Controlling the Reactivity of the Boronyl Group in Platinum Complexes towards Cyclodimerization: A Theoretical Survey

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Supporting Information

Table S1: Comparing selected experimental bond distances (Å) with theoretical results.

Table S2: Some predicted natural charges for monomers, dimers, and transition states.

Table S3: Specific solvation energy contributions (in kcal/mol) for monomers, dimers, and transition states.

Tables S4-S19: The theoretical Cartesian coordinates for monomers (7 structures), dimers (5 structures), and transition states (4 structures) in gas phase and dichloromethane.

Complete Gaussian 09 reference (Reference 33)

Table S1. Comparing selected experimental bond distances (Å) with theoretical results.

	Pt1-B1	Pt2-B2	Ave	B1-O1	B1-O2	B2-O1	B2-O2	B1-B2	Ave	Pt1-H1	Pt2-H2
Exp.[a]	1.946	1.953	1.950	1.424	1.410	1.413	1.404	1.845	1.413	2.239	2.351
Gas	1.952	1.951	1.952	1.417	1.414	1.418	1.416	1.828	1.416	2.365	2.346
Sol.	1.945	1.947	1.946	1.419	1.416	1.418	1.416	1.832	1.417	2.559	2.639

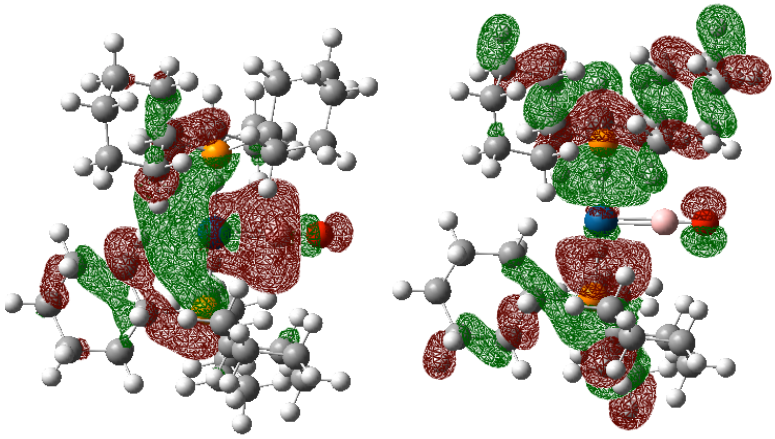
[a] The experimental results come from Ref. 1.

Table S2. Some predicted natural charges for monomers, dimers, and transition states.

	1	**2**	**2ts**	**1Br**	**2Br**	**2Brts**	**1Ir**	**2Ir**
Pt1	-0.59	-0.59	-0.65	-0.61	-0.56	-0.61	-1.27(Ir)	-1.12(Ir)
Pt2		-0.57	-0.56		-0.50	-0.53		-0.11(Ir)
B1	0.75	0.92	0.83	0.65	0.84	0.80	1.02	1.18
O1	-0.87	-1.04	-1.01	-0.98	-1.09	-1.10	-0.89	-1.06
B2		0.91	0.83		0.82	0.80		1.19
O2		-1.04	-1.05		-1.09	-1.04		-1.06
Br1				-0.58	-0.71	-0.76	-0.27	-0.45
Br2					-0.66	-0.57	-0.44(Cl)	-0.44

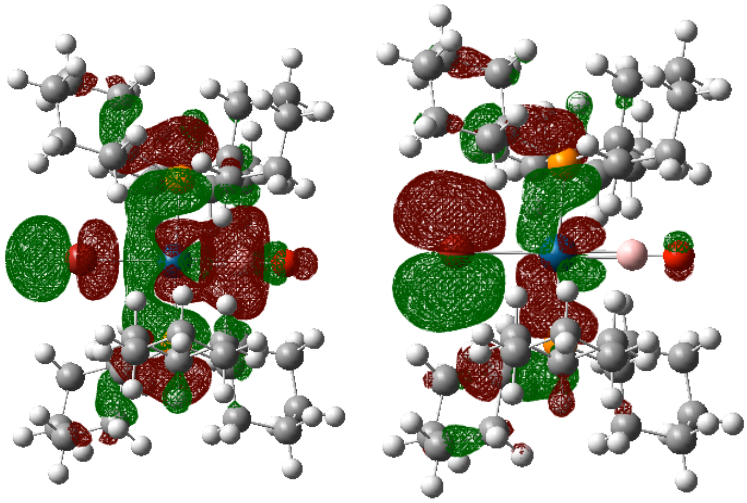
Table S3. Specific solvation energy contributions (in kcal/mol) for monomers, dimers, and transition states.

	1	**2**	**2ts**	**1Br**	**2Br**	**2Brts**
G_{es}	-33.4	-82.2	-82.2	-13.5	-40.7	-40.1
G_{Cav}	57.2	97.3	97.3	58.1	98.5	99.5
G_{Dis}	-37.3	-57.3	-57.4	-38.2	-58.9	-59.4
G_{Rep}	1.7	2.3	2.3	1.7	2.5	2.6
$G_{non\text{-}es}$	21.5	42.4	42.3	21.6	42.1	42.8
G_{Sol}	-11.9	-39.8	-39.9	8.1	1.4	2.7



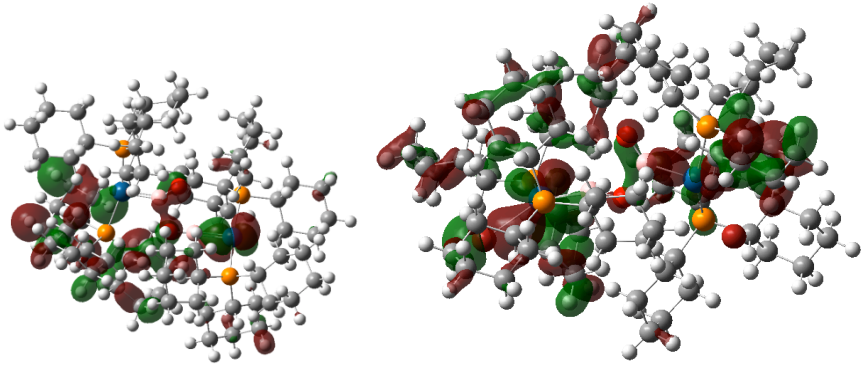
1

LUMO(-0.176) HOMO(-0.305) Gap:0.129



1Br

LUMO(-0.011) HOMO(-0.168) Gap:0.157



2ts HOMO-48(-0.424) **2Brts** HOMO-45(-0.255)

Figure S1. Important molecular orbitals as well as orbital energies (in a.u.) for momomers and transition states.

Table S4. The theoretical Cartesian coordinates (in Å) for the structure **1** in the gas phase.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.346637	-0.487135	-0.221423
2	6	0	2.862138	-2.249846	-0.391573
3	1	0	3.858887	-2.277357	-0.882703
4	6	0	1.829903	-3.004380	-1.288528
5	1	0	0.830661	-2.919715	-0.810952
6	1	0	1.767871	-2.533124	-2.288287
7	6	0	2.212959	-4.500550	-1.428835
8	1	0	1.454015	-5.009253	-2.049578
9	1	0	3.183521	-4.579274	-1.953332
10	6	0	2.312729	-5.172769	-0.037352
11	1	0	1.320488	-5.153564	0.451960
12	1	0	2.608848	-6.230702	-0.151224
13	6	0	3.337737	-4.430644	0.853921
14	1	0	4.346208	-4.506597	0.406332
15	1	0	3.378536	-4.893052	1.856088
16	6	0	2.960171	-2.933442	1.008649
17	1	0	3.709610	-2.421090	1.636324
18	1	0	1.978107	-2.856286	1.520827
19	6	0	3.300034	0.314055	1.137546
20	1	0	2.965126	-0.247323	2.037001
21	6	0	4.853463	0.199632	1.046940
22	1	0	5.156281	-0.852539	0.899704
23	1	0	5.222478	0.784356	0.187324
24	6	0	5.477536	0.756208	2.356473
25	1	0	5.151306	0.129656	3.207488
26	1	0	6.578213	0.687166	2.291721
27	6	0	5.047656	2.226150	2.593780
28	1	0	5.446028	2.860244	1.780051
29	1	0	5.477788	2.593251	3.542460
30	6	0	3.503228	2.355831	2.636912
31	1	0	3.212330	3.414160	2.761617
32	1	0	3.105932	1.792038	3.502106
33	6	0	2.861159	1.796378	1.340273
34	1	0	3.182100	2.405151	0.473487
35	1	0	1.754023	1.849930	1.409692
36	6	0	2.547291	0.339977	-1.876518
37	1	0	2.333962	-0.467701	-2.610056
38	6	0	3.938325	0.945044	-2.215753

39	1	0	4.172423	1.755995	-1.501590
40	1	0	4.718418	0.168092	-2.121843
41	6	0	3.923057	1.520624	-3.657744
42	1	0	4.910473	1.960299	-3.885341
43	1	0	3.748989	0.698239	-4.376654
44	6	0	2.816581	2.594275	-3.816240
45	1	0	2.810097	2.980583	-4.851161
46	1	0	3.026378	3.445888	-3.142039
47	6	0	1.420280	2.009629	-3.478912
48	1	0	1.166714	1.205131	-4.195919
49	1	0	0.643295	2.792052	-3.550980
50	6	0	1.427488	1.417928	-2.042478
51	1	0	0.400980	0.956707	-1.887824
52	1	0	1.554126	2.221823	-1.291433
53	8	0	-0.186343	-1.779806	2.705118
54	5	0	-0.091662	-1.142306	1.662219
55	78	0	0.037233	-0.119229	0.041174
56	15	0	-2.268927	0.406541	0.199949
57	6	0	-2.406708	2.007493	1.114508
58	1	0	-3.469241	2.327988	1.136809
59	6	0	-1.898480	1.803391	2.577257
60	1	0	-0.853024	1.429914	2.534356
61	1	0	-2.507651	1.041815	3.096591
62	6	0	-1.930363	3.135989	3.369778
63	1	0	-1.546310	2.956131	4.389503
64	1	0	-2.976821	3.481961	3.460852
65	6	0	-1.082871	4.217663	2.657076
66	1	0	-0.023325	3.896772	2.632859
67	1	0	-1.130464	5.168010	3.217717
68	6	0	-1.586968	4.434128	1.209672
69	1	0	-2.624469	4.817232	1.230277
70	1	0	-0.963414	5.184399	0.691514
71	6	0	-1.557352	3.107522	0.406726
72	1	0	-1.924486	3.283100	-0.621083
73	1	0	-0.506342	2.744665	0.338688
74	6	0	-2.865717	0.667510	-1.533960
75	1	0	-2.386155	1.624086	-1.836393
76	6	0	-4.406364	0.832873	-1.694828
77	1	0	-4.789274	1.597576	-0.994652
78	1	0	-4.898577	-0.128042	-1.460484
79	6	0	-4.731543	1.235267	-3.159838
80	1	0	-4.281880	2.223245	-3.371969
81	1	0	-5.825789	1.334838	-3.274719
82	6	0	-4.184269	0.185448	-4.160235

83	1	0	-4.706474	-0.776803	-4.004722
84	1	0	-4.390018	0.511580	-5.195218
85	6	0	-2.659906	-0.026124	-3.972027
86	1	0	-2.295880	-0.810701	-4.658978
87	1	0	-2.120538	0.911063	-4.211696
88	6	0	-2.337919	-0.429873	-2.509785
89	1	0	-2.810131	-1.401397	-2.274310
90	1	0	-1.238862	-0.560977	-2.386892
91	6	0	-3.225251	-0.868225	1.130180
92	1	0	-2.651510	-0.961094	2.078166
93	6	0	-4.693125	-0.497515	1.509261
94	1	0	-5.320885	-0.460473	0.602722
95	1	0	-4.730528	0.494813	1.992945
96	6	0	-5.241966	-1.581280	2.479003
97	1	0	-6.286581	-1.336566	2.742696
98	1	0	-4.646516	-1.563456	3.410842
99	6	0	-5.167820	-2.991815	1.840724
100	1	0	-5.529882	-3.745242	2.562478
101	1	0	-5.833198	-3.029671	0.958188
102	6	0	-3.719803	-3.336785	1.406874
103	1	0	-3.061431	-3.386711	2.295048
104	1	0	-3.694461	-4.324294	0.912502
105	6	0	-3.164952	-2.262010	0.436059
106	1	0	-2.118305	-2.500200	0.156961
107	1	0	-3.774726	-2.244522	-0.487420

Sum of electronic and zero-point Energies= -2295.308564
Sum of electronic and thermal Energies= -2295.265489
Sum of electronic and thermal Enthalpies= -2295.264545
Sum of electronic and thermal Free Energies= -2295.385500

Table S5. The theoretical Cartesian coordinates (in Å) for the structure **1Br** in the gas phase.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.000000	0.000000	2.676216
2	15	0	0.000000	2.368915	-0.113155
3	6	0	-1.754887	2.929329	-0.327357
4	1	0	-1.784595	4.038930	-0.315306
5	6	0	-2.598892	2.383307	0.864993
6	1	0	-2.516844	1.275767	0.869915
7	1	0	-2.188975	2.745997	1.824948
8	6	0	-4.086527	2.792894	0.730382
9	1	0	-4.657362	2.370161	1.576191
10	1	0	-4.170888	3.894834	0.785356
11	6	0	-4.670126	2.294370	-0.614614
12	1	0	-4.637767	1.187428	-0.636018
13	1	0	-5.727715	2.599798	-0.709339
14	6	0	-3.844837	2.848981	-1.801508
15	1	0	-3.919229	3.952570	-1.820743
16	1	0	-4.245865	2.468845	-2.757987
17	6	0	-2.355942	2.435057	-1.676429
18	1	0	-1.782311	2.840857	-2.528082
19	1	0	-2.283374	1.329614	-1.713398
20	6	0	0.935539	2.936446	-1.605320
21	1	0	0.338754	2.520759	-2.444991
22	6	0	1.038385	4.476932	-1.817096
23	1	0	0.047425	4.954456	-1.712272
24	1	0	1.710139	4.909194	-1.053890
25	6	0	1.615178	4.754798	-3.233826
26	1	0	0.907489	4.365587	-3.989579
27	1	0	1.704189	5.845478	-3.388530
28	6	0	2.995775	4.074941	-3.419564
29	1	0	3.723008	4.533849	-2.723970
30	1	0	3.362276	4.250805	-4.446755
31	6	0	2.912830	2.551484	-3.138593
32	1	0	3.913868	2.093290	-3.228827
33	1	0	2.249706	2.066182	-3.879983
34	6	0	2.346405	2.288436	-1.721329
35	1	0	3.027067	2.720322	-0.964314
36	1	0	2.275956	1.199446	-1.533422
37	6	0	0.615672	3.179414	1.428868
38	1	0	0.073368	2.629174	2.222896

39	6	0	0.312219	4.697122	1.617780
40	1	0	0.896927	5.299122	0.900969
41	1	0	-0.758155	4.905152	1.446016
42	6	0	0.693777	5.099275	3.070182
43	1	0	0.491154	6.175590	3.219265
44	1	0	0.053003	4.536347	3.774613
45	6	0	2.183086	4.788961	3.369864
46	1	0	2.413964	5.048914	4.418449
47	1	0	2.823082	5.417129	2.722507
48	6	0	2.503619	3.294039	3.110010
49	1	0	1.928092	2.659302	3.810733
50	1	0	3.576980	3.098377	3.282641
51	6	0	2.128148	2.898164	1.660291
52	1	0	2.336948	1.823779	1.494534
53	1	0	2.730828	3.492655	0.949176
54	8	0	0.000000	0.000000	-3.192501
55	5	0	0.000000	0.000000	-1.959305
56	78	0	0.000000	0.000000	0.002580
57	15	0	0.000000	-2.368915	-0.113155
58	6	0	1.754887	-2.929329	-0.327357
59	1	0	1.784595	-4.038930	-0.315306
60	6	0	2.355942	-2.435057	-1.676429
61	1	0	2.283374	-1.329614	-1.713398
62	1	0	1.782311	-2.840857	-2.528082
63	6	0	3.844837	-2.848981	-1.801508
64	1	0	4.245865	-2.468845	-2.757987
65	1	0	3.919229	-3.952570	-1.820743
66	6	0	4.670126	-2.294370	-0.614614
67	1	0	4.637767	-1.187428	-0.636018
68	1	0	5.727715	-2.599798	-0.709339
69	6	0	4.086527	-2.792894	0.730382
70	1	0	4.170888	-3.894834	0.785356
71	1	0	4.657362	-2.370161	1.576191
72	6	0	2.598892	-2.383307	0.864993
73	1	0	2.188975	-2.745997	1.824948
74	1	0	2.516844	-1.275767	0.869915
75	6	0	-0.615672	-3.179414	1.428868
76	1	0	-0.073368	-2.629174	2.222896
77	6	0	-0.312219	-4.697122	1.617780
78	1	0	0.758155	-4.905152	1.446016
79	1	0	-0.896927	-5.299122	0.900969
80	6	0	-0.693777	-5.099275	3.070182
81	1	0	-0.053003	-4.536347	3.774613
82	1	0	-0.491154	-6.175590	3.219265

