Supporting Information:

Structures and Dynamic Stereochemistry of 9-Arylselanyltriptycenes: X-ray Crystallographic, Spectroscopic and Theoretical Investigations

Takashi Nakamoto,[a] Satoko Hayashi,[a] Waro Nakanishi,*[a] Mao Minoura[b] and Gaku Yamamoto[b]

[a] *Department of Material Science and Chemistry, Faculty of Systems Engineering, Wakayama University, 930 Sakaedani, Wakayama 640-8510, JAPAN*
Fax: +81-73-457-8253
E-mail: nakanisi@sys.wakayama-u.ac.jp

[b] *Department of Chemistry, School of Science, Kitasato University, Kitasato, Sagamihara, Kanagawa 228-8555, JAPAN*

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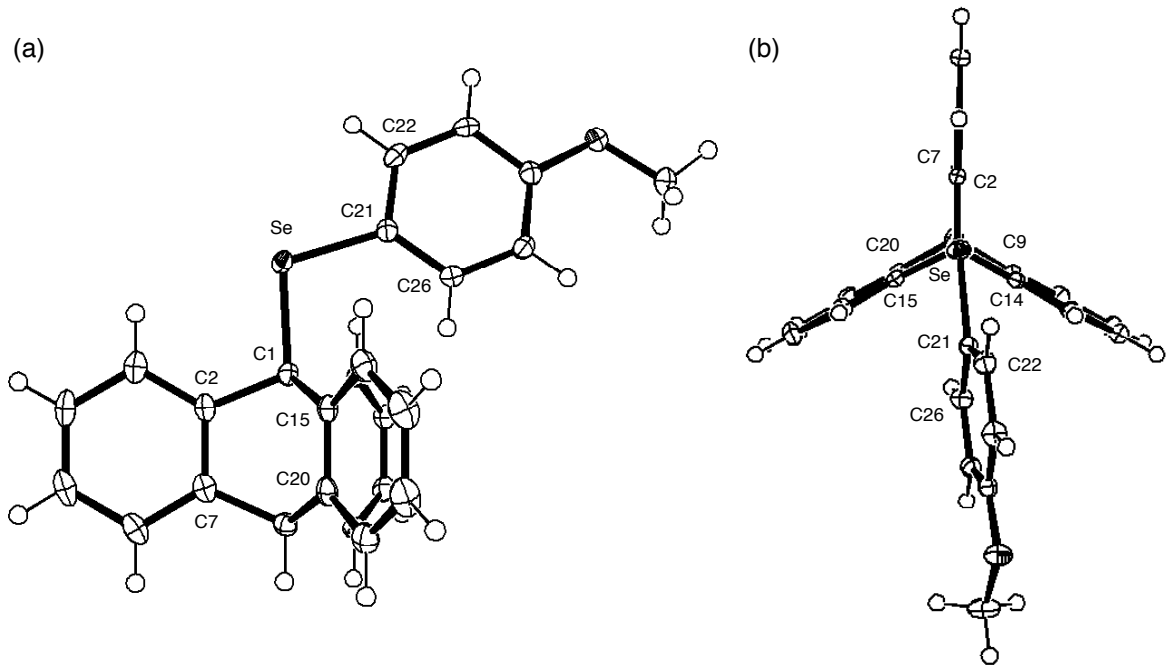

Fig. S1 ORTEP drawing of **1c** with atomic numbering scheme for selected atoms (50% probability thermal level): (a) side view and (b) top view.

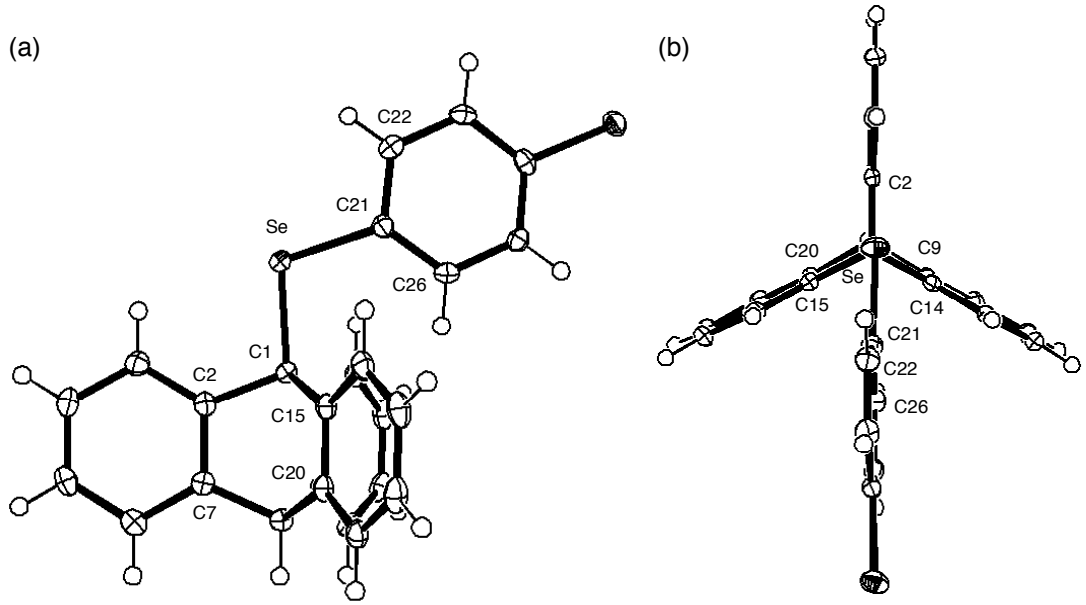

Fig. S2 ORTEP drawing of **1d** with atomic numbering scheme for selected atoms (50% probability thermal level): (a) side view and (b) top view.

