000000
6	0	1.459898	2.560687	1.217207
6	0	1.459898	2.560687	-1.217207
6	0	1.459898	3.958333	1.211171
6	0	1.459898	3.958333	-1.211171
6	0	1.460877	4.656437	0.000000
1	0	1.458522	2.014860	2.153405
1	0	1.458522	2.014860	-2.153405
1	0	1.462964	4.499395	2.150080
1	0	1.462964	4.499395	-2.150080
1	0	1.462723	5.739800	0.000000

1b' (A): MP2 = -7282.0654295 a.u.

6	0	-1.781438	0.509175	-0.252867
6	0	-2.853606	1.222817	0.386998
6	0	-1.077351	1.151122	-1.305702
6	0	-1.447610	2.409030	-1.743154
6	0	-2.503868	3.106552	-1.115751

6	0	-3.209566	2.511108	-0.089937
1	0	-0.274193	0.618491	-1.799717
1	0	-0.903897	2.874448	-2.556975
1	0	-2.782712	4.093496	-1.465582
1	0	-4.028155	3.036182	0.391424
6	0	-1.426191	-0.778965	0.261572
6	0	-2.163186	-1.350972	1.293016
6	0	-3.251123	-0.660839	1.874146
6	0	-3.594430	0.596756	1.423224
1	0	-1.878107	-2.324151	1.676273
1	0	-3.815202	-1.129043	2.672489
1	0	-4.416055	1.139509	1.879282
52	0	0.176278	-1.904706	-0.531569
6	0	1.675202	-0.517245	-0.013992
6	0	1.796794	-0.065448	1.309703
6	0	2.551755	-0.019998	-0.990919
6	0	2.770993	0.872551	1.644293
6	0	3.541246	0.900231	-0.646044
6	0	3.649094	1.376795	0.669932
1	0	1.130643	-0.445645	2.076418
1	0	2.461852	-0.350740	-2.019966
1	0	2.854918	1.219981	2.669053
1	0	4.217878	1.275077	-1.407279
7	0	4.676815	2.257532	1.028220
1	0	4.463571	2.825472	1.835730
1	0	5.005019	2.832899	0.265767

1b' (B'): MP2 = -7282.065225 a.u.

6	0	2.429295	0.221775	0.017894
6	0	3.202648	1.432779	-0.015674
6	0	3.118796	-1.019828	0.004972
6	0	4.499732	-1.069748	0.025537
6	0	5.257353	0.122689	0.012171
6	0	4.618734	1.346443	0.014690
1	0	2.554389	-1.946788	0.019596
1	0	5.003158	-2.029308	0.023574
1	0	6.339653	0.074397	0.028655
1	0	5.195369	2.265660	0.003794
6	0	1.004507	0.322621	-0.013788
6	0	0.387480	1.565114	-0.013237
6	0	1.161500	2.747660	-0.022532
6	0	2.539694	2.686785	-0.003074
1	0	-0.693779	1.636247	-0.030076
1	0	0.658081	3.707846	-0.020506
1	0	3.133083	3.594978	-0.013909
52	0	-0.149313	-1.457783	-0.008638
6	0	-2.019856	-0.508784	-0.000048
6	0	-2.661331	-0.188317	-1.208940
6	0	-2.649942	-0.188281	1.214855
6	0	-3.896335	0.456902	-1.200434
6	0	-3.884918	0.456819	1.217882
6	0	-4.533776	0.770780	0.011728
1	0	-2.186339	-0.431855	-2.152261
1	0	-2.165969	-0.431509	2.153670
1	0	-4.382173	0.704293	-2.138690
1	0	-4.361967	0.704168	2.160649
7	0	-5.739715	1.476762	0.017484
1	0	-6.300317	1.343399	-0.811672
1	0	-6.292375	1.343383	0.851953

1b' (B_o): MP2 = -7282.0651953 a.u.

6	0	-1.320878	-2.051062	0.000000
6	0	-2.752851	-2.175363	0.000000
6	0	-0.539614	-3.237216	0.000000
6	0	-1.135223	-4.484306	0.000000
6	0	-2.543065	-4.603408	0.000000
6	0	-3.332123	-3.470789	0.000000
1	0	0.543465	-3.166332	0.000000
1	0	-0.518074	-5.375010	0.000000
1	0	-3.001394	-5.585207	0.000000
1	0	-4.413961	-3.556044	0.000000
6	0	-0.751051	-0.740877	0.000000

6	0	-1.566722	0.381277	0.000000
6	0	-2.973305	0.242612	0.000000
6	0	-3.557641	-1.007212	0.000000
1	0	-1.129235	1.372789	0.000000
1	0	-3.591349	1.133358	0.000000
1	0	-4.637428	-1.112788	0.000000
52	0	1.361163	-0.542454	0.000000
6	0	1.386068	1.554933	0.000000
6	0	1.396520	2.266841	1.211915
6	0	1.396520	2.266841	-1.211915
6	0	1.396520	3.660206	1.209172
6	0	1.396520	3.660206	-1.209172
6	0	1.416155	4.375614	0.000000
1	0	1.390170	1.729152	2.152989
1	0	1.390170	1.729152	-2.152989
1	0	1.400272	4.201477	2.149693
1	0	1.400272	4.201477	-2.149693
7	0	1.348847	5.771402	0.000000
1	0	1.724846	6.202991	0.831817
1	0	1.724846	6.202991	-0.831817

1c (A): MP2 = -7266.0487383 a.u.

6	0	-1.783272	0.510263	-0.271962
6	0	-2.867159	1.238804	0.330097
6	0	-1.052725	1.130112	-1.320020
6	0	-1.409234	2.380446	-1.789395
6	0	-2.478844	3.091555	-1.201062
6	0	-3.209192	2.518117	-0.180055
1	0	-0.236665	0.588966	-1.783205
1	0	-0.844247	2.829729	-2.597661
1	0	-2.746490	4.072310	-1.575977
1	0	-4.036665	3.054519	0.272661
6	0	-1.444334	-0.768314	0.276471
6	0	-2.200525	-1.315376	1.307675
6	0	-3.298579	-0.610701	1.850926
6	0	-3.630314	0.636710	1.364375
1	0	-1.924586	-2.279933	1.718317
1	0	-3.878828	-1.059445	2.648760
1	0	-4.460337	1.190511	1.790931
52	0	0.157813	-1.919465	-0.472327
6	0	1.660057	-0.516633	0.008018
6	0	1.615552	0.185682	1.221761
6	0	2.708564	-0.280159	-0.893371
6	0	2.608737	1.120952	1.516513
6	0	3.708294	0.640783	-0.569861
6	0	3.670249	1.361004	0.631439
1	0	0.807234	0.009472	1.923300
1	0	2.737716	-0.801203	-1.844409
1	0	2.559278	1.670639	2.451210
1	0	4.515355	0.818195	-1.273539
6	0	4.762483	2.335891	0.984621
1	0	5.550211	1.849789	1.563383
1	0	5.219627	2.753734	0.088025
1	0	4.373539	3.160090	1.582219

1c (B): MP2 = -7266.0476169 a.u.

6	0	2.429708	0.230770	0.020972
6	0	3.195684	1.446276	-0.017659
6	0	3.127273	-1.006242	0.035755
6	0	4.508057	-1.046712	0.076699
6	0	5.258104	0.150373	0.057252
6	0	4.611694	1.369786	0.034181
1	0	2.569095	-1.936855	0.057803
1	0	5.017509	-2.002857	0.095989
1	0	6.340312	0.109442	0.089754
1	0	5.182423	2.292579	0.019170
6	0	1.004879	0.322371	-0.034294
6	0	0.380106	1.560796	-0.060525
6	0	1.146927	2.748005	-0.072465
6	0	2.524914	2.696091	-0.031455
1	0	-0.700878	1.626004	-0.097079
1	0	0.637683	3.704907	-0.090967

1	0	3.112761	3.607795	-0.045366
52	0	-0.132612	-1.467655	-0.028031
6	0	-2.012546	-0.526669	0.000587
6	0	-2.664804	-0.213312	-1.203474
6	0	-2.617738	-0.195654	1.224476
6	0	-3.904378	0.429401	-1.174487
6	0	-3.857087	0.447449	1.234141
6	0	-4.516873	0.770756	0.039697
1	0	-2.200494	-0.465471	-2.149867
1	0	-2.117034	-0.434298	2.155682
1	0	-4.399754	0.673134	-2.108799
1	0	-4.315813	0.705118	2.183317
6	0	-5.872517	1.426177	0.061580
1	0	-6.667118	0.678196	0.087381
1	0	-6.024751	2.041152	-0.824944
1	0	-5.986509	2.061241	0.939659

1c (B₀): MP2 = -7266.0475868 a.u.

6	0	-1.322702	-2.052037	0.000000
6	0	-2.755046	-2.171610	0.000000
6	0	-0.545422	-3.240740	0.000000
6	0	-1.145148	-4.485846	0.000000
6	0	-2.553338	-4.600271	0.000000
6	0	-3.338640	-3.465076	0.000000
1	0	0.537959	-3.174054	0.000000
1	0	-0.530908	-5.378519	0.000000
1	0	-3.014873	-5.580530	0.000000
1	0	-4.420722	-3.546673	0.000000
6	0	-0.749039	-0.743386	0.000000
6	0	-1.561208	0.381401	0.000000
6	0	-2.968208	0.246939	0.000000
6	0	-3.556262	-1.001024	0.000000
1	0	-1.121920	1.371930	0.000000
1	0	-3.583545	1.139524	0.000000
1	0	-4.636331	-1.103289	0.000000
52	0	1.363609	-0.557511	0.000000
6	0	1.393809	1.544756	0.000000
6	0	1.397435	2.251274	1.214242
6	0	1.397435	2.251274	-1.214242
6	0	1.397435	3.647686	1.204584
6	0	1.397435	3.647686	-1.204584
6	0	1.395414	4.365464	0.000000
1	0	1.393017	1.709900	2.153235
1	0	1.393017	1.709900	-2.153235
1	0	1.394609	4.186649	2.146529
1	0	1.394609	4.186649	-2.146529
6	0	1.437876	5.870795	0.000000
1	0	2.467945	6.232028	0.000000
1	0	0.944264	6.276670	0.882566
1	0	0.944264	6.276670	-0.882566

1f (A): MP2 = -7685.8834751 a.u.

6	0	-1.942946	0.671342	-0.272094
6	0	-2.878488	1.581074	0.332245
6	0	-1.184540	1.122318	-1.384617
6	0	-1.379410	2.386004	-1.909851
6	0	-2.303883	3.275733	-1.318572
6	0	-3.057142	2.869107	-0.236028
1	0	-0.480844	0.443585	-1.851260
1	0	-0.797150	2.705458	-2.766093
1	0	-2.444833	4.264921	-1.737556
1	0	-3.774230	3.543937	0.219624
6	0	-1.765216	-0.612478	0.336601
6	0	-2.537531	-0.988937	1.430453
6	0	-3.493637	-0.103418	1.977255
6	0	-3.666348	1.151981	1.432210
1	0	-2.382893	-1.960904	1.884824
1	0	-4.090837	-0.419659	2.824472
1	0	-4.385179	1.842918	1.860422
52	0	-0.385346	-2.022193	-0.410090
6	0	1.323445	-0.835853	-0.054831
6	0	1.403028	-0.022752	1.086118

6	0	2.391824	-0.863512	-0.964101
6	0	2.532676	0.765879	1.308162
6	0	3.534500	-0.094606	-0.732069
6	0	3.594164	0.719271	0.400692
1	0	0.583363	0.002829	1.795729
1	0	2.332239	-1.473385	-1.858980
1	0	2.596216	1.402162	2.182043
1	0	4.362518	-0.113680	-1.429472
17	0	5.005685	1.693466	0.683030

1f (B'): MP2 = -7685.8818274 a.u.