83	6	0	-2.183086	-4.788961	3.369864
84	1	0	-2.823082	-5.417129	2.722507
85	1	0	-2.413964	-5.048914	4.418449
86	6	0	-2.503619	-3.294039	3.110010
87	1	0	-3.576980	-3.098377	3.282641
88	1	0	-1.928092	-2.659302	3.810733
89	6	0	-2.128148	-2.898164	1.660291
90	1	0	-2.730828	-3.492655	0.949176
91	1	0	-2.336948	-1.823779	1.494534
92	6	0	-0.935539	-2.936446	-1.605320
93	1	0	-0.338754	-2.520759	-2.444991
94	6	0	-1.038385	-4.476932	-1.817096
95	1	0	-1.710139	-4.909194	-1.053890
96	1	0	-0.047425	-4.954456	-1.712272
97	6	0	-1.615178	-4.754798	-3.233826
98	1	0	-1.704189	-5.845478	-3.388530
99	1	0	-0.907489	-4.365587	-3.989579
100	6	0	-2.995775	-4.074941	-3.419564
101	1	0	-3.362276	-4.250805	-4.446755
102	1	0	-3.723008	-4.533849	-2.723970
103	6	0	-2.912830	-2.551484	-3.138593
104	1	0	-2.249706	-2.066182	-3.879983
105	1	0	-3.913868	-2.093290	-3.228827
106	6	0	-2.346405	-2.288436	-1.721329
107	1	0	-2.275956	-1.199446	-1.533422
108	1	0	-3.027067	-2.720322	-0.964314

Sum of electronic and zero-point Energies= -4869.545208

Sum of electronic and thermal Energies= -4869.500697

Sum of electronic and thermal Enthalpies= -4869.499752

Sum of electronic and thermal Free Energies= -4869.622745

Table S6. The theoretical Cartesian coordinates (in Å) for the structure **1Me** in the gas phase.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	0.000000	0.000000	0.258385
2	8	0	0.000000	0.000000	-2.884752
3	5	0	0.000000	0.000000	-1.664016
4	15	0	0.000000	2.374662	0.159699
5	15	0	0.000000	-2.374662	0.159699
6	6	0	1.443308	3.035739	-0.713174
7	1	0	1.409955	4.128673	-0.740400
8	1	0	2.363711	2.719956	-0.217771
9	1	0	1.460316	2.656615	-1.738222
10	6	0	-1.443308	3.035739	-0.713174
11	1	0	-2.363711	2.719956	-0.217771
12	1	0	-1.409955	4.128673	-0.740400
13	1	0	-1.460316	2.656615	-1.738222
14	6	0	0.000000	3.165496	1.794860
15	1	0	0.886890	2.876290	2.362684
16	1	0	0.000000	4.253923	1.682885
17	1	0	-0.886890	2.876290	2.362684
18	6	0	1.443308	-3.035739	-0.713174
19	1	0	1.409955	-4.128673	-0.740400
20	1	0	1.460316	-2.656615	-1.738222
21	1	0	2.363711	-2.719956	-0.217771
22	6	0	-1.443308	-3.035739	-0.713174
23	1	0	-1.460316	-2.656615	-1.738222
24	1	0	-1.409955	-4.128673	-0.740400
25	1	0	-2.363711	-2.719956	-0.217771
26	6	0	0.000000	-3.165496	1.794860
27	1	0	-0.886890	-2.876290	2.362684
28	1	0	0.000000	-4.253923	1.682885
29	1	0	0.886890	-2.876290	2.362684

Sum of electronic and zero-point Energies= -1141.123270

Sum of electronic and thermal Energies= -1141.104490

Sum of electronic and thermal Enthalpies= -1141.103545

Sum of electronic and thermal Free Energies= -1141.170620

Table S7. The theoretical Cartesian coordinates (in Å) for the structure **1MeBr** in the gas phase.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	0.000000	0.000000	0.313120
2	8	0	0.000000	0.000000	3.514115
3	5	0	0.000000	0.000000	2.285657
4	15	0	0.000000	2.334965	0.259008
5	15	0	0.000000	-2.334965	0.259008
6	6	0	0.000000	3.217362	1.846873
7	1	0	0.000000	4.301727	1.694318
8	1	0	-0.877543	2.933207	2.431032
9	1	0	0.877543	2.933207	2.431032
10	6	0	1.432045	3.004502	-0.632666
11	1	0	1.456199	2.563559	-1.632492
12	1	0	1.374227	4.095380	-0.709134
13	1	0	2.353840	2.729648	-0.114742
14	6	0	-1.432045	3.004502	-0.632666
15	1	0	-2.353840	2.729648	-0.114742
16	1	0	-1.374227	4.095380	-0.709134
17	1	0	-1.456199	2.563559	-1.632492
18	6	0	0.000000	-3.217362	1.846873
19	1	0	0.000000	-4.301727	1.694318
20	1	0	0.877543	-2.933207	2.431032
21	1	0	-0.877543	-2.933207	2.431032
22	6	0	1.432045	-3.004502	-0.632666
23	1	0	2.353840	-2.729648	-0.114742
24	1	0	1.374227	-4.095380	-0.709134
25	1	0	1.456199	-2.563559	-1.632492
26	6	0	-1.432045	-3.004502	-0.632666
27	1	0	-1.456199	-2.563559	-1.632492
28	1	0	-1.374227	-4.095380	-0.709134
29	1	0	-2.353840	-2.729648	-0.114742
30	35	0	0.000000	0.000000	-2.342872

Sum of electronic and zero-point Energies= -3715.399781

Sum of electronic and thermal Energies= -3715.378984

Sum of electronic and thermal Enthalpies= -3715.378039

Sum of electronic and thermal Free Energies= -3715.449877

Table S8. The theoretical Cartesian coordinates (in Å) for the structure **1Ir** in the gas phase.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.000009	0.301629	0.109432
2	15	0	2.384581	0.120298	0.002391
3	15	0	-2.384586	0.120414	0.002540
4	6	0	3.092539	-0.871197	1.342703
5	1	0	2.647800	-1.870086	1.307543
6	1	0	4.179531	-0.951668	1.243630
7	1	0	2.841202	-0.430438	2.311023
8	6	0	2.974286	-0.633441	-1.531273
9	1	0	4.068154	-0.684001	-1.531778
10	1	0	2.554568	-1.638018	-1.621869
11	1	0	2.616761	-0.042861	-2.378005
12	6	0	3.225952	1.727094	0.078030
13	1	0	4.310201	1.608835	-0.008652
14	1	0	2.870291	2.355562	-0.743464
15	1	0	2.999434	2.230125	1.021859
16	6	0	-3.092526	-0.871582	1.342484
17	1	0	-2.841105	-0.431290	2.310994
18	1	0	-4.179529	-0.951915	1.243410
19	1	0	-2.647889	-1.870494	1.306798
20	6	0	-3.225990	1.727164	0.078734
21	1	0	-2.870063	2.356078	-0.742304
22	1	0	-4.310203	1.608926	-0.008397
23	1	0	-2.999826	2.229708	1.022908
24	6	0	-2.974313	-0.632823	-1.531365
25	1	0	-4.068169	-0.683624	-1.531804
26	1	0	-2.616991	-0.041842	-2.377903
27	1	0	-2.554375	-1.637268	-1.622415
28	17	0	-0.000044	0.845937	-2.380385
29	35	0	-0.000135	-2.285519	-0.286415
30	6	0	0.000071	2.121885	0.434221
31	8	0	0.000100	3.264608	0.629836
32	8	0	0.000413	-0.391722	3.267227
33	5	0	0.000168	-0.153058	2.066310

Sum of electronic and zero-point Energies= -4274.518502

Sum of electronic and thermal Energies= -4274.494218

Sum of electronic and thermal Enthalpies= -4274.493274

Sum of electronic and thermal Free Energies= -4274.572639

Table S9. The theoretical Cartesian coordinates (in Å) for the structure **2** in gas phase.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.846663	0.001662	-0.091045
2	8	0	-0.060618	1.067045	-0.314041
3	5	0	-0.981504	0.016821	-0.069968
4	8	0	-0.071885	-1.048395	0.138859
5	78	0	2.796757	-0.030115	-0.162764
6	15	0	3.099371	2.047513	-1.256517
7	6	0	4.731624	1.760676	-2.106324
8	1	0	4.468330	1.354740	-3.107896
9	6	0	5.502142	0.639118	-1.339697
10	1	0	5.723520	0.969945	-0.304930
11	1	0	4.860854	-0.280792	-1.289076
12	6	0	6.821250	0.249750	-2.059391
13	1	0	7.357162	-0.508031	-1.459201
14	1	0	6.574379	-0.201107	-3.039476
15	6	0	7.707880	1.504134	-2.264375
16	1	0	8.624699	1.221990	-2.812007
17	1	0	8.015940	1.897758	-1.277071
18	6	0	6.942586	2.602739	-3.044293
19	1	0	7.583493	3.493842	-3.167459
20	1	0	6.687014	2.232554	-4.054897
21	6	0	5.640327	3.010723	-2.303709
22	1	0	5.105035	3.787263	-2.876174
23	1	0	5.900723	3.439470	-1.318734
24	6	0	3.290689	3.418546	-0.030067
25	1	0	3.634514	4.331767	-0.559655
26	6	0	4.344711	3.031430	1.052705
27	1	0	4.015279	2.082176	1.530933
28	1	0	5.330020	2.852246	0.589205
29	6	0	4.469050	4.136595	2.132073
30	1	0	5.208208	3.820048	2.889525
31	1	0	4.848442	5.061394	1.658557
32	6	0	3.099464	4.412838	2.796111
33	1	0	3.197416	5.216420	3.547593
34	1	0	2.761832	3.499868	3.323361
35	6	0	2.050002	4.807671	1.728180
36	1	0	2.351989	5.754418	1.242675
37	1	0	1.066717	4.976300	2.203049
38	6	0	1.916794	3.700686	0.649436

39	1	0	1.170118	3.999095	-0.107467
40	1	0	1.566370	2.759349	1.121794
41	6	0	1.871663	2.573936	-2.525258
42	1	0	0.984816	2.916939	-1.954677
43	6	0	2.380724	3.737763	-3.433252
44	1	0	2.695649	4.599197	-2.816634
45	1	0	3.256756	3.387045	-4.008233
46	6	0	1.265214	4.174448	-4.422123
47	1	0	0.424758	4.609751	-3.852978
48	1	0	1.662216	4.963462	-5.085882
49	6	0	0.762477	2.975055	-5.263726
50	1	0	1.579537	2.615449	-5.916241
51	1	0	-0.065595	3.300468	-5.918322
52	6	0	0.286809	1.812427	-4.355081
53	1	0	-0.582579	2.138731	-3.751118
54	1	0	-0.035602	0.956668	-4.974450
55	6	0	1.416507	1.363912	-3.391402
56	1	0	2.275622	0.966948	-3.970533
57	1	0	1.060165	0.551752	-2.725343
58	15	0	3.080406	-2.050623	1.030013
59	6	0	1.803625	-2.642309	2.220030
60	1	0	0.988783	-2.975445	1.543976
61	6	0	1.169784	-1.561169	3.142332
62	1	0	1.893065	-1.233831	3.912136
63	1	0	0.881880	-0.671248	2.544439
64	6	0	-0.081677	-2.182350	3.820559
65	1	0	-0.555375	-1.441806	4.487156
66	1	0	-0.813506	-2.441583	3.032689
67	6	0	0.284477	-3.451234	4.634767
68	1	0	0.932413	-3.163083	5.483033
69	1	0	-0.634179	-3.897715	5.056409
70	6	0	1.022873	-4.496190	3.762045
71	1	0	0.344511	-4.881626	2.977967
72	1	0	1.340118	-5.353836	4.382150
73	6	0	2.264908	-3.866506	3.075929
74	1	0	2.770389	-4.621839	2.447991
75	1	0	2.982573	-3.523271	3.842562
76	6	0	3.441019	-3.501797	-0.065099
77	1	0	3.995150	-4.245002	0.544197
78	6	0	2.148898	-4.186405	-0.600126
79	1	0	1.571750	-3.455301	-1.200454
80	1	0	1.511693	-4.521892	0.235976
81	6	0	2.531693	-5.409238	-1.476572
82	1	0	3.071355	-6.143652	-0.850194

83	1	0	1.614314	-5.901977	-1.844405
84	6	0	3.427966	-4.981815	-2.663940
85	1	0	2.867517	-4.286093	-3.316628
86	1	0	3.699117	-5.864030	-3.270642
87	6	0	4.709667	-4.281827	-2.149372
88	1	0	5.329975	-3.939346	-2.996755
89	1	0	5.312898	-4.996584	-1.558800
90	6	0	4.351829	-3.066203	-1.254307
91	1	0	5.276395	-2.592739	-0.873256
92	1	0	3.801064	-2.311602	-1.859207
93	6	0	4.696878	-1.614125	1.840995
94	1	0	5.253086	-1.083290	1.032910
95	6	0	5.608634	-2.789055	2.312951
96	1	0	5.128768	-3.312734	3.158891
97	6	0	6.981735	-2.212172	2.755405
98	1	0	7.624169	-3.037228	3.112100
99	1	0	7.478798	-1.761135	1.874613
100	6	0	6.820711	-1.144921	3.866868
101	1	0	7.808793	-0.726090	4.127484
102	1	0	6.411892	-1.622534	4.776589
103	6	0	5.867138	-0.007539	3.419143
104	1	0	6.307378	0.535773	2.558678
105	1	0	5.724674	0.719727	4.238089
106	6	0	4.494662	-0.589613	2.996335
107	1	0	3.807984	0.219890	2.670445
108	1	0	4.031247	-1.103227	3.859053
109	78	0	-2.930679	0.041108	0.005476
110	15	0	-3.024385	2.098565	1.140148
111	6	0	-4.865641	2.363701	1.216267
112	1	0	-5.120120	2.898541	0.274927
113	6	0	-5.590977	0.985318	1.181646
114	1	0	-5.232752	0.380521	0.305195
115	1	0	-5.354525	0.412544	2.099600
116	6	0	-7.124564	1.165417	1.038750
117	1	0	-7.339422	1.652707	0.067924
118	1	0	-7.614766	0.175206	1.041337
119	6	0	-7.665913	2.037873	2.201169
120	1	0	-8.749560	2.202905	2.064892
121	1	0	-7.528860	1.493864	3.154728
122	6	0	-6.928422	3.399152	2.272547
123	1	0	-7.302215	3.985164	3.131099
124	1	0	-7.132845	3.983321	1.355592
125	6	0	-5.394882	3.200684	2.417069
126	1	0	-4.887933	4.180325	2.460700

127	1	0	-5.180681	2.662772	3.359749
128	6	0	-2.307433	3.484224	0.161327
129	1	0	-1.208358	3.363242	0.245673
130	6	0	-2.668829	3.347438	-1.347660
131	1	0	-3.767440	3.412021	-1.483744
132	1	0	-2.337439	2.353535	-1.713529
133	6	0	-1.973268	4.475293	-2.153957
134	1	0	-0.878973	4.341859	-2.063570
135	1	0	-2.239273	4.384716	-3.222538
136	6	0	-2.359983	5.876554	-1.616139
137	1	0	-1.833461	6.656909	-2.193930
138	1	0	-3.445360	6.036434	-1.752653
139	6	0	-2.006836	6.001814	-0.113270
140	1	0	-2.317468	6.989691	0.271730
141	1	0	-0.912403	5.917234	0.024730
142	6	0	-2.713246	4.889065	0.707480
143	1	0	-3.807861	5.011328	0.613278
144	1	0	-2.448610	4.980151	1.776621
145	6	0	-2.355289	2.206197	2.854530
146	1	0	-2.843175	3.072433	3.347951
147	6	0	-2.695976	0.918343	3.663122
148	1	0	-2.195741	0.056969	3.172369
149	1	0	-3.785656	0.728647	3.647821
150	6	0	-2.207386	1.068433	5.129067
151	1	0	-2.777516	1.883965	5.611852
152	1	0	-2.424538	0.138179	5.684273
153	6	0	-0.691503	1.387395	5.193385
154	1	0	-0.393016	1.560007	6.242786
155	1	0	-0.115290	0.520798	4.823124
156	6	0	-0.335349	2.625447	4.334766
157	1	0	0.756348	2.793730	4.342485
158	1	0	-0.815234	3.527545	4.758046
159	6	0	-0.816360	2.445321	2.870047
160	1	0	-0.303448	1.571957	2.409232
161	1	0	-0.557234	3.338085	2.277637
162	15	0	-3.190165	-1.986638	-1.211307
163	6	0	-1.701743	-2.586704	-2.121302
164	1	0	-0.940271	-2.785861	-1.340531
165	6	0	-1.129765	-1.479397	-3.055898
166	1	0	-0.952765	-0.546988	-2.475484
167	1	0	-1.867240	-1.228965	-3.845584
168	6	0	0.190644	-1.966433	-3.708390
169	1	0	0.578604	-1.185599	-4.385244
170	1	0	0.945989	-2.124693	-2.910899

