Supporting Information

Cage Complexes of Carba- and Silylium Cations with an Aromatic Base. Is η^6 Coordination Type Realizable?

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Table S1. NBO charges on selected atoms of the cations **1a**(C_1) and **2a**(C_1)

Cation	q_E	q_{C^1}	q_{C^2}	q_{C^3}	q_{C^4}	q_{C^5}	q_{C^6}
1a(C_1)	0.027	–0.355	0.232	–0.350	0.297	–0.340	0.206
2a(C_1)	2.181	–0.502	0.075	–0.267	0.099	–0.267	0.054

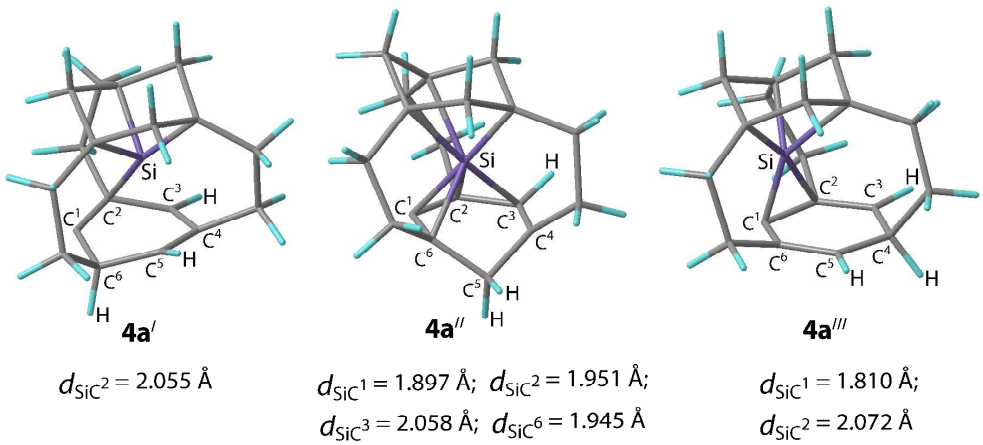

Figure S1. Optimized geometries of the unsymmetrical isomers **4a**$^{/}$, **4a**$^{//}$, and **4a**$^{///}$.

Table S2. MP2/6-311++G(d,p), MP2/6-31+G(d,p) [italic type], and B3LYP/6-31+G(d,p) [boldface type] selected geometrical parameters[a] and the relative stability[b] of the C_3 symmetrical (η^6) and C_1 unsymmetrical (η^1) forms of the cage cations **1**, **2a**, and **4a**.

Cation	d_{EAr}	d_{EC^1}	d_{EC^2}	$\sum\angle$(E)	α	$\sum\angle(C^1)$	A	ΔE	ΔG
1a(C_1)	-	1.673	-	330.5	90.0	346.8	0.876	0.00	0.00
	-	*1.663*	-	*330.4*	*90.7*	*345.6*	*0.870*	*0.00*	*0.00*
	-	**1.656**	-	**330.6**	**93.3**	**342.6**	**0.780**	**0.00**	**0.00**
1a(C_3)	2.609	2.971	2.953	356.1	-	-	0.999	9.69	9.58
	2.615	*2.976*	*2.958*	*355.8*	-	-	*0.999*	*10.01*	*9.74*
	2.722	**3.079**	**3.045**	**356.7**	-	-	**0.999**	**5.67**	**5.02**
1c(C_1)	-	1.935	-	337.2	83.2	354.9	0.952	1.99	1.96
	-	*1.907*	-	*336.8*	*84.1*	*353.7*	*0.945*	*2.48*	*2.79*
	-	**1.680**	-	**330.5**	**91.8**	**342.0**	**0.743**	**7.87**	**7.93**
1c(C_3)	2.620	2.966	2.972	356.7	-	-	0.999	0.00	0.00
	2.633	*2.975*	*2.985*	*356.7*	-	-	*1.000*	*0.00*	*0.00*
	2.738	**3.076**	**3.068**	**357.3**	-	-	**0.999**	**0.00**	**0.00**
2a(C_1)	-	2.209	-	345.1	77.5	359.3	0.987	0.00	0.00
	-	*2.202*	-	*344.7*	*77.6*	*359.1*	*0.988*	*0.00*	*0.00*
	-	**2.174**	-	**345.0**	**80.8**	**357.9**	**0.967**	**0.00**	**0.00**
2a(C_3)[c]	2.375	2.760	2.762	347.4	-	-	1.000	3.17	4.44
	2.383	*2.767*	*2.768*	*347.4*	-	-	*1.000*	*4.10*	*5.48*
	2.472	**2.847**	**2.841**	**348.9**	-	-	**0.999**	**4.79**	**6.05**
4a(C_3)	1.805	2.303	2.297	264.3	-	-	0.999	-	-
	1.805	*2.301*	*2.296*	*264.0*	-	-	*0.999*	-	-
	1.851	**2.338**	**2.330**	**265.5**	-	-	**1.000**	-	-

[a] The distance from the cationic center E to the central point of the benzene ring (d_{EAr}, Å) and to its carbon atoms C^1 (d_{EC^1}, Å) и C^2 (d_{EC^2}, Å); the sum of the bond angles at the central atom E ($\sum\angle$(E), deg); the angle between the EC^1 bond and the vector C^1C^4 (α, deg); the sum of the bond angles at the arene atom C^1 ($\sum\angle(C^1)$, deg); *A* is a Julg parameter. [b] The difference in internal energies of the η^1 and η^6 forms of cations **1** and **2** corrected for the zero-point vibrational energies (ΔE, kcal/mol) and in Gibbs free energies (ΔG, kcal/mol) calculated at the normal conditions (298.15 K, 1 Atm). [c] The structure has two imaginary frequencies.