6	0	2.690065	0.295722	0.032596
6	0	3.397846	1.545168	-0.029093
6	0	3.443655	-0.902081	0.152594
6	0	4.820463	-0.870362	0.267549
6	0	5.512400	0.360527	0.221972
6	0	4.810876	1.543111	0.100894
1	0	2.929924	-1.856935	0.202842
1	0	5.373014	-1.797079	0.367140
1	0	6.591889	0.375969	0.312901
1	0	5.336787	2.491612	0.067331
6	0	1.268359	0.313540	-0.107003
6	0	0.587454	1.515343	-0.235883
6	0	1.295711	2.738111	-0.263356
6	0	2.669997	2.757245	-0.144402
1	0	-0.490839	1.524520	-0.342066
1	0	0.743460	3.665840	-0.360614
1	0	3.213508	3.695648	-0.173416
52	0	0.221335	-1.530709	-0.084667
6	0	-1.700466	-0.680787	-0.009687
6	0	-2.424940	-0.461638	-1.193354
6	0	-2.267257	-0.327827	1.226955
6	0	-3.697476	0.111568	-1.144088
6	0	-3.537017	0.249250	1.279672
6	0	-4.243018	0.463032	0.092810
1	0	-1.993303	-0.733764	-2.149330
1	0	-1.714392	-0.498788	2.143117
1	0	-4.261120	0.283722	-2.052329
1	0	-3.978926	0.525566	2.228681
17	0	-5.824669	1.177708	0.157023

1f (B_o): MP2 = -7685.8817941 a.u.

6	0	-1.373449	-2.338282	0.000000
6	0	-2.804804	-2.468830	0.000000
6	0	-0.586708	-3.520692	0.000000
6	0	-1.176644	-4.770445	0.000000
6	0	-2.583896	-4.895703	0.000000
6	0	-3.378220	-3.766807	0.000000
1	0	0.496285	-3.446419	0.000000
1	0	-0.555486	-5.658262	0.000000
1	0	-3.037665	-5.879526	0.000000
1	0	-4.459560	-3.856929	0.000000
6	0	-0.811190	-1.024910	0.000000
6	0	-1.631573	0.093745	0.000000
6	0	-3.037518	-0.051788	0.000000
6	0	-3.615169	-1.304529	0.000000
1	0	-1.201445	1.088183	0.000000
1	0	-3.659789	0.835862	0.000000
1	0	-4.694340	-1.415282	0.000000
52	0	1.300551	-0.828121	0.000000
6	0	1.318229	1.274379	0.000000
6	0	1.324059	1.981010	1.214600
6	0	1.324059	1.981010	-1.214600
6	0	1.324059	3.377143	1.216507
6	0	1.324059	3.377143	-1.216507
6	0	1.324855	4.064218	0.000000
1	0	1.322689	1.440761	2.153942
1	0	1.322689	1.440761	-2.153942
1	0	1.327249	3.928068	2.148555
1	0	1.327249	3.928068	-2.148555
17	0	1.326035	5.801001	0.000000

1j (A): MP2 = -7430.8557595 a.u.

6	0	-2.114350	0.707275	-0.295604
6	0	-2.995464	1.684628	0.284555
6	0	-1.373905	1.066916	-1.452628
6	0	-1.536831	2.307047	-2.041020
6	0	-2.409273	3.262708	-1.473924
6	0	-3.143313	2.945850	-0.349056
1	0	-0.710827	0.336734	-1.901306
1	0	-0.969817	2.556548	-2.930040
1	0	-2.525572	4.232406	-1.942878
1	0	-3.819767	3.672179	0.089001
6	0	-1.965916	-0.546250	0.380494
6	0	-2.713393	-0.831325	1.518445
6	0	-3.616847	0.120411	2.042840
6	0	-3.761281	1.348626	1.431474
1	0	-2.580657	-1.782036	2.021880
1	0	-4.196360	-0.123791	2.925310
1	0	-4.439681	2.089688	1.841297
52	0	-0.672548	-2.049572	-0.333377
6	0	1.104893	-0.949680	-0.053214
6	0	1.186925	0.052836	0.926971
6	0	2.222758	-1.234382	-0.855008
6	0	2.368043	0.774050	1.098807
6	0	3.416627	-0.534723	-0.678383
6	0	3.463410	0.462110	0.294564
1	0	0.329297	0.272601	1.552641
1	0	2.161314	-1.994770	-1.625918
1	0	2.452382	1.554179	1.842426
1	0	4.288940	-0.737628	-1.283656
7	0	4.711700	1.215802	0.475482
8	0	4.727488	2.102247	1.346554
8	0	5.673620	0.919559	-0.253732

1j (B'): MP2 = -7430.8557595 a.u.

6	0	-2.114345	0.707264	-0.295613
6	0	-2.995457	1.684624	0.284539
6	0	-1.373888	1.066901	-1.452632
6	0	-1.536797	2.307035	-2.041021
6	0	-2.409232	3.262704	-1.473927
6	0	-3.143287	2.945849	-0.349069
1	0	-0.710820	0.336711	-1.901310
1	0	-0.969775	2.556533	-2.930037
1	0	-2.525513	4.232407	-1.942876
1	0	-3.819740	3.672182	0.088982
6	0	-1.965922	-0.546260	0.380489
6	0	-2.713413	-0.831331	1.518431
6	0	-3.616870	0.120407	2.042814
6	0	-3.761291	1.348624	1.431447
1	0	-2.580685	-1.782041	2.021870
1	0	-4.196397	-0.123793	2.925276
1	0	-4.439693	2.089689	1.841260
52	0	-0.672544	-2.049585	-0.333361
6	0	1.104890	-0.949680	-0.053205
6	0	2.222755	-1.234375	-0.855001
6	0	1.186919	0.052837	0.926980
6	0	3.416624	-0.534715	-0.678372
6	0	2.368028	0.774071	1.098801
6	0	3.463398	0.462128	0.294565
1	0	2.161310	-1.994754	-1.625920
1	0	0.329296	0.272588	1.552662
1	0	4.288946	-0.737634	-1.283629
1	0	2.452354	1.554220	1.842400
7	0	4.711683	1.215831	0.475475
8	0	5.673884	0.918976	-0.253118
8	0	4.727184	2.102898	1.345919

1j (B_o): MP2 = -7430.8527357 a.u.

6	0	-1.411863	-2.544714	0.000000
6	0	-2.842787	-2.679790	0.000000
6	0	-0.621065	-3.724330	0.000000
6	0	-1.206771	-4.976042	0.000000
6	0	-2.613592	-5.105771	0.000000

6	0	-3.411839	-3.979660	0.000000
1	0	0.461829	-3.647275	0.000000
1	0	-0.582694	-5.861751	0.000000
1	0	-3.064005	-6.091082	0.000000
1	0	-4.492801	-4.073414	0.000000
6	0	-0.855181	-1.229132	0.000000
6	0	-1.678815	-0.112875	0.000000
6	0	-3.084277	-0.263445	0.000000
6	0	-3.657154	-1.518264	0.000000
1	0	-1.253620	0.883526	0.000000
1	0	-3.709613	0.621960	0.000000
1	0	-4.735875	-1.632708	0.000000
52	0	1.256623	-1.031966	0.000000
6	0	1.268857	1.072722	0.000000
6	0	1.275397	1.778193	1.216484
6	0	1.275397	1.778193	-1.216484
6	0	1.275458	3.173955	1.223577
6	0	1.275458	3.173955	-1.223577
6	0	1.277170	3.841844	0.000000
1	0	1.273963	1.234127	2.153378
1	0	1.273963	1.234127	-2.153378
1	0	1.278659	3.739142	2.144978
1	0	1.278659	3.739142	-2.144978
7	0	1.276206	5.314414	0.000000
8	0	1.275458	5.887907	1.102159
8	0	1.275458	5.887907	-1.102159

2a (A): MP2 = -3015.0773862 a.u.

6	0	-1.471896	0.180864	-0.305195
6	0	-2.712002	0.430858	0.376658
6	0	-0.899626	1.225236	-1.077432
6	0	-3.355127	1.684236	0.204032
6	0	-1.548532	2.437238	-1.216895
6	0	-2.773433	2.678853	-0.555169
6	0	-0.835008	-1.082527	-0.094768
6	0	-3.318715	-0.604762	1.134728
6	0	-1.447348	-2.066608	0.668227
6	0	-2.693380	-1.824570	1.288906
1	0	0.034242	1.045530	-1.594265
1	0	-4.298616	1.859192	0.710444
1	0	-1.099980	3.218516	-1.819144
1	0	-3.270911	3.634342	-0.671771
34	0	0.840020	-1.515968	-0.925128
1	0	-4.267213	-0.407467	1.623378
1	0	-0.942611	-3.014250	0.815394
1	0	-3.157857	-2.607359	1.876943
6	0	1.940158	-0.238912	0.000640
6	0	1.758193	0.009731	1.367073
6	0	2.942320	0.430696	-0.713370
6	0	2.579228	0.935867	2.013118
6	0	3.774906	1.336977	-0.050980
6	0	3.590198	1.597672	1.309040
1	0	0.983369	-0.514895	1.914442
1	0	3.064695	0.248140	-1.775278
1	0	2.433991	1.133627	3.068722
1	0	4.552238	1.851998	-0.603101
1	0	4.228348	2.310447	1.816920

2a (TS-AB'): MP2 = -3015.0751277 a.u.

6	0	1.904254	-0.093940	-0.064995
6	0	2.805614	1.023672	0.025498
6	0	2.354427	-1.364167	0.385671
6	0	4.133871	0.803421	0.475739
6	0	3.651021	-1.540046	0.828134
6	0	4.546689	-0.448080	0.883560
6	0	0.578819	0.151600	-0.536698
6	0	2.377471	2.308728	-0.393600
6	0	0.193507	1.419895	-0.944240
6	0	1.086206	2.507235	-0.839825
1	0	1.672831	-2.205491	0.360226
1	0	4.812349	1.648787	0.524538
1	0	3.974593	-2.518648	1.162606

1	0	5.562012	-0.599323	1.230337
34	0	-0.676178	-1.304511	-0.701083
1	0	3.071000	3.140162	-0.324591
1	0	-0.810954	1.581411	-1.318928
1	0	0.763436	3.492288	-1.156425
6	0	-2.198053	-0.399662	0.036725
6	0	-3.302718	-0.123632	-0.779790
6	0	-2.209214	-0.034121	1.390969
6	0	-4.421356	0.516023	-0.236218
6	0	-3.322786	0.621081	1.918555
6	0	-4.430640	0.893250	1.108483
1	0	-3.280553	-0.402425	-1.826666
1	0	-1.353908	-0.262137	2.016216
1	0	-5.277097	0.727675	-0.866333
1	0	-3.330633	0.908393	2.963359
1	0	-5.295670	1.395149	1.524676

2a (B¹): MP2 = -3015.075142 a.u.

6	0	1.948579	-0.068650	-0.047081
6	0	2.832906	1.063143	0.019508
6	0	2.462129	-1.349585	0.290621
6	0	4.201917	0.849849	0.328299
6	0	3.798378	-1.519450	0.596808
6	0	4.674892	-0.411347	0.626851
6	0	0.578504	0.167663	-0.374010
6	0	2.343602	2.357071	-0.292113
6	0	0.132460	1.444152	-0.678815
6	0	1.012192	2.545054	-0.603191
1	0	1.798827	-2.206278	0.288570
1	0	4.866564	1.706985	0.358899
1	0	4.169728	-2.506417	0.846153
1	0	5.721467	-0.556851	0.866608
34	0	-0.628360	-1.332554	-0.502597
1	0	3.023976	3.200680	-0.244531
1	0	-0.905023	1.603965	-0.948344
1	0	0.641526	3.536218	-0.837887
6	0	-2.232157	-0.426042	0.025317
6	0	-3.221076	-0.150150	-0.928657
6	0	-2.421630	-0.063457	1.367234
6	0	-4.400135	0.491513	-0.536320
6	0	-3.595601	0.589963	1.745377
6	0	-4.586571	0.864597	0.796774
1	0	-3.061895	-0.429982	-1.963246
1	0	-1.654625	-0.291421	2.097883
1	0	-5.166075	0.703966	-1.272705
1	0	-3.741653	0.874206	2.780759
1	0	-5.498901	1.365813	1.096541

2a (TS-B¹B¹): MP2 = -3015.0750215 a.u.