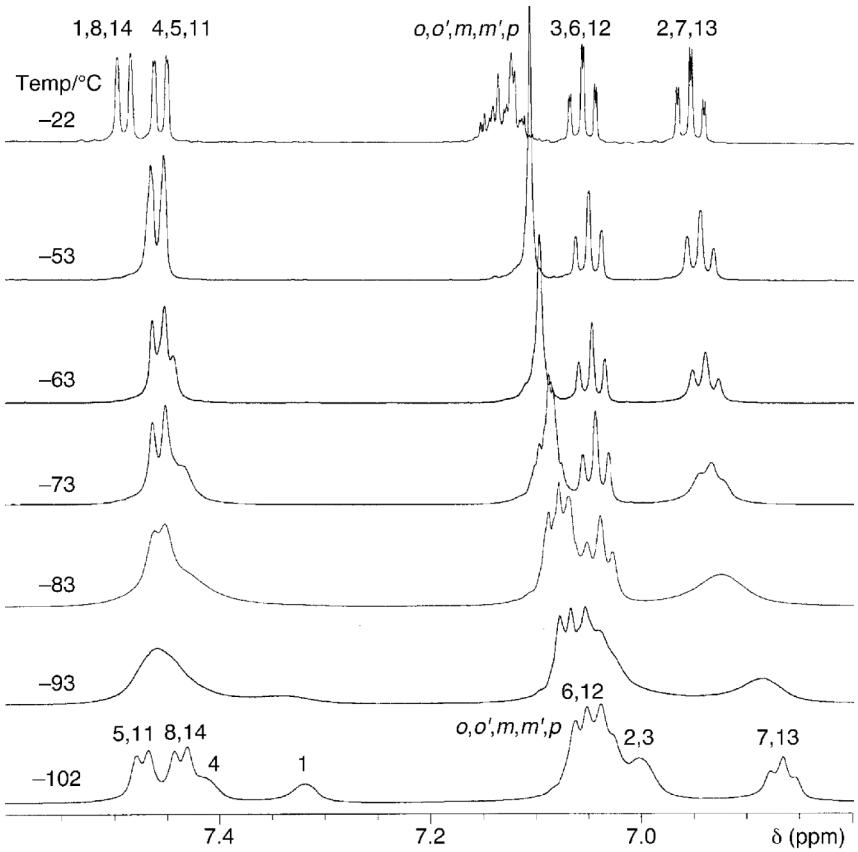

Fig. S3 NMR spectra (600 MHz) due to the aromatic protons of **1a** in CD_2Cl_2 at various temperatures.

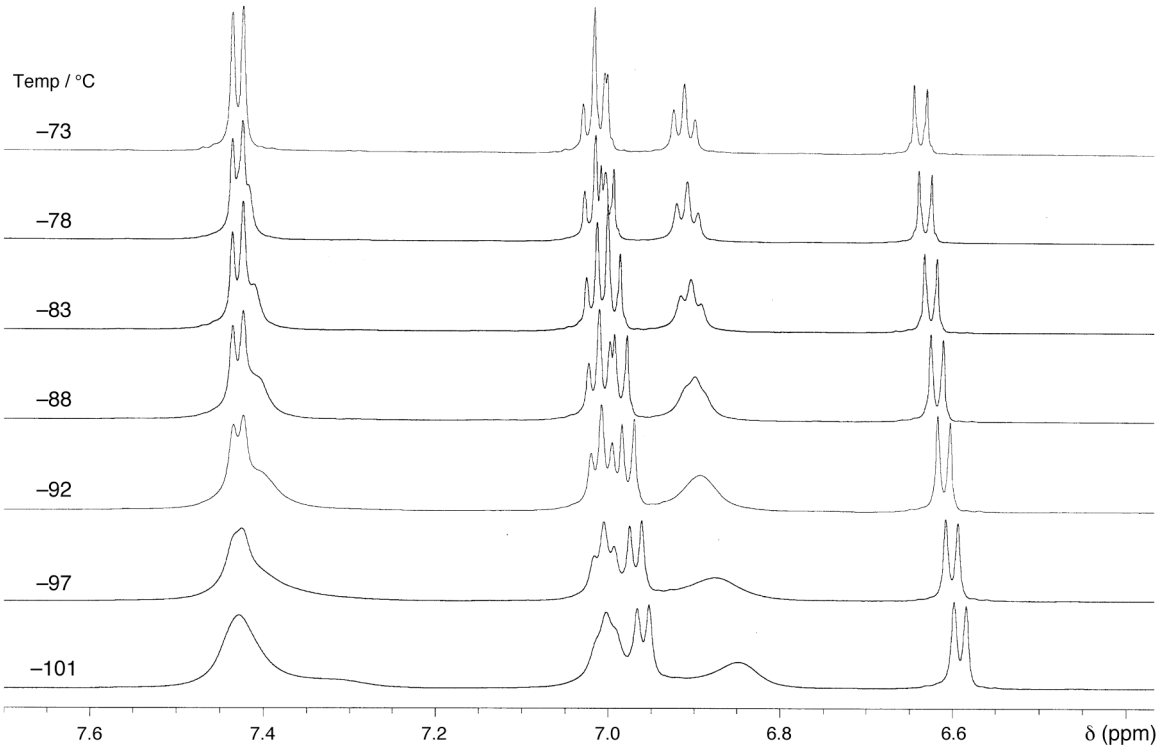

Fig. S4 NMR spectra (600 MHz) due to the aromatic protons of **1c** in CD_2Cl_2 at various temperatures.