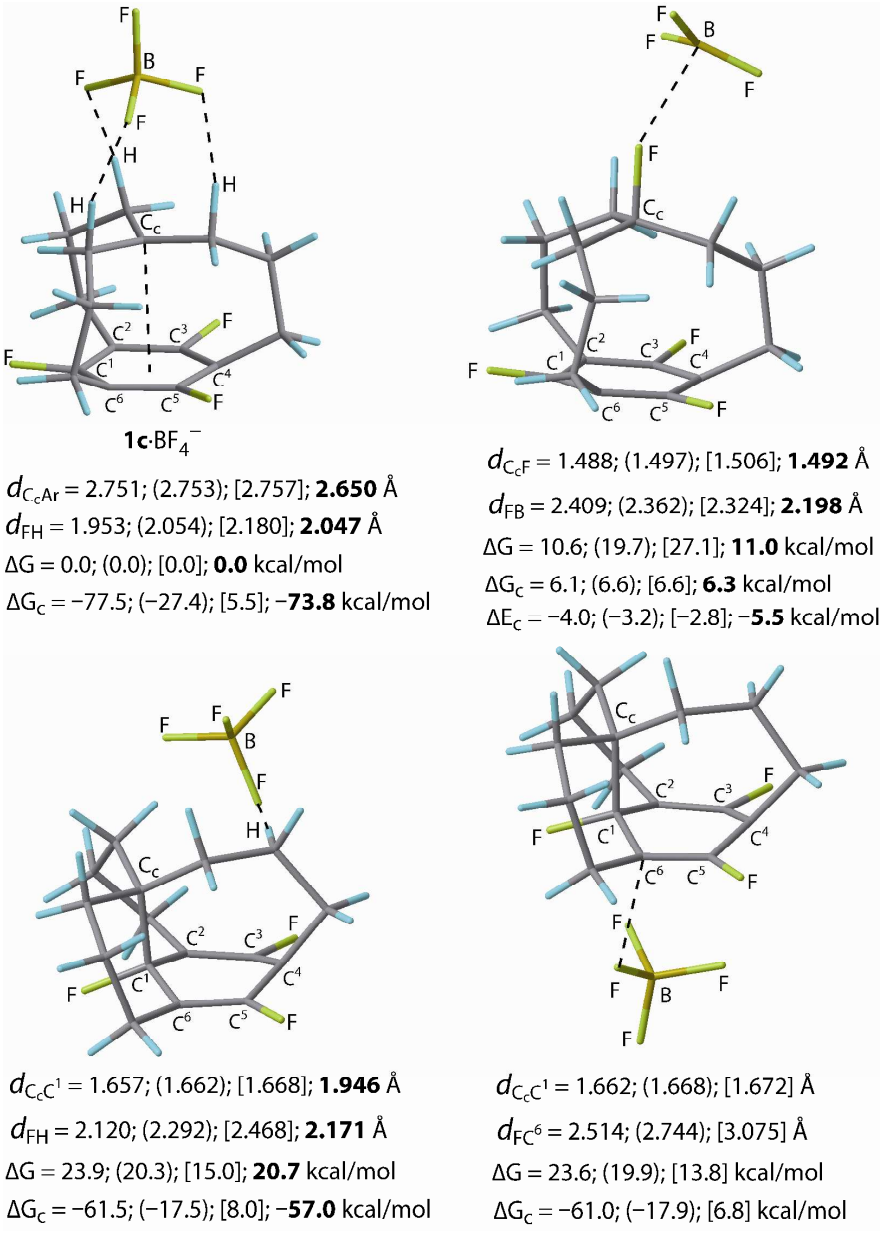

Figure S2. B3LYP/6-31+G(d,p) and MP2/6-31+G(d,p) [boldface type] optimized geometries of the possible structures of complexes **1c**·BF_4^- in the isolated state and in solvents (toluene [in parentheses], DMSO [in brackets]), as well as their relative stability (ΔG) and the complexation energy (ΔE_c, ΔG_c).