6	0	-1.992134	-0.040059	-0.021226
6	0	-2.870165	1.096016	0.018995
6	0	-2.564234	-1.339485	0.014958
6	0	-4.273012	0.881790	0.003096
6	0	-3.934977	-1.512370	0.010083
6	0	-4.798242	-0.394126	0.022677
6	0	-0.582455	0.193764	0.000113
6	0	-2.325650	2.405441	-0.014153
6	0	-0.080762	1.484413	-0.023833
6	0	-0.959027	2.590725	-0.008326
1	0	-1.921177	-2.212197	0.004030
1	0	-4.929662	1.745533	0.014697
1	0	-4.349449	-2.513360	0.027719
1	0	-5.871769	-0.540498	0.018374
34	0	0.578380	-1.347718	-0.015163
1	0	-2.999246	3.255538	0.000252
1	0	0.988601	1.653772	-0.018810
1	0	-0.544602	3.592222	-0.025793
6	0	2.269730	-0.450903	0.000587
6	0	2.883777	-0.139917	1.222548
6	0	2.902001	-0.134661	-1.210649
6	0	4.125421	0.500599	1.227580
6	0	4.144003	0.505085	-1.194387

6	0	4.756199	0.821395	0.021919
1	0	2.386786	-0.392614	2.151481
1	0	2.418520	-0.382391	-2.148013
1	0	4.600726	0.743027	2.170609
1	0	4.633584	0.751159	-2.129131
1	0	5.719948	1.315963	0.030234

2a (B_o): MP2 = -3015.0749573 a.u.

6	0	-0.876811	-1.789400	0.000000
6	0	-2.289642	-2.049299	0.000000
6	0	0.016182	-2.893879	0.000000
6	0	-2.742208	-3.394410	0.000000
6	0	-0.459004	-4.191248	0.000000
6	0	-1.848654	-4.445987	0.000000
6	0	-0.439071	-0.428909	0.000000
6	0	-3.204336	-0.965013	0.000000
6	0	-1.356564	0.608538	0.000000
6	0	-2.742432	0.334481	0.000000
1	0	1.086639	-2.722159	0.000000
1	0	-3.810939	-3.582182	0.000000
1	0	0.240517	-5.018761	0.000000
1	0	-2.210482	-5.467262	0.000000
34	0	1.463060	-0.103175	0.000000
1	0	-4.268674	-1.174460	0.000000
1	0	-1.017311	1.636744	0.000000
1	0	-3.442728	1.161926	0.000000
6	0	1.440862	1.811139	0.000000
6	0	1.447769	2.508727	1.216643
6	0	1.447769	2.508727	-1.216643
6	0	1.447769	3.905868	1.211026
6	0	1.447769	3.905868	-1.211026
6	0	1.449424	4.604253	0.000000
1	0	1.445515	1.958293	2.149803
1	0	1.445515	1.958293	-2.149803
1	0	1.451781	4.446625	2.149938
1	0	1.451781	4.446625	-2.149938
1	0	1.451407	5.687523	0.000000

2a (A_o): MP2 = -3015.076251 a.u.

6	0	-1.570138	0.093104	-0.297230
6	0	-2.803116	0.260939	0.421826
6	0	-1.146067	1.129403	-1.170158
6	0	-3.593411	1.414771	0.177829
6	0	-1.934783	2.244710	-1.376143
6	0	-3.156695	2.400757	-0.682794
6	0	-0.781024	-1.066104	-0.013432
6	0	-3.252373	-0.765370	1.293038
6	0	-1.242684	-2.042179	0.858228
6	0	-2.479977	-1.885768	1.521337
1	0	-0.215449	1.008758	-1.711074
1	0	-4.531560	1.525679	0.711412
1	0	-1.599183	3.020191	-2.054504
1	0	-3.765107	3.280978	-0.853242
34	0	0.880070	-1.389965	-0.913448
1	0	-4.197516	-0.635049	1.809850
1	0	-0.627031	-2.912206	1.053116
1	0	-2.825726	-2.660166	2.195809
6	0	2.006903	-0.123551	-0.004264
6	0	1.541574	0.716404	1.014039
6	0	3.340288	-0.042754	-0.431158
6	0	2.422897	1.618383	1.616679
6	0	4.210599	0.861039	0.180184
6	0	3.753897	1.699617	1.201056
1	0	0.513520	0.655902	1.348302
1	0	3.698357	-0.688532	-1.226169
1	0	2.060616	2.264785	2.407645
1	0	5.241210	0.915783	-0.150205
1	0	4.430162	2.402284	1.672083

2b' (A): MP2 = -3070.2796795 a.u.

6	0	-1.703529	0.310429	-0.272069
6	0	-2.794388	0.873610	0.475267

6	0	-1.045656	1.125353	-1.230080
6	0	-3.214872	2.199267	0.191994
6	0	-1.476485	2.415266	-1.475355
6	0	-2.553922	2.966066	-0.745723
6	0	-1.288041	-1.020604	0.046523
6	0	-3.489707	0.070905	1.417272
6	0	-1.980560	-1.771318	0.985872
6	0	-3.084560	-1.222043	1.675746
1	0	-0.224106	0.708562	-1.797661
1	0	-4.048171	2.611644	0.751408
1	0	-0.967162	3.017786	-2.218378
1	0	-2.881028	3.979275	-0.947208
34	0	0.186558	-1.864257	-0.851282
1	0	-4.325685	0.503872	1.956820
1	0	-1.644964	-2.776572	1.212579
1	0	-3.614858	-1.826757	2.402092
6	0	1.584479	-0.717727	-0.203886
6	0	1.712985	-0.446196	1.164324
6	0	2.487323	-0.145596	-1.108922
6	0	2.733387	0.385753	1.618463
6	0	3.523112	0.666283	-0.647251
6	0	3.643509	0.965423	0.718436
1	0	1.020200	-0.888570	1.871346
1	0	2.385727	-0.339892	-2.170980
1	0	2.826035	0.594289	2.679387
1	0	4.222598	1.101298	-1.353632
7	0	4.714179	1.738222	1.189544
1	0	4.518278	2.211704	2.060100
1	0	5.072451	2.391313	0.507221

2b' (B'): MP2 = -3070.2785101 a.u.

6	0	-2.325885	0.015471	0.022317
6	0	-3.138497	1.199427	-0.016294
6	0	-2.972469	-1.248476	0.063678
6	0	-4.548796	1.068792	0.074243
6	0	-4.348964	-1.339993	0.139675
6	0	-5.146558	-0.173949	0.125024
6	0	-0.908310	0.164137	-0.078975
6	0	-2.518490	2.474694	-0.054679
6	0	-0.332950	1.422865	-0.127921
6	0	-1.145333	2.578396	-0.133810
1	0	-2.379425	-2.155708	0.084154
1	0	-5.154821	1.968848	0.062954
1	0	-4.820377	-2.314786	0.181278
1	0	-6.225226	-0.256555	0.185476
34	0	0.167805	-1.438569	-0.086012
1	0	-3.141915	3.362365	-0.065265
1	0	0.742823	1.525747	-0.198325
1	0	-0.673675	3.553713	-0.172101
6	0	1.902056	-0.642860	-0.016774
6	0	2.611073	-0.387250	-1.199381
6	0	2.493354	-0.344872	1.219779
6	0	3.882726	0.180044	-1.145253
6	0	3.763816	0.223833	1.269441
6	0	4.484721	0.473364	0.089458
1	0	2.158541	-0.616552	-2.156886
1	0	1.950224	-0.543207	2.136211
1	0	4.424452	0.378652	-2.064106
1	0	4.213956	0.455768	2.229034
7	0	5.733226	1.101998	0.139800
1	0	6.238073	0.943961	0.999982
1	0	6.320474	0.913359	-0.659773

2b' (A₀): MP2 = -3070.2777182 a.u.

6	0	-1.829099	0.187503	-0.276953
6	0	-2.958411	0.669274	0.469854
6	0	-1.315012	0.993214	-1.326867
6	0	-3.570554	1.891113	0.085199
6	0	-1.928925	2.182768	-1.668163
6	0	-3.051235	2.647538	-0.945195
6	0	-1.215648	-1.033989	0.146155
6	0	-3.496329	-0.123168	1.517179

6	0	-1.757852	-1.774718	1.186812
6	0	-2.897870	-1.312089	1.880829
1	0	-0.461404	0.634971	-1.889146
1	0	-4.433771	2.239196	0.642804
1	0	-1.528634	2.778569	-2.480011
1	0	-3.522858	3.582622	-1.223244
34	0	0.295806	-1.766768	-0.777048
1	0	-4.364471	0.242423	2.055796
1	0	-1.275665	-2.697535	1.486506
1	0	-3.308718	-1.906424	2.688420
6	0	1.673554	-0.578486	-0.150526
6	0	1.433361	0.475391	0.737576
6	0	2.963305	-0.764096	-0.666802
6	0	2.483310	1.303828	1.134626
6	0	4.007400	0.066040	-0.263760
6	0	3.776965	1.130930	0.621043
1	0	0.444150	0.633852	1.148650
1	0	3.162669	-1.571910	-1.363363
1	0	2.288986	2.113853	1.830329
1	0	5.003974	-0.093373	-0.662354
7	0	4.841604	1.927870	1.074604
1	0	4.550156	2.848841	1.371373
1	0	5.595194	2.003618	0.405609

2b' (B₀): MP2 = -3070.2784431 a.u.

6	0	0.962021	-2.120816	0.000000
6	0	2.375362	-2.378306	0.000000
6	0	0.070924	-3.226899	0.000000
6	0	2.830174	-3.722690	0.000000
6	0	0.548300	-4.523476	0.000000
6	0	1.938440	-4.775859	0.000000
6	0	0.521123	-0.761515	0.000000
6	0	3.287803	-1.292125	0.000000
6	0	1.436612	0.277590	0.000000
6	0	2.823006	0.006523	0.000000
1	0	-0.999679	-3.056198	0.000000
1	0	3.899262	-3.908740	0.000000
1	0	-0.149758	-5.352283	0.000000
1	0	2.302080	-5.796537	0.000000
34	0	-1.381262	-0.432880	0.000000
1	0	4.352623	-1.499392	0.000000
1	0	1.093106	1.304625	0.000000
1	0	3.521691	0.835403	0.000000
6	0	-1.362570	1.476246	0.000000
6	0	-1.375184	2.183262	1.211213
6	0	-1.375184	2.183262	-1.211213
6	0	-1.375184	3.576416	1.209021
6	0	-1.375184	3.576416	-1.209021
6	0	-1.397355	4.291564	0.000000
1	0	-1.367182	1.641081	2.149370
1	0	-1.367182	1.641081	-2.149370
1	0	-1.381046	4.117425	2.149496
1	0	-1.381046	4.117425	-2.149496
7	0	-1.332899	5.688793	0.000000
1	0	-1.714143	6.117457	-0.831056
1	0	-1.714143	6.117457	0.831056

2c (A): MP2 = -3054.2633367 a.u.

6	0	-1.713960	0.304463	-0.284775
6	0	-2.807434	0.892225	0.439231
6	0	-1.046493	1.089595	-1.260833
6	0	-3.224718	2.208755	0.112123
6	0	-1.473633	2.371991	-1.548152
6	0	-2.555522	2.945887	-0.843314
6	0	-1.300814	-1.015259	0.080885
6	0	-3.509265	0.120011	1.401717
6	0	-1.998384	-1.735575	1.040072
6	0	-3.105570	-1.163453	1.705832
1	0	-0.221796	0.654876	-1.810637
1	0	-4.060629	2.639361	0.653518
1	0	-0.956959	2.951618	-2.304090
1	0	-2.879301	3.953051	-1.077556

34	0	0.170201	-1.888118	-0.790227
1	0	-4.347852	0.570655	1.922358
1	0	-1.663288	-2.732318	1.302152
1	0	-3.640257	-1.743922	2.448462
6	0	1.572154	-0.724031	-0.178615
6	0	1.608522	-0.275222	1.147487
6	0	2.579283	-0.342843	-1.073593
6	0	2.644795	0.560858	1.563333
6	0	3.623216	0.474209	-0.633416
6	0	3.670777	0.942681	0.686038
1	0	0.833627	-0.576399	1.843505
1	0	2.544343	-0.678042	-2.104489
1	0	2.666027	0.908067	2.591435
1	0	4.404468	0.759871	-1.330362
6	0	4.767159	1.870418	1.139465
1	0	4.474396	2.914987	1.017046
1	0	5.001462	1.714328	2.192343
1	0	5.678241	1.711630	0.563117

2c (B'): MP2 = -3054.2611318 a.u.