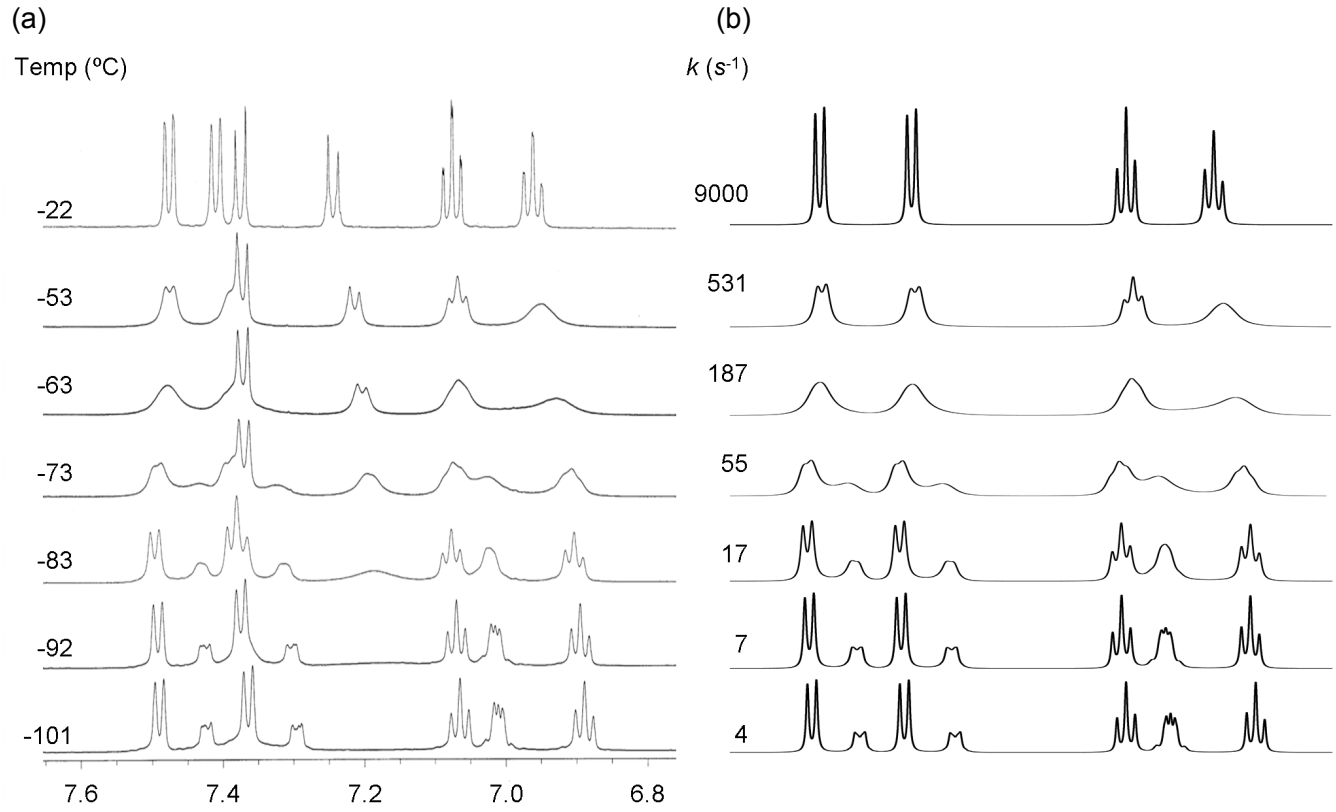

Fig. S5 The observed ^{1}H NMR spectra (600 MHz) due to the aromatic protons region of **1e** in CD_2Cl_2 at various temperatures (a) and the calculated spectra with the best-fit rate constants for the inter-conversion (b).

Table S1 shows the results of QC calculations on **1a** employing the 6-311+G(d) basis sets for Se and the 4-31G(d) basis sets for C and H (basis sets-A) at the MP2 level. **1a** (**A**: **pd**) and **1a** (**B**: **pd**) are optimized to be less stable than **1a** (**A**: **pl**) by 19.4 and 30.2 kJ mol^{-1}, respectively, on the potential energy surface. Frequency analysis is applied on the optimized structures of **1a** with the same method. Whereas all frequencies are positive for **1a** (**A**: **pl**), only one imaginary frequency is predicted for each of **1a** (**A**: **pd**) and **1a** (**B**: **pd**). The sum of electronic and thermal Gibbs free energies at 298.15 K for **1a** (**A**: **pd**) and **1a** (**B**: **pd**) relative to **1a** (**A**: **pl**) amount to 27.0 and 37.0 kJ mol^{-1}, respectively. The evaluated energy difference for **1a** (**B**: **pd**) on the potential energy surface (30.2 kJ mol^{-1}) is about 6 kJ mol^{-1} smaller than the observed activation energy for GR (36.4 kJ mol^{-1}). However, the calculated activation energy (37.0 kJ mol^{-1}) is very close to the observed value for GR if the sum of electronic and thermal Gibbs free energy at 298.15 K is considered.

Table S1 Results of QC calculations with and without the frequency analysis on **1a** (**A**: **pl**), **1a** (**A**: **pd**), and **1a** (**B**: **pd**) at the MP2 level.[a]

Compd	**1a** (**A**: **pl**)	**1a** (**A**: **pd**)	**1a** (**B**: **pd**)
Symmetry	C_s	C_s	C_s
E^b/au	–3396.0128	–3396.0054	–3396.0013
ΔE^b/kJ mol^{-1}	0.0[c]	19.4	30.2
$\nu_1{}^d$ (character)/cm^{-1}	8.5 (A")	–41.2 (A")	–34.4 (A")
$\nu_2{}^e$ (character)/cm^{-1}	48.6 (A')	33.6 (A')	44.4 (A')
ZPC[f]/au	0.3533	0.3537	0.3534
TCF[g]/au	0.3031	0.3060	0.3057
$E_F{}^h$/au	–3395.7097	–3395.6994	–3395.6956
$\Delta E_F{}^h$/kJ mol^{-1}	0.0[c]	27.0	37.0
Meaning	minimum	TS for IR	TS for GR

[a] The 6-311+G(d) basis sets being employed for Se and the 4-31G basis sets for C and H (basis sets-A). [b] Values on the energy potential surface. [c] Taken as the standard. [d] Lowest frequency obtained by the frequency analysis. [e] Second-lowest frequency obtained by the frequency analysis. [f] Zero-point correction. [g] Thermal correction to Gibbs free energy at 298.15 K. [h] Sum of electronic and thermal Gibbs free energies at 298.15 K.