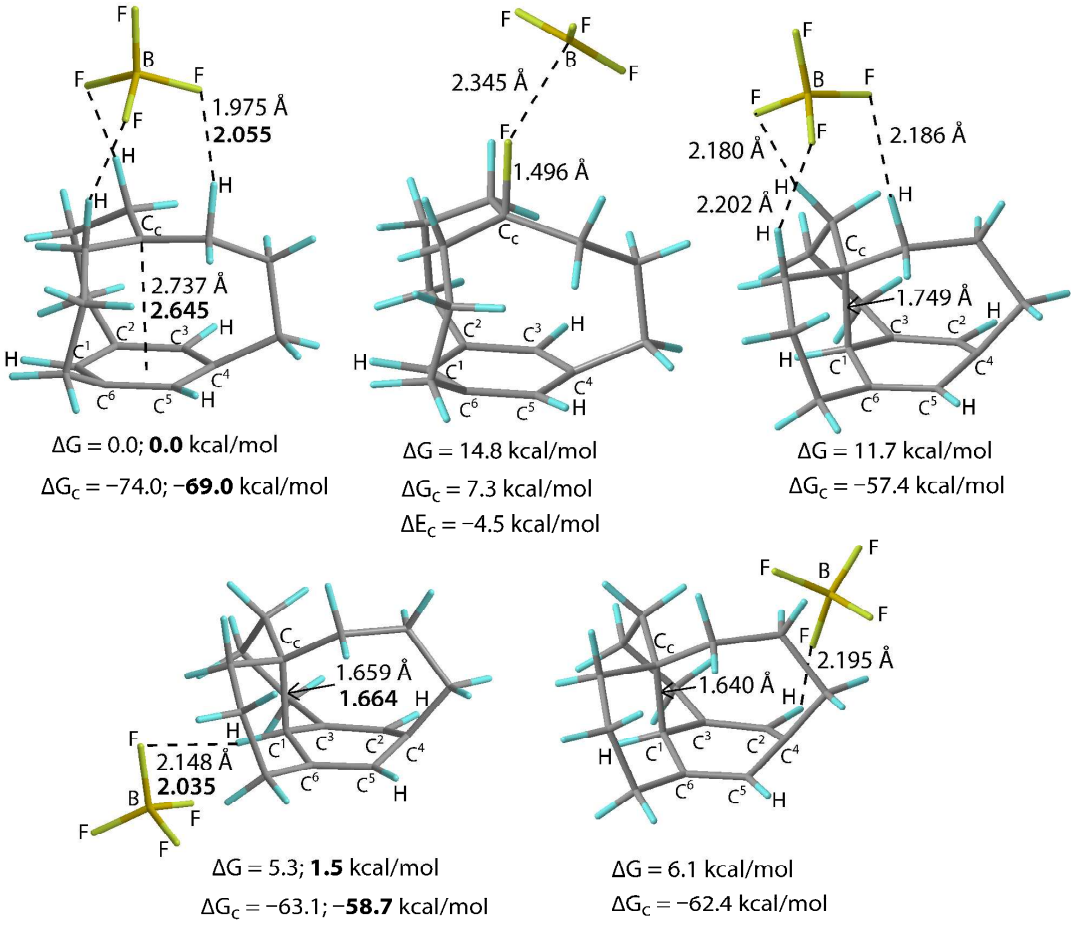

Figure S3. B3LYP/6-31+G(d,p) and MP2/6-31+G(d,p) [boldface type] optimized geometries of the possible structures of complexes **1a**·BF_4^-, as well as their relative stability (ΔG) and the complexation energy (ΔE_c, ΔG_c).

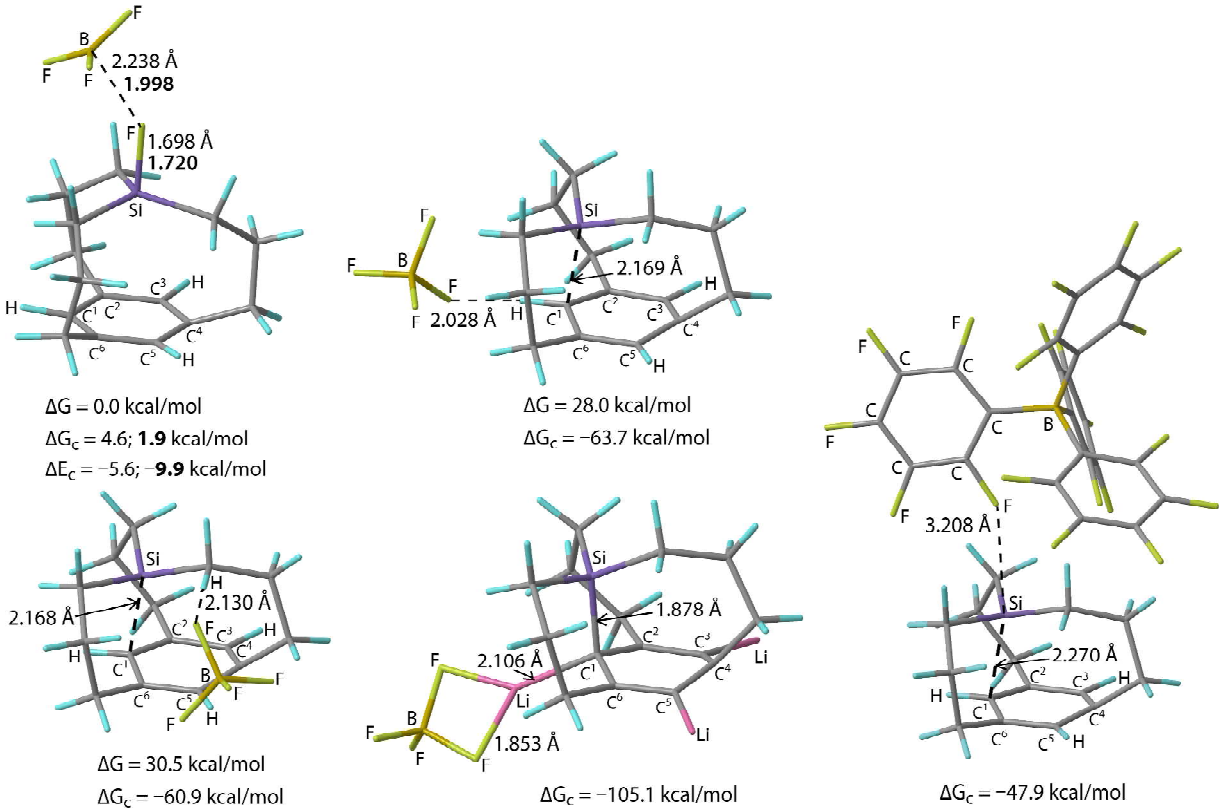

Figure S4. B3LYP/6-31+G(d,p) optimized geometries of the possible structures of complexes **2a**·BF_4^-, **2a**·$B(C_6F_5)_4^-$, and **2b**·BF_4^-, as well as their relative stability (ΔG) and the complexation energy (ΔE_c, ΔG_c).