6	0	2.332610	0.020744	-0.000073
6	0	3.136408	1.211374	-0.000087
6	0	2.987232	-1.239732	-0.000120
6	0	4.550209	1.087576	-0.000147
6	0	4.366336	-1.323681	-0.000178
6	0	5.156134	-0.152235	-0.000192
6	0	0.910649	0.163970	-0.000011
6	0	2.508892	2.483595	-0.000042
6	0	0.327259	1.420064	0.000033
6	0	1.133095	2.580363	0.000017
1	0	2.401124	-2.151776	-0.000111
1	0	5.150165	1.991752	-0.000157
1	0	4.844614	-2.295988	-0.000214
1	0	6.236862	-0.229519	-0.000237
34	0	-0.150739	-1.447905	0.000013
1	0	3.126853	3.375135	-0.000053
1	0	-0.750911	1.520071	0.000081
1	0	0.655202	3.553378	0.000052
6	0	-1.894500	-0.660937	0.000059
6	0	-2.538191	-0.381355	1.213747
6	0	-2.538242	-0.381325	-1.213598
6	0	-3.814941	0.183083	1.204643
6	0	-3.814987	0.183115	-1.204427
6	0	-4.470760	0.474988	0.000126
1	0	-2.036720	-0.597347	2.149731
1	0	-2.036809	-0.597294	-2.149607
1	0	-4.306804	0.402759	2.146569
1	0	-4.306887	0.402818	-2.146329
6	0	-5.864886	1.044592	0.000148
1	0	-6.612114	0.248848	-0.000277
1	0	-6.036812	1.660025	0.882769
1	0	-6.036558	1.660718	-0.882039

2c (A_o): MP2 = -3054.2620552 a.u.

6	0	-1.841097	0.191975	-0.272463
6	0	-2.963100	0.680537	0.481072
6	0	-1.335246	0.989639	-1.332471
6	0	-3.576836	1.900607	0.093495
6	0	-1.950333	2.177856	-1.676297
6	0	-3.065497	2.649153	-0.946590
6	0	-1.225787	-1.026965	0.154857
6	0	-3.492504	-0.103566	1.538927
6	0	-1.759388	-1.759894	1.205433
6	0	-2.892452	-1.290610	1.906185
1	0	-0.487247	0.626855	-1.900333
1	0	-4.434404	2.253918	0.656448
1	0	-1.556094	2.767666	-2.495386
1	0	-3.537832	3.583259	-1.226559
34	0	0.276617	-1.768898	-0.775988
1	0	-4.355340	0.267125	2.082523
1	0	-1.276140	-2.681507	1.507192
1	0	-3.297023	-1.878468	2.721615

6	0	1.664254	-0.584836	-0.167116
6	0	1.433082	0.473681	0.718037
6	0	2.953538	-0.801112	-0.673432
6	0	2.496963	1.293231	1.102333
6	0	4.003161	0.027173	-0.276283
6	0	3.794086	1.089270	0.614658
1	0	0.443267	0.647096	1.121581
1	0	3.139968	-1.618145	-1.362902
1	0	2.309932	2.107077	1.795746
1	0	4.998849	-0.155378	-0.667524
6	0	4.923076	2.007273	1.003217
1	0	5.021876	2.833085	0.295964
1	0	4.756520	2.435913	1.991239
1	0	5.873176	1.473563	1.022637

2c (B₀): MP2 = -3054.2611318 a.u.

6	0	0.962128	-2.125045	0.000000
6	0	2.376095	-2.378799	0.000000
6	0	0.073967	-3.233423	0.000000
6	0	2.834514	-3.721933	0.000000
6	0	0.554803	-4.528711	0.000000
6	0	1.945563	-4.777416	0.000000
6	0	0.518179	-0.766593	0.000000
6	0	3.285958	-1.290464	0.000000
6	0	1.431134	0.274863	0.000000
6	0	2.818184	0.006982	0.000000
1	0	-0.997182	-3.066130	0.000000
1	0	3.904065	-3.905073	0.000000
1	0	-0.141097	-5.359286	0.000000
1	0	2.311851	-5.797112	0.000000
34	0	-1.385214	-0.447567	0.000000
1	0	4.351233	-1.495180	0.000000
1	0	1.086662	1.301406	0.000000
1	0	3.514887	0.837491	0.000000
6	0	-1.370506	1.465494	0.000000
6	0	-1.375063	2.167295	1.213673
6	0	-1.375063	2.167295	-1.213673
6	0	-1.375063	3.563245	1.204535
6	0	-1.375063	3.563245	-1.204535
6	0	-1.373263	4.281064	0.000000
1	0	-1.369845	1.621333	2.149669
1	0	-1.369845	1.621333	-2.149669
1	0	-1.373019	4.101953	2.146449
1	0	-1.373019	4.101953	-2.146449
6	0	-1.415998	5.786457	0.000000
1	0	-2.445926	6.148129	0.000000
1	0	-0.922265	6.192570	0.882404
1	0	-0.922265	6.192570	-0.882404

2f (A): MP2 = -3474.0981486 a.u.

6	0	-1.954696	0.382629	-0.279635
6	0	-2.940082	1.133485	0.448736
6	0	-1.270436	1.018263	-1.348390
6	0	-3.243171	2.457513	0.037109
6	0	-1.584244	2.312472	-1.717204
6	0	-2.560514	3.046928	-1.007197
6	0	-1.652804	-0.939813	0.173924
6	0	-3.657232	0.513177	1.505287
6	0	-2.360120	-1.510197	1.222675
6	0	-3.364964	-0.777782	1.893679
1	0	-0.528887	0.459112	-1.904395
1	0	-3.998964	3.012199	0.583191
1	0	-1.057756	2.776688	-2.542746
1	0	-2.795296	4.061711	-1.305524
34	0	-0.327039	-2.021998	-0.694474
1	0	-4.415413	1.086228	2.028770
1	0	-2.109713	-2.512937	1.548657
1	0	-3.910170	-1.241429	2.707273
6	0	1.214797	-0.973718	-0.232909
6	0	1.334823	-0.382342	1.031276
6	0	2.235814	-0.815298	-1.178868
6	0	2.467190	0.368363	1.346486

6	0	3.382136	-0.085515	-0.858332
6	0	3.485771	0.509307	0.400300
1	0	0.547633	-0.506330	1.766116
1	0	2.136780	-1.255505	-2.164818
1	0	2.564936	0.833919	2.319087
1	0	4.176278	0.039345	-1.583442
17	0	4.900959	1.438242	0.796372

2f (B'): MP2 = -3474.0965958 a.u.

6	0	2.234988	0.127141	-0.137122
6	0	3.153103	0.738587	0.786549
6	0	2.241436	0.567652	-1.488415
6	0	3.990593	1.792260	0.334728
6	0	3.075290	1.591398	-1.895296
6	0	3.965203	2.201692	-0.982365
6	0	1.396986	-0.924057	0.350209
6	0	3.165048	0.325777	2.143549
6	0	1.446418	-1.313603	1.681067
6	0	2.340168	-0.691319	2.579255
1	0	1.566594	0.098466	-2.193869
1	0	4.671813	2.254325	1.041535
1	0	3.061014	1.914209	-2.929626
1	0	4.613298	3.003917	-1.314497
34	0	0.139079	-1.820180	-0.799984
1	0	3.855912	0.805361	2.829098
1	0	0.800063	-2.113183	2.023303
1	0	2.361137	-1.006323	3.615877
6	0	-1.394564	-0.737968	-0.386601
6	0	-1.314880	0.661635	-0.376158
6	0	-2.616967	-1.370864	-0.125733
6	0	-2.448549	1.422720	-0.091536
6	0	-3.758998	-0.610778	0.134838
6	0	-3.665309	0.781666	0.155620
1	0	-0.373644	1.156368	-0.584359
1	0	-2.676185	-2.453004	-0.114748
1	0	-2.394099	2.503922	-0.074749
1	0	-4.706841	-1.093031	0.337383
17	0	-5.080443	1.731969	0.498152

2f (A₀): MP2 = -3474.0970925 a.u.

6	0	-2.091570	0.272750	-0.261484
6	0	-3.122875	0.925803	0.497118
6	0	-1.557633	0.938148	-1.396359
6	0	-3.627990	2.173111	0.044917
6	0	-2.065239	2.157096	-1.802506
6	0	-3.092258	2.790763	-1.066418
6	0	-1.582649	-0.969624	0.232700
6	0	-3.678923	0.276013	1.629748
6	0	-2.137483	-1.569516	1.354247
6	0	-3.184838	-0.938103	2.060893
1	0	-0.778877	0.450762	-1.970204
1	0	-4.418761	2.651512	0.613094
1	0	-1.652237	2.644570	-2.677654
1	0	-3.480270	3.747298	-1.395620
34	0	-0.204211	-1.924351	-0.695848
1	0	-4.474428	0.770746	2.177186
1	0	-1.735510	-2.512653	1.704775
1	0	-3.608536	-1.422605	2.932531
6	0	1.315818	-0.849174	-0.222708
6	0	1.225232	0.285268	0.592273
6	0	2.555134	-1.222320	-0.762743
6	0	2.371497	1.026968	0.884859
6	0	3.701256	-0.483909	-0.470177
6	0	3.601075	0.643806	0.347643
1	0	0.274959	0.583107	1.017096
1	0	2.633096	-2.095350	-1.402008
1	0	2.307543	1.903187	1.517738
1	0	4.660133	-0.772137	-0.881820
17	0	5.026162	1.572767	0.708923

2f (B₀): MP2 = -3474.0953860 a.u.

6	0	-1.021198	-2.435347	0.000000
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6	0	-2.433502	-2.698029	0.000000
6	0	-0.125676	-3.537745	0.000000
6	0	-2.883235	-4.044061	0.000000
6	0	-0.598194	-4.836071	0.000000
6	0	-1.987318	-5.093618	0.000000
6	0	-0.587421	-1.073853	0.000000
6	0	-3.350460	-1.615625	0.000000
6	0	-1.506503	-0.038033	0.000000
6	0	-2.891856	-0.315012	0.000000
1	0	0.944587	-3.364443	0.000000
1	0	-3.951507	-4.234138	0.000000
1	0	0.103002	-5.662116	0.000000
1	0	-2.346903	-6.115641	0.000000
34	0	1.315265	-0.746634	0.000000
1	0	-4.414303	-1.827343	0.000000
1	0	-1.170411	0.991195	0.000000
1	0	-3.593892	0.510862	0.000000
6	0	1.290635	1.165451	0.000000
6	0	1.297835	1.867294	1.214168
6	0	1.297835	1.867294	-1.214168
6	0	1.297835	3.262914	1.216443
6	0	1.297835	3.262914	-1.216443
6	0	1.299629	3.950155	0.000000
1	0	1.295639	1.322325	2.150435
1	0	1.295639	1.322325	-2.150435
1	0	1.302201	3.813629	2.148426
1	0	1.302201	3.813629	-2.148426
17	0	1.302194	5.687264	0.000000

2j (A): MP2 = -3219.0709093 a.u.

