# Ring-opening polymerization of glycolide and *rac*-lactide, catalyzed by aryloxy magnesium complexes: DFT study of reaction profile and stereocontrol mechanism

Pavel V. Ivchenko, Andrey V. Shlyakhtin and Ilya E. Nifant'ev

Thermodinamic parameters and Cartesian coordinates for key intermediates and transition states.

I-0c1_DBP_Mg_MeG

E = -1163.593853   E0 = -1163.203047   ZPVE = 0.390806 a.u. = 245.2346 kcal/mol
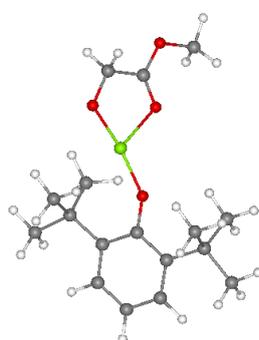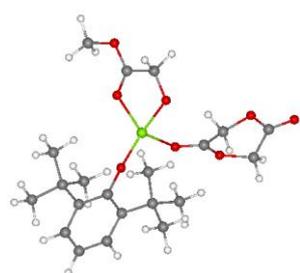
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	19.2222	43.1666	0.8887	1.4812	-11.3889
rotational	16.0706	34.9165	0.8887	0.8887	-9.5216
vibrational	23.6633	95.1124	259.5721	259.5721	231.2143
total	58.9560	173.1956	261.3496	261.9421	210.3038

```
8  -0.06439924  -0.19607472   0.52372980          1  -4.15914345  -2.75575686   1.06346226
6  -1.26652205   0.12441468   0.03290093          1  -3.64487553  -3.30761337  -0.55264431
6  -1.52854621   1.43502736  -0.48827052          1  -3.08705139  -4.15947247   0.89997029
6  -2.79981565   1.72326016  -0.99953926          6  -0.94428241  -2.98576355  -0.21866083
1  -3.01090479   2.71472406  -1.39860582          1  -0.00567436  -2.42305136  -0.17060089
6  -3.81122160   0.76674461  -1.00890422          1  -0.77164400  -3.99587107   0.18493104
6  -3.55427408  -0.50523245  -0.49696618          1  -1.23623574  -3.08887243  -1.27425396
1  -4.35749674  -1.24009454  -0.50982934          6  -1.67261326  -2.20605803   2.08102942
6  -2.30606842  -0.86104870   0.02773070          1  -2.48561525  -1.75344551   2.66755271
6  -0.42715681   2.51029706  -0.46249628          1  -1.49594390  -3.21961069   2.47405076
6  -2.06145382  -2.27894831   0.58535409          1  -0.76625741  -1.60822022   2.22576118
6  -0.04009926   2.82956219   1.00850987         12   1.67447484   0.49118376   0.59855771
1   0.87819439   3.43319178   1.06832814          8   3.09516811   1.23743844   1.61664844
1  -0.85009134   3.40363693   1.47854590          6   5.34164143  -1.94749224  -1.14086580
1   0.07439649   1.93390477   1.63797951          8   5.40819740  -0.93278372  -0.09551013
6   0.80062509   2.03623080  -1.30720305          1   5.08005190   1.44483709   1.00357223
1   0.83715296   0.94103336  -1.43632495          6   4.32838964   0.69554305   1.34255338
1   0.72885698   2.41661930  -2.33511376          1   4.79987812   0.19185281   2.21755147
1   1.75846970   2.43074894  -0.91577071          6   4.25844145  -0.35819125   0.24035728
6  -0.87375152   3.84972477  -1.07968974          1   6.37048769  -2.29617023  -1.26141918
1  -1.17101514   3.73462772  -2.13134360          1   4.96512365  -1.50405538  -2.06974196
1  -1.71498859   4.28949499  -0.52748477          8   3.17736936  -0.65528309  -0.30524588
1  -0.03964937   4.56669521  -1.04176116          1  -4.79535484   1.00957727  -1.41090059
6  -3.31727600  -3.16624928   0.48746765          1   4.68250990  -2.76501322  -0.82739961
```

I-0c1_DBP_Mg_MeG

E = -1619.037478   E0 = -1618.564342   ZPVE = 0.473136 a.u. = 296.8974 kcal/mol

	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	19.6885	44.0933	0.8887	1.4812	-11.6652
rotational	16.9969	36.7573	0.8887	0.8887	-10.0705
vibrational	36.0053	137.7863	316.6456	316.6456	275.5646
total	72.6907	218.6369	318.4231	319.0156	253.8290