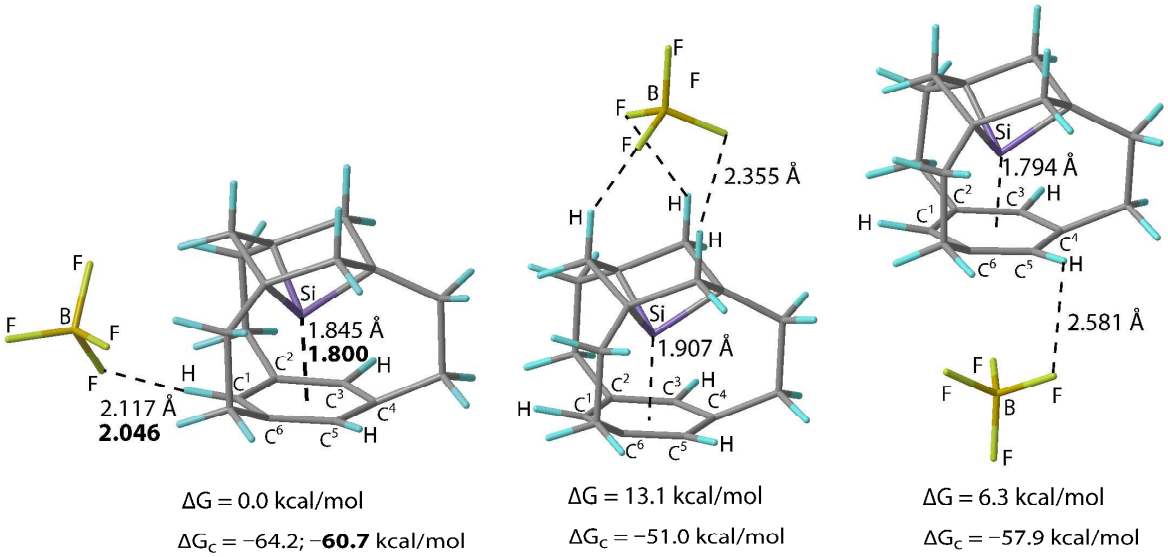

Figure S5. B3LYP/6-31+G(d,p) optimized geometries of the possible structures of the ionic pair **4a**·BF_4^-, as well as their relative stability (ΔG) and the complexation energy (ΔG_c).

Cartesian coordinates and total energies of the structures calculated at the MP2/6-311++G(d,p) theoretical levels.

Molecule 1a(C_1)

6	-0.297478	-0.739544	0.717761
6	-1.705952	-1.355091	0.871140
6	-2.838759	-0.484977	0.301091
6	-2.560485	0.049792	-1.138983
6	-1.133606	0.473204	-1.199095
6	-0.175995	-0.592546	-0.944573
6	-0.258232	0.579716	1.566931
6	0.935285	1.579264	1.630971
6	0.985069	2.722728	0.541253
6	0.689401	1.907916	-0.662551
6	-0.667341	1.761880	-1.038338
6	0.825374	-1.702933	1.175063
6	1.454662	-2.518588	0.037766
6	2.110657	-1.568757	-0.998108
6	1.253408	-0.348608	-1.118391
6	1.681001	0.951014	-1.007953
1	-1.890503	-1.516978	1.941611
1	-1.706005	-2.345270	0.396356
1	-3.769844	-1.059916	0.286895
1	-3.014410	0.372325	0.958126
1	-2.727201	-0.755203	-1.864459
1	-3.240626	0.874399	-1.371372
1	-0.498968	-1.563668	-1.323578
1	-0.353462	0.179701	2.586958
1	-1.172280	1.158855	1.398879
1	0.881694	2.074039	2.607293
1	1.888087	1.041871	1.587072
1	0.218646	3.477821	0.736239
1	1.978687	3.180119	0.546248
1	-1.350764	2.601854	-0.929601
1	0.412915	-2.372700	1.939583
1	1.622140	-1.122519	1.657370

1	2.210357	-3.200491	0.437902
1	0.696205	-3.144800	-0.444894
1	3.126864	-1.293590	-0.697551
1	2.173183	-2.069154	-1.974251
1	2.733228	1.196491	-0.878745

E = -620.2991846 a.u.