6	0	-2.156453	0.393653	-0.305924
6	0	-3.100234	1.231713	0.381227
6	0	-1.477261	0.920025	-1.435614
6	0	-3.373472	2.527382	-0.129706
6	0	-1.760943	2.189678	-1.901254
6	0	-2.697572	3.009181	-1.231943
6	0	-1.881529	-0.894870	0.250657
6	0	-3.808815	0.721630	1.500683
6	0	-2.578025	-1.357132	1.358157
6	0	-3.543893	-0.541208	1.988667
1	0	-0.768934	0.293359	-1.962681
1	0	-4.098758	3.147955	0.385800
1	0	-1.240459	2.569461	-2.772418
1	0	-2.908503	4.003789	-1.606130
34	0	-0.614937	-2.084626	-0.560505
1	0	-4.536701	1.358638	1.992138
1	0	-2.347971	-2.336786	1.760269
1	0	-4.081899	-0.919484	2.849704
6	0	0.979093	-1.082787	-0.196695
6	0	1.079258	-0.244488	0.922803
6	0	2.064143	-1.212868	-1.076223
6	0	2.254760	0.464080	1.163803
6	0	3.253099	-0.526431	-0.833821
6	0	3.322040	0.308442	0.280085
1	0	0.243096	-0.149711	1.605439
1	0	1.979655	-1.846534	-1.951967
1	0	2.355485	1.119226	2.017609
1	0	4.102634	-0.611164	-1.496565
7	0	4.564041	1.050305	0.532343
8	0	4.600487	1.789512	1.530990
8	0	5.501605	0.893037	-0.268474

2j (B'): MP2 = -3219.0709093 a.u.

6	0	-2.156463	0.393661	-0.305857
6	0	-3.100225	1.231695	0.381354
6	0	-1.477308	0.920074	-1.435551
6	0	-3.373463	2.527391	-0.129511
6	0	-1.760993	2.189751	-1.901125
6	0	-2.697593	3.009232	-1.231747
6	0	-1.881529	-0.894886	0.250662
6	0	-3.808774	0.721569	1.500809
6	0	-2.577997	-1.357193	1.358161

6	0	-3.543849	-0.541293	1.988729
1	0	-0.769005	0.293422	-1.962669
1	0	-4.098728	3.147948	0.386045
1	0	-1.240537	2.569565	-2.772292
1	0	-2.908522	4.003862	-1.605881
34	0	-0.614948	-2.084604	-0.560573
1	0	-4.536647	1.358558	1.992309
1	0	-2.347933	-2.336863	1.760228
1	0	-4.081834	-0.919603	2.849764
6	0	0.979085	-1.082774	-0.196760
6	0	2.064131	-1.212860	-1.076293
6	0	1.079263	-0.244480	0.922741
6	0	3.253092	-0.526431	-0.833895
6	0	2.254771	0.464078	1.163738
6	0	3.322046	0.308436	0.280014
1	0	1.979635	-1.846523	-1.952039
1	0	0.243104	-0.149697	1.605380
1	0	4.102624	-0.611169	-1.496643
1	0	2.355505	1.119220	2.017546
7	0	4.564055	1.050286	0.532272
8	0	5.501615	0.893013	-0.268550
8	0	4.600514	1.789485	1.530924

2j (A_o): MP2 = -3219.0703265 a.u.

6	0	-2.278983	0.301083	-0.275000
6	0	-3.263206	1.050633	0.456583
6	0	-1.735316	0.866068	-1.458667
6	0	-3.715731	2.290453	-0.066293
6	0	-2.191034	2.080550	-1.933855
6	0	-3.171794	2.809351	-1.223196
6	0	-1.821351	-0.929732	0.292079
6	0	-3.828090	0.502106	1.637427
6	0	-2.382572	-1.430792	1.457972
6	0	-3.385126	-0.704952	2.138343
1	0	-0.993357	0.305433	-2.014230
1	0	-4.471365	2.842360	0.482571
1	0	-1.772239	2.490593	-2.845148
1	0	-3.518834	3.761419	-1.606426
34	0	-0.505801	-2.007055	-0.592826
1	0	-4.588414	1.069063	2.164309
1	0	-2.020062	-2.368430	1.862231
1	0	-3.815220	-1.111527	3.045849
6	0	1.068182	-0.983148	-0.209872
6	0	1.043734	0.204343	0.534300
6	0	2.280618	-1.452708	-0.740440
6	0	2.225081	0.907789	0.767096
6	0	3.466421	-0.759216	-0.512253
6	0	3.415156	0.417710	0.233927
1	0	0.113437	0.571238	0.948577
1	0	2.301977	-2.367352	-1.323055
1	0	2.230983	1.823742	1.341074
1	0	4.410572	-1.105937	-0.907729
7	0	4.658704	1.158811	0.474604
8	0	4.586103	2.206105	1.140328
8	0	5.708008	0.693942	-0.003213

2j (B_o): MP2 = -3219.0667322 a.u.

6	0	-1.063485	-2.659383	0.000000
6	0	-2.474957	-2.926407	0.000000
6	0	-0.164226	-3.758668	0.000000
6	0	-2.920324	-4.273862	0.000000
6	0	-0.632558	-5.058485	0.000000
6	0	-2.020844	-5.320338	0.000000
6	0	-0.635499	-1.296229	0.000000
6	0	-3.395596	-1.847094	0.000000
6	0	-1.557474	-0.263018	0.000000
6	0	-2.941928	-0.544887	0.000000
1	0	0.905669	-3.582730	0.000000
1	0	-3.987901	-4.467401	0.000000
1	0	0.071263	-5.882230	0.000000
1	0	-2.377028	-6.343500	0.000000
34	0	1.267479	-0.967882	0.000000

1	0	-4.458650	-2.062416	0.000000
1	0	-1.226708	0.767805	0.000000
1	0	-3.646729	0.278523	0.000000
6	0	1.237324	0.945049	0.000000
6	0	1.245130	1.645498	1.216298
6	0	1.245130	1.645498	-1.216298
6	0	1.245130	3.040525	1.223725
6	0	1.245130	3.040525	-1.223725
6	0	1.247602	3.708513	0.000000
1	0	1.242973	1.096541	2.150001
1	0	1.242973	1.096541	-2.150001
1	0	1.249242	3.605526	2.145043
1	0	1.249242	3.605526	-2.145043
7	0	1.247608	5.180452	0.000000
8	0	1.247299	5.754326	1.102064
8	0	1.247299	5.754326	-1.102064

3a (A): MP2 = -1012.6770442 a.u.

6	0	-1.325896	0.129770	-0.371071
6	0	-2.560510	0.234442	0.354265
6	0	-0.733855	1.312490	-0.885033
6	0	-3.181189	1.504611	0.480381
6	0	-1.362477	2.534338	-0.738227
6	0	-2.582674	2.637126	-0.032832
6	0	-0.709650	-1.159427	-0.468170
6	0	-3.183393	-0.939360	0.854752
6	0	-1.338272	-2.282862	0.051167
6	0	-2.579426	-2.171957	0.716097
1	0	0.198720	1.242314	-1.429594
1	0	-4.120906	1.574297	1.018193
1	0	-0.901403	3.426279	-1.145797
1	0	-3.063013	3.602184	0.076580
16	0	0.816081	-1.391867	-1.341059
1	0	-4.128682	-0.846290	1.379215
1	0	-0.848023	-3.245533	-0.035603
1	0	-3.056359	-3.062148	1.108800
6	0	1.953185	-0.497826	-0.307304
6	0	1.849233	-0.520326	1.090601
6	0	2.996278	0.206963	-0.924608
6	0	2.781640	0.174135	1.862107
6	0	3.940020	0.875531	-0.141304
6	0	3.830724	0.868904	1.251499
1	0	1.044232	-1.072903	1.561011
1	0	3.059557	0.231742	-2.006913
1	0	2.694567	0.162913	2.942252
1	0	4.746358	1.417310	-0.621368
1	0	4.555216	1.400384	1.856248

3a (TS-AB'): MP2 = -1012.6743666 a.u.

6	0	1.754155	-0.215243	-0.193949
6	0	2.675865	0.839773	0.129132
6	0	2.175375	-1.561665	-0.024762
6	0	3.997400	0.502542	0.523721
6	0	3.466753	-1.852533	0.369596
6	0	4.383540	-0.815160	0.655460
6	0	0.433931	0.147317	-0.605549
6	0	2.271525	2.192209	-0.002705
6	0	0.074462	1.482362	-0.731414
6	0	0.985024	2.504573	-0.396066
1	0	1.477047	-2.362972	-0.231373
1	0	4.692388	1.304316	0.750557
1	0	3.770442	-2.885880	0.488767
1	0	5.394143	-1.057174	0.962305
16	0	-0.725796	-1.128033	-1.051549
1	0	2.979037	2.977242	0.242457
1	0	-0.926241	1.734540	-1.063492
1	0	0.680877	3.540250	-0.493586
6	0	-2.186940	-0.545385	-0.230354
6	0	-2.209228	-0.395726	1.165616
6	0	-3.337699	-0.282206	-0.985678
6	0	-3.376966	0.034710	1.794217
6	0	-4.510511	0.125202	-0.342682

6	0	-4.530665	0.290115	1.043774
1	0	-1.316160	-0.612348	1.740320
1	0	-3.304338	-0.392144	-2.063201
1	0	-3.392494	0.155893	2.870893
1	0	-5.400260	0.326261	-0.927376
1	0	-5.437832	0.615229	1.538371

3a (B'): MP2 = -1012.6744674 a.u.

6	0	1.835097	-0.211310	-0.080038
6	0	2.727156	0.907645	0.036792
6	0	2.366937	-1.522128	0.047764
6	0	4.117034	0.664566	0.190933
6	0	3.725100	-1.721633	0.204391
6	0	4.607409	-0.621356	0.290231
6	0	0.437753	0.049423	-0.245476
6	0	2.218606	2.227257	-0.072459
6	0	-0.026087	1.352010	-0.352520
6	0	0.865282	2.439843	-0.235398
1	0	1.703128	-2.376622	-0.006059
1	0	4.787468	1.514704	0.262678
1	0	4.111970	-2.729897	0.293375
1	0	5.670648	-0.789927	0.413088
16	0	-0.642845	-1.355838	-0.408467
1	0	2.903907	3.063859	0.011335
1	0	-1.082450	1.538697	-0.500289
1	0	0.478059	3.449041	-0.315950
6	0	-2.228575	-0.635505	-0.081245
6	0	-3.112404	-0.391495	-1.142007
6	0	-2.614282	-0.353402	1.238843
6	0	-4.379314	0.137509	-0.879932
6	0	-3.876171	0.186496	1.488708
6	0	-4.760979	0.428381	0.432128
1	0	-2.799422	-0.611551	-2.155680
1	0	-1.923661	-0.555170	2.049066
1	0	-5.063197	0.324522	-1.699157
1	0	-4.173868	0.406964	2.506885
1	0	-5.742425	0.840993	0.631896

3a (B₀): MP2 = -1012.6744034 a.u.

6	0	-0.537956	-1.781745	0.000000
6	0	-1.923029	-2.157723	0.000000
6	0	0.446678	-2.805249	0.000000
6	0	-2.260715	-3.536170	0.000000
6	0	0.081362	-4.137913	0.000000
6	0	-1.281846	-4.508865	0.000000
6	0	-0.211437	-0.387633	0.000000
6	0	-2.925637	-1.153866	0.000000
6	0	-1.215144	0.568538	0.000000
6	0	-2.572488	0.179119	0.000000
1	0	1.497463	-2.540576	0.000000
1	0	-3.309847	-3.813215	0.000000
1	0	0.847846	-4.903867	0.000000
1	0	-1.556425	-5.556998	0.000000
16	0	1.519016	0.029224	0.000000
1	0	-3.968858	-1.450857	0.000000
1	0	-0.962429	1.620967	0.000000
1	0	-3.338793	0.945787	0.000000
6	0	1.480597	1.800518	0.000000
6	0	1.485324	2.499617	1.216453
6	0	1.485324	2.499617	-1.216453
6	0	1.485324	3.896034	1.211182
6	0	1.485324	3.896034	-1.211182
6	0	1.486990	4.594472	0.000000
1	0	1.483553	1.945427	2.147467
1	0	1.483553	1.945427	-2.147467
1	0	1.489032	4.436945	2.149910
1	0	1.489032	4.436945	-2.149910
1	0	1.489583	5.677719	0.000000

3b' (B'): MP2 = 1067.8779173 a.u.