171	6	0	-0.035155	-3.285654	-4.492064
172	1	0	-0.729355	-3.093295	-5.330981
173	1	0	0.919058	-3.633325	-4.925976
174	6	0	-0.629475	-4.381534	-3.574061
175	1	0	0.093253	-4.631237	-2.776852
176	1	0	-0.821185	-5.301611	-4.154890
177	6	0	-1.954879	-3.901407	-2.924299
178	1	0	-2.355980	-4.687360	-2.259317
179	1	0	-2.698435	-3.708282	-3.718279
180	6	0	-3.664389	-3.268450	0.035089
181	1	0	-4.004807	-4.190805	-0.478719
182	6	0	-2.432997	-3.595684	0.932075
183	1	0	-2.064589	-2.640985	1.363797
184	1	0	-1.618427	-4.027943	0.323845
185	6	0	-2.815660	-4.575498	2.072446
186	1	0	-3.114361	-5.545111	1.632248
187	1	0	-1.929999	-4.755124	2.707129
188	6	0	-3.976857	-4.014595	2.928700
189	1	0	-4.247999	-4.738283	3.717825
190	1	0	-3.647059	-3.081923	3.428839
191	6	0	-5.206973	-3.712249	2.039461
192	1	0	-6.026077	-3.284626	2.644638
193	1	0	-5.579195	-4.648250	1.582497
194	6	0	-4.825594	-2.713871	0.917783
195	1	0	-4.474055	-1.769390	1.394287
196	1	0	-5.707324	-2.470366	0.295943
197	6	0	-4.542583	-1.828555	-2.481421
198	1	0	-4.007991	-1.621630	-3.433384
199	6	0	-5.480587	-0.615536	-2.203825
200	1	0	-6.053936	-0.803805	-1.275281
201	1	0	-4.871429	0.305667	-2.059391
202	6	0	-6.467942	-0.415697	-3.383536
203	1	0	-7.135819	0.435878	-3.162142
204	1	0	-5.892623	-0.166495	-4.294940
205	6	0	-7.299686	-1.701525	-3.623197
206	1	0	-7.941500	-1.889859	-2.742325
207	1	0	-7.963567	-1.559348	-4.494332
208	6	0	-6.377931	-2.924588	-3.858505
209	1	0	-5.797030	-2.781652	-4.788772
210	1	0	-6.985192	-3.839195	-3.981495
211	6	0	-5.395483	-3.121570	-2.672256
212	1	0	-4.746406	-3.994606	-2.858332
213	1	0	-5.969098	-3.318363	-1.747589
214	1	0	5.761933	-3.518260	1.498640

Sum of electronic and zero-point Energies=	-4590.649959
Sum of electronic and thermal Energies=	-4590.564464
Sum of electronic and thermal Enthalpies=	-4590.563519
Sum of electronic and thermal Free Energies=	-4590.772333

Table S10. The theoretical Cartesian coordinates (in Å) for the structure **2Br** in gas phase.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.825608	0.109451	0.182163
2	8	0	-0.132097	1.013514	-0.331796
3	5	0	-1.036583	-0.003885	0.132413
4	8	0	-0.069775	-0.863230	0.719770
5	15	0	2.963596	2.032120	-1.313963
6	6	0	4.690755	2.091937	-2.012149
7	1	0	4.628532	1.442143	-2.908531
8	6	0	5.723930	1.420889	-1.049952
9	1	0	5.902334	2.061568	-0.167280
10	1	0	5.335985	0.445421	-0.694399
11	6	0	7.059303	1.193855	-1.798405
12	1	0	7.783397	0.702363	-1.123985
13	1	0	6.875055	0.513683	-2.651087
14	6	0	7.625436	2.545181	-2.307666
15	1	0	8.552961	2.375131	-2.883356
16	1	0	7.883929	3.182240	-1.440891
17	6	0	6.588657	3.283287	-3.193457
18	1	0	6.987955	4.265293	-3.506672
19	1	0	6.401735	2.690597	-4.108465
20	6	0	5.239863	3.486296	-2.446655
21	1	0	4.529308	4.010113	-3.105684
22	1	0	5.403135	4.121767	-1.557770
23	6	0	2.837125	3.546686	-0.234627
24	1	0	2.977766	4.429000	-0.894914
25	6	0	3.941461	3.564987	0.860854
26	1	0	3.862737	2.626236	1.444106
27	1	0	4.937993	3.589553	0.395839
28	6	0	3.810450	4.786370	1.806521
29	1	0	4.590760	4.723944	2.586006
30	1	0	3.990416	5.711687	1.227410
31	6	0	2.406755	4.853324	2.449089
32	1	0	2.324774	5.739720	3.103637
33	1	0	2.245176	3.955103	3.075617
34	6	0	1.329852	4.894539	1.340458
35	1	0	1.464181	5.804966	0.726470
36	1	0	0.322241	4.942877	1.790927
37	6	0	1.440618	3.639795	0.436026
38	1	0	0.647211	3.649606	-0.329500

39	1	0	1.296120	2.728565	1.050943
40	6	0	1.708888	2.307388	-2.656238
41	1	0	0.792536	2.606104	-2.106603
42	6	0	2.050066	3.412451	-3.700875
43	1	0	2.264260	4.373131	-3.198051
44	1	0	2.949629	3.108833	-4.266594
45	6	0	0.867108	3.592627	-4.692903
46	1	0	-0.015747	3.962930	-4.141560
47	1	0	1.136766	4.357682	-5.443552
48	6	0	0.513645	2.256884	-5.393725
49	1	0	1.368910	1.933021	-6.015646
50	1	0	-0.351827	2.404514	-6.064367
51	6	0	0.198571	1.155298	-4.349413
52	1	0	-0.705023	1.437264	-3.772397
53	1	0	-0.010926	0.198195	-4.859335
54	6	0	1.385834	0.968977	-3.373873
55	1	0	2.280704	0.607877	-3.917955
56	1	0	1.140851	0.206474	-2.611910
57	15	0	3.148776	-1.685332	1.484056
58	6	0	1.791310	-2.644540	2.354085
59	1	0	1.044556	-2.856699	1.561676
60	6	0	1.084346	-1.785454	3.442905
61	1	0	1.801365	-1.577379	4.258566
62	1	0	0.759501	-0.823733	3.006152
63	6	0	-0.136999	-2.534427	4.033107
64	1	0	-0.613313	-1.911047	4.809751
65	1	0	-0.877198	-2.694111	3.230500
66	6	0	0.288052	-3.897312	4.633303
67	1	0	0.969221	-3.725535	5.487401
68	1	0	-0.595857	-4.437554	5.017510
69	6	0	1.014241	-4.751669	3.566419
70	1	0	0.317120	-4.985030	2.739864
71	1	0	1.345810	-5.710779	4.004161
72	6	0	2.244179	-4.000070	2.989438
73	1	0	2.734857	-4.642558	2.241669
74	1	0	2.969321	-3.806363	3.800227
75	6	0	4.385808	-2.994721	1.017921
76	1	0	4.564797	-3.614987	1.919512
77	6	0	3.780564	-3.892013	-0.100386
78	1	0	3.578521	-3.255827	-0.980116
79	1	0	2.821943	-4.328664	0.232988
80	6	0	4.762070	-5.022948	-0.495482
81	1	0	4.917437	-5.698713	0.367682
82	1	0	4.316862	-5.618096	-1.312928

83	6	0	6.117640	-4.427321	-0.947121
84	1	0	5.953133	-3.800879	-1.844864
85	1	0	6.819954	-5.236305	-1.218332
86	6	0	6.726075	-3.549616	0.174268
87	1	0	7.680655	-3.108865	-0.164719
88	1	0	6.940382	-4.174487	1.062561
89	6	0	5.756770	-2.406415	0.572036
90	1	0	6.206023	-1.812691	1.390412
91	1	0	5.601528	-1.745200	-0.300734
92	6	0	4.087375	-0.652863	2.727603
93	1	0	4.917812	-0.254245	2.103448
94	6	0	4.728856	-1.446466	3.906559
95	1	0	3.934304	-1.782006	4.597878
96	6	0	5.730597	-0.534116	4.666316
97	1	0	6.166549	-1.089644	5.516375
98	1	0	6.558915	-0.269334	3.981907
99	6	0	5.043467	0.760689	5.170394
100	1	0	5.786652	1.412669	5.663520
101	1	0	4.278518	0.497745	5.924799
102	6	0	4.361333	1.516618	4.000691
103	1	0	5.131531	1.843652	3.275245
104	1	0	3.849454	2.419324	4.378949
105	6	0	3.341657	0.595965	3.283040
106	1	0	2.840574	1.131084	2.453037
107	1	0	2.568767	0.293075	4.008551
108	15	0	-3.183768	1.961996	1.029502
109	6	0	-4.983774	2.320501	1.395999
110	1	0	-5.361040	2.755170	0.447064
111	6	0	-5.822438	1.035530	1.669371
112	1	0	-5.616198	0.277474	0.896607
113	1	0	-5.552702	0.616161	2.658026
114	6	0	-7.330725	1.390249	1.653571
115	1	0	-7.589903	1.773166	0.648603
116	1	0	-7.926657	0.476858	1.828940
117	6	0	-7.660754	2.458742	2.727944
118	1	0	-8.725430	2.746886	2.664132
119	1	0	-7.492823	2.028179	3.732849
120	6	0	-6.764428	3.710884	2.557776
121	1	0	-6.960716	4.433467	3.370920
122	1	0	-7.002470	4.211714	1.600770
123	6	0	-5.259641	3.323002	2.563105
124	1	0	-4.641189	4.231119	2.483128
125	1	0	-5.017034	2.832710	3.524014
126	6	0	-2.454402	3.426148	0.150708

127	1	0	-1.361666	3.264786	0.240836
128	6	0	-2.795994	3.376788	-1.366691
129	1	0	-3.889539	3.458859	-1.510025
130	1	0	-2.485121	2.397191	-1.775366
131	6	0	-2.076635	4.519920	-2.124808
132	1	0	-0.982070	4.375422	-2.044710
133	1	0	-2.345622	4.471185	-3.195068
134	6	0	-2.450381	5.903028	-1.536298
135	1	0	-1.920486	6.706381	-2.079011
136	1	0	-3.535716	6.072958	-1.661270
137	6	0	-2.090002	5.954514	-0.031381
138	1	0	-2.374516	6.931113	0.400531
139	1	0	-0.997216	5.842550	0.085115
140	6	0	-2.812721	4.820843	0.747694
141	1	0	-3.902962	4.979121	0.663664
142	1	0	-2.539163	4.867175	1.817746
143	6	0	-2.396708	1.927366	2.713665
144	1	0	-2.877273	2.741219	3.292439
145	6	0	-2.676757	0.585497	3.450336
146	1	0	-2.109244	-0.222279	2.939311
147	1	0	-3.748497	0.323908	3.394250
148	6	0	-2.238444	0.704954	4.934193
149	1	0	-2.855357	1.481143	5.425341
150	1	0	-2.429352	-0.249756	5.456649
151	6	0	-0.739389	1.081476	5.049472
152	1	0	-0.472064	1.242860	6.109486
153	1	0	-0.127850	0.241500	4.678231
154	6	0	-0.398532	2.345726	4.221225
155	1	0	0.692132	2.524515	4.245060
156	1	0	-0.891849	3.231263	4.664278
157	6	0	-0.865458	2.195048	2.747655
158	1	0	-0.324883	1.341566	2.283859
159	1	0	-0.613103	3.102903	2.180141
160	15	0	-3.049324	-2.218185	-1.107377
161	6	0	-1.363672	-2.889025	-1.468111
162	1	0	-0.823286	-2.666264	-0.525208
163	6	0	-0.644138	-2.066066	-2.572128
164	1	0	-0.761502	-0.982478	-2.363014
165	1	0	-1.103142	-2.261697	-3.561497
166	6	0	0.857897	-2.442571	-2.592725
167	1	0	1.378786	-1.899918	-3.399879
168	1	0	1.322891	-2.110609	-1.637703
169	6	0	1.082204	-3.965734	-2.754662
170	1	0	0.733965	-4.284902	-3.754969

171	1	0	2.165289	-4.177804	-2.695238
172	6	0	0.312506	-4.765363	-1.673013
173	1	0	0.701393	-4.508972	-0.668517
174	1	0	0.454761	-5.851426	-1.821507
175	6	0	-1.200026	-4.420561	-1.732655
176	1	0	-1.764332	-5.015241	-0.993145
177	1	0	-1.581017	-4.682179	-2.731385
178	6	0	-3.682769	-3.254795	0.312869
179	1	0	-4.078214	-4.212786	-0.086254
180	6	0	-2.538059	-3.551757	1.326380
181	1	0	-2.140098	-2.575595	1.674538
182	1	0	-1.710930	-4.100244	0.849469
183	6	0	-3.063207	-4.373853	2.533356
184	1	0	-3.443530	-5.346626	2.168258
185	1	0	-2.228567	-4.582527	3.225070
186	6	0	-4.195489	-3.622470	3.270905
187	1	0	-4.568853	-4.226972	4.117136
188	1	0	-3.793417	-2.676847	3.686137
189	6	0	-5.344306	-3.301764	2.285783
190	1	0	-6.132459	-2.714809	2.791070
191	1	0	-5.802922	-4.243096	1.928705
192	6	0	-4.808580	-2.494268	1.077683
193	1	0	-4.364813	-1.547201	1.451229
194	1	0	-5.636978	-2.222879	0.403197
195	6	0	-4.170757	-2.484723	-2.585089
196	1	0	-4.116254	-1.517911	-3.125127
197	6	0	-5.660314	-2.700087	-2.177066
198	1	0	-5.767242	-3.672406	-1.658960
199	1	0	-5.982217	-1.893998	-1.500279
200	6	0	-6.565314	-2.672399	-3.434627
201	1	0	-7.617433	-2.813748	-3.129580
202	1	0	-6.482402	-1.672453	-3.901016
203	6	0	-6.147751	-3.762125	-4.452159
204	1	0	-6.307227	-4.762215	-4.007784
205	1	0	-6.774510	-3.696423	-5.359570
206	6	0	-4.655483	-3.598009	-4.827461
207	1	0	-4.512666	-2.634516	-5.351161
208	1	0	-4.340288	-4.403001	-5.516154
209	6	0	-3.746549	-3.619240	-3.567379
210	1	0	-2.700929	-3.482155	-3.885690
211	1	0	-3.829880	-4.599935	-3.063810
212	1	0	5.256073	-2.341888	3.534742
213	78	0	2.760210	-0.070958	-0.223909
214	78	0	-2.983838	0.010723	-0.265103

215	35	0	-5.219825	0.741122	-1.770117
216	35	0	4.194729	-1.245090	-2.582685

Sum of electronic and zero-point Energies= -9739.079337
Sum of electronic and thermal Energies= -9738.990711
Sum of electronic and thermal Enthalpies= -9738.989767
Sum of electronic and thermal Free Energies= -9739.204091

Table S11. The theoretical Cartesian coordinates (in Å) for the structure **2Ir** in gas phase.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.030649	-1.135012	0.454857
2	8	0	-0.020641	1.013388	0.333440
3	5	0	-0.911809	-0.086888	0.333162
4	5	0	0.923724	-0.038426	0.320633
5	15	0	2.570584	1.892624	-1.440165
6	15	0	3.303028	-1.708718	1.616653
7	15	0	-2.966928	1.981512	1.329847
8	15	0	-2.895575	-1.983864	-1.348578
9	77	0	2.922922	-0.017054	-0.033035
10	77	0	-2.934777	-0.089048	0.123179
11	6	0	-3.188346	-1.079560	1.653801
12	6	0	2.733117	-1.203890	-1.427639
13	17	0	-2.506688	1.138602	-1.979622
14	17	0	3.113787	1.483582	1.917205
15	35	0	5.628591	-0.031126	-0.552433
16	35	0	-5.667563	-0.045317	-0.193141
17	8	0	-3.337452	-1.705516	2.621521
18	8	0	2.588031	-1.960079	-2.298773
19	6	0	2.034776	-1.749244	2.913768
20	1	0	1.061912	-1.989724	2.478036
21	1	0	2.287853	-2.488324	3.680651
22	1	0	1.980398	-0.755947	3.369377
23	6	0	3.323004	-3.387978	0.927051
24	1	0	4.115267	-3.461842	0.176743
25	1	0	3.495730	-4.138232	1.704450
26	1	0	2.363371	-3.592000	0.441610
27	6	0	4.858335	-1.531756	2.522141
28	1	0	4.928246	-2.292900	3.306477
29	1	0	5.698772	-1.614600	1.830047
30	1	0	4.888100	-0.532529	2.964305
31	6	0	2.092654	3.377850	-0.525881
32	1	0	2.913350	3.684552	0.125627
33	1	0	1.839711	4.183218	-1.223518
34	1	0	1.235214	3.140944	0.107955
35	6	0	1.246548	1.653821	-2.661817
36	1	0	0.281888	1.503229	-2.162655
37	1	0	1.164428	2.527328	-3.316549
38	1	0	1.462195	0.777514	-3.280749