Molecule 1a(C_3)

6	0.000000	0.000000	1.316955
6	0.385705	1.428622	1.490449
6	-0.388632	2.585288	0.813001
6	0.000000	2.785142	-0.677787
6	0.005243	1.409859	-1.277683
6	-1.207468	0.699314	-1.306545
6	1.044371	-1.048341	1.490449
6	2.433241	-0.956079	0.813001
6	2.412003	-1.392571	-0.677787
6	1.218352	-0.709470	-1.277683
6	1.209358	0.696041	-1.306545
6	-1.430075	-0.380281	1.490449
6	-2.044609	-1.629209	0.813001
6	-2.412003	-1.392571	-0.677787
6	-1.223595	-0.700389	-1.277683
6	-0.001889	-1.395355	-1.306545
1	-1.465397	2.407818	0.887132
1	-0.177619	3.496366	1.383262
1	-0.728606	3.456778	-1.144147
1	0.989200	3.248886	-0.751640
1	2.817930	0.065162	0.887132
1	3.116751	-1.594361	1.383262
1	3.357961	-1.097398	-1.144147
1	2.319018	-2.481115	-0.751640
1	-1.352533	-2.472980	0.887132
1	-2.939132	-1.902005	1.383262
1	-2.629355	-2.359381	-1.144147

1	-3.308217	-0.767771	-0.751640
1	-2.146256	1.242585	-1.196967
1	2.149238	1.237420	-1.196967
1	-0.002982	-2.480005	-1.196967
1	0.194648	1.529435	2.581796
1	1.227206	-0.933288	2.581796
1	-1.421854	-0.596147	2.581796
1	1.463260	1.550299	1.358042
1	0.610968	-2.042370	1.358042
1	-2.074229	0.492071	1.358042

E = -620.2804472 a.u.

Molecule 1c(C_1)

6	-0.334022	-0.750663	1.002503
6	-1.757676	-1.302630	1.145192
6	-2.882011	-0.413320	0.598337
6	-2.670397	0.020816	-0.888899
6	-1.227549	0.345090	-1.048800
6	-0.310784	-0.745335	-0.932808
6	-0.207261	0.621654	1.720256
6	1.053880	1.543658	1.723074
6	1.124423	2.595839	0.567614
6	0.726821	1.728597	-0.591991
6	-0.645219	1.586237	-0.855805
6	0.773569	-1.724908	1.422310
6	1.301497	-2.691850	0.353816
6	1.909542	-1.895727	-0.835414
6	1.118098	-0.643079	-1.001666
6	1.588422	0.644051	-0.848764
1	-1.902195	-1.414233	2.230541
1	-1.809842	-2.311357	0.725125
1	-3.830916	-0.953327	0.670281
1	-2.985134	0.484907	1.213900
1	-2.940220	-0.801357	-1.557081
1	-3.295626	0.885626	-1.119942

9	-0.808666	-1.942649	-1.301581
1	-0.316114	0.280284	2.763210
1	-1.093355	1.235309	1.531956
1	1.050945	2.078579	2.678856
1	1.967996	0.941605	1.698830
1	0.411588	3.407286	0.722868
1	2.130460	3.009818	0.484549
9	-1.434586	2.644221	-0.664825
1	0.367167	-2.307805	2.260588
1	1.620990	-1.147453	1.809899
1	2.077194	-3.321715	0.797917
1	0.507869	-3.354483	0.004241
1	2.955654	-1.641521	-0.647440
1	1.860508	-2.499721	-1.749059
9	2.893810	0.844982	-0.666145

E = -917.5057255 a.u.

Molecule 1c(C_3)

6	0.000000	0.000000	1.516953
6	0.427886	1.417789	1.672922
6	-0.347889	2.590568	1.025245
6	0.000000	2.796764	-0.475648
6	0.005726	1.427588	-1.089697
6	-1.180105	0.685099	-1.116657
6	1.013898	-1.079454	1.672922
6	2.417442	-0.994003	1.025245
6	2.422069	-1.398382	-0.475648
6	1.233465	-0.718753	-1.089697
6	1.183365	0.679451	-1.116657
6	-1.441784	-0.338334	1.672922
6	-2.069553	-1.596565	1.025245
6	-2.422069	-1.398382	-0.475648
6	-1.239190	-0.708836	-1.089697
6	-0.003261	-1.364550	-1.116657
1	-1.425063	2.443312	1.135517

1	-0.094828	3.495899	1.586133
1	-0.747820	3.451850	-0.929362
1	0.978831	3.268000	-0.582177
1	2.828501	0.012485	1.135517
1	3.074951	-1.665826	1.586133
1	3.363300	-1.078294	-0.929362
1	2.340756	-2.481693	-0.582177
1	-1.403439	-2.455797	1.135517
1	-2.980123	-1.830073	1.586133
1	-2.615480	-2.373556	-0.929362
1	-3.319587	-0.786307	-0.582177
9	-2.332486	1.366771	-0.957598
9	2.349901	1.336606	-0.957598
9	-0.017416	-2.703377	-0.957598
1	0.285925	1.520671	2.772155
1	1.173977	-1.007954	2.772155
1	-1.459902	-0.512717	2.772155
1	1.502962	1.517392	1.505219
1	0.562619	-2.060299	1.505219
1	-2.065581	0.542907	1.505219

E = -917.5066888 a.u.