6	0	2.242354	-0.179698	-0.021353
6	0	3.088157	0.979021	0.020311

6	0	2.846120	-1.464883	0.008236
6	0	4.496231	0.801615	0.010479
6	0	4.221243	-1.600603	0.008197
6	0	5.054896	-0.460139	0.026523
6	0	0.823638	0.012082	-0.010376
6	0	2.508648	2.273699	-0.007779
6	0	0.289359	1.291048	-0.028565
6	0	1.137260	2.419883	-0.007798
1	0	2.222868	-2.351115	-0.006884
1	0	5.129980	1.682307	0.025971
1	0	4.662387	-2.590282	0.022325
1	0	6.131989	-0.578189	0.025848
16	0	-0.188483	-1.452552	-0.023809
1	0	3.158281	3.142148	0.010764
1	0	-0.784415	1.428484	-0.028583
1	0	0.694997	3.409484	-0.022266
6	0	-1.825414	-0.786834	-0.008644
6	0	-2.499054	-0.536482	-1.213658
6	0	-2.481670	-0.547455	1.208190
6	0	-3.798810	-0.037037	-1.200344
6	0	-3.781119	-0.047362	1.217982
6	0	-4.465339	0.194155	0.014723
1	0	-1.993369	-0.720592	-2.154244
1	0	-1.962769	-0.740720	2.139687
1	0	-4.312614	0.156218	-2.136134
1	0	-4.281340	0.137645	2.162758
7	0	-5.746141	0.755815	0.026529
1	0	-6.289261	0.557849	-0.801446
1	0	-6.277011	0.550837	0.860720

3b' (B_o): MP2 = -1067.8778826 a.u.

6	0	-0.636671	-2.157546	0.000000
6	0	-2.022455	-2.531222	0.000000
6	0	0.346187	-3.182861	0.000000
6	0	-2.362419	-3.909147	0.000000
6	0	-0.021364	-4.514917	0.000000
6	0	-1.385250	-4.883593	0.000000
6	0	-0.306908	-0.764330	0.000000
6	0	-3.023052	-1.525378	0.000000
6	0	-1.308907	0.193563	0.000000
6	0	-2.666982	-0.192979	0.000000
1	0	1.397196	-2.919195	0.000000
1	0	-3.412056	-4.184499	0.000000
1	0	0.743784	-5.282276	0.000000
1	0	-1.661688	-5.931287	0.000000
16	0	1.423423	-0.345342	0.000000
1	0	-4.066915	-1.820299	0.000000
1	0	-1.051851	1.245144	0.000000
1	0	-3.431849	0.575213	0.000000
6	0	1.389727	1.421518	0.000000
6	0	1.399850	2.130066	1.210968
6	0	1.399850	2.130066	-1.210968
6	0	1.399850	3.522499	1.209207
6	0	1.399850	3.522499	-1.209207
6	0	1.421666	4.237727	0.000000
1	0	1.392053	1.584163	2.147043
1	0	1.392053	1.584163	-2.147043
1	0	1.405309	4.063633	2.149522
1	0	1.405309	4.063633	-2.149522
7	0	1.357162	5.634832	0.000000
1	0	1.737964	6.063733	0.831112
1	0	1.737964	6.063733	-0.831112

3c (B_o): MP2 = -1051.8605551 a.u.

6	0	0.635421	-2.164779	0.000000
6	0	2.021869	-2.535736	0.000000
6	0	-0.345471	-3.191883	0.000000
6	0	2.364550	-3.912958	0.000000
6	0	0.024680	-4.523213	0.000000
6	0	1.389238	-4.889233	0.000000
6	0	0.303535	-0.771952	0.000000
6	0	3.020743	-1.528174	0.000000

6	0	1.303785	0.187863	0.000000
6	0	2.662541	-0.196482	0.000000
1	0	-1.397142	-2.930783	0.000000
1	0	3.414692	-4.186215	0.000000
1	0	-0.739011	-5.291970	0.000000
1	0	1.667644	-5.936369	0.000000
16	0	-1.428110	-0.360032	0.000000
1	0	4.065076	-1.821290	0.000000
1	0	1.046446	1.239237	0.000000
1	0	3.426078	0.572984	0.000000
6	0	-1.395818	1.410222	0.000000
6	0	-1.398738	2.113531	1.213461
6	0	-1.398738	2.113531	-1.213461
6	0	-1.398738	3.508756	1.204677
6	0	-1.398738	3.508756	-1.204677
6	0	-1.397379	4.226691	0.000000
1	0	-1.393742	1.563839	2.147351
1	0	-1.393742	1.563839	-2.147351
1	0	-1.396706	4.047602	2.146412
1	0	-1.396706	4.047602	-2.146412
6	0	-1.440752	5.732063	0.000000
1	0	-2.470786	6.093408	0.000000
1	0	-0.947135	6.138308	0.882407
1	0	-0.947135	6.138308	-0.882407

3f (B'): MP2 = -1471.6978029 a.u.

6	0	-1.965208	0.171700	0.337616
6	0	-3.019280	0.652281	-0.510513
6	0	-1.297482	1.092932	1.185484
6	0	-3.402104	2.016599	-0.429615
6	0	-1.691887	2.416430	1.234502
6	0	-2.735336	2.888541	0.406635
6	0	-1.584097	-1.203802	0.221294
6	0	-3.717852	-0.257388	-1.347689
6	0	-2.276477	-2.060822	-0.623126
6	0	-3.347373	-1.584829	-1.411440
1	0	-0.501397	0.738661	1.827417
1	0	-4.208361	2.370119	-1.063655
1	0	-1.178062	3.104455	1.895384
1	0	-3.031890	3.929579	0.453518
16	0	-0.289585	-1.891051	1.219311
1	0	-4.528651	0.116901	-1.963902
1	0	-1.964851	-3.096636	-0.690965
1	0	-3.879514	-2.270895	-2.059608
6	0	1.132633	-1.046084	0.574842
6	0	1.261968	-0.751016	-0.789680
6	0	2.164210	-0.706106	1.461456
6	0	2.406092	-0.109113	-1.260705
6	0	3.322705	-0.088293	0.988802
6	0	3.432558	0.214829	-0.369464
1	0	0.468406	-1.019188	-1.477269
1	0	2.057814	-0.920541	2.519000
1	0	2.508650	0.128702	-2.311934
1	0	4.122474	0.175334	1.669057
17	0	4.862959	1.007363	-0.959789

3f (B_o): MP2 = -1471.6947975 a.u.

6	0	-0.706905	-2.508658	0.000000
6	0	-2.091543	-2.886197	0.000000
6	0	0.279234	-3.530682	0.000000
6	0	-2.427522	-4.265033	0.000000
6	0	-0.084510	-4.863762	0.000000
6	0	-1.447273	-5.236324	0.000000
6	0	-0.383319	-1.114151	0.000000
6	0	-3.095388	-1.883543	0.000000
6	0	-1.387613	-0.158874	0.000000
6	0	-2.744540	-0.549999	0.000000
1	0	1.329887	-3.265309	0.000000
1	0	-3.476236	-4.543449	0.000000
1	0	0.682871	-5.628764	0.000000
1	0	-1.720426	-6.284787	0.000000
16	0	1.348030	-0.696818	0.000000

1	0	-4.138178	-2.181888	0.000000
1	0	-1.137320	0.894140	0.000000
1	0	-3.511819	0.215584	0.000000
6	0	1.308344	1.072161	0.000000
6	0	1.313502	1.775333	1.214106
6	0	1.313502	1.775333	-1.214106
6	0	1.313502	3.170205	1.216609
6	0	1.313502	3.170205	-1.216609
6	0	1.315413	3.857543	0.000000
1	0	1.311555	1.226535	2.148195
1	0	1.311555	1.226535	-2.148195
1	0	1.317764	3.721076	2.148410
1	0	1.317764	3.721076	-2.148410
17	0	1.318458	5.594529	0.000000

3j (B'): MP2 = -1216.6707500 a.u.

6	0	-2.204402	0.150885	-0.354988
6	0	-3.233089	0.731260	0.461259
6	0	-1.542942	0.970324	-1.306027
6	0	-3.602532	2.084748	0.246303
6	0	-1.923728	2.286514	-1.484979
6	0	-2.943326	2.855892	-0.689015
6	0	-1.834618	-1.208586	-0.099201
6	0	-3.921136	-0.076636	1.404766
6	0	-2.514294	-1.964349	0.845964
6	0	-3.561575	-1.393983	1.602472
1	0	-0.768438	0.539160	-1.927500
1	0	-4.390333	2.513279	0.856667
1	0	-1.416529	2.895394	-2.223904
1	0	-3.228759	3.890349	-0.837901
16	0	-0.574005	-2.011869	-1.050929
1	0	-4.713730	0.370524	1.995455
1	0	-2.210961	-2.990656	1.016837
1	0	-4.085324	-2.000652	2.331432
6	0	0.884067	-1.161570	-0.515315
6	0	1.981255	-1.134616	-1.391569
6	0	0.982142	-0.553845	0.745939
6	0	3.171874	-0.518749	-1.012877
6	0	2.160364	0.084180	1.126241
6	0	3.236891	0.088552	0.240210
1	0	1.897773	-1.592685	-2.370732
1	0	0.139279	-0.583251	1.425591
1	0	4.027548	-0.485796	-1.672194
1	0	2.257091	0.562750	2.090536
7	0	4.480622	0.757824	0.639461
8	0	5.426105	0.745536	-0.167508
8	0	4.511695	1.295289	1.759915

3j (B_o): MP2 = -1216.6661046 a.u.

6	0	-0.757866	-2.754930	0.000000
6	0	-2.141867	-3.134713	0.000000
6	0	0.230290	-3.774908	0.000000
6	0	-2.475389	-4.514114	0.000000
6	0	-0.131104	-5.108614	0.000000
6	0	-1.493212	-5.483428	0.000000
6	0	-0.438264	-1.359708	0.000000
6	0	-3.147643	-2.133952	0.000000
6	0	-1.443743	-0.405760	0.000000
6	0	-2.799950	-0.799715	0.000000
1	0	1.280732	-3.508457	0.000000
1	0	-3.523521	-4.794419	0.000000
1	0	0.637599	-5.872211	0.000000
1	0	-1.764385	-6.532350	0.000000
16	0	1.294077	-0.943221	0.000000
1	0	-4.189794	-2.434297	0.000000
1	0	-1.197497	0.648112	0.000000
1	0	-3.568681	-0.035714	0.000000
6	0	1.250865	0.826144	0.000000
6	0	1.256475	1.527921	1.216283
6	0	1.256475	1.527921	-1.216283
6	0	1.256475	2.922221	1.223825
6	0	1.256475	2.922221	-1.223825

6	0	1.259073	3.590462	0.000000
1	0	1.254652	0.975206	2.147822
1	0	1.254652	0.975206	-2.147822
1	0	1.260424	3.487291	2.145019
1	0	1.260424	3.487291	-2.145019
7	0	1.259560	5.062274	0.000000
8	0	1.259418	5.636105	1.102102
8	0	1.259418	5.636105	-1.102102

4a (A): MP2 = -690.0839115 a.u.

6	0	1.279207	-0.107026	-0.377768
6	0	2.537489	0.153068	0.257052
6	0	0.394313	0.988623	-0.568390
6	0	0.756394	2.282049	-0.255838
6	0	2.014797	2.529316	0.338428
6	0	2.895767	1.491243	0.569501
1	0	0.051784	3.082811	-0.443877
1	0	2.296224	3.546265	0.583944
1	0	3.858697	1.682182	1.030764
6	0	0.915155	-1.438662	-0.702599
6	0	1.802081	-2.471766	-0.471762
6	0	3.055147	-2.222286	0.136160
6	0	3.424843	-0.934564	0.468999
1	0	-0.040776	-1.623230	-1.176531
1	0	1.525821	-3.486664	-0.732191
1	0	3.739734	-3.043709	0.311237
1	0	4.386976	-0.742138	0.931989
8	0	-0.818459	0.764441	-1.199658
6	0	-1.866524	0.310044	-0.419253
6	0	-3.067443	0.083161	-1.097982
6	0	-4.174288	-0.380206	-0.388484
6	0	-4.084093	-0.621820	0.986393
6	0	-2.876464	-0.391506	1.647481
6	0	-1.754727	0.072335	0.953253
1	0	-3.111293	0.278278	-2.162208
1	0	-5.106727	-0.554330	-0.911907
1	0	-4.945483	-0.981976	1.534531
1	0	-2.796793	-0.576247	2.712183
1	0	-0.820411	0.251211	1.468179

4a (TS-AB'): MP2 = -690.0833142 a.u.