39	6	0	4.008976	2.385392	-2.423303
40	1	0	3.767976	3.257934	-3.040081
41	1	0	4.844921	2.609889	-1.756914
42	1	0	4.327547	1.556724	-3.060793
43	6	0	-1.919629	1.958104	2.817154
44	1	0	-0.875043	1.802126	2.530746
45	1	0	-1.999292	2.903818	3.362529
46	1	0	-2.227651	1.145417	3.481494
47	6	0	-4.596420	2.481226	1.942436
48	1	0	-4.524473	3.423437	2.496328
49	1	0	-5.285716	2.585301	1.101471
50	1	0	-5.003475	1.702301	2.592916
51	6	0	-2.356662	3.387305	0.370613
52	1	0	-3.000492	3.546045	-0.496486
53	1	0	-2.333463	4.286608	0.994626
54	1	0	-1.353157	3.155319	0.003952
55	6	0	-4.063803	-1.871624	-2.725368
56	1	0	-3.974620	-2.757122	-3.363706
57	1	0	-5.080063	-1.777974	-2.336894
58	1	0	-3.837799	-0.970478	-3.300748
59	6	0	-3.289801	-3.547917	-0.514999
60	1	0	-4.279685	-3.471750	-0.056194
61	1	0	-3.287452	-4.384169	-1.220793
62	1	0	-2.556756	-3.745742	0.272461
63	6	0	-1.296600	-2.271483	-2.157560
64	1	0	-0.530134	-2.494873	-1.412204
65	1	0	-1.371024	-3.096306	-2.873326
66	1	0	-1.008207	-1.359482	-2.691148

Sum of electronic and zero-point Energies= -8549.086062
Sum of electronic and thermal Energies= -8549.037681
Sum of electronic and thermal Enthalpies= -8549.036737
Sum of electronic and thermal Free Energies= -8549.170428

Table S12. The theoretical Cartesian coordinates (in Å) for the structure **2ts** in gas phase.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.036573	0.392300	0.528371
2	8	0	-0.391681	1.339013	1.044575
3	5	0	1.280570	-0.460684	-0.023215
4	8	0	0.126047	-0.939650	0.064412
5	78	0	-2.864549	-0.185808	0.034246
6	15	0	-3.702767	1.783210	0.969614
7	6	0	-5.494854	1.292306	1.153321
8	1	0	-5.553148	0.799165	2.148511
9	6	0	-5.882059	0.224871	0.081932
10	1	0	-5.849212	0.676340	-0.928532
11	1	0	-5.159377	-0.633849	0.095265
12	6	0	-7.294487	-0.352570	0.362478
13	1	0	-7.550544	-1.099271	-0.410603
14	1	0	-7.282653	-0.864990	1.344047
15	6	0	-8.339884	0.791836	0.376666
16	1	0	-9.335709	0.381186	0.621390
17	1	0	-8.401765	1.237298	-0.634255
18	6	0	-7.953187	1.887752	1.402288
19	1	0	-8.687235	2.712476	1.366880
20	1	0	-7.974457	1.465274	2.424425
21	6	0	-6.534568	2.450861	1.114589
22	1	0	-6.276703	3.229578	1.853268
23	1	0	-6.523540	2.915501	0.110438
24	6	0	-3.666027	3.298629	-0.090575
25	1	0	-4.508702	3.949670	0.221572
26	6	0	-3.876206	2.877386	-1.577447
27	1	0	-3.042949	2.201570	-1.857495
28	1	0	-4.818840	2.309948	-1.685976
29	6	0	-3.894144	4.110079	-2.515775
30	1	0	-3.998626	3.769140	-3.561517
31	1	0	-4.775306	4.734037	-2.276768
32	6	0	-2.604124	4.950932	-2.351353
33	1	0	-2.661671	5.853420	-2.985748
34	1	0	-1.732027	4.360866	-2.690035
35	6	0	-2.399692	5.358498	-0.871845
36	1	0	-3.233977	6.008167	-0.548478
37	1	0	-1.468115	5.941198	-0.766099
38	6	0	-2.345719	4.111183	0.053302

39	1	0	-2.199837	4.423504	1.101904
40	1	0	-1.490992	3.462674	-0.224415
41	6	0	-3.043650	2.187702	2.638582
42	1	0	-2.022994	2.576478	2.445237
43	6	0	-3.868974	3.267877	3.407463
44	1	0	-3.995210	4.176509	2.791545
45	1	0	-4.873119	2.865616	3.635156
46	6	0	-3.144653	3.620401	4.735274
47	1	0	-2.158771	4.064072	4.501617
48	1	0	-3.733616	4.378710	5.281993
49	6	0	-2.956359	2.356349	5.610262
50	1	0	-3.947275	1.965429	5.906673
51	1	0	-2.412828	2.618399	6.535345
52	6	0	-2.180873	1.257053	4.839774
53	1	0	-1.158019	1.613383	4.610483
54	1	0	-2.093807	0.348092	5.461579
55	6	0	-2.885150	0.901882	3.504613
56	1	0	-3.880282	0.455826	3.709805
57	1	0	-2.284937	0.153615	2.948178
58	15	0	-2.717460	-2.425814	-0.808359
59	6	0	-1.163852	-3.094946	-1.543533
60	1	0	-0.428618	-2.932718	-0.732389
61	6	0	-0.693687	-2.238470	-2.750447
62	1	0	-1.343076	-2.432547	-3.625019
63	1	0	-0.773646	-1.165575	-2.489973
64	6	0	0.771039	-2.606833	-3.099868
65	1	0	1.108773	-2.025933	-3.977628
66	1	0	1.421071	-2.318144	-2.242848
67	6	0	0.914361	-4.126041	-3.382425
68	1	0	0.360548	-4.368146	-4.308516
69	1	0	1.975866	-4.375924	-3.558601
70	6	0	0.356648	-4.985200	-2.218328
71	1	0	0.967228	-4.825956	-1.309872
72	1	0	0.419108	-6.057119	-2.479772
73	6	0	-1.117834	-4.613979	-1.897757
74	1	0	-1.483306	-5.226602	-1.055055
75	1	0	-1.752425	-4.824934	-2.774273
76	6	0	-3.143559	-3.556747	0.599487
77	1	0	-3.300908	-4.585475	0.214476
78	6	0	-1.956198	-3.552191	1.609452
79	1	0	-1.784498	-2.500171	1.918690
80	1	0	-1.033129	-3.917223	1.124120
81	6	0	-2.271406	-4.418496	2.855242
82	1	0	-2.384361	-5.474537	2.546561

83	1	0	-1.421126	-4.364445	3.557807
84	6	0	-3.567763	-3.937874	3.551036
85	1	0	-3.421750	-2.903849	3.921684
86	1	0	-3.789943	-4.577762	4.423455
87	6	0	-4.753709	-3.963685	2.556866
88	1	0	-5.673432	-3.592520	3.043228
89	1	0	-4.943455	-5.002255	2.226901
90	6	0	-4.444139	-3.083727	1.319436
91	1	0	-5.301625	-3.098221	0.621807
92	1	0	-4.292589	-2.033976	1.660811
93	6	0	-4.135398	-2.479875	-2.012360
94	1	0	-5.036473	-2.385703	-1.367739
95	6	0	-4.291685	-3.788768	-2.841619
96	1	0	-3.443268	-3.879795	-3.543008
97	6	0	-5.617643	-3.731637	-3.649285
98	1	0	-5.723442	-4.656504	-4.244135
99	1	0	-6.469437	-3.688319	-2.944634
100	6	0	-5.645200	-2.493425	-4.580676
101	1	0	-6.607358	-2.451913	-5.121451
102	1	0	-4.842787	-2.584652	-5.336206
103	6	0	-5.441372	-1.184512	-3.775138
104	1	0	-6.291661	-1.044136	-3.079414
105	1	0	-5.416854	-0.315658	-4.456527
106	6	0	-4.126157	-1.237976	-2.956451
107	1	0	-4.013571	-0.305230	-2.358565
108	1	0	-3.255832	-1.292572	-3.638505
109	78	0	3.058568	0.173719	-0.194709
110	15	0	2.488278	2.211186	-1.266811
111	6	0	4.215124	2.812223	-1.606610
112	1	0	4.508885	3.362059	-0.685612
113	6	0	5.171593	1.586621	-1.739945
114	1	0	5.085760	0.910631	-0.835155
115	1	0	4.897836	0.977699	-2.623921
116	6	0	6.652962	2.039412	-1.820220
117	1	0	6.924537	2.548189	-0.874724
118	1	0	7.305094	1.155118	-1.936754
119	6	0	6.837214	3.012034	-3.014836
120	1	0	7.885126	3.360437	-3.043124
121	1	0	6.640101	2.467472	-3.957526
122	6	0	5.878843	4.225700	-2.904185
123	1	0	6.006299	4.886257	-3.780294
124	1	0	6.127796	4.815922	-2.002228
125	6	0	4.396599	3.769104	-2.820568
126	1	0	3.732684	4.645392	-2.716395

127	1	0	4.119874	3.242824	-3.752587
128	6	0	1.729841	3.361247	-0.043819
129	1	0	0.679632	3.024363	0.067676
130	6	0	2.410292	3.165137	1.346937
131	1	0	3.489389	3.415773	1.285180
132	1	0	2.308543	2.100955	1.650353
133	6	0	1.729095	4.069291	2.405802
134	1	0	0.671759	3.755914	2.505165
135	1	0	2.223253	3.922728	3.382877
136	6	0	1.804316	5.555653	1.976587
137	1	0	1.312231	6.192264	2.733183
138	1	0	2.862969	5.869358	1.914623
139	6	0	1.116699	5.751936	0.603602
140	1	0	1.180099	6.808551	0.286618
141	1	0	0.048237	5.490504	0.699070
142	6	0	1.760752	4.855774	-0.491566
143	1	0	2.807947	5.173846	-0.650705
144	1	0	1.213688	4.976664	-1.445518
145	6	0	1.515538	2.159473	-2.828003
146	1	0	1.560284	3.166890	-3.295760
147	6	0	2.122065	1.113501	-3.814110
148	1	0	2.076155	0.115268	-3.330926
149	1	0	3.182584	1.341750	-4.022463
150	6	0	1.319244	1.103019	-5.141984
151	1	0	1.418009	2.091486	-5.628060
152	1	0	1.756805	0.351056	-5.822911
153	6	0	-0.175481	0.788219	-4.890340
154	1	0	-0.734584	0.851394	-5.840743
155	1	0	-0.271783	-0.246261	-4.517426
156	6	0	-0.793817	1.764471	-3.858518
157	1	0	-1.831233	1.456465	-3.627996
158	1	0	-0.833115	2.782757	-4.287800
159	6	0	0.024096	1.802616	-2.538544
160	1	0	-0.017180	0.803696	-2.052315
161	1	0	-0.420211	2.531596	-1.836491
162	15	0	3.872951	-1.567785	1.216954
163	6	0	2.541320	-2.241105	2.302963
164	1	0	1.793121	-2.685791	1.608670
165	6	0	1.833231	-1.099136	3.099434
166	1	0	1.477851	-0.300489	2.415262
167	1	0	2.552345	-0.634319	3.803429
168	6	0	0.634776	-1.679292	3.892476
169	1	0	0.159319	-0.867707	4.470492
170	1	0	-0.112421	-2.064455	3.173515

171	6	0	1.090336	-2.819587	4.840289
172	1	0	1.768307	-2.404987	5.608993
173	1	0	0.215686	-3.242977	5.365230
174	6	0	1.827766	-3.935534	4.057728
175	1	0	1.134877	-4.414078	3.340394
176	1	0	2.185039	-4.716930	4.752387
177	6	0	3.038525	-3.353699	3.278212
178	1	0	3.554380	-4.157358	2.722370
179	1	0	3.757127	-2.913983	3.993640
180	6	0	4.641323	-2.918116	0.224624
181	1	0	5.280364	-3.531879	0.892340
182	6	0	3.555704	-3.831684	-0.415504
183	1	0	2.881806	-3.203312	-1.035162
184	1	0	2.948818	-4.311495	0.372282
185	6	0	4.219413	-4.916091	-1.306714
186	1	0	4.838313	-5.574830	-0.669304
187	1	0	3.432874	-5.541266	-1.764998
188	6	0	5.104941	-4.273264	-2.402376
189	1	0	5.582544	-5.061899	-3.010430
190	1	0	4.472387	-3.666458	-3.079592
191	6	0	6.188409	-3.368283	-1.766874
192	1	0	6.796581	-2.884599	-2.551754
193	1	0	6.867982	-3.977908	-1.142249
194	6	0	5.532400	-2.276409	-0.884630
195	1	0	4.881070	-1.637687	-1.524395
196	1	0	6.306206	-1.628375	-0.431275
197	6	0	5.164160	-0.831028	2.340072
198	1	0	4.613703	-0.569463	3.268806
199	6	0	5.756365	0.489139	1.761716
200	1	0	6.319142	0.261272	0.835302
201	1	0	4.931644	1.196666	1.509617
202	6	0	6.705082	1.156631	2.792430
203	1	0	7.127830	2.079624	2.356508
204	1	0	6.119145	1.440966	3.686797
205	6	0	7.840769	0.182632	3.195286
206	1	0	8.472648	-0.028306	2.312240
207	1	0	8.483284	0.657493	3.957861
208	6	0	7.263045	-1.144658	3.746866
209	1	0	6.700635	-0.949247	4.678955
210	1	0	8.082225	-1.844488	3.991053
211	6	0	6.317328	-1.814862	2.712412
212	1	0	5.907711	-2.753383	3.126929
213	1	0	6.890207	-2.067071	1.800403
214	1	0	-4.287614	-4.671244	-2.176603

Sum of electronic and zero-point Energies=	-4590.595265
Sum of electronic and thermal Energies=	-4590.509561
Sum of electronic and thermal Enthalpies=	-4590.508617
Sum of electronic and thermal Free Energies=	-4590.716893

Table S13. The theoretical Cartesian coordinates (in Å) for the structure **2Brts** in gas phase.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.920816	-0.020697	0.670002
2	8	0	-0.119937	0.688525	-0.369967
3	5	0	-1.310489	0.281062	-0.143349
4	8	0	0.305668	-0.571046	1.642213
5	15	0	2.799975	2.143242	-1.157538
6	6	0	4.514827	2.317498	-1.883611
7	1	0	4.439503	1.749033	-2.832209
8	6	0	5.579404	1.575433	-1.014679
9	1	0	5.745098	2.112764	-0.062185
10	1	0	5.219803	0.554088	-0.778479
11	6	0	6.912427	1.459247	-1.793584
12	1	0	7.658499	0.934341	-1.169939
13	1	0	6.737035	0.846740	-2.698310
14	6	0	7.435666	2.862045	-2.196998
15	1	0	8.359176	2.764515	-2.795507
16	1	0	7.688567	3.434744	-1.284840
17	6	0	6.364400	3.638171	-3.004900
18	1	0	6.734087	4.650071	-3.252724
19	1	0	6.168306	3.109912	-3.956679
20	6	0	5.033613	3.752595	-2.209788
21	1	0	4.299092	4.319969	-2.801192
22	1	0	5.217099	4.315548	-1.277912
23	6	0	2.631682	3.579473	0.019290
24	1	0	2.664124	4.506857	-0.591039
25	6	0	3.796494	3.621224	1.047855
26	1	0	3.789671	2.667786	1.607923
27	1	0	4.764135	3.697774	0.531334
28	6	0	3.662487	4.812845	2.029259
29	1	0	4.491670	4.775518	2.758450
30	1	0	3.756414	5.759526	1.464425
31	6	0	2.301555	4.784106	2.761263
32	1	0	2.205473	5.658301	3.430310
33	1	0	2.244655	3.873265	3.388324
34	6	0	1.149895	4.766987	1.727880
35	1	0	1.186374	5.693288	1.123692
36	1	0	0.173989	4.745651	2.244261
37	6	0	1.280933	3.539251	0.786840
38	1	0	0.433019	3.511587	0.078993