Molecule 2a(C_1)

14	0.177145	-0.589363	0.941375
6	-0.904936	-2.119536	1.085163
6	-2.238683	-1.974179	0.322983
6	-2.057858	-1.656131	-1.187579
6	-1.108467	-0.503284	-1.325549
6	0.285801	-0.774481	-1.256861
6	-0.715295	0.910906	1.684462
6	-0.387515	2.400278	1.402334
6	-0.919586	2.934046	0.035013
6	-0.561676	1.835812	-0.918964
6	-1.512135	0.829961	-1.164705
6	2.012437	-0.727390	1.328830

6	2.856006	-1.137657	0.103815
6	2.711871	-0.129834	-1.063409
6	1.267958	0.258290	-1.223862
6	0.812477	1.570060	-1.078463
1	-1.112551	-2.301958	2.149016
1	-0.348566	-2.994782	0.723700
1	-2.821300	-2.896320	0.416223
1	-2.838071	-1.175899	0.776732
1	-1.659655	-2.535097	-1.706247
1	-3.029975	-1.413524	-1.627896
1	0.616135	-1.804639	-1.389632
1	-0.512878	0.731012	2.756566
1	-1.794035	0.741661	1.568372
1	-0.817092	3.006282	2.207498
1	0.698263	2.548934	1.432261
1	-2.002935	3.085041	0.078092
1	-0.438726	3.889172	-0.198066
1	-2.571250	1.059954	-1.056170
1	2.156506	-1.449819	2.142734
1	2.356242	0.247430	1.702269
1	3.911959	-1.209845	0.381227
1	2.556288	-2.137287	-0.231635
1	3.305469	0.768045	-0.861195
1	3.092502	-0.579998	-1.987841
1	1.531246	2.371560	-0.914516

E = -871.3882929 a.u.

Molecule 2a(C_3)

14	0.000000	0.000000	1.099109
6	0.600623	1.732319	1.488585
6	0.000000	2.889231	0.666297
6	0.400955	2.825068	-0.832161
6	0.205806	1.404083	-1.269987
6	-1.097291	0.865641	-1.280767
6	1.199921	-1.386314	1.488585

6	2.502147	-1.444615	0.666297
6	2.246103	-1.759771	-0.832161
6	1.113068	-0.880275	-1.269987
6	1.298313	0.517461	-1.280767
6	-1.800544	-0.346005	1.488585
6	-2.502147	-1.444615	0.666297
6	-2.647058	-1.065297	-0.832161
6	-1.318874	-0.523808	-1.269987
6	-0.201022	-1.383103	-1.280767
1	-1.093774	2.865959	0.743941
1	0.328896	3.844441	1.087641
1	-0.220017	3.519072	-1.407681
1	1.448268	3.120167	-0.955181
1	3.028880	-0.485744	0.743941
1	3.164935	-2.207053	1.087641
1	3.157614	-1.568996	-1.407681
1	1.978010	-2.814321	-0.955181
1	-1.935106	-2.380216	0.743941
1	-3.493831	-1.637388	1.087641
1	-2.937597	-1.950076	-1.407681
1	-3.426278	-0.305847	-0.955181
1	-1.951005	1.537744	-1.201807
1	2.307228	0.920748	-1.201807
1	-0.356223	-2.458492	-1.201807
1	0.352749	1.879146	2.553240
1	1.451013	-1.245062	2.553240
1	-1.803762	-0.634083	2.553240
1	1.696839	1.741700	1.418875
1	0.659936	-2.340356	1.418875
1	-2.356776	0.598656	1.418875

E = -871.3818156 a.u.

Molecule 2b(C_1)

14	0.014699	-0.911789	0.797090
6	1.747561	-1.561309	1.225129

6	2.553174	-1.797490	-0.069541
6	2.616466	-0.545580	-0.977337
6	1.283392	0.184250	-1.083457
6	1.210760	1.590397	-0.940070
6	-1.497363	-2.045267	0.966340
6	-2.694629	-1.413444	0.212355
6	-2.365661	-0.942345	-1.227433
6	-1.163318	-0.016772	-1.247962
6	0.115060	-0.659193	-1.084459
6	-0.436970	0.642156	1.831073
6	0.262778	2.024058	1.763613
6	-0.190369	2.922191	0.574439
6	-0.117989	2.020017	-0.632020
6	-1.327552	1.373864	-1.020475
1	3.575516	-2.122135	0.158532
1	2.115873	-2.654330	-0.615047
1	3.367538	0.137425	-0.559062
1	2.976242	-0.840827	-1.975369
1	-3.537268	-2.115887	0.181695
1	-3.036937	-0.534547	0.773046
1	-2.198336	-1.827157	-1.865004
1	-3.244810	-0.428984	-1.641255
1	0.081370	2.562991	2.703716
1	1.346474	1.880007	1.673636
1	-1.217225	3.272417	0.759260
1	0.470651	3.801333	0.522462
3	2.753952	2.907608	-1.008738
3	0.291292	-2.549880	-1.823841
3	-3.038361	2.462460	-1.105927
1	1.723167	-2.476076	1.830440
1	2.264185	-0.801541	1.827925
1	-1.779855	-2.213110	2.014002
1	-1.276396	-3.041915	0.550614
1	-0.309642	0.263594	2.861001
1	-1.519027	0.790041	1.714491

E = -892.0001894 a.u.