6	0	1.449965	-0.217889	-0.265808
6	0	2.607910	0.518443	0.149686
6	0	0.298188	0.517520	-0.649876
6	0	0.254404	1.896081	-0.582576
6	0	1.394273	2.606514	-0.146028
6	0	2.542017	1.933950	0.227573
1	0	-0.648355	2.412965	-0.885346
1	0	1.356873	3.688058	-0.093329
1	0	3.417716	2.483701	0.555151
6	0	1.497969	-1.633964	-0.333232
6	0	2.645357	-2.302733	0.044729
6	0	3.789700	-1.586139	0.468860
6	0	3.764892	-0.207581	0.536593
1	0	0.618654	-2.171347	-0.665015
1	0	2.678156	-3.384864	-0.001541
1	0	4.682476	-2.125658	0.762111
1	0	4.642455	0.341477	0.861535
8	0	-0.779863	-0.199099	-1.139951
6	0	-1.954632	-0.170342	-0.410128
6	0	-3.114081	-0.522403	-1.105728
6	0	-4.330592	-0.564651	-0.424819
6	0	-1.992651	0.139012	0.952484
6	0	-3.221372	0.095032	1.616890
6	0	-4.390685	-0.253112	0.937041
1	0	-5.231894	-0.834936	-0.961714
1	0	-3.040813	-0.754535	-2.160773
1	0	-3.258187	0.331613	2.673622
1	0	-1.085102	0.403474	1.478866
1	0	-5.337046	-0.283591	1.462080

4a (B'): MP2 = -690.0835 a.u.

1	6	0	-0.030064	-1.649056	0.000000
2	6	0	-1.181832	-2.496049	0.000000
3	6	0	-0.231405	-0.235557	0.000000
4	6	0	-1.496549	0.303173	0.000000
5	6	0	-2.622997	-0.552008	0.000000
6	6	0	-2.478107	-1.915182	0.000000
7	1	0	-1.632879	1.376201	0.000000
8	1	0	-3.612579	-0.108964	0.000000
9	1	0	-3.346238	-2.564835	0.000000
10	6	0	1.261915	-2.232214	0.000000
11	6	0	1.411293	-3.599005	0.000000
12	6	0	0.277356	-4.441549	0.000000
13	6	0	-0.985919	-3.901392	0.000000
14	1	0	2.127527	-1.582989	0.000000
15	1	0	2.403994	-4.034871	0.000000
16	1	0	0.407972	-5.518000	0.000000
17	1	0	-1.858343	-4.546494	0.000000
18	8	0	0.923673	0.516352	0.000000
19	6	0	0.842292	1.902852	0.000000
20	6	0	0.843011	2.587331	1.211508
21	6	0	0.843011	3.980630	1.206199
22	6	0	0.843011	2.587331	-1.211508
23	6	0	0.843011	3.980630	-1.206199
24	6	0	0.841732	4.679216	0.000000
25	1	0	0.848401	4.519663	2.146759
26	1	0	0.850547	2.025958	2.138019
27	1	0	0.848401	4.519663	-2.146759
28	1	0	0.850547	2.025958	-2.138019
29	1	0	0.844715	5.763006	0.000000

4a (TS-B'B'): MP2 = -690.0831199 a.u.

6	0	1.623481	-0.258202	-0.024048
6	0	2.633463	0.755666	0.013972
6	0	0.260043	0.153619	-0.005241
6	0	-0.094903	1.488807	-0.028450
6	0	0.920252	2.474225	-0.015096
6	0	2.253740	2.123864	-0.019054
1	0	-1.136929	1.778798	-0.023357
1	0	0.633532	3.519165	-0.032674
1	0	3.024629	2.886327	-0.004739
6	0	1.996188	-1.625938	0.008428
6	0	3.331978	-1.978786	0.007197
6	0	4.337806	-0.985239	0.020491
6	0	3.993816	0.351790	0.001330
1	0	1.221794	-2.381686	-0.003644
1	0	3.611850	-3.025570	0.023137
1	0	5.381680	-1.275966	0.018283
1	0	4.764163	1.115800	0.012736
8	0	-0.653650	-0.881183	-0.004493
6	0	-1.998014	-0.540658	0.001192
6	0	-2.675035	-0.435086	-1.213969
6	0	-4.043956	-0.157339	-1.201355
6	0	-4.718157	0.008265	0.012290
6	0	-4.023444	-0.104840	1.220506
6	0	-2.654625	-0.382879	1.222100
1	0	-2.126817	-0.572506	-2.137712
1	0	-4.582730	-0.075414	-2.137510
1	0	-5.779983	0.220790	0.016680
1	0	-4.546452	0.017472	2.161191
1	0	-2.091344	-0.481352	2.141782

4a (B₀): MP2 = -690.0831199 a.u.

6	0	1.623481	-0.258202	-0.024048
6	0	2.633463	0.755666	0.013972
6	0	0.260043	0.153619	-0.005241
6	0	-0.094903	1.488807	-0.028450
6	0	0.920252	2.474225	-0.015096
6	0	2.253740	2.123864	-0.019054
1	0	-1.136929	1.778798	-0.023357
1	0	0.633532	3.519165	-0.032674
1	0	3.024629	2.886327	-0.004739
6	0	1.996188	-1.625938	0.008428

6	0	3.331978	-1.978786	0.007197
6	0	4.337806	-0.985239	0.020491
6	0	3.993816	0.351790	0.001330
1	0	1.221794	-2.381686	-0.003644
1	0	3.611850	-3.025570	0.023137
1	0	5.381680	-1.275966	0.018283
1	0	4.764163	1.115800	0.012736
8	0	-0.653650	-0.881183	-0.004493
6	0	-1.998014	-0.540658	0.001192
6	0	-2.675035	-0.435086	-1.213969
6	0	-4.043956	-0.157339	-1.201355
6	0	-4.718157	0.008265	0.012290
6	0	-4.023444	-0.104840	1.220506
6	0	-2.654625	-0.382879	1.222100
1	0	-2.126817	-0.572506	-2.137712
1	0	-4.582730	-0.075414	-2.137510
1	0	-5.779983	0.220790	0.016680
1	0	-4.546452	0.017472	2.161191
1	0	-2.091344	-0.481352	2.141782

4a (A_o): MP2 = -690.0839115 a.u.

6	0	1.279207	-0.107026	-0.377768
6	0	2.537489	0.153068	0.257052
6	0	0.394313	0.988623	-0.568390
6	0	0.756394	2.282049	-0.255838
6	0	2.014797	2.529316	0.338428
6	0	2.895767	1.491243	0.569501
1	0	0.051784	3.082811	-0.443877
1	0	2.296224	3.546265	0.583944
1	0	3.858697	1.682182	1.030764
6	0	0.915155	-1.438662	-0.702599
6	0	1.802081	-2.471766	-0.471762
6	0	3.055147	-2.222286	0.136160
6	0	3.424843	-0.934564	0.468999
1	0	-0.040776	-1.623230	-1.176531
1	0	1.525821	-3.486664	-0.732191
1	0	3.739734	-3.043709	0.311237
1	0	4.386976	-0.742138	0.931989
8	0	-0.818459	0.764441	-1.199658
6	0	-1.866524	0.310044	-0.419253
6	0	-3.067443	0.083161	-1.097982
6	0	-4.174288	-0.380206	-0.388484
6	0	-4.084093	-0.621820	0.986393
6	0	-2.876464	-0.391506	1.647481
6	0	-1.754727	0.072335	0.953253
1	0	-3.111293	0.278278	-2.162208
1	0	-5.106727	-0.554330	-0.911907
1	0	-4.945483	-0.981976	1.534531
1	0	-2.796793	-0.576247	2.712183
1	0	-0.820411	0.251211	1.468179

4b' (B'): MP2 = -745.2844940 a.u.

6	0	-2.034134	-0.252988	-0.000017
6	0	-3.032124	0.773577	-0.000027
6	0	-2.423553	-1.616567	-0.000022
6	0	-4.397297	0.385888	-0.000041
6	0	-3.763671	-1.952694	-0.000036
6	0	-4.757586	-0.946996	-0.000046
6	0	-0.665411	0.142184	-0.000003
6	0	-2.635900	2.137468	-0.000022
6	0	-0.294507	1.473352	0.000001
6	0	-1.297892	2.470735	-0.000009
1	0	-1.657728	-2.381139	-0.000015
1	0	-5.158525	1.159178	-0.000048
1	0	-4.056587	-2.996082	-0.000040
1	0	-5.804949	-1.225080	-0.000057
1	0	-3.397747	2.909189	-0.000029
1	0	0.751368	1.749377	0.000012
1	0	-0.998270	3.512272	-0.000005
8	0	0.235378	-0.903046	0.000006
6	0	1.584373	-0.575490	0.000016
6	0	2.262244	-0.456841	1.213105

6	0	2.262264	-0.456851	-1.213062
6	0	3.630430	-0.188550	1.209130
6	0	3.630449	-0.188559	-1.209068
6	0	4.335648	-0.072770	0.000037
1	0	1.712503	-0.562284	2.140331
1	0	1.712538	-0.562302	-2.140296
1	0	4.163141	-0.093264	2.149179
1	0	4.163176	-0.093280	-2.149108
7	0	5.699039	0.264761	0.000044
1	0	6.187386	-0.047445	0.827659
1	0	6.187404	-0.047478	-0.827549

4b' (B₀): MP2 = -745.2844941 a.u.

6	0	-0.143152	-2.044802	0.000000
6	0	-1.342570	-2.826605	0.000000
6	0	1.120010	-2.689330	0.000000
6	0	-1.224820	-4.240865	0.000000
6	0	1.191983	-4.069082	0.000000
6	0	0.013826	-4.850902	0.000000
6	0	-0.267563	-0.625617	0.000000
6	0	-2.604729	-2.175338	0.000000
6	0	-1.502482	-0.005493	0.000000
6	0	-2.674302	-0.798206	0.000000
1	0	2.017657	-2.084940	0.000000
1	0	-2.130138	-4.839066	0.000000
1	0	2.159508	-4.557298	0.000000
1	0	0.085174	-5.932201	0.000000
1	0	-3.508626	-2.774449	0.000000
1	0	-1.572096	1.073950	0.000000
1	0	-3.638720	-0.303766	0.000000
8	0	0.931466	0.057212	0.000000
6	0	0.869608	1.444026	0.000000
6	0	0.883611	2.132068	1.213084
6	0	0.883611	2.132068	-1.213084
6	0	0.883611	3.526311	1.209099
6	0	0.883611	3.526311	-1.209099
6	0	0.905684	4.240620	0.000000
1	0	0.881308	1.572318	2.140314
1	0	0.881308	1.572318	-2.140314
1	0	0.892605	4.067409	2.149144
1	0	0.892605	4.067409	-2.149144
7	0	0.836818	5.643480	0.000000
1	0	1.237173	6.062632	0.827604
1	0	1.237173	6.062632	-0.827604

4c (B₁): MP2 = -729.2690181 a.u.