39	1	0	1.249321	2.605268	1.387447
40	6	0	1.546651	2.534982	-2.479198
41	1	0	0.635643	2.818947	-1.911964
42	6	0	1.912446	3.701098	-3.448243
43	1	0	2.149205	4.622682	-2.886364
44	1	0	2.805490	3.412405	-4.031471
45	6	0	0.741009	3.981938	-4.431176
46	1	0	-0.128552	4.357231	-3.863379
47	1	0	1.044458	4.778625	-5.134677
48	6	0	0.337107	2.707553	-5.214777
49	1	0	1.174526	2.401715	-5.869001
50	1	0	-0.531055	2.926556	-5.862271
51	6	0	0.006233	1.544074	-4.244639
52	1	0	-0.887228	1.804945	-3.641337
53	1	0	-0.232097	0.631289	-4.819541
54	6	0	1.200327	1.264683	-3.299724
55	1	0	2.083372	0.948757	-3.886872
56	1	0	0.962815	0.445997	-2.602403
57	15	0	3.502950	-1.680390	1.371107
58	6	0	2.318603	-2.687431	2.419996
59	1	0	1.416328	-2.776104	1.781139
60	6	0	1.878831	-1.947077	3.718154
61	1	0	2.722338	-1.932847	4.434065
62	1	0	1.587356	-0.915466	3.474603
63	6	0	0.672609	-2.678698	4.356046
64	1	0	0.355970	-2.143763	5.269575
65	1	0	-0.169454	-2.642744	3.639628
66	6	0	1.035454	-4.145638	4.700481
67	1	0	1.801633	-4.149164	5.497773
68	1	0	0.150340	-4.680247	5.090902
69	6	0	1.594623	-4.887105	3.459902
70	1	0	0.798503	-4.989711	2.698536
71	1	0	1.918361	-5.906023	3.740807
72	6	0	2.788163	-4.123305	2.821318
73	1	0	3.146739	-4.694740	1.951053
74	1	0	3.619320	-4.051739	3.546474
75	6	0	4.664381	-2.945919	0.638520
76	1	0	4.973661	-3.629568	1.455580
77	6	0	3.890710	-3.761117	-0.434784
78	1	0	3.539856	-3.059581	-1.213853
79	1	0	3.005893	-4.238506	0.021723
80	6	0	4.791352	-4.841265	-1.083002
81	1	0	5.090137	-5.584708	-0.318799
82	1	0	4.213905	-5.372254	-1.861355

83	6	0	6.048764	-4.188030	-1.703683
84	1	0	5.730734	-3.485106	-2.497582
85	1	0	6.694823	-4.958069	-2.162666
86	6	0	6.837209	-3.404188	-0.626582
87	1	0	7.718986	-2.918402	-1.081886
88	1	0	7.201851	-4.100641	0.153181
89	6	0	5.948126	-2.313566	0.027894
90	1	0	6.529404	-1.787323	0.807186
91	1	0	5.653807	-1.583856	-0.747839
92	6	0	4.624492	-0.674206	2.471612
93	1	0	5.303600	-0.202671	1.727153
94	6	0	5.514027	-1.478490	3.467796
95	1	0	4.884700	-1.879766	4.283165
96	6	0	6.598984	-0.532809	4.054991
97	1	0	7.222551	-1.086489	4.780319
98	1	0	7.261375	-0.202846	3.231948
99	6	0	5.967258	0.708079	4.737827
100	1	0	6.764926	1.383943	5.095339
101	1	0	5.388078	0.380755	5.621380
102	6	0	5.020686	1.461382	3.766156
103	1	0	5.606585	1.863870	2.916680
104	1	0	4.544568	2.314626	4.281905
105	6	0	3.934727	0.494001	3.231687
106	1	0	3.225543	1.012081	2.557131
107	1	0	3.362836	0.102768	4.088612
108	15	0	-3.567887	1.953942	1.022923
109	6	0	-5.374597	2.248412	1.351593
110	1	0	-5.800782	2.494399	0.357250
111	6	0	-6.082875	0.954327	1.858779
112	1	0	-5.805544	0.093735	1.225421
113	1	0	-5.765548	0.748446	2.899022
114	6	0	-7.617236	1.162058	1.825202
115	1	0	-7.926134	1.355317	0.780290
116	1	0	-8.122075	0.238498	2.160054
117	6	0	-8.025698	2.353589	2.729584
118	1	0	-9.113183	2.532634	2.654524
119	1	0	-7.801550	2.102553	3.783011
120	6	0	-7.253144	3.638814	2.338905
121	1	0	-7.500227	4.458279	3.038260
122	1	0	-7.557358	3.960891	1.325556
123	6	0	-5.716391	3.401446	2.350015
124	1	0	-5.198018	4.336773	2.089858
125	1	0	-5.398932	3.110804	3.367842
126	6	0	-2.825972	3.393775	0.125369

127	1	0	-1.737610	3.165242	0.151423
128	6	0	-3.257242	3.389245	-1.371705
129	1	0	-4.337743	3.616217	-1.451391
130	1	0	-3.097490	2.383263	-1.805339
131	6	0	-2.427587	4.438202	-2.152262
132	1	0	-1.361542	4.145025	-2.104083
133	1	0	-2.730315	4.432847	-3.214637
134	6	0	-2.591209	5.855457	-1.547895
135	1	0	-1.963951	6.576966	-2.101662
136	1	0	-3.643613	6.178897	-1.650588
137	6	0	-2.198149	5.853847	-0.048906
138	1	0	-2.352047	6.856137	0.390085
139	1	0	-1.125815	5.604467	0.052272
140	6	0	-3.042907	4.812251	0.734336
141	1	0	-4.109135	5.083828	0.640623
142	1	0	-2.776026	4.828371	1.806548
143	6	0	-2.772279	1.818718	2.698614
144	1	0	-3.342281	2.481926	3.382025
145	6	0	-2.849582	0.354715	3.228776
146	1	0	-2.251775	-0.285900	2.547815
147	1	0	-3.892228	-0.011667	3.218994
148	6	0	-2.259240	0.257403	4.657963
149	1	0	-2.860147	0.876606	5.351049
150	1	0	-2.317824	-0.789932	5.004319
151	6	0	-0.786309	0.729401	4.656057
152	1	0	-0.359999	0.668956	5.673812
153	1	0	-0.204195	0.063296	3.993220
154	6	0	-0.674465	2.173162	4.113598
155	1	0	0.388311	2.473198	4.066138
156	1	0	-1.195197	2.879138	4.788831
157	6	0	-1.285645	2.270397	2.691482
158	1	0	-0.711873	1.598129	2.022164
159	1	0	-1.197061	3.300315	2.312338
160	15	0	-2.991608	-2.259207	-1.065833
161	6	0	-1.252749	-2.676266	-1.537386
162	1	0	-0.667956	-2.287282	-0.671100
163	6	0	-0.778111	-1.873090	-2.782190
164	1	0	-1.010400	-0.798411	-2.639540
165	1	0	-1.317288	-2.213052	-3.687910
166	6	0	0.748775	-2.067946	-2.956939
167	1	0	1.102592	-1.531908	-3.853789
168	1	0	1.269899	-1.611747	-2.088781
169	6	0	1.153184	-3.556598	-3.037265
170	1	0	0.732245	-4.017412	-3.950841

171	1	0	2.254971	-3.615452	-3.103708
172	6	0	0.643164	-4.322752	-1.793337
173	1	0	1.098555	-3.889209	-0.882308
174	1	0	0.926751	-5.389687	-1.843109
175	6	0	-0.898047	-4.191986	-1.688819
176	1	0	-1.282836	-4.776522	-0.835421
177	1	0	-1.349870	-4.600499	-2.605045
178	6	0	-3.351088	-3.265610	0.463239
179	1	0	-3.616655	-4.295243	0.139625
180	6	0	-2.118435	-3.341000	1.418182
181	1	0	-1.857340	-2.314722	1.749351
182	1	0	-1.236087	-3.754728	0.905669
183	6	0	-2.460785	-4.231319	2.641175
184	1	0	-2.697503	-5.253046	2.288008
185	1	0	-1.579478	-4.303782	3.300958
186	6	0	-3.665605	-3.664086	3.428752
187	1	0	-3.908427	-4.321588	4.282907
188	1	0	-3.394309	-2.671492	3.836810
189	6	0	-4.894470	-3.513911	2.500593
190	1	0	-5.732350	-3.041915	3.044612
191	1	0	-5.232300	-4.511780	2.162500
192	6	0	-4.541297	-2.651152	1.264398
193	1	0	-4.227663	-1.641637	1.606890
194	1	0	-5.429579	-2.519892	0.626200
195	6	0	-4.178904	-2.769593	-2.423994
196	1	0	-4.294176	-1.845888	-3.027149
197	6	0	-5.590716	-3.150829	-1.878203
198	1	0	-5.516361	-4.077321	-1.276761
199	1	0	-5.978832	-2.340531	-1.242163
200	6	0	-6.581646	-3.366226	-3.051268
201	1	0	-7.574374	-3.625253	-2.642206
202	1	0	-6.685166	-2.413320	-3.604290
203	6	0	-6.085400	-4.474523	-4.010536
204	1	0	-6.056993	-5.441496	-3.474823
205	1	0	-6.783052	-4.583523	-4.860013
206	6	0	-4.669648	-4.130793	-4.529853
207	1	0	-4.714178	-3.207051	-5.136177
208	1	0	-4.289382	-4.939916	-5.179651
209	6	0	-3.673257	-3.913480	-3.357561
210	1	0	-2.686341	-3.663365	-3.777313
211	1	0	-3.576965	-4.848591	-2.775747
212	1	0	6.001786	-2.330616	2.964560
213	78	0	2.767078	-0.027287	-0.172332
214	78	0	-3.210575	0.001088	-0.296936

215	35	0	-5.558910	0.340323	-1.550574
216	35	0	4.073518	-0.957877	-2.850672

Sum of electronic and zero-point Energies= -9739.031755
Sum of electronic and thermal Energies= -9738.943254
Sum of electronic and thermal Enthalpies= -9738.942310
Sum of electronic and thermal Free Energies= -9739.156207

Table S14. The theoretical Cartesian coordinates (in Å) for the structure **1** in dichloromethane.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.360326	0.456323	0.182226
2	6	0	2.878519	2.216271	0.362931
3	1	0	3.862292	2.239817	0.878420
4	6	0	1.830185	2.981897	1.230272
5	1	0	0.842314	2.908715	0.727978
6	1	0	1.736280	2.513324	2.228262
7	6	0	2.224247	4.473845	1.377301
8	1	0	1.456974	4.991299	1.980361
9	1	0	3.184814	4.543890	1.920609
10	6	0	2.359626	5.141640	-0.013508
11	1	0	1.378100	5.125070	-0.524583
12	1	0	2.659170	6.198569	0.102373
13	6	0	3.400033	4.388782	-0.877875
14	1	0	4.396770	4.456324	-0.403846
15	1	0	3.470937	4.848556	-1.879687
16	6	0	3.016044	2.894023	-1.035659
17	1	0	3.776081	2.374527	-1.644557
18	1	0	2.044776	2.820562	-1.569234
19	6	0	3.364797	-0.357103	-1.130639
20	1	0	3.056317	0.178816	-2.054033
21	6	0	4.912459	-0.224274	-0.988879
22	1	0	5.200191	0.833481	-0.854712
23	1	0	5.256576	-0.786241	-0.104305
24	6	0	5.586417	-0.803758	-2.262917
25	1	0	5.281494	-0.201320	-3.138871
26	1	0	6.683509	-0.720484	-2.162906
27	6	0	5.180917	-2.283967	-2.479552
28	1	0	5.555001	-2.892183	-1.635180
29	1	0	5.648758	-2.669668	-3.402849
30	6	0	3.640420	-2.430660	-2.572317
31	1	0	3.362781	-3.494126	-2.682580
32	1	0	3.268215	-1.888994	-3.462367
33	6	0	2.952252	-1.849786	-1.309970
34	1	0	3.259942	-2.430072	-0.419835
35	1	0	1.848862	-1.927354	-1.410247
36	6	0	2.495983	-0.360731	1.845302
37	1	0	2.170192	0.431198	2.554513
38	6	0	3.904591	-0.853233	2.283294

39	1	0	4.240855	-1.659478	1.605611
40	1	0	4.630456	-0.022423	2.220599
41	6	0	3.837990	-1.400273	3.734656
42	1	0	4.838543	-1.761129	4.032705
43	1	0	3.557989	-0.579094	4.420647
44	6	0	2.804596	-2.549766	3.848362
45	1	0	2.755424	-2.911870	4.890857
46	1	0	3.122497	-3.396921	3.212058
47	6	0	1.396846	-2.077746	3.401561
48	1	0	1.038539	-1.274678	4.073922
49	1	0	0.673876	-2.911885	3.445178
50	6	0	1.456367	-1.523479	1.953298
51	1	0	0.407184	-1.165504	1.717743
52	1	0	1.698128	-2.328323	1.233011
53	8	0	-0.305605	2.042184	-2.604080
54	5	0	-0.148033	1.296759	-1.634917
55	78	0	0.049538	0.115358	-0.144136
56	15	0	-2.272229	-0.372642	-0.212041
57	6	0	-2.487024	-1.925839	-1.191389
58	1	0	-3.563470	-2.195530	-1.214746
59	6	0	-1.991366	-1.681777	-2.652058
60	1	0	-0.925906	-1.369245	-2.613102
61	1	0	-2.568081	-0.865875	-3.124702
62	6	0	-2.112786	-2.974386	-3.499721
63	1	0	-1.736780	-2.773583	-4.518647
64	1	0	-3.179194	-3.255434	-3.582590
65	6	0	-1.317156	-4.132958	-2.850246
66	1	0	-0.240979	-3.872772	-2.831537
67	1	0	-1.428280	-5.052478	-3.452036
68	6	0	-1.809721	-4.384505	-1.404422
69	1	0	-2.867973	-4.705766	-1.422927
70	1	0	-1.221005	-5.190741	-0.931717
71	6	0	-1.689023	-3.099655	-0.545219
72	1	0	-2.057198	-3.300724	0.476706
73	1	0	-0.615973	-2.811421	-0.475339
74	6	0	-2.752353	-0.716878	1.544363
75	1	0	-2.218468	-1.663162	1.779645
76	6	0	-4.276008	-0.956878	1.769290
77	1	0	-4.654953	-1.713482	1.058467
78	1	0	-4.821680	-0.011999	1.595547
79	6	0	-4.516780	-1.428525	3.229182
80	1	0	-4.014478	-2.401934	3.382382
81	1	0	-5.599725	-1.580834	3.386019
82	6	0	-3.969538	-0.392645	4.243450

83	1	0	-4.532469	0.553592	4.140462
84	1	0	-4.119414	-0.760793	5.274054
85	6	0	-2.463736	-0.119888	3.997610
86	1	0	-2.093449	0.646983	4.700927
87	1	0	-1.884767	-1.047394	4.171165
88	6	0	-2.218501	0.358089	2.542775
89	1	0	-2.733215	1.321194	2.371987
90	1	0	-1.129864	0.531678	2.391899
91	6	0	-3.288806	0.940923	-1.016685
92	1	0	-2.763139	1.103330	-1.982849
93	6	0	-4.765412	0.559191	-1.348008
94	1	0	-5.345597	0.448125	-0.416080
95	1	0	-4.804979	-0.399874	-1.893430
96	6	0	-5.387906	1.686255	-2.217614
97	1	0	-6.438302	1.430225	-2.445140
98	1	0	-4.839672	1.743497	-3.176505
99	6	0	-5.316313	3.054902	-1.493927
100	1	0	-5.734430	3.843602	-2.144555
101	1	0	-5.933572	3.015685	-0.577335
102	6	0	-3.856204	3.408490	-1.111044
103	1	0	-3.246979	3.528326	-2.027199
104	1	0	-3.826543	4.364294	-0.557988
105	6	0	-3.230905	2.289251	-0.238273
106	1	0	-2.180598	2.539798	0.012692
107	1	0	-3.799654	2.196846	0.706124

Sum of electronic and zero-point Energies= -2295.360649
Sum of electronic and thermal Energies= -2295.318049
Sum of electronic and thermal Enthalpies= -2295.317105
Sum of electronic and thermal Free Energies= -2295.436417