Molecule 2b(C_3)

14	0.000000	0.000000	0.916823
6	0.316486	1.759236	1.561755
6	-0.380355	2.876380	0.772930
6	0.000000	2.842064	-0.732933
6	0.011788	1.392929	-1.154917
6	-1.267566	0.746476	-1.154671
6	1.365300	-1.153703	1.561755
6	2.681195	-1.108793	0.772930
6	2.461299	-1.421032	-0.732933
6	1.200418	-0.706673	-1.154917
6	1.280250	0.724506	-1.154671
6	-1.681786	-0.605533	1.561755
6	-2.300840	-1.767587	0.772930
6	-2.461299	-1.421032	-0.732933
6	-1.212206	-0.686256	-1.154917
6	-0.012684	-1.470982	-1.154671
1	-1.465681	2.733356	0.857536
1	-0.151171	3.860678	1.198448
1	-0.717310	3.441415	-1.310994
1	0.991659	3.298999	-0.866192
1	3.099996	-0.097361	0.857536
1	3.419030	-1.799421	1.198448
1	3.339008	-1.099498	-1.310994
1	2.361188	-2.508302	-0.866192
1	-1.634315	-2.635995	0.857536
1	-3.267860	-2.061257	1.198448
1	-2.621698	-2.341916	-1.310994
1	-3.352847	-0.790698	-0.866192
3	-3.035276	1.726363	-1.359194
3	3.012712	1.765444	-1.359194
3	0.022564	-3.491808	-1.359194
1	-0.007972	1.785543	2.613189
1	1.550311	-0.885867	2.613189

1	-1.542339	-0.899676	2.613189
1	1.404835	1.914663	1.554104
1	0.955730	-2.173955	1.554104
1	-2.360565	0.259291	1.554104

E = -891.9723998 a.u.

Molecule 2c(C_1)

14	0.327632	-0.427179	1.228662
6	-0.287738	-2.189864	1.395356
6	-1.638319	-2.464703	0.700593
6	-1.599749	-2.267359	-0.840772
6	-0.930119	-0.955282	-1.119456
6	0.475588	-0.885407	-1.158886
6	-0.929783	0.842287	1.827538
6	-0.930199	2.334060	1.407635
6	-1.518681	2.588354	-0.011195
6	-0.918419	1.506092	-0.864513
6	-1.580057	0.279545	-0.991580
6	2.135571	-0.062309	1.548750
6	3.072185	-0.481933	0.396919
6	2.727285	0.252662	-0.924783
6	1.235446	0.305682	-1.088875
6	0.476518	1.479739	-0.988416
9	1.153205	-2.032722	-1.307113
9	-2.902686	0.252618	-0.793799
9	1.135776	2.630060	-0.814016
1	-0.397570	-2.367273	2.477078
1	0.481926	-2.889567	1.047278
1	-1.947244	-3.494193	0.906886
1	-2.412671	-1.812202	1.119782
1	-1.041153	-3.078409	-1.314057
1	-2.617345	-2.271444	-1.238035
1	-0.724157	0.801171	2.914531
1	-1.934625	0.415571	1.712062
1	-1.523766	2.895402	2.136317

1	0.088189	2.734216	1.451073
1	-2.606984	2.505848	-0.000539
1	-1.249266	3.589239	-0.355025
1	2.425632	-0.585215	2.471356
1	2.238700	1.014096	1.744185
1	4.108068	-0.254422	0.664152
1	3.011167	-1.563262	0.243043
1	3.116847	1.273070	-0.906154
1	3.183571	-0.271130	-1.770751

E = -1168.6024335 a.u.

Molecule 2c(C_3)

14	0.000000	0.000000	1.352701
6	-0.428071	1.792406	1.669192
6	0.349905	2.862147	0.872895
6	0.000000	2.863750	-0.640042
6	-0.005537	1.434514	-1.095486
6	-1.188059	0.680952	-1.109695
6	1.766304	-0.525483	1.669192
6	2.303740	-1.734101	0.872895
6	2.480080	-1.431875	-0.640042
6	1.245094	-0.712462	-1.095486
6	1.183751	0.688413	-1.109695
6	-1.338233	-1.266923	1.669192
6	-2.653645	-1.128047	0.872895
6	-2.480080	-1.431875	-0.640042
6	-1.239557	-0.722052	-1.095486
6	0.004307	-1.369365	-1.109695
1	0.121258	3.849076	1.286421
1	1.427493	2.707008	0.993376
1	-0.983192	3.309601	-0.804614
1	0.740573	3.451506	-1.188335
1	3.272769	-2.029551	1.286421
1	1.630591	-2.589750	0.993376
1	3.357794	-0.803331	-0.804614

1	2.618805	-2.367108	-1.188335
1	-3.394027	-1.819526	1.286421
1	-3.058085	-0.117259	0.993376
1	-2.374603	-2.506269	-0.804614
1	-3.359378	-1.084398	-1.188335
9	-2.351605	1.338166	-1.008339
9	2.334688	1.367467	-1.008339
9	0.016917	-2.705633	-1.008339
1	-0.217827	1.925869	2.744851
1	-1.510671	1.929992	1.549569
1	1.776765	-0.774291	2.744851
1	2.426758	0.343284	1.549569
1	-1.558938	-1.151578	2.744851
1	-0.916086	-2.273276	1.549569

E = -1168.6003448 a.u.