6	0	2.007658	-0.258393	-0.069338
6	0	3.049749	0.720497	0.019480
6	0	2.322115	-1.636259	0.049881
6	0	4.368926	0.276576	0.297062
6	0	3.621041	-2.028621	0.308605
6	0	4.654370	-1.068964	0.415756
6	0	0.688622	0.192757	-0.354113
6	0	2.725096	2.098413	-0.086783
6	0	0.390508	1.537461	-0.468980
6	0	1.427745	2.489960	-0.347099
1	0	1.525213	-2.364027	-0.030270
1	0	5.160433	1.014012	0.380577
1	0	3.855297	-3.082001	0.407779
1	0	5.668667	-1.391180	0.619679
1	0	3.516179	2.835153	-0.000929
1	0	-0.622194	1.851561	-0.686178
1	0	1.186343	3.542382	-0.439230
8	0	-0.250865	-0.804034	-0.523813
6	0	-1.575740	-0.498590	-0.258407
6	0	-1.962213	0.014659	0.982635
6	0	-2.519542	-0.797848	-1.239095
6	0	-3.317704	0.230050	1.229664
6	0	-3.872540	-0.582077	-0.967559
6	0	-4.292684	-0.059772	0.262762
1	0	-1.210299	0.236269	1.730048
1	0	-2.184112	-1.193736	-2.189504

1	0	-3.622907	0.629430	2.191146
1	0	-4.609479	-0.811565	-1.729763
6	0	-5.756088	0.137421	0.561616
1	0	-6.179815	-0.740159	1.053389
1	0	-5.909911	0.991919	1.220347
1	0	-6.322410	0.310583	-0.353100

4c (A_g): MP2 = -729.2692708 a.u.

6	0	1.662024	0.108442	0.365638
6	0	2.875242	-0.002470	-0.389108
6	0	0.875467	-1.063603	0.532366
6	0	1.298595	-2.296091	0.080936
6	0	2.514642	-2.397647	-0.632375
6	0	3.297561	-1.279853	-0.843703
1	0	0.670605	-3.161051	0.255642
1	0	2.843948	-3.367075	-0.986596
1	0	4.227630	-1.358717	-1.396181
6	0	1.235604	1.377880	0.832591
6	0	2.024908	2.491179	0.620930
6	0	3.234640	2.388253	-0.105688
6	0	3.662805	1.163554	-0.577355
1	0	0.313794	1.449801	1.396115
1	0	1.702249	3.457732	0.989524
1	0	3.842489	3.271183	-0.263898
1	0	4.592045	1.083305	-1.131605
8	0	-0.289949	-0.984737	1.276725
6	0	-1.429117	-0.544682	0.625495
6	0	-2.580099	-0.453819	1.412978
6	0	-3.768937	-0.013498	0.835296
6	0	-3.830666	0.354758	-0.517267
6	0	-2.660734	0.253952	-1.279039
6	0	-1.454913	-0.183500	-0.723448
1	0	-2.524020	-0.734059	2.457628
1	0	-4.660412	0.056737	1.449746
1	0	-2.681074	0.536126	-2.326575
1	0	-0.560846	-0.249284	-1.329085
6	0	-5.130073	0.792810	-1.141085
1	0	-5.716922	-0.063810	-1.478125
1	0	-5.738647	1.349690	-0.428554
1	0	-4.952934	1.433325	-2.004808

4c (B_g): MP2 = -729.2686899 a.u.

6	0	0.134770	-2.054236	0.000000
6	0	1.332128	-2.839103	0.000000
6	0	-1.130163	-2.695146	0.000000
6	0	1.210695	-4.253011	0.000000
6	0	-1.205708	-4.074708	0.000000
6	0	-0.029636	-4.859614	0.000000
6	0	0.263539	-0.635591	0.000000
6	0	2.596073	-2.191192	0.000000
6	0	1.499885	-0.018458	0.000000
6	0	2.669639	-0.814357	0.000000
1	0	-2.026378	-2.088629	0.000000
1	0	2.114379	-4.853619	0.000000
1	0	-2.174501	-4.560327	0.000000
1	0	-0.103924	-5.940687	0.000000
1	0	3.498305	-2.792760	0.000000
1	0	1.573284	1.060709	0.000000
1	0	3.635407	-0.322630	0.000000
8	0	-0.933932	0.050643	0.000000
6	0	-0.870993	1.436193	0.000000
6	0	-0.871884	2.120042	1.215479
6	0	-0.871884	2.120042	-1.215479
6	0	-0.871884	3.515931	1.204928
6	0	-0.871884	3.515931	-1.204928
6	0	-0.867970	4.233622	0.000000
1	0	-0.873774	1.556498	2.140458
1	0	-0.873774	1.556498	-2.140458
1	0	-0.871492	4.054669	2.146475
1	0	-0.871492	4.054669	-2.146475
6	0	-0.911486	5.739626	0.000000
1	0	-1.940622	6.103315	0.000000

1	0	-0.416685	6.145658	0.881904
1	0	-0.416685	6.145658	-0.881904

4f (B'): MP2 = -1149.1037083 a.u.

6	0	2.330118	-0.255461	0.116185
6	0	3.390742	0.677624	-0.125976
6	0	1.074504	0.260093	0.535970
6	0	0.842975	1.617586	0.648878
6	0	1.891455	2.523911	0.374850
6	0	3.133438	2.069548	-0.022157
1	0	-0.126365	1.973888	0.974860
1	0	1.704844	3.587463	0.464350
1	0	3.936249	2.770208	-0.223584
6	0	2.573298	-1.648018	-0.001251
6	0	3.816523	-2.099764	-0.398402
6	0	4.866076	-1.186458	-0.654459
6	0	4.650388	0.172394	-0.541580
1	0	1.764536	-2.339605	0.196208
1	0	3.996835	-3.163886	-0.494835
1	0	5.835908	-1.556120	-0.965637
1	0	5.454494	0.873401	-0.739267
8	0	0.112794	-0.680288	0.860538
6	0	-1.192610	-0.427528	0.488656
6	0	-1.515150	0.095026	-0.767766
6	0	-2.856061	0.254394	-1.116105
6	0	-2.190515	-0.799345	1.390329
6	0	-3.531369	-0.646266	1.036160
6	0	-3.856486	-0.115987	-0.213728
1	0	-3.124539	0.654553	-2.085283
1	0	-0.728703	0.369572	-1.459062
1	0	-4.316514	-0.928451	1.725438
1	0	-1.905832	-1.203613	2.353370
17	0	-5.526895	0.085553	-0.654617

4f (A₀): MP2 = 1149.1043637 a.u.

6	0	2.000250	0.113322	0.357549
6	0	3.178759	0.088970	-0.457734
6	0	1.268011	-1.096438	0.496049
6	0	1.712978	-2.287130	-0.038173
6	0	2.896548	-2.303549	-0.810716
6	0	3.625700	-1.145857	-0.998373
1	0	1.126743	-3.184122	0.119269
1	0	3.244373	-3.239615	-1.230588
1	0	4.530340	-1.159332	-1.596535
6	0	1.550371	1.339312	0.910646
6	0	2.286361	2.492415	0.721004
6	0	3.461848	2.474538	-0.066252
6	0	3.912058	1.293431	-0.621218
1	0	0.656737	1.346542	1.522141
1	0	1.946695	3.425223	1.155228
1	0	4.027613	3.387886	-0.206337
1	0	4.815495	1.278438	-1.221656
8	0	0.133819	-1.101795	1.294783
6	0	-1.046358	-0.677691	0.718576
6	0	-2.165404	-0.683360	1.556711
6	0	-3.399857	-0.267592	1.063695
6	0	-3.504956	0.157225	-0.263517
6	0	-2.387703	0.163718	-1.098028
6	0	-1.146779	-0.251371	-0.608593
1	0	-2.053192	-1.018081	2.580279
1	0	-4.273419	-0.269921	1.702609
1	0	-2.481843	0.495528	-2.124040
1	0	-0.278987	-0.248087	-1.254250
17	0	-5.046004	0.678838	-0.880832

4j (B'): MP2 = -894.2173413 a.u.

6	0	-2.673582	-0.243359	0.000033
6	0	-3.657127	0.797048	-0.000186
6	0	-1.302758	0.138589	-0.000116
6	0	-0.910818	1.462732	-0.000450
6	0	-1.901107	2.473725	-0.000659
6	0	-3.242545	2.155723	-0.000529

1	0	0.137770	1.728895	-0.000561
1	0	-1.588221	3.511036	-0.000922
1	0	-3.994331	2.937042	-0.000691
6	0	-3.079947	-1.601809	0.000381
6	0	-4.424625	-1.919166	0.000510
6	0	-5.404607	-0.900000	0.000297
6	0	-5.027326	0.428151	-0.000042
1	0	-2.326017	-2.378149	0.000545
1	0	-4.731687	-2.958309	0.000777
1	0	-6.455360	-1.164312	0.000402
1	0	-5.778064	1.211343	-0.000205
8	0	-0.411002	-0.922433	0.000095
6	0	0.934056	-0.619681	0.000077
6	0	1.607970	-0.510879	1.219243
6	0	2.981844	-0.275083	1.225565
6	0	1.608124	-0.511809	-1.219082
6	0	2.982005	-0.276041	-1.225412
6	0	3.640008	-0.165280	0.000075
1	0	3.539884	-0.186146	2.146729
1	0	1.049459	-0.610692	2.141329
1	0	3.540162	-0.187828	-2.146576
1	0	1.049725	-0.612301	-2.141162
7	0	5.088026	0.083941	0.000056
8	0	5.652954	0.182893	1.093657
8	0	5.653437	0.180123	-1.093538

4j (A_o): MP2 = -894.2488580 a.u.

6	0	2.237461	0.108271	0.361747
6	0	3.405550	0.149273	-0.467865
6	0	1.535839	-1.123335	0.443311
6	0	1.987236	-2.275417	-0.164056
6	0	3.160981	-2.226350	-0.950262
6	0	3.863975	-1.045158	-1.084594
1	0	1.421957	-3.191590	-0.043061
1	0	3.518371	-3.130078	-1.428652
1	0	4.760291	-1.008842	-1.694152
6	0	1.772307	1.292774	0.988089
6	0	2.483718	2.468586	0.849952
6	0	3.647093	2.515715	0.046088
6	0	4.111689	1.375671	-0.578750
1	0	0.888799	1.250375	1.612897
1	0	2.133649	3.369829	1.338936
1	0	4.192247	3.446656	-0.053258
1	0	5.005943	1.411144	-1.191763
8	0	0.412732	-1.192117	1.259044
6	0	-0.780900	-0.768424	0.734439
6	0	-1.880572	-0.841544	1.599387
6	0	-3.134171	-0.430803	1.160468
6	0	-3.257285	0.057855	-0.142119
6	0	-2.172246	0.136383	-1.013446
6	0	-0.916655	-0.276002	-0.569568
1	0	-1.731877	-1.227319	2.600084
1	0	-4.001743	-0.477625	1.803195
1	0	-2.314054	0.520261	-2.013914
1	0	-0.059980	-0.223959	-1.227825
7	0	-4.573724	0.492909	-0.612702
8	0	-4.662626	0.914279	-1.772070
8	0	-5.522812	0.416064	0.176712

4j (B_o): MP2 = -894.2173413 a.u.

6	0	-0.210935	-2.676332	0.000000
6	0	-1.402283	-3.470371	0.000000
6	0	-0.356277	-1.260734	0.000000
6	0	-1.595377	-0.651139	0.000000
6	0	-2.758868	-1.456786	0.000000
6	0	-2.671602	-2.832636	0.000000
1	0	-1.680928	0.427313	0.000000
1	0	-3.728572	-0.973476	0.000000
1	0	-3.568494	-3.441919	0.000000
6	0	1.059547	-3.305930	0.000000
6	0	1.145632	-4.684865	0.000000
6	0	-0.024178	-5.478973	0.000000

6	0	-1.269699	-4.883153	0.000000
1	0	1.951894	-2.693694	0.000000
1	0	2.118124	-5.162742	0.000000
1	0	0.059181	-6.559248	0.000000
1	0	-2.168261	-5.491087	0.000000
8	0	0.839916	-0.560650	0.000000
6	0	0.768311	0.816197	0.000000
6	0	0.775057	1.498804	1.219165
6	0	0.774430	2.892767	1.225490
6	0	0.775057	1.498804	-1.219165
6	0	0.774430	2.892767	-1.225490
6	0	0.776519	3.560017	0.000000
1	0	0.781145	3.457811	2.146655
1	0	0.779685	0.931457	2.141247
1	0	0.781145	3.457811	-2.146655
1	0	0.779685	0.931457	-2.141247
7	0	0.775231	5.029318	0.000000
8	0	0.774430	5.602854	1.093596
8	0	0.774430	5.602854	-1.093596