Table S2 Results of QC calculations on **1a**, **1b'**, **1e** and **1f** at the MP2 level.[a,b]

Compd	E(**A**: **pl**)	ΔE(**A**: **pd**)[c]	ΔE(**B**: **pd**)[c]	$\Delta\Delta E$[d]
	au (kJ mol^{-1})	kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}
1a	–3398.4101 (0.0)[e]	25.1	34.0	8.9
1b'	–3453.6003 (0.0)[e]	20.4[f]	29.0	8.6
1e	–3490.4203 (0.0)[e]	29.6	39.1	9.5
1f	–3602.4129 (0.0)[e]	30.0	39.9	9.9

[a] The 6-311+G(d) basis sets being employed for Se and the 6-31G(d) basis sets for H, C, N and O (basis sets-B). [b] The C_s symmetry being assumed. [c] $\Delta E = E$(**A** or **B**: **pd**) – ΔE(**A**: **pl**). [d] $\Delta\Delta E = \Delta E$(**B**: **pd**) – ΔE(**A**: **pd**). [e] Taken as the standard. [f] The C_1 symmetry being assumed.

Optimized structures given by Cartesian coordinates for **1a**, **1b**', **1e** and **1f**, together with the total energies and the method for the calculations.

The 6-311+G(d) basis sets being employed for Se and the 6-31G(d) basis sets for C and H at the MP2 level.

1a (**A**: **pl**)

Total energy: -3398.4100806 hartrees

6	0	0.393830	-0.413937	0.000000
6	0	1.066958	-1.791925	0.000000
6	0	2.854369	-3.414596	0.000000
6	0	2.432996	-2.078218	0.000000
6	0	0.129146	-2.842537	0.000000
6	0	1.922314	-4.455267	0.000000
6	0	0.551708	-4.169643	0.000000
1	0	3.918531	-3.639442	0.000000
1	0	3.176635	-1.284563	0.000000
1	0	2.261585	-5.488649	0.000000
1	0	-0.180865	-4.975536	0.000000
6	0	-0.513039	-0.423964	1.234660
6	0	-1.372460	0.259103	3.384253
6	0	-0.465413	0.437770	2.332521
6	0	-1.445546	-1.477363	1.211875
6	0	-2.313875	-0.773884	3.348097
6	0	-2.348414	-1.652144	2.259207
1	0	-1.339725	0.932729	4.237719
1	0	0.267411	1.239131	2.372769
1	0	-3.013643	-0.901329	4.171092
1	0	-3.064055	-2.472761	2.232202
6	0	-0.513039	-0.423964	-1.234660
6	0	-1.372460	0.259103	-3.384253
6	0	-0.465413	0.437770	-2.332521
6	0	-1.445546	-1.477363	-1.211875
6	0	-2.313875	-0.773884	-3.348097
6	0	-2.348414	-1.652144	-2.259207
1	0	-1.339725	0.932729	-4.237719
1	0	0.267411	1.239131	-2.372769
1	0	-3.013643	-0.901329	-4.171092
1	0	-3.064055	-2.472761	-2.232202
6	0	-1.313453	-2.373362	0.000000
1	0	-2.031487	-3.202647	0.000000
34	0	1.758545	0.999225	0.000000
6	0	0.701623	2.607529	0.000000
6	0	-0.699200	2.652325	0.000000
6	0	-1.345883	3.892697	0.000000
6	0	-0.614752	5.082380	0.000000
6	0	0.782607	5.030974	0.000000
6	0	1.441641	3.800846	0.000000
1	0	-1.287737	1.741674	0.000000
1	0	-2.433540	3.920502	0.000000
1	0	-1.127704	6.041071	0.000000
1	0	1.365143	5.949686	0.000000
1	0	2.530477	3.770877	0.000000

1a (**A**: **pd**)
Total energy: -3398.4005081 hartrees

6	0	0.415064	0.000000	0.321209
6	0	1.740164	0.000000	1.104015
6	0	3.226278	0.000000	3.010579
6	0	1.925949	0.000000	2.488402
6	0	2.862852	0.000000	0.252039
6	0	4.335803	0.000000	2.162314
6	0	4.153926	0.000000	0.774611
1	0	3.367596	0.000000	4.089067
1	0	1.081967	0.000000	3.173275
1	0	5.340272	0.000000	2.579514
1	0	5.012277	0.000000	0.104208
6	0	0.506616	-1.230613	-0.585492
6	0	-0.083050	-3.391056	-1.499997
6	0	-0.335263	-2.341158	-0.608303
6	0	1.632384	-1.206802	-1.431099
6	0	1.014611	-3.343702	-2.362649
6	0	1.884905	-2.248990	-2.320568
1	0	-0.748818	-4.251344	-1.515181
1	0	-1.168098	-2.402039	0.077377
1	0	1.201750	-4.162429	-3.053876
1	0	2.761503	-2.213204	-2.965993
6	0	0.506616	1.230613	-0.585492
6	0	-0.083050	3.391056	-1.499997
6	0	-0.335263	2.341158	-0.608303
6	0	1.632384	1.206802	-1.431099
6	0	1.014611	3.343702	-2.362649
6	0	1.884905	2.248990	-2.320568
1	0	-0.748818	4.251344	-1.515181
1	0	-1.168098	2.402039	0.077377
1	0	1.201750	4.162429	-3.053876
1	0	2.761503	2.213204	-2.965993
6	0	2.515814	0.000000	-1.223943
1	0	3.402124	0.000000	-1.870251
34	0	-1.080214	0.000000	1.647553
6	0	-2.747314	0.000000	0.658990
6	0	-3.415690	1.209356	0.406383
6	0	-4.679386	1.206655	-0.189681
6	0	-5.309521	0.000000	-0.502771
6	0	-3.415690	-1.209356	0.406383
6	0	-4.679386	-1.206655	-0.189681
1	0	-2.968020	2.154014	0.697129
1	0	-5.178577	2.152213	-0.389310
1	0	-6.292050	0.000000	-0.968690
1	0	-2.968020	-2.154014	0.697129
1	0	-5.178577	-2.152213	-0.389310

1a (**B**: **pd**)
Total energy: -3398.3971336 hartrees

6	0	-0.313295	-0.399054	0.000000
6	0	1.202874	-0.136629	0.000000
6	0	3.302064	1.073806	0.000000
6	0	1.900745	1.074338	0.000000