Molecule 3a(C_1)

6	-0.533747	-0.017328	0.039300
6	0.317052	-0.136224	1.395434
6	1.815920	-0.328865	1.775702
6	2.999675	0.061051	0.791456
6	2.315228	0.080558	-0.534483
6	1.745440	1.323776	-0.878036
6	-1.496042	-1.129319	0.471304
6	-1.701902	-2.192174	-0.598079
6	-0.377148	-2.421512	-1.429265
6	0.486384	-1.183668	-1.470694
6	1.790519	-1.148635	-0.990667
6	-1.425270	1.088471	0.634790
6	-1.654889	2.295081	-0.263529
6	-0.421420	2.581236	-1.215050
6	0.450047	1.367310	-1.366053
6	-0.216514	0.088279	-1.533995
1	1.968698	0.210134	2.719768
1	1.947539	-1.394478	1.989303

1	3.414633	1.041540	1.038449
1	3.787523	-0.692947	0.874911
1	-2.026212	-3.154642	-0.187707
1	-2.491392	-1.855086	-1.280563
1	0.208070	-3.243207	-1.004479
1	-0.660146	-2.716068	-2.448154
1	-2.534247	2.101993	-0.888166
1	-1.866968	3.203619	0.310423
1	-0.811233	2.893383	-2.191736
1	0.185161	3.403745	-0.824861
1	2.214149	2.233972	-0.509067
1	2.283376	-2.073368	-0.694641
1	-1.185288	0.096460	-2.039827
6	-0.422892	1.170072	1.822733
6	-0.557013	-1.407185	1.670411
6	-2.534911	-0.008350	0.795629
1	-0.839237	1.190716	2.837052
1	-1.022206	-1.481066	2.660486
1	-3.041369	-0.071290	1.764114
1	0.241302	2.033875	1.687070
1	0.040902	-2.307800	1.485615
1	-3.284155	0.085077	0.000549

E = -734.231643 a.u.

Molecule 3a(C_3)

6	0.000000	0.000000	0.497647
6	-0.446746	1.258667	1.192782
6	-0.876638	2.559300	0.527945
6	-1.445347	2.375684	-0.931036
6	-0.740936	1.209835	-1.570536
6	-1.398133	-0.031658	-1.605254
6	1.313411	-0.242440	1.192782
6	2.654737	-0.520459	0.527945
6	2.780077	0.063865	-0.931036
6	1.418216	0.036752	-1.570536

6	0.671650	1.226648	-1.605254
6	-0.866664	-1.016227	1.192782
6	-1.778100	-2.038840	0.527945
6	-1.334729	-2.439550	-0.931036
6	-0.677280	-1.246587	-1.570536
6	0.726483	-1.194990	-1.605254
1	-1.620581	3.071917	1.148476
1	0.000000	3.213555	0.474327
1	-2.523177	2.187232	-0.899430
1	-1.284862	3.316841	-1.468047
1	3.470649	-0.132494	1.148476
1	2.783020	-1.606778	0.474327
1	3.155787	1.091519	-0.899430
1	3.514899	-0.545697	-1.468047
1	-1.850068	-2.939423	1.148476
1	-2.783020	-1.606778	0.474327
1	-0.632610	-3.278752	-0.899430
1	-2.230037	-2.771143	-1.468047
1	-2.477569	-0.055293	-1.453346
1	1.190900	2.173284	-1.453346
1	1.286669	-2.117992	-1.453346
6	-1.487809	0.279309	1.852756
6	0.985793	1.148826	1.852756
6	0.502015	-1.428135	1.852756
1	-1.483293	0.283219	2.947495
1	0.986921	1.142960	2.947495
1	0.496372	-1.426178	2.947495
1	-2.490683	0.461478	1.455291
1	1.644993	1.926256	1.455291
1	0.845690	-2.387734	1.455291

E = -734.196708 a.u.

Molecule 4a(C_3)

14	0.000000	0.000000	0.183110
6	-0.012446	1.448846	1.260031

6	0.000000	2.819715	0.602021
6	-0.368577	2.800730	-0.980471
6	-0.186823	1.431478	-1.603263
6	-1.296468	0.542701	-1.640884
6	1.260960	-0.713644	1.260031
6	2.441944	-1.409857	0.602021
6	2.609791	-1.081168	-0.980471
6	1.333108	-0.553946	-1.603263
6	1.118227	0.851423	-1.640884
6	-1.248514	-0.735202	1.260031
6	-2.441944	-1.409857	0.602021
6	-2.241215	-1.719561	-0.980471
6	-1.146285	-0.877532	-1.603263
6	0.178241	-1.394124	-1.640884
1	-0.686743	3.536140	1.066957
1	1.005470	3.247011	0.691549
1	-1.411027	3.106793	-1.111318
1	0.260588	3.540572	-1.485460
1	3.405758	-1.173333	1.066957
1	2.309259	-2.494268	0.691549
1	3.396075	-0.331411	-1.111318
1	2.935931	-1.995962	-1.485460
1	-2.719015	-2.362806	1.066957
1	-3.314729	-0.752743	0.691549
1	-1.985048	-2.775382	-1.111318
1	-3.196520	-1.544610	-1.485460
1	-2.287319	0.954193	-1.448972
1	1.970015	1.503779	-1.448972
1	0.317304	-2.457973	-1.448972
6	-1.313024	0.744502	1.861562
6	1.301269	0.764861	1.861562
6	0.011755	-1.509363	1.861562
1	-1.332221	0.761524	2.959110
1	1.325610	0.772976	2.959110
1	0.006612	-1.534500	2.959110
1	-2.209205	1.249541	1.479648

1	2.186736	1.288457	1.479648
1	0.022469	-2.537998	1.479648

E = -985.235803 a.u.