Table S15. The theoretical Cartesian coordinates (in Å) for the structure **1Br** in dichloromethane.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.000000	0.000000	2.718172
2	15	0	0.000000	2.385127	-0.114593
3	6	0	-1.749592	2.954465	-0.340319
4	1	0	-1.762283	4.064373	-0.356705
5	6	0	-2.605806	2.454828	0.863262
6	1	0	-2.550309	1.345685	0.893904
7	1	0	-2.191987	2.836332	1.814300
8	6	0	-4.084060	2.893200	0.713586
9	1	0	-4.666086	2.506214	1.568937
10	1	0	-4.141042	3.997766	0.739007
11	6	0	-4.675830	2.372621	-0.619213
12	1	0	-4.671092	1.264909	-0.611678
13	1	0	-5.725234	2.701640	-0.724505
14	6	0	-3.836108	2.877260	-1.818118
15	1	0	-3.884557	3.981222	-1.866283
16	1	0	-4.242839	2.480557	-2.765481
17	6	0	-2.356153	2.436460	-1.677885
18	1	0	-1.772556	2.812361	-2.536877
19	1	0	-2.306628	1.328113	-1.684450
20	6	0	0.944440	2.939213	-1.606677
21	1	0	0.345504	2.526859	-2.446804
22	6	0	1.050615	4.479783	-1.819450
23	1	0	0.059256	4.957531	-1.720828
24	1	0	1.719800	4.910945	-1.053670
25	6	0	1.635518	4.755480	-3.232785
26	1	0	0.931697	4.368278	-3.993261
27	1	0	1.726838	5.846197	-3.384808
28	6	0	3.016958	4.075360	-3.408787
29	1	0	3.738667	4.530905	-2.705536
30	1	0	3.392458	4.251427	-4.432678
31	6	0	2.929658	2.551694	-3.131503
32	1	0	3.929900	2.090403	-3.215848
33	1	0	2.270398	2.072215	-3.880381
34	6	0	2.353988	2.286875	-1.717854
35	1	0	3.033062	2.716858	-0.958616
36	1	0	2.282240	1.197107	-1.529709
37	6	0	0.618471	3.201455	1.424404
38	1	0	0.075038	2.661590	2.224822

39	6	0	0.316077	4.722337	1.596648
40	1	0	0.898210	5.313991	0.869814
41	1	0	-0.754850	4.929062	1.427494
42	6	0	0.707033	5.142827	3.041140
43	1	0	0.505641	6.221290	3.174537
44	1	0	0.070314	4.591257	3.758298
45	6	0	2.198719	4.838152	3.334275
46	1	0	2.438326	5.113433	4.376989
47	1	0	2.833688	5.454699	2.671292
48	6	0	2.517221	3.339666	3.094986
49	1	0	1.945698	2.719268	3.812295
50	1	0	3.591699	3.145216	3.262712
51	6	0	2.132228	2.923721	1.652995
52	1	0	2.344120	1.848066	1.495675
53	1	0	2.730772	3.510947	0.933046
54	8	0	0.000000	0.000000	-3.175712
55	5	0	0.000000	0.000000	-1.938901
56	78	0	0.000000	0.000000	0.011635
57	15	0	0.000000	-2.385127	-0.114593
58	6	0	1.749592	-2.954465	-0.340319
59	1	0	1.762283	-4.064373	-0.356705
60	6	0	2.356153	-2.436460	-1.677885
61	1	0	2.306628	-1.328113	-1.684450
62	1	0	1.772556	-2.812361	-2.536877
63	6	0	3.836108	-2.877260	-1.818118
64	1	0	4.242839	-2.480557	-2.765481
65	1	0	3.884557	-3.981222	-1.866283
66	6	0	4.675830	-2.372621	-0.619213
67	1	0	4.671092	-1.264909	-0.611678
68	1	0	5.725234	-2.701640	-0.724505
69	6	0	4.084060	-2.893200	0.713586
70	1	0	4.141042	-3.997766	0.739007
71	1	0	4.666086	-2.506214	1.568937
72	6	0	2.605806	-2.454828	0.863262
73	1	0	2.191987	-2.836332	1.814300
74	1	0	2.550309	-1.345685	0.893904
75	6	0	-0.618471	-3.201455	1.424404
76	1	0	-0.075038	-2.661590	2.224822
77	6	0	-0.316077	-4.722337	1.596648
78	1	0	0.754850	-4.929062	1.427494
79	1	0	-0.898210	-5.313991	0.869814
80	6	0	-0.707033	-5.142827	3.041140
81	1	0	-0.070314	-4.591257	3.758298
82	1	0	-0.505641	-6.221290	3.174537

83	6	0	-2.198719	-4.838152	3.334275
84	1	0	-2.833688	-5.454699	2.671292
85	1	0	-2.438326	-5.113433	4.376989
86	6	0	-2.517221	-3.339666	3.094986
87	1	0	-3.591699	-3.145216	3.262712
88	1	0	-1.945698	-2.719268	3.812295
89	6	0	-2.132228	-2.923721	1.652995
90	1	0	-2.730772	-3.510947	0.933046
91	1	0	-2.344120	-1.848066	1.495675
92	6	0	-0.944440	-2.939213	-1.606677
93	1	0	-0.345504	-2.526859	-2.446804
94	6	0	-1.050615	-4.479783	-1.819450
95	1	0	-1.719800	-4.910945	-1.053670
96	1	0	-0.059256	-4.957531	-1.720828
97	6	0	-1.635518	-4.755480	-3.232785
98	1	0	-1.726838	-5.846197	-3.384808
99	1	0	-0.931697	-4.368278	-3.993261
100	6	0	-3.016958	-4.075360	-3.408787
101	1	0	-3.392458	-4.251427	-4.432678
102	1	0	-3.738667	-4.530905	-2.705536
103	6	0	-2.929658	-2.551694	-3.131503
104	1	0	-2.270398	-2.072215	-3.880381
105	1	0	-3.929900	-2.090403	-3.215848
106	6	0	-2.353988	-2.286875	-1.717854
107	1	0	-2.282240	-1.197107	-1.529709
108	1	0	-3.033062	-2.716858	-0.958616

Sum of electronic and zero-point Energies= -4869.566024

Sum of electronic and thermal Energies= -4869.522201

Sum of electronic and thermal Enthalpies= -4869.521257

Sum of electronic and thermal Free Energies= -4869.642451

Table S16. The theoretical Cartesian coordinates (in Å) for the structure **2** in dichloromethane.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.840104	0.009638	-0.119629
2	8	0	-0.067383	1.078412	-0.338119
3	5	0	-0.991857	0.033072	-0.087235
4	8	0	-0.085760	-1.034517	0.122476
5	78	0	2.784977	-0.019115	-0.136698
6	15	0	3.097113	2.040918	-1.273617
7	6	0	4.652714	1.795747	-2.263932
8	1	0	4.303212	1.554003	-3.291011
9	6	0	5.428813	0.549989	-1.737621
10	1	0	5.761128	0.725346	-0.693171
11	1	0	4.746435	-0.330768	-1.749657
12	6	0	6.657521	0.237013	-2.631092
13	1	0	7.206737	-0.625148	-2.211906
14	1	0	6.300361	-0.042946	-3.640141
15	6	0	7.584565	1.474627	-2.731000
16	1	0	8.436367	1.249410	-3.397368
17	1	0	7.993641	1.705131	-1.729138
18	6	0	6.805962	2.703919	-3.264892
19	1	0	7.472827	3.583220	-3.314448
20	1	0	6.444694	2.497679	-4.289775
21	6	0	5.593942	3.034277	-2.353803
22	1	0	5.045938	3.905736	-2.751206
23	1	0	5.960012	3.297436	-1.344916
24	6	0	3.382631	3.349019	0.000140
25	1	0	3.744330	4.275317	-0.492170
26	6	0	4.456904	2.859029	1.020056
27	1	0	4.097781	1.908273	1.473981
28	1	0	5.413777	2.646847	0.511179
29	6	0	4.670542	3.902346	2.144952
30	1	0	5.425216	3.519571	2.855057
31	1	0	5.064656	4.835995	1.701822
32	6	0	3.338396	4.189433	2.878415
33	1	0	3.494409	4.946170	3.667882
34	1	0	2.991213	3.259912	3.369794
35	6	0	2.259583	4.678414	1.880133
36	1	0	2.573233	5.642290	1.437831
37	1	0	1.301275	4.846005	2.404541
38	6	0	2.045466	3.644169	0.744203

39	1	0	1.285433	4.015966	0.034267
40	1	0	1.670740	2.691235	1.173694
41	6	0	1.811434	2.637846	-2.453629
42	1	0	0.948917	2.950482	-1.831079
43	6	0	2.290590	3.845560	-3.320169
44	1	0	2.601161	4.684380	-2.671684
45	1	0	3.162498	3.534559	-3.923037
46	6	0	1.159114	4.312125	-4.276508
47	1	0	0.326199	4.726727	-3.682213
48	1	0	1.546356	5.124629	-4.917419
49	6	0	0.644754	3.143999	-5.155086
50	1	0	1.453078	2.812257	-5.832834
51	1	0	-0.195625	3.491884	-5.782189
52	6	0	0.188959	1.943853	-4.285682
53	1	0	-0.674589	2.239700	-3.659117
54	1	0	-0.134760	1.109760	-4.933448
55	6	0	1.335838	1.466245	-3.359608
56	1	0	2.182870	1.091492	-3.969747
57	1	0	0.991636	0.630496	-2.718743
58	15	0	3.023972	-2.026329	1.098674
59	6	0	1.722403	-2.629225	2.256176
60	1	0	0.929835	-2.972546	1.559926
61	6	0	1.050136	-1.559858	3.162685
62	1	0	1.747818	-1.221431	3.950334
63	1	0	0.763801	-0.675510	2.557126
64	6	0	-0.207576	-2.201904	3.809222
65	1	0	-0.713749	-1.470188	4.461237
66	1	0	-0.913418	-2.475737	3.003588
67	6	0	0.160581	-3.462421	4.634590
68	1	0	0.788384	-3.161605	5.493665
69	1	0	-0.759987	-3.921723	5.038132
70	6	0	0.931997	-4.496775	3.777909
71	1	0	0.275340	-4.889059	2.979168
72	1	0	1.247732	-5.350868	4.403636
73	6	0	2.179476	-3.849552	3.119423
74	1	0	2.705771	-4.596719	2.499348
75	1	0	2.876915	-3.501391	3.901997
76	6	0	3.406005	-3.492333	0.026781
77	1	0	3.970603	-4.216298	0.648794
78	6	0	2.122914	-4.204815	-0.493414
79	1	0	1.538152	-3.495185	-1.111945
80	1	0	1.487231	-4.530454	0.347083
81	6	0	2.521758	-5.443819	-1.338754
82	1	0	3.067409	-6.155584	-0.691712

83	1	0	1.609797	-5.953734	-1.696962
84	6	0	3.417631	-5.036825	-2.533697
85	1	0	2.848692	-4.366107	-3.205095
86	1	0	3.701957	-5.931163	-3.116297
87	6	0	4.687383	-4.304552	-2.033021
88	1	0	5.305861	-3.975505	-2.887141
89	1	0	5.297202	-4.993315	-1.418862
90	6	0	4.302763	-3.070534	-1.175852
91	1	0	5.213493	-2.555912	-0.815923
92	1	0	3.727561	-2.357887	-1.804937
93	6	0	4.609268	-1.586078	1.967601
94	1	0	5.172724	-1.006651	1.200796
95	6	0	5.528184	-2.767476	2.406879
96	1	0	5.028295	-3.349892	3.200985
97	6	0	6.873662	-2.198807	2.934306
98	1	0	7.513716	-3.034497	3.269960
99	1	0	7.396473	-1.691708	2.101028
100	6	0	6.653786	-1.195543	4.093898
101	1	0	7.624815	-0.781131	4.418578
102	1	0	6.210362	-1.725336	4.957404
103	6	0	5.706932	-0.046805	3.661872
104	1	0	6.175833	0.536361	2.844542
105	1	0	5.525985	0.641583	4.506431
106	6	0	4.356294	-0.622202	3.164449
107	1	0	3.671936	0.196286	2.860085
108	1	0	3.875506	-1.182521	3.986937
109	78	0	-2.938540	0.046924	-0.049478
110	15	0	-3.033653	2.081841	1.146354
111	6	0	-4.851697	2.463417	1.343433
112	1	0	-5.110873	3.096632	0.467937
113	6	0	-5.697338	1.158290	1.244867
114	1	0	-5.486431	0.648844	0.278860
115	1	0	-5.425667	0.470344	2.068950
116	6	0	-7.217331	1.464627	1.289974
117	1	0	-7.488408	2.060427	0.398002
118	1	0	-7.780447	0.515119	1.249423
119	6	0	-7.575871	2.254569	2.572190
120	1	0	-8.653574	2.496869	2.573259
121	1	0	-7.371725	1.624927	3.458450
122	6	0	-6.740172	3.556734	2.659484
123	1	0	-6.984217	4.104895	3.587142
124	1	0	-6.987091	4.214610	1.805428
125	6	0	-5.218864	3.245558	2.640370
126	1	0	-4.641921	4.184993	2.698680

127	1	0	-4.962546	2.632861	3.524276
128	6	0	-2.304433	3.456794	0.162212
129	1	0	-1.214532	3.251515	0.139636
130	6	0	-2.811945	3.399744	-1.308417
131	1	0	-3.907932	3.561709	-1.341395
132	1	0	-2.600794	2.393186	-1.725295
133	6	0	-2.092029	4.486259	-2.145480
134	1	0	-1.010492	4.257276	-2.144676
135	1	0	-2.446532	4.449342	-3.191331
136	6	0	-2.311799	5.897549	-1.544609
137	1	0	-1.768798	6.647651	-2.147082
138	1	0	-3.387426	6.150450	-1.583546
139	6	0	-1.824129	5.946838	-0.074778
140	1	0	-2.017377	6.944224	0.359379
141	1	0	-0.732607	5.769797	-0.037626
142	6	0	-2.543779	4.868893	0.780693
143	1	0	-3.628093	5.082066	0.796086
144	1	0	-2.171965	4.903610	1.820677
145	6	0	-2.274297	2.131299	2.824256
146	1	0	-2.700873	3.009034	3.350867
147	6	0	-2.627105	0.849738	3.635048
148	1	0	-2.146356	-0.018924	3.138539
149	1	0	-3.719506	0.674657	3.637300
150	6	0	-2.112972	1.000656	5.091783
151	1	0	-2.662760	1.830575	5.573794
152	1	0	-2.336450	0.078539	5.658247
153	6	0	-0.589770	1.291306	5.134013
154	1	0	-0.280697	1.491161	6.175565
155	1	0	-0.035865	0.400220	4.792389
156	6	0	-0.201085	2.490773	4.234605
157	1	0	0.897921	2.601237	4.212547
158	1	0	-0.624389	3.425972	4.646475
159	6	0	-0.728661	2.308089	2.786003
160	1	0	-0.266857	1.406962	2.324875
161	1	0	-0.449432	3.180476	2.172751
162	15	0	-3.146285	-1.982044	-1.296300
163	6	0	-1.632054	-2.565714	-2.172228
164	1	0	-0.886009	-2.748214	-1.373414
165	6	0	-1.062111	-1.450003	-3.096584
166	1	0	-0.917089	-0.513978	-2.514438
167	1	0	-1.786234	-1.217184	-3.903628
168	6	0	0.281806	-1.910672	-3.718245
169	1	0	0.670556	-1.121180	-4.384815
170	1	0	1.021980	-2.060600	-2.904753

171	6	0	0.097517	-3.233071	-4.507074
172	1	0	-0.587061	-3.053706	-5.356728
173	1	0	1.067181	-3.560878	-4.922330
174	6	0	-0.491745	-4.339547	-3.598221
175	1	0	0.220900	-4.571773	-2.787078
176	1	0	-0.652477	-5.264887	-4.180005
177	6	0	-1.840328	-3.886688	-2.976462
178	1	0	-2.237154	-4.679428	-2.317260
179	1	0	-2.570506	-3.711471	-3.786637
180	6	0	-3.638586	-3.269703	-0.063890
181	1	0	-3.952469	-4.195797	-0.587291
182	6	0	-2.429155	-3.588962	0.863760
183	1	0	-2.087473	-2.635862	1.319429
184	1	0	-1.589790	-4.002886	0.276520
185	6	0	-2.834157	-4.587910	1.978535
186	1	0	-3.111738	-5.552801	1.514925
187	1	0	-1.966335	-4.769172	2.636783
188	6	0	-4.026284	-4.049014	2.806457
189	1	0	-4.310705	-4.782730	3.581653
190	1	0	-3.722156	-3.116742	3.322909
191	6	0	-5.233863	-3.751770	1.884738
192	1	0	-6.075758	-3.341938	2.470648
193	1	0	-5.578242	-4.686862	1.404531
194	6	0	-4.832945	-2.734581	0.787027
195	1	0	-4.516164	-1.790155	1.286698
196	1	0	-5.698321	-2.498412	0.140937
197	6	0	-4.474949	-1.853351	-2.599963
198	1	0	-3.921203	-1.657323	-3.542862
199	6	0	-5.438806	-0.648292	-2.371323
200	1	0	-6.013184	-0.806517	-1.437395
201	1	0	-4.847512	0.286552	-2.264726
202	6	0	-6.418255	-0.504688	-3.565549
203	1	0	-7.105359	0.339052	-3.375505
204	1	0	-5.836893	-0.270464	-4.477029
205	6	0	-7.219450	-1.812780	-3.782639
206	1	0	-7.857814	-2.000740	-2.899294
207	1	0	-7.883484	-1.704080	-4.658687
208	6	0	-6.263668	-3.014088	-3.989737
209	1	0	-5.671838	-2.864954	-4.912101
210	1	0	-6.843773	-3.946594	-4.109717
211	6	0	-5.296989	-3.167136	-2.785122
212	1	0	-4.625596	-4.027615	-2.947482
213	1	0	-5.882888	-3.363893	-1.868673
214	1	0	5.726605	-3.442680	1.556904