6	0	1.939607	-1.342217	0.000000
6	0	4.021502	-0.121676	0.000000
6	0	3.332511	-1.338392	0.000000
1	0	3.829006	2.025651	0.000000
1	0	1.383024	2.020947	0.000000
1	0	5.109146	-0.108475	0.000000
1	0	3.875344	-2.282677	0.000000
6	0	-0.565290	-1.294951	1.230002
6	0	-1.503044	-1.994148	3.348633
6	0	-1.412542	-1.052677	2.314884
6	0	0.194392	-2.479913	1.206377
6	0	-0.752526	-3.171470	3.312958
6	0	0.106010	-3.414483	2.235637
1	0	-2.166625	-1.799479	4.188421
1	0	-2.000639	-0.141733	2.362885
1	0	-0.831365	-3.894767	4.121556
1	0	0.705025	-4.323384	2.197914
6	0	-0.565290	-1.294951	-1.230002
6	0	-1.503044	-1.994148	-3.348633
6	0	-1.412542	-1.052677	-2.314884
6	0	0.194392	-2.479913	-1.206377
6	0	-0.752526	-3.171470	-3.312958
6	0	0.106010	-3.414483	-2.235637
1	0	-2.166625	-1.799479	-4.188421
1	0	-2.000639	-0.141733	-2.362885
1	0	-0.831365	-3.894767	-4.121556
1	0	0.705025	-4.323384	-2.197914
6	0	1.094010	-2.595415	0.000000
1	0	1.695642	-3.512706	0.000000
34	0	-1.642206	1.109062	0.000000
6	0	-0.712648	2.788025	0.000000
6	0	0.206174	4.671145	-1.211142
6	0	-0.421612	3.423091	-1.216989
6	0	0.522453	5.295078	0.000000
6	0	0.206174	4.671145	1.211142
6	0	-0.421612	3.423091	1.216989
1	0	0.441813	5.159521	-2.154132
1	0	-0.661839	2.928277	-2.154884
1	0	1.012431	6.265972	0.000000
1	0	0.441813	5.159521	2.154132
1	0	-0.661839	2.928277	2.154884

1b' (**A**: **pl**)

Total energy: -3453.6003225 hartrees

6	0	0.679940	-0.361982	-0.181122
6	0	2.088974	-0.965463	-0.229768
6	0	3.811370	-2.609011	-0.630892
6	0	2.459784	-2.240335	-0.660097
6	0	3.071129	-0.066026	0.228377
6	0	4.783914	-1.714893	-0.176500
6	0	4.413433	-0.436341	0.257432
1	0	4.101838	-3.602266	-0.965782
1	0	1.718286	-2.955171	-1.009376
1	0	5.829823	-2.012849	-0.157705
1	0	5.165479	0.265477	0.615313

6	0	0.779717	0.920864	-1.014770
6	0	0.296063	2.465818	-2.806887
6	0	0.054119	1.245832	-2.163158
6	0	1.763033	1.806269	-0.537035
6	0	1.259728	3.352473	-2.317170
6	0	2.001550	3.020795	-1.177851
1	0	-0.271529	2.720957	-3.699161
1	0	-0.693730	0.558535	-2.551111
1	0	1.438574	4.297219	-2.825888
1	0	2.766987	3.696909	-0.799289
6	0	0.486541	0.055387	1.279733
6	0	-0.478076	0.084427	3.492546
6	0	-0.479309	-0.401808	2.179307
6	0	1.473051	0.959947	1.715389
6	0	0.483462	1.007792	3.913116
6	0	1.471053	1.443107	3.022699
1	0	-1.234834	-0.265979	4.190978
1	0	-1.225491	-1.127135	1.869793
1	0	0.471570	1.378823	4.935625
1	0	2.241782	2.140647	3.348001
6	0	2.513902	1.276224	0.663395
1	0	3.289622	1.963835	1.022338
34	0	-0.635355	-1.658922	-0.856932
6	0	-2.306385	-0.802166	-0.436526
6	0	-2.469920	0.567188	-0.189060
6	0	-3.738824	1.077208	0.087895
6	0	-4.874492	0.253906	0.071461
6	0	-4.698922	-1.117507	-0.170632
6	0	-3.432602	-1.638696	-0.430152
1	0	-1.617398	1.237850	-0.175221
1	0	-3.849454	2.141336	0.293873
1	0	-5.562154	-1.781822	-0.163762
1	0	-3.321746	-2.709173	-0.597485
7	0	-6.138870	0.765834	0.409596
1	0	-6.906576	0.243350	-0.000604
1	0	-6.240279	1.753906	0.199627

1b' (**A**: **pd**)

Total energy: -3453.5925584 hartrees

6	0	0.332464	-0.683015	0.000000
6	0	1.042651	-2.048181	0.000000
6	0	2.868204	-3.633038	0.000000
6	0	2.415364	-2.306966	0.000000
6	0	0.133021	-3.124608	0.000000
6	0	1.962675	-4.696398	0.000000
6	0	0.586505	-4.441568	0.000000
1	0	3.937766	-3.831056	0.000000
1	0	3.143394	-1.500012	0.000000
1	0	2.326304	-5.721513	0.000000
1	0	-0.128266	-5.263387	0.000000
6	0	-0.579196	-0.726334	1.229562
6	0	-1.464779	-0.085033	3.387254
6	0	-0.560497	0.119099	2.337601
6	0	-1.482508	-1.806419	1.206774
6	0	-2.381965	-1.137733	3.342030