Sum of electronic and zero-point Energies=	-4590.784270
Sum of electronic and thermal Energies=	-4590.699973
Sum of electronic and thermal Enthalpies=	-4590.699028
Sum of electronic and thermal Free Energies=	-4590.902538

Table S17. The theoretical Cartesian coordinates (in Å) for the structure **2Br** in dichloromethane.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.792971	-0.251101	0.190922
2	8	0	0.145929	-0.783410	-0.709481
3	5	0	1.046139	-0.086996	0.169055
4	8	0	0.084725	0.365656	1.112985
5	15	0	-2.855148	-1.052671	-2.129299
6	6	0	-4.440387	-0.405006	-2.856293
7	1	0	-4.158465	0.531328	-3.384911
8	6	0	-5.404204	0.005672	-1.703277
9	1	0	-5.604932	-0.867310	-1.049171
10	1	0	-4.903547	0.798984	-1.102738
11	6	0	-6.739863	0.583286	-2.239668
12	1	0	-7.416726	0.787082	-1.390804
13	1	0	-6.519820	1.545016	-2.740462
14	6	0	-7.406021	-0.389345	-3.243362
15	1	0	-8.334073	0.061673	-3.638212
16	1	0	-7.682265	-1.326119	-2.722962
17	6	0	-6.436522	-0.714257	-4.406635
18	1	0	-6.917089	-1.401936	-5.125723
19	1	0	-6.181955	0.216745	-4.947676
20	6	0	-5.135619	-1.365473	-3.867035
21	1	0	-4.453903	-1.603024	-4.701114
22	1	0	-5.392256	-2.314735	-3.363378
23	6	0	-2.979119	-2.898058	-2.011714
24	1	0	-3.199336	-3.320684	-3.013675
25	6	0	-4.127696	-3.286698	-1.030405
26	1	0	-3.935485	-2.786132	-0.053025
27	1	0	-5.099129	-2.920339	-1.406690
28	6	0	-4.192333	-4.819066	-0.813064
29	1	0	-5.000162	-5.050000	-0.095930
30	1	0	-4.442678	-5.309758	-1.772392
31	6	0	-2.838442	-5.357281	-0.291985
32	1	0	-2.894215	-6.450992	-0.147264
33	1	0	-2.615529	-4.898798	0.691136
34	6	0	-1.702600	-5.005323	-1.281809
35	1	0	-1.884131	-5.505974	-2.251216
36	1	0	-0.734125	-5.367849	-0.891843
37	6	0	-1.624895	-3.472230	-1.499793
38	1	0	-0.819887	-3.228214	-2.214949

39	1	0	-1.380581	-2.977721	-0.535706
40	6	0	-1.500862	-0.601588	-3.296543
41	1	0	-0.605184	-1.158202	-2.956885
42	6	0	-1.777434	-0.943543	-4.793443
43	1	0	-1.965558	-2.026233	-4.914382
44	1	0	-2.673804	-0.394523	-5.133476
45	6	0	-0.561494	-0.518494	-5.664496
46	1	0	0.316449	-1.124853	-5.381811
47	1	0	-0.787755	-0.729939	-6.725146
48	6	0	-0.223896	0.982128	-5.480287
49	1	0	-1.066588	1.597753	-5.846980
50	1	0	0.666832	1.240082	-6.080782
51	6	0	0.027126	1.312076	-3.986025
52	1	0	0.913507	0.756330	-3.615349
53	1	0	0.225282	2.391917	-3.861703
54	6	0	-1.201857	0.914181	-3.135170
55	1	0	-2.085039	1.509520	-3.443258
56	1	0	-1.020234	1.126841	-2.066443
57	15	0	-3.147773	0.280250	2.383148
58	6	0	-1.826447	1.020552	3.464074
59	1	0	-1.207520	1.629014	2.772295
60	6	0	-0.902605	-0.078837	4.068188
61	1	0	-1.484229	-0.709995	4.764818
62	1	0	-0.513913	-0.718954	3.255329
63	6	0	0.273761	0.572642	4.837013
64	1	0	0.924143	-0.216760	5.255497
65	1	0	0.871646	1.165052	4.123505
66	6	0	-0.250959	1.498482	5.963059
67	1	0	-0.814655	0.897733	6.700613
68	1	0	0.596348	1.970140	6.492368
69	6	0	-1.175292	2.587999	5.368802
70	1	0	-0.591391	3.226551	4.679384
71	1	0	-1.571697	3.236369	6.170927
72	6	0	-2.363472	1.960472	4.590372
73	1	0	-2.969270	2.773374	4.156334
74	1	0	-3.003158	1.386505	5.284831
75	6	0	-4.564434	1.487812	2.404562
76	1	0	-4.721719	1.823884	3.448913
77	6	0	-4.176727	2.720077	1.532603
78	1	0	-3.989376	2.383528	0.489963
79	1	0	-3.237891	3.167070	1.908104
80	6	0	-5.310368	3.774193	1.519893
81	1	0	-5.464665	4.159424	2.546008
82	1	0	-5.012810	4.624432	0.880348

83	6	0	-6.621512	3.141950	0.994282
84	1	0	-6.474555	2.818895	-0.054600
85	1	0	-7.433526	3.890710	1.000598
86	6	0	-7.022679	1.925069	1.863675
87	1	0	-7.945774	1.460085	1.473836
88	1	0	-7.229594	2.265963	2.895612
89	6	0	-5.899074	0.855919	1.910885
90	1	0	-6.206701	0.039748	2.587713
91	1	0	-5.753299	0.422282	0.901414
92	6	0	-3.839220	-1.285744	3.099829
93	1	0	-4.708336	-1.479846	2.433743
94	6	0	-4.380323	-1.179491	4.558171
95	1	0	-3.534119	-1.066733	5.259602
96	6	0	-5.174565	-2.469152	4.902315
97	1	0	-5.539595	-2.409497	5.943525
98	1	0	-6.058934	-2.531485	4.240223
99	6	0	-4.296308	-3.732615	4.717548
100	1	0	-4.894476	-4.637287	4.927721
101	1	0	-3.462867	-3.707578	5.444225
102	6	0	-3.714931	-3.807079	3.281723
103	1	0	-4.540020	-3.913169	2.550747
104	1	0	-3.063212	-4.693364	3.184350
105	6	0	-2.909296	-2.525352	2.948519
106	1	0	-2.518595	-2.573705	1.911371
107	1	0	-2.049104	-2.445776	3.634450
108	15	0	3.132653	-2.203426	-0.149142
109	6	0	4.939773	-2.698686	-0.153147
110	1	0	5.212903	-2.689053	-1.230102
111	6	0	5.868672	-1.673628	0.565295
112	1	0	5.664361	-0.652846	0.200356
113	1	0	5.680944	-1.700228	1.656766
114	6	0	7.354103	-2.021691	0.286008
115	1	0	7.540921	-1.937722	-0.801396
116	1	0	8.003711	-1.288264	0.796497
117	6	0	7.692863	-3.458560	0.758122
118	1	0	8.734916	-3.709002	0.489946
119	1	0	7.609549	-3.509795	1.859552
120	6	0	6.721032	-4.487095	0.127533
121	1	0	6.930881	-5.499050	0.518796
122	1	0	6.864222	-4.514804	-0.968840
123	6	0	5.245969	-4.113442	0.436893
124	1	0	4.571928	-4.883923	0.030194
125	1	0	5.105191	-4.083034	1.533048
126	6	0	2.316287	-3.061629	-1.579959

127	1	0	1.231824	-2.950990	-1.380733
128	6	0	2.623171	-2.316854	-2.910475
129	1	0	3.713208	-2.327812	-3.096850
130	1	0	2.313262	-1.258672	-2.812179
131	6	0	1.883127	-2.983202	-4.098473
132	1	0	0.790942	-2.878335	-3.951394
133	1	0	2.149866	-2.456404	-5.032226
134	6	0	2.235754	-4.486494	-4.214533
135	1	0	1.680649	-4.940583	-5.054898
136	1	0	3.315394	-4.595846	-4.426417
137	6	0	1.893510	-5.218100	-2.894539
138	1	0	2.163070	-6.287342	-2.965131
139	1	0	0.805597	-5.157813	-2.711921
140	6	0	2.657782	-4.579095	-1.703108
141	1	0	3.741648	-4.691400	-1.884292
142	1	0	2.405008	-5.110505	-0.767522
143	6	0	2.442475	-3.002544	1.378755
144	1	0	2.929800	-3.996106	1.440145
145	6	0	2.818537	-2.206048	2.663160
146	1	0	2.252089	-1.249326	2.669494
147	1	0	3.895347	-1.956059	2.664521
148	6	0	2.465755	-3.040559	3.922172
149	1	0	3.084030	-3.957943	3.925370
150	1	0	2.717606	-2.462498	4.829532
151	6	0	0.963831	-3.422225	3.936164
152	1	0	0.752051	-4.082995	4.796003
153	1	0	0.361136	-2.505998	4.067066
154	6	0	0.543097	-4.124079	2.619870
155	1	0	-0.543792	-4.321988	2.624320
156	1	0	1.058983	-5.098809	2.534794
157	6	0	0.906681	-3.260732	1.379789
158	1	0	0.361922	-2.292629	1.441585
159	1	0	0.587229	-3.773811	0.457978
160	15	0	3.011854	2.517280	0.239442
161	6	0	1.302168	3.183785	0.518108
162	1	0	0.885743	2.466310	1.253439
163	6	0	0.454823	3.019449	-0.773779
164	1	0	0.601807	1.994803	-1.173663
165	1	0	0.800651	3.723348	-1.556722
166	6	0	-1.040213	3.271509	-0.464330
167	1	0	-1.637345	3.188775	-1.391099
168	1	0	-1.398641	2.484372	0.236062
169	6	0	-1.248525	4.665336	0.179862
170	1	0	-0.961679	5.444895	-0.550571

171	1	0	-2.318112	4.809633	0.415952
172	6	0	-0.385702	4.818985	1.459469
173	1	0	-0.702569	4.072415	2.213090
174	1	0	-0.528166	5.822200	1.900694
175	6	0	1.118862	4.610382	1.128375
176	1	0	1.731567	4.729448	2.038869
177	1	0	1.431179	5.384803	0.411828
178	6	0	3.893503	2.672851	1.879677
179	1	0	4.231854	3.723420	2.005084
180	6	0	2.930096	2.297215	3.045696
181	1	0	2.591750	1.253523	2.875358
182	1	0	2.041529	2.948748	3.054233
183	6	0	3.642661	2.388510	4.419397
184	1	0	3.962210	3.433302	4.592735
185	1	0	2.926386	2.120429	5.215983
186	6	0	4.874028	1.454682	4.467508
187	1	0	5.385830	1.543885	5.442503
188	1	0	4.538471	0.403594	4.359868
189	6	0	5.844967	1.799980	3.313772
190	1	0	6.703421	1.104309	3.311622
191	1	0	6.240135	2.824091	3.451868
192	6	0	5.118136	1.710087	1.949183
193	1	0	4.732435	0.676255	1.821912
194	1	0	5.829055	1.902597	1.130023
195	6	0	3.907373	3.570922	-1.028667
196	1	0	3.706411	3.054322	-1.990496
197	6	0	5.451000	3.563366	-0.808030
198	1	0	5.690895	4.079201	0.141197
199	1	0	5.812488	2.524340	-0.751946
200	6	0	6.168863	4.276296	-1.982550
201	1	0	7.259758	4.250612	-1.810653
202	1	0	5.961299	3.718790	-2.915991
203	6	0	5.678038	5.736566	-2.131057
204	1	0	5.948049	6.308981	-1.224326
205	1	0	6.172752	6.219894	-2.992578
206	6	0	4.142700	5.762475	-2.318656
207	1	0	3.878317	5.256956	-3.266163
208	1	0	3.780292	6.804542	-2.382841
209	6	0	3.414083	5.046037	-1.148211
210	1	0	2.330078	5.073896	-1.341036
211	1	0	3.614037	5.582500	-0.202249
212	1	0	-5.034441	-0.296125	4.667090
213	78	0	-2.754223	-0.238861	0.098187
214	78	0	2.953616	0.157708	-0.233897

215	35	0	4.993436	0.371702	-2.303292
216	35	0	-4.305962	3.722670	-2.820240

Sum of electronic and zero-point Energies= -9739.133037
Sum of electronic and thermal Energies= -9739.044958
Sum of electronic and thermal Enthalpies= -9739.044014
Sum of electronic and thermal Free Energies= -9739.257365

Table S18. The theoretical Cartesian coordinates (in Å) for the structure **2ts** in dichloromethane.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.084607	0.428098	0.626023
2	8	0	-0.439260	1.305278	1.244568
3	5	0	1.313730	-0.457345	-0.041633
4	8	0	0.154437	-0.910430	0.065463
5	78	0	-2.861815	-0.148152	-0.006434
6	15	0	-3.761282	1.786356	0.956029
7	6	0	-5.555869	1.287756	1.071532
8	1	0	-5.650483	0.792437	2.062415
9	6	0	-5.900877	0.219939	-0.012188
10	1	0	-5.811774	0.658688	-1.025002
11	1	0	-5.190040	-0.642010	0.057913
12	6	0	-7.329810	-0.344568	0.202771
13	1	0	-7.555563	-1.088191	-0.582359
14	1	0	-7.364417	-0.859195	1.182238
15	6	0	-8.366285	0.807152	0.174889
16	1	0	-9.376150	0.403290	0.368343
17	1	0	-8.374018	1.262406	-0.833455
18	6	0	-8.018888	1.890438	1.227727
19	1	0	-8.747768	2.718760	1.173346
20	1	0	-8.080446	1.454253	2.242362
21	6	0	-6.588342	2.450579	1.002284
22	1	0	-6.356824	3.219699	1.759385
23	1	0	-6.535997	2.926457	0.005211
24	6	0	-3.692776	3.335102	-0.049322
25	1	0	-4.524348	3.992667	0.278933
26	6	0	-3.903716	2.965097	-1.549816
27	1	0	-3.087324	2.277200	-1.848441
28	1	0	-4.860868	2.428425	-1.681556
29	6	0	-3.880214	4.225120	-2.449994
30	1	0	-3.985707	3.917243	-3.505872
31	1	0	-4.744633	4.866386	-2.195940
32	6	0	-2.566779	5.020286	-2.250478
33	1	0	-2.586626	5.939429	-2.862820
34	1	0	-1.709589	4.410638	-2.592339
35	6	0	-2.369636	5.384201	-0.758887
36	1	0	-3.192995	6.043528	-0.426798
37	1	0	-1.424922	5.939635	-0.628616
38	6	0	-2.356265	4.112549	0.133244

39	1	0	-2.220241	4.395494	1.191387
40	1	0	-1.510618	3.454106	-0.150173
41	6	0	-3.168179	2.133495	2.663886
42	1	0	-2.139951	2.524867	2.527378
43	6	0	-4.019314	3.189822	3.436091
44	1	0	-4.102049	4.125116	2.853750
45	1	0	-5.038283	2.792572	3.595643
46	6	0	-3.359184	3.476572	4.812845
47	1	0	-2.357973	3.916372	4.647744
48	1	0	-3.967441	4.218640	5.360845
49	6	0	-3.226439	2.175268	5.643040
50	1	0	-4.234533	1.779059	5.865833
51	1	0	-2.732974	2.393926	6.606891
52	6	0	-2.415330	1.106505	4.866940
53	1	0	-1.382571	1.469888	4.704658
54	1	0	-2.357623	0.169987	5.450427
55	6	0	-3.057758	0.814558	3.486777
56	1	0	-4.064728	0.371028	3.627448
57	1	0	-2.438920	0.081623	2.931258
58	15	0	-2.669689	-2.397577	-0.830198
59	6	0	-1.110203	-3.058089	-1.562781
60	1	0	-0.378952	-2.904659	-0.745808
61	6	0	-0.636646	-2.190863	-2.760424
62	1	0	-1.282821	-2.376858	-3.638727
63	1	0	-0.716563	-1.121232	-2.488386
64	6	0	0.827344	-2.555317	-3.113999
65	1	0	1.162290	-1.966301	-3.987355
66	1	0	1.479896	-2.275882	-2.257010
67	6	0	0.969066	-4.071639	-3.411527
68	1	0	0.414120	-4.303319	-4.339599
69	1	0	2.030664	-4.320955	-3.588190
70	6	0	0.409782	-4.941783	-2.256418
71	1	0	1.018919	-4.792907	-1.345978
72	1	0	0.470814	-6.011005	-2.528890
73	6	0	-1.064139	-4.573018	-1.932586
74	1	0	-1.428626	-5.194138	-1.095841
75	1	0	-1.696942	-4.774082	-2.812924
76	6	0	-3.068620	-3.522747	0.590187
77	1	0	-3.090284	-4.570939	0.227914
78	6	0	-1.954988	-3.379278	1.670796
79	1	0	-1.920063	-2.315127	1.985209
80	1	0	-0.968043	-3.637087	1.244367
81	6	0	-2.251642	-4.277838	2.898475
82	1	0	-2.230333	-5.338531	2.586002