6	0	-2.384437	-2.011002	2.248824
1	0	-1.446599	0.582546	4.246161
1	0	0.164915	0.917853	2.395119
1	0	-3.081970	-1.287943	4.160986
1	0	-3.074392	-2.853102	2.214180
6	0	-0.579196	-0.726334	-1.229562
6	0	-1.464779	-0.085033	-3.387254
6	0	-0.560497	0.119099	-2.337601
6	0	-1.482508	-1.806419	-1.206774
6	0	-2.381965	-1.137733	-3.342030
6	0	-2.384437	-2.011002	-2.248824
1	0	-1.446599	0.582546	-4.246161
1	0	0.164915	0.917853	-2.395119
1	0	-3.081970	-1.287943	-4.160986
1	0	-3.074392	-2.853102	-2.214180
6	0	-1.322372	-2.699823	0.000000
1	0	-2.014839	-3.550633	0.000000
34	0	1.735337	0.741746	0.000000
6	0	0.836526	2.451212	0.000000
6	0	0.617977	3.141547	-1.203827
6	0	0.092549	4.431793	-1.204646
6	0	-0.208278	5.086267	0.000000
6	0	0.617977	3.141547	1.203827
6	0	0.092549	4.431793	1.204646
1	0	0.885712	2.688078	-2.152979
1	0	-0.072196	4.944385	-2.151436
1	0	0.885712	2.688078	2.152979
1	0	-0.072196	4.944385	2.151436
7	0	-0.682464	6.403215	0.000000
1	0	-1.202902	6.653406	-0.834179
1	0	-1.202902	6.653406	0.834179

1b' (**B**: **pd**)

Total energy: -3453.5892781 hartrees

6	0	-0.325827	-0.665599	0.000000
6	0	1.173036	-0.316249	0.000000
6	0	3.198870	1.013487	0.000000
6	0	1.799813	0.933389	0.000000
6	0	1.978467	-1.477118	0.000000
6	0	3.986248	-0.138446	0.000000
6	0	3.368855	-1.393014	0.000000
1	0	3.669483	1.994432	0.000000
1	0	1.228110	1.848480	0.000000
1	0	5.071373	-0.062397	0.000000
1	0	3.965360	-2.304412	0.000000
6	0	-0.524857	-1.575331	1.229465
6	0	-1.420698	-2.327875	3.348212
6	0	-1.384730	-1.382765	2.314436
6	0	0.302090	-2.714412	1.206228
6	0	-0.603261	-3.459784	3.312711
6	0	0.267990	-3.652615	2.235438
1	0	-2.094512	-2.171985	4.188007
1	0	-2.024224	-0.507120	2.361946
1	0	-0.640091	-4.186429	4.121369
1	0	0.918764	-4.525251	2.197798

6	0	-0.524857	-1.575331	-1.229465
6	0	-1.420698	-2.327875	-3.348212
6	0	-1.384730	-1.382765	-2.314436
6	0	0.302090	-2.714412	-1.206228
6	0	-0.603261	-3.459784	-3.312711
6	0	0.267990	-3.652615	-2.235438
1	0	-2.094512	-2.171985	-4.188007
1	0	-2.024224	-0.507120	-2.361946
1	0	-0.640091	-4.186429	-4.121369
1	0	0.918764	-4.525251	-2.197798
6	0	1.207003	-2.777348	0.000000
1	0	1.860884	-3.658223	0.000000
34	0	-1.739494	0.765786	0.000000
6	0	-0.905111	2.486743	0.000000
6	0	-0.071535	4.415156	-1.209003
6	0	-0.643028	3.144709	-1.211269
6	0	0.207218	5.075500	0.000000
6	0	-0.071535	4.415156	1.209003
6	0	-0.643028	3.144709	1.211269
1	0	0.140543	4.913273	-2.154214
1	0	-0.851755	2.644702	-2.154215
1	0	0.140543	4.913273	2.154214
1	0	-0.851755	2.644702	2.154215
7	0	0.843989	6.321738	0.000000
1	0	0.673563	6.872896	-0.834642
1	0	0.673563	6.872896	0.834642

1e (**A**: **pl**)

Total energy: -3490.4202495 hartrees

6	0	0.401925	-0.839073	0.000000
6	0	0.926626	-2.279620	0.000000
6	0	2.530998	-4.082686	0.000000
6	0	2.254537	-2.709000	0.000000
6	0	-0.118501	-3.223490	0.000000
6	0	1.493045	-5.017749	0.000000
6	0	0.160552	-4.587968	0.000000
1	0	3.564997	-4.419826	0.000000
1	0	3.079424	-1.999893	0.000000
1	0	1.720218	-6.081329	0.000000
1	0	-0.653409	-5.311455	0.000000
6	0	-0.499030	-0.750733	1.235875
6	0	-1.279673	0.018206	3.386916
6	0	-0.358043	0.098468	2.335690
6	0	-1.539421	-1.697756	1.211689
6	0	-2.328066	-0.905809	3.348108
6	0	-2.456438	-1.774427	2.258494
1	0	-1.173934	0.682313	4.241812
1	0	0.460354	0.812124	2.381682
1	0	-3.038234	-0.957297	4.170304
1	0	-3.256513	-2.512797	2.230590
6	0	-0.499030	-0.750733	-1.235875
6	0	-1.279673	0.018206	-3.386916
6	0	-0.358043	0.098468	-2.335690
6	0	-1.539421	-1.697756	-1.211689
6	0	-2.328066	-0.905809	-3.348108

6	0	-2.456438	-1.774427	-2.258494
1	0	-1.173934	0.682313	-4.241812
1	0	0.460354	0.812124	-2.381682
1	0	-3.038234	-0.957297	-4.170304
1	0	-3.256513	-2.512797	-2.230590
6	0	-1.503117	-2.602958	0.000000
1	0	-2.305412	-3.350853	0.000000
34	0	1.907445	0.423231	0.000000
6	0	1.018731	2.123021	0.000000
6	0	-0.372583	2.307131	0.000000
6	0	-0.901858	3.597755	0.000000
6	0	-0.049456	4.712527	0.000000
6	0	1.344011	4.529993	0.000000
6	0	1.870268	3.241688	0.000000
1	0	-1.048110	1.459278	0.000000
1	0	-1.979914	3.741795	0.000000
1	0	2.004617	5.393703	0.000000
1	0	2.950917	3.107354	0.000000
6	0	-0.599727	6.037476	0.000000
7	0	-1.053493	7.132146	0.000000

1e (**A**: **pd**)

Total energy: -3490.4089826 hartrees

6	0	0.343181	-0.839535	0.000000
6	0	0.971881	-2.242597	0.000000
6	0	2.696449	-3.934195	0.000000
6	0	2.325909	-2.582680	0.000000
6	0	-0.005188	-3.258914	0.000000
6	0	1.726304	-4.938921	0.000000
6	0	0.367828	-4.600736	0.000000
1	0	3.751515	-4.198351	0.000000
1	0	3.101732	-1.820804	0.000000
1	0	2.026022	-5.984401	0.000000
1	0	-0.395031	-5.377992	0.000000
6	0	-0.560956	-0.830474	1.235700
6	0	-1.367912	-0.172886	3.420046
6	0	-0.460499	-0.018861	2.364710
6	0	-1.537147	-1.844584	1.207433
6	0	-2.369223	-1.145030	3.360251
6	0	-2.444422	-1.997792	2.253690
1	0	-1.286231	0.469341	4.294293
1	0	0.343439	0.699220	2.444233
1	0	-3.073115	-1.255140	4.182029
1	0	-3.193031	-2.787756	2.213414
6	0	-0.560956	-0.830474	-1.235700
6	0	-1.367912	-0.172886	-3.420046
6	0	-0.460499	-0.018861	-2.364710
6	0	-1.537147	-1.844584	-1.207433
6	0	-2.369223	-1.145030	-3.360251
6	0	-2.444422	-1.997792	-2.253690
1	0	-1.286231	0.469341	-4.294293
1	0	0.343439	0.699220	-2.444233
1	0	-3.073115	-1.255140	-4.182029
1	0	-3.193031	-2.787756	-2.213414
6	0	-1.433543	-2.744383	0.000000

1	0	-2.176548	-3.551210	0.000000
34	0	1.811707	0.514901	0.000000
6	0	0.954666	2.253962	0.000000
6	0	0.748934	2.941064	-1.209019
6	0	0.243269	4.240194	-1.215250
6	0	-0.024611	4.889247	0.000000
6	0	0.748934	2.941064	1.209019
6	0	0.243269	4.240194	1.215250
1	0	1.002364	2.475315	-2.154720
1	0	0.075602	4.760073	-2.155430
1	0	1.002364	2.475315	2.154720
1	0	0.075602	4.760073	2.155430
6	0	-0.551352	6.224523	0.000000
7	0	-0.985348	7.327118	0.000000

1e (**B**: **pd**)

Total energy: -3490.4053554 hartrees

6	0	-0.319662	-0.825636	0.000000
6	0	1.168337	-0.436574	0.000000
6	0	3.160234	0.944701	0.000000
6	0	1.763882	0.827543	0.000000
6	0	2.002178	-1.577050	0.000000
6	0	3.975689	-0.187401	0.000000
6	0	3.389937	-1.457045	0.000000
1	0	3.606862	1.936706	0.000000
1	0	1.169965	1.728134	0.000000
1	0	5.058362	-0.084007	0.000000
1	0	4.009457	-2.352781	0.000000
6	0	-0.498804	-1.737507	1.230779
6	0	-1.376342	-2.512971	3.348444
6	0	-1.364051	-1.566807	2.315101
6	0	0.356812	-2.855190	1.206487
6	0	-0.530206	-3.623470	3.312642
6	0	0.345978	-3.793924	2.235655
1	0	-2.054372	-2.374757	4.187781
1	0	-2.027205	-0.709013	2.364294
1	0	-0.548822	-4.350984	4.120974
1	0	1.018366	-4.649879	2.197994
6	0	-0.498804	-1.737507	-1.230779
6	0	-1.376342	-2.512971	-3.348444
6	0	-1.364051	-1.566807	-2.315101
6	0	0.356812	-2.855190	-1.206487
6	0	-0.530206	-3.623470	-3.312642
6	0	0.345978	-3.793924	-2.235655
1	0	-2.054372	-2.374757	-4.187781
1	0	-2.027205	-0.709013	-2.364294
1	0	-0.548822	-4.350984	-4.120974
1	0	1.018366	-4.649879	-2.197994
6	0	1.262947	-2.895751	0.000000
1	0	1.938252	-3.760106	0.000000
34	0	-1.770818	0.565995	0.000000
6	0	-0.986633	2.316817	0.000000
6	0	-0.249059	4.277288	-1.220034
6	0	-0.756828	2.979202	-1.216874
6	0	0.008013	4.926250	0.000000

6	0	-0.249059	4.277288	1.220034
6	0	-0.756828	2.979202	1.216874
1	0	-0.056828	4.793646	-2.157556
1	0	-0.951146	2.466015	-2.155314
1	0	-0.056828	4.793646	2.157556
1	0	-0.951146	2.466015	2.155314
6	0	0.533937	6.262126	0.000000
7	0	0.968827	7.364405	0.000000

1f (**A**: **pl**)

Total energy: -3602.412882 hartrees

6	0	0.410229	-1.112686	0.000000
6	0	0.908586	-2.562441	0.000000
6	0	2.479505	-4.394658	0.000000
6	0	2.228402	-3.016118	0.000000
6	0	-0.153826	-3.486829	0.000000
6	0	1.424480	-5.310422	0.000000
6	0	0.100118	-4.856203	0.000000
1	0	3.507113	-4.750791	0.000000
1	0	3.066311	-2.322426	0.000000
1	0	1.632038	-6.378000	0.000000
1	0	-0.727018	-5.564585	0.000000
6	0	-0.488716	-1.007584	1.236022
6	0	-1.255129	-0.224563	3.387142
6	0	-0.331943	-0.161477	2.336113
6	0	-1.546533	-1.935098	1.211631
6	0	-2.320723	-1.128632	3.347902
6	0	-2.465011	-1.994676	2.258252
1	0	-1.137174	0.437362	4.242120
1	0	0.500032	0.536267	2.382931
1	0	-3.032018	-1.166734	4.169836
1	0	-3.278780	-2.717901	2.230074
6	0	-0.488716	-1.007584	-1.236022
6	0	-1.255129	-0.224563	-3.387142
6	0	-0.331943	-0.161477	-2.336113
6	0	-1.546533	-1.935098	-1.211631
6	0	-2.320723	-1.128632	-3.347902
6	0	-2.465011	-1.994676	-2.258252
1	0	-1.137174	0.437362	-4.242120
1	0	0.500032	0.536267	-2.382931
1	0	-3.032018	-1.166734	-4.169836
1	0	-3.278780	-2.717901	-2.230074
6	0	-1.526810	-2.840873	0.000000
1	0	-2.342763	-3.573835	0.000000
34	0	1.938340	0.122070	0.000000
6	0	1.080143	1.836051	0.000000
6	0	-0.308102	2.044804	0.000000
6	0	-0.818957	3.343590	0.000000
6	0	0.066543	4.418500	0.000000
6	0	1.449944	4.239914	0.000000
6	0	1.950323	2.940673	0.000000
1	0	-0.998308	1.209043	0.000000
1	0	-1.889137	3.523177	0.000000
1	0	2.109870	5.100960	0.000000
1	0	3.028416	2.788035	0.000000