83	1	0	-1.459264	-4.134823	3.654114
84	6	0	-3.635624	-3.943353	3.506589
85	1	0	-3.628013	-2.901047	3.880675
86	1	0	-3.842488	-4.605612	4.366123
87	6	0	-4.744869	-4.096094	2.437880
88	1	0	-5.729070	-3.829149	2.862568
89	1	0	-4.796130	-5.148862	2.102508
90	6	0	-4.456988	-3.188444	1.215200
91	1	0	-5.260397	-3.309582	0.466289
92	1	0	-4.454325	-2.127376	1.550945
93	6	0	-4.105872	-2.511151	-2.008816
94	1	0	-4.983979	-2.305315	-1.360733
95	6	0	-4.336073	-3.903841	-2.666251
96	1	0	-3.523202	-4.109932	-3.384247
97	6	0	-5.692644	-3.895487	-3.420808
98	1	0	-5.857990	-4.882768	-3.888309
99	1	0	-6.509943	-3.726126	-2.694180
100	6	0	-5.713467	-2.783364	-4.499799
101	1	0	-6.692803	-2.771948	-5.010686
102	1	0	-4.940935	-2.999270	-5.261017
103	6	0	-5.434998	-1.394924	-3.869131
104	1	0	-6.253285	-1.139442	-3.168538
105	1	0	-5.407940	-0.617217	-4.652772
106	6	0	-4.091313	-1.391950	-3.094751
107	1	0	-3.938570	-0.398767	-2.620425
108	1	0	-3.253663	-1.556639	-3.797954
109	78	0	3.088777	0.183298	-0.192415
110	15	0	2.516626	2.236639	-1.231390
111	6	0	4.231143	2.862366	-1.592717
112	1	0	4.539705	3.391465	-0.664869
113	6	0	5.204957	1.656455	-1.785486
114	1	0	5.174437	0.964426	-0.896791
115	1	0	4.913797	1.062263	-2.673438
116	6	0	6.673531	2.140426	-1.905000
117	1	0	6.966113	2.628771	-0.955297
118	1	0	7.334034	1.269102	-2.062566
119	6	0	6.806580	3.145275	-3.077157
120	1	0	7.847510	3.510992	-3.131753
121	1	0	6.581728	2.624871	-4.027217
122	6	0	5.834303	4.339448	-2.896453
123	1	0	5.922884	5.032034	-3.752437
124	1	0	6.101869	4.900258	-1.981230
125	6	0	4.362913	3.856229	-2.783366
126	1	0	3.691004	4.719336	-2.633771

127	1	0	4.067663	3.355112	-3.723035
128	6	0	1.762870	3.352877	0.028495
129	1	0	0.725333	2.984116	0.165888
130	6	0	2.491803	3.173017	1.396715
131	1	0	3.561382	3.447167	1.300171
132	1	0	2.428686	2.107942	1.703722
133	6	0	1.828287	4.060361	2.480287
134	1	0	0.780878	3.729022	2.617658
135	1	0	2.360146	3.922506	3.438636
136	6	0	1.854651	5.548131	2.052146
137	1	0	1.378996	6.173282	2.828732
138	1	0	2.903252	5.883233	1.946317
139	6	0	1.107699	5.725783	0.708059
140	1	0	1.127326	6.783654	0.389820
141	1	0	0.052125	5.433943	0.848348
142	6	0	1.732557	4.848530	-0.412322
143	1	0	2.763027	5.196604	-0.611214
144	1	0	1.144710	4.953272	-1.343217
145	6	0	1.512464	2.219322	-2.772919
146	1	0	1.537090	3.238669	-3.215795
147	6	0	2.112368	1.205163	-3.794574
148	1	0	2.080919	0.193734	-3.339354
149	1	0	3.167591	1.446927	-4.012569
150	6	0	1.290066	1.225860	-5.109312
151	1	0	1.369448	2.231010	-5.563532
152	1	0	1.724552	0.499701	-5.819446
153	6	0	-0.196302	0.885455	-4.842372
154	1	0	-0.774084	0.968710	-5.779996
155	1	0	-0.272806	-0.160462	-4.497799
156	6	0	-0.807976	1.824950	-3.773229
157	1	0	-1.838314	1.498579	-3.535752
158	1	0	-0.864460	2.854525	-4.172508
159	6	0	0.031027	1.838834	-2.466393
160	1	0	0.008629	0.828825	-2.002492
161	1	0	-0.409220	2.548983	-1.742281
162	15	0	3.896027	-1.577228	1.197100
163	6	0	2.563961	-2.226470	2.297596
164	1	0	1.801598	-2.662395	1.613440
165	6	0	1.886607	-1.064054	3.089512
166	1	0	1.536387	-0.273089	2.396419
167	1	0	2.622807	-0.601944	3.776954
168	6	0	0.687116	-1.608721	3.904090
169	1	0	0.231408	-0.780542	4.475602
170	1	0	-0.073702	-1.990961	3.198174

171	6	0	1.137383	-2.742483	4.862117
172	1	0	1.839882	-2.327547	5.608443
173	1	0	0.265759	-3.140965	5.411113
174	6	0	1.838764	-3.883432	4.082128
175	1	0	1.122979	-4.354805	3.382959
176	1	0	2.190126	-4.663445	4.781334
177	6	0	3.049723	-3.339037	3.276658
178	1	0	3.535815	-4.161073	2.721424
179	1	0	3.789658	-2.909194	3.975997
180	6	0	4.634430	-2.945314	0.205240
181	1	0	5.257998	-3.570241	0.876985
182	6	0	3.542835	-3.845463	-0.441610
183	1	0	2.904019	-3.216764	-1.094875
184	1	0	2.902065	-4.294047	0.337368
185	6	0	4.209543	-4.965432	-1.286252
186	1	0	4.792281	-5.620468	-0.612157
187	1	0	3.423915	-5.583102	-1.756448
188	6	0	5.145597	-4.373324	-2.369196
189	1	0	5.629446	-5.190116	-2.933842
190	1	0	4.547339	-3.779456	-3.087022
191	6	0	6.220208	-3.462459	-1.726920
192	1	0	6.860339	-3.012550	-2.506392
193	1	0	6.867867	-4.058292	-1.056856
194	6	0	5.544177	-2.335509	-0.906771
195	1	0	4.906324	-1.731433	-1.590178
196	1	0	6.308611	-1.668331	-0.466661
197	6	0	5.218369	-0.874026	2.309428
198	1	0	4.687428	-0.610521	3.248763
199	6	0	5.837346	0.438539	1.740238
200	1	0	6.371410	0.215819	0.796068
201	1	0	5.037375	1.183205	1.530590
202	6	0	6.827101	1.060726	2.760168
203	1	0	7.268382	1.974910	2.324183
204	1	0	6.266006	1.352326	3.667842
205	6	0	7.939352	0.050776	3.136451
206	1	0	8.547612	-0.175622	2.240751
207	1	0	8.609365	0.499013	3.891618
208	6	0	7.324822	-1.260162	3.686900
209	1	0	6.775552	-1.050740	4.623710
210	1	0	8.122328	-1.988276	3.919797
211	6	0	6.350385	-1.891330	2.655813
212	1	0	5.921509	-2.823537	3.064147
213	1	0	6.907798	-2.146188	1.735565
214	1	0	-4.331190	-4.698455	-1.899000

Sum of electronic and zero-point Energies=	-4590.730047
Sum of electronic and thermal Energies=	-4590.645009
Sum of electronic and thermal Enthalpies=	-4590.644065
Sum of electronic and thermal Free Energies=	-4590.850188

Table S19. The theoretical Cartesian coordinates (in Å) for the structure **2Brts** in dichloromethane.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.866755	-0.109251	0.695504
2	8	0	-0.066086	0.525578	-0.332808
3	5	0	-1.287760	0.184998	-0.107790
4	8	0	0.311267	-0.736195	1.659921
5	15	0	2.650359	2.016981	-1.304104
6	6	0	4.214234	2.102115	-2.322238
7	1	0	3.959565	1.601360	-3.279719
8	6	0	5.338296	1.261197	-1.651922
9	1	0	5.555578	1.666758	-0.642460
10	1	0	4.976423	0.216645	-1.545553
11	6	0	6.634236	1.246579	-2.504658
12	1	0	7.420003	0.692664	-1.959860
13	1	0	6.429752	0.703270	-3.446800
14	6	0	7.108621	2.685224	-2.828979
15	1	0	8.007443	2.647248	-3.470254
16	1	0	7.386703	3.202398	-1.891305
17	6	0	5.982658	3.478493	-3.537603
18	1	0	6.321692	4.505630	-3.763815
19	1	0	5.730064	2.987711	-4.496154
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21	1	0	3.926218	4.123497	-3.151142
22	1	0	4.967820	4.070140	-1.707232
23	6	0	2.599409	3.557049	-0.271997
24	1	0	2.687805	4.440652	-0.936465
25	6	0	3.778750	3.572382	0.747261
26	1	0	3.688253	2.674073	1.396217
27	1	0	4.748884	3.507160	0.224938
28	6	0	3.735399	4.853062	1.619587
29	1	0	4.573825	4.835825	2.338448
30	1	0	3.868847	5.737012	0.967797
31	6	0	2.386820	4.960487	2.371590
32	1	0	2.354998	5.891748	2.965187
33	1	0	2.294328	4.112085	3.076004
34	6	0	1.202798	4.924912	1.374567
35	1	0	1.247543	5.811457	0.714590
36	1	0	0.244335	4.963457	1.923300
37	6	0	1.254022	3.641725	0.503914

38	1	0	0.403844	3.628771	-0.202167
39	1	0	1.172695	2.746449	1.156180
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41	1	0	0.345823	2.286669	-1.949288
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43	1	0	1.454283	4.242055	-3.112307
44	1	0	2.318806	3.101724	-4.189978
45	6	0	0.174715	3.213809	-4.563989
46	1	0	-0.744292	3.434241	-3.993448
47	1	0	0.291871	4.003452	-5.328138
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52	1	0	-1.008131	0.870267	-3.563687
53	1	0	-0.169659	-0.276741	-4.654683
54	6	0	1.144013	0.738034	-3.238374
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57	15	0	3.552989	-1.315720	1.872939
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61	1	0	2.489352	-2.026499	4.747505
62	1	0	1.304730	-1.116588	3.746646
63	6	0	0.626606	-3.092028	4.338415
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66	6	0	1.193562	-4.515837	4.563774
67	1	0	1.883651	-4.501369	5.427558
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69	6	0	1.957270	-5.003544	3.306754
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73	1	0	3.582748	-4.391160	1.991069
74	1	0	3.830119	-3.932070	3.700018
75	6	0	5.021844	-2.232752	1.191036
76	1	0	5.326375	-3.008380	1.922383
77	6	0	4.599115	-2.928261	-0.138503
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79	1	0	3.733674	-3.592433	0.037667
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81	1	0	6.070439	-4.535431	-0.056239

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83	6	0	6.982764	-2.787773	-1.005928
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86	6	0	7.414644	-2.082158	0.303086
87	1	0	8.249406	-1.385855	0.105735
88	1	0	7.773047	-2.838138	1.027109
89	6	0	6.240340	-1.296967	0.942407
90	1	0	6.580518	-0.846061	1.890218
91	1	0	5.931777	-0.474630	0.266596
92	6	0	4.261423	-0.169549	3.155299
93	1	0	4.974351	0.432899	2.550047
94	6	0	5.076091	-0.841372	4.301704
95	1	0	4.390440	-1.383031	4.977310
96	6	0	5.829897	0.259215	5.098020
97	1	0	6.395996	-0.205246	5.925599
98	1	0	6.560312	0.749743	4.426871
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103	1	0	4.656984	2.502568	3.826725
104	1	0	3.272693	2.668028	4.945345
105	6	0	3.236533	0.848138	3.736566
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107	1	0	2.536499	0.340389	4.420783
108	15	0	-3.571544	2.000784	0.810915
109	6	0	-5.408442	2.217260	1.035929
110	1	0	-5.755760	2.631816	0.065203
111	6	0	-6.164680	0.872435	1.266838
112	1	0	-5.862434	0.123692	0.514346
113	1	0	-5.919119	0.476091	2.270596
114	6	0	-7.692429	1.114430	1.169992
115	1	0	-7.932182	1.483766	0.154734
116	1	0	-8.224038	0.156977	1.315636
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118	1	0	-9.230446	2.359804	2.107347
119	1	0	-8.004864	1.726098	3.237733
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122	1	0	-7.568406	3.954269	1.137095
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124	1	0	-5.263743	4.146725	2.131144
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127	1	0	-1.784357	3.372346	0.050248
128	6	0	-3.210800	3.473288	-1.572356
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135	1	0	-2.372781	6.839528	-2.158571
136	1	0	-3.989743	6.184764	-1.779503
137	6	0	-2.562074	6.018219	-0.138688
138	1	0	-2.860097	6.975888	0.324596
139	1	0	-1.470435	5.903577	-0.005797
140	6	0	-3.293976	4.854880	0.583303
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142	1	0	-3.058549	4.870454	1.662723
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147	1	0	-4.162955	0.383393	3.233964
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153	1	0	-0.462301	0.096760	3.989113
154	6	0	-0.712257	2.252698	3.933096
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156	1	0	-1.163913	3.056991	4.544408
157	6	0	-1.310538	2.297473	2.502475
158	1	0	-0.793528	1.526704	1.893016
159	1	0	-1.121265	3.284328	2.049908
160	15	0	-2.866958	-2.425142	-0.801388
161	6	0	-1.083441	-2.916427	-0.964096
162	1	0	-0.598530	-2.406791	-0.098445
163	6	0	-0.465509	-2.318423	-2.260236
164	1	0	-0.683881	-1.233719	-2.306557
165	1	0	-0.929096	-2.784257	-3.151007
166	6	0	1.065877	-2.557235	-2.285362
167	1	0	1.482825	-2.169557	-3.231871
168	1	0	1.539872	-1.982261	-1.456975
169	6	0	1.411830	-4.056154	-2.125038

170	1	0	1.019018	-4.619482	-2.992082
171	1	0	2.509553	-4.180736	-2.114882
172	6	0	0.788773	-4.618132	-0.823546
173	1	0	1.202941	-4.076122	0.049511
174	1	0	1.033579	-5.689166	-0.703595
175	6	0	-0.754255	-4.440997	-0.848297
176	1	0	-1.203124	-4.875515	0.060623
177	1	0	-1.158534	-4.988818	-1.713265
178	6	0	-3.491206	-3.255799	0.747867
179	1	0	-3.707754	-4.315880	0.492976
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184	1	0	-3.137736	-5.017809	2.888576
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196	1	0	-3.739053	-2.228998	-3.021740
197	6	0	-5.358785	-3.192529	-1.940328
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199	1	0	-5.738211	-2.261550	-1.488893
200	6	0	-6.166580	-3.491450	-3.228269
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202	1	0	-6.055815	-2.640046	-3.926582
203	6	0	-5.664961	-4.788771	-3.908444
204	1	0	-5.847953	-5.649022	-3.238255
205	1	0	-6.222747	-4.967836	-4.845029
206	6	0	-4.150800	-4.680803	-4.206920
207	1	0	-3.975933	-3.873445	-4.942254
208	1	0	-3.776871	-5.622276	-4.648368
209	6	0	-3.333826	-4.371366	-2.921864
210	1	0	-2.270671	-4.286504	-3.197008
211	1	0	-3.442412	-5.202125	-2.200249
212	1	0	5.795647	-1.572256	3.892199
213	78	0	2.816099	0.156341	0.180797

214	78	0	-3.146911	-0.058404	-0.353800
215	35	0	-5.193172	0.372812	-2.149870
216	35	0	4.426531	-1.718145	-4.401331

Sum of electronic and zero-point Energies= -9739.084621
Sum of electronic and thermal Energies= -9738.996454
Sum of electronic and thermal Enthalpies= -9738.995510
Sum of electronic and thermal Free Energies= -9739.207212

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