7	0	-0.472084	5.783293	0.000000
8	0	-1.708258	5.916241	0.000000
8	0	0.341201	6.723951	0.000000

1f (**A**: **pd**)

Total energy: -3602.4014637 hartrees

6	0	0.349607	-1.120350	0.000000
6	0	0.945828	-2.537311	0.000000
6	0	2.630782	-4.268158	0.000000
6	0	2.291615	-2.908413	0.000000
6	0	-0.054782	-3.530562	0.000000
6	0	1.637561	-5.250080	0.000000
6	0	0.287215	-4.880612	0.000000
1	0	3.679429	-4.556738	0.000000
1	0	3.084745	-2.164507	0.000000
1	0	1.912983	-6.302221	0.000000
1	0	-0.493331	-5.640103	0.000000
6	0	-0.553357	-1.090908	1.236276
6	0	-1.341208	-0.418477	3.423201
6	0	-0.431127	-0.285080	2.367356
6	0	-1.553642	-2.081197	1.207517
6	0	-2.366920	-1.364754	3.361988
6	0	-2.463739	-2.213682	2.254172
1	0	-1.242448	0.219401	4.298856
1	0	0.392306	0.410382	2.449044
1	0	-3.072823	-1.458743	4.184037
1	0	-3.231280	-2.985237	2.213375
6	0	-0.553357	-1.090908	-1.236276
6	0	-1.341208	-0.418477	-3.423201
6	0	-0.431127	-0.285080	-2.367356
6	0	-1.553642	-2.081197	-1.207517
6	0	-2.366920	-1.364754	-3.361988
6	0	-2.463739	-2.213682	-2.254172
1	0	-1.242448	0.219401	-4.298856
1	0	0.392306	0.410382	-2.449044
1	0	-3.072823	-1.458743	-4.184037
1	0	-3.231280	-2.985237	-2.213375
6	0	-1.471031	-2.982971	0.000000
1	0	-2.232472	-3.772418	0.000000
34	0	1.846053	0.202418	0.000000
6	0	1.020565	1.956336	0.000000
6	0	0.826106	2.647557	-1.208885
6	0	0.342880	3.956078	-1.219345
6	0	0.096451	4.582324	0.000000
6	0	0.826106	2.647557	1.208885
6	0	0.342880	3.956078	1.219345
1	0	1.070100	2.177455	-2.154649
1	0	0.178530	4.491584	-2.148449
1	0	1.070100	2.177455	2.154649
1	0	0.178530	4.491584	2.148449
7	0	-0.417375	5.959776	0.000000
8	0	-0.618442	6.498124	1.102056
8	0	-0.618442	6.498124	-1.102056

1f (**B**: **pd**)

Total energy: -3602.3976815 hartrees

6	0	-0.323424	-1.108304	0.000000
6	0	1.157829	-0.694422	0.000000
6	0	3.126459	0.719898	0.000000
6	0	1.732265	0.579356	0.000000
6	0	2.010543	-1.820832	0.000000
6	0	3.960635	-0.398448	0.000000
6	0	3.396103	-1.677680	0.000000
1	0	3.556534	1.719182	0.000000
1	0	1.123128	1.469687	0.000000
1	0	5.041426	-0.277022	0.000000
1	0	4.030488	-2.562945	0.000000
6	0	-0.487465	-2.022956	1.230817
6	0	-1.351907	-2.812823	3.348500
6	0	-1.355447	-1.866624	2.315102
6	0	0.386740	-3.126149	1.206518
6	0	-0.487358	-3.909031	3.312715
6	0	0.391540	-4.064894	2.235713
1	0	-2.032083	-2.685842	4.187869
1	0	-2.032904	-1.020087	2.364447
1	0	-0.493817	-4.636721	4.121074
1	0	1.078144	-4.909487	2.198133
6	0	-0.487465	-2.022956	-1.230817
6	0	-1.351907	-2.812823	-3.348500
6	0	-1.355447	-1.866624	-2.315102
6	0	0.386740	-3.126149	-1.206518
6	0	-0.487358	-3.909031	-3.312715
6	0	0.391540	-4.064894	-2.235713
1	0	-2.032083	-2.685842	-4.187869
1	0	-2.032904	-1.020087	-2.364447
1	0	-0.493817	-4.636721	-4.121074
1	0	1.078144	-4.909487	-2.198133
6	0	1.293412	-3.151666	0.000000
1	0	1.983065	-4.004599	0.000000
34	0	-1.797439	0.258373	0.000000
6	0	-1.043829	2.022212	0.000000
6	0	-0.344973	3.998924	-1.223769
6	0	-0.826697	2.690029	-1.216520
6	0	-0.112369	4.626370	0.000000
6	0	-0.344973	3.998924	1.223769
6	0	-0.826697	2.690029	1.216520
1	0	-0.158268	4.531783	-2.150246
1	0	-1.010749	2.173682	-2.155151
1	0	-0.158268	4.531783	2.150246
1	0	-1.010749	2.173682	2.155151
7	0	0.399613	6.005647	0.000000
8	0	0.600087	6.544264	1.101971
8	0	0.600087	6.544264	-1.101971