8	0.18910377	0.43227997	-0.56518972	1	2.60605979	0.40693063	-3.32346392
6	-0.31260377	1.18683851	-1.54039013	6	-0.09707987	-1.73462284	-2.72014356
6	-1.01534259	2.39938998	-1.22692990	1	-1.09261990	-1.84773517	-3.17327857
6	-1.53133357	3.16620803	-2.27946568	1	0.48213413	-2.64502621	-2.93998694
1	-2.06658578	4.08851194	-2.06037164	1	-0.23592955	-1.66200793	-1.63598132
6	-1.37992179	2.78794885	-3.61103439	6	-3.31786990	-2.72113991	3.75221229
6	-0.69252193	1.61441708	-3.91101217	8	-2.48773503	-2.82862616	2.55896759
1	-0.57845175	1.33319354	-4.95652771	6	-1.49482107	-1.94075727	2.45203042
6	-0.14830615	0.79684991	-2.91268349	6	-1.17819476	-1.09754753	3.66229844
6	-1.20684052	2.86835384	0.23191725	8	-1.38825178	-1.79486823	4.91435146
6	0.61421305	-0.48902833	-3.29958534	6	-2.52800655	-2.52835202	5.03788614
6	-2.04141164	1.82962906	1.01989353	8	-0.88493282	-1.86426425	1.38611019
1	-1.59595811	0.83025664	0.94987893	1	-4.02548981	-1.88733637	3.61839318
1	-2.11393738	2.12463689	2.07957911	1	-3.87604189	-3.65872669	3.81109881
1	-3.06036353	1.76931322	0.61041558	12	0.74255693	-0.67679375	0.80855858
6	0.16106702	3.10291743	0.91462553	8	1.52642095	-0.35291529	2.55617452
1	0.78771484	2.20484138	0.90573299	6	2.76067233	-0.93973547	2.72885108
1	0.70916897	3.90122294	0.39379081	6	3.12929559	-1.83696473	1.55006576
1	0.01800348	3.41708183	1.96039248	8	4.29409981	-2.46997428	1.64635336
6	-1.97568405	4.20148468	0.32672384	6	4.66631317	-3.30583310	0.51052302
1	-1.44264317	5.01901102	-0.17852801	1	3.59363174	-0.20677686	2.82680321
1	-2.98558903	4.12949705	-0.10148448	1	2.83094478	-1.57700515	3.63909984
1	-2.08191824	4.48048830	1.38571668	1	-0.10954942	-0.80564702	3.60915375
6	0.67810947	-0.69904339	-4.82585430	1	-1.79099309	-0.17952244	3.62981057
1	-0.32147032	-0.80460030	-5.27089834	8	-2.87445545	-2.99048495	6.09748697
1	1.19870639	0.12499822	-5.33390665	8	2.38271284	-1.95615780	0.56154811
1	1.23467851	-1.62422895	-5.03758240	1	4.72106361	-2.69720340	-0.39925528
6	2.07924676	-0.40955493	-2.80843401	1	5.64589596	-3.71500015	0.77056795
1	2.13676882	-0.21895193	-1.73166192	1	3.92839551	-4.10510111	0.37689352
1	2.60828900	-1.35000455	-3.03026152	1	-1.79242539	3.40523171	-4.41000366

I-1om-si_DBP_Mg_MeG_GL_GL

E = -2074.458201   E0 = -2073.903042   ZPVE = 0.555159 a.u. = 348.3676 kcal/mol
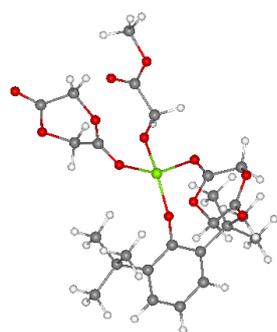
	ln(Q)	S,	U,	H,	G,
		cal/mol·K	kcal/mol	kcal/mol	kcal/mol
translational	20.0437	44.7992	0.8887	1.4812	-11.8756
rotational	17.6461	38.0474	0.8887	0.8887	-10.4551
vibrational	51.9117	188.7560	373.8881	373.8881	317.6105
total	89.6015	271.6026	375.6656	376.2581	295.2798

|							
8	-0.57529879	0.50862128	-0.80747902	6	1.71731639	-2.84985423	1.00742114
6	-0.82355642	1.19555461	-1.92343676	6	3.08167839	-2.52838707	0.44900811
6	-1.25226474	2.56648636	-1.84995162	8	3.93984747	-3.69840527	0.37560546
6	-1.52370858	3.25391531	-3.03973722	6	4.00517416	-4.46543121	1.49874413
1	-1.84561980	4.29303122	-2.99803877	6	2.97697592	-4.11898899	2.56168532
6	-1.39382720	2.64986968	-4.28712177	8	0.66121161	-2.36261678	0.59825134
6	-0.98091030	1.32211256	-4.35719633	1	3.34335995	-3.28075457	3.17556214
1	-0.88334191	0.86169255	-5.33870983	1	2.78326750	-4.99638367	3.18243980
6	-0.68910038	0.57099068	-3.21142006	6	-4.29506159	-1.47630310	0.40170288
6	-1.42304480	3.28901434	-0.49593723	8	-2.86926317	-1.42055190	0.70561641
6	-0.22169966	-0.89342529	-3.35813189	6	-2.51555634	-0.77406132	1.81315637
6	-2.48703861	2.55475211	0.35537130	6	-3.61615372	-0.39651933	2.77595949
1	-2.22481108	1.49505734	0.44292259	8	-4.71309233	-1.33274102	2.80652380
1	-2.55443048	3.00215483	1.36044896	6	-5.16813803	-1.79924130	1.60319710
1	-3.47400951	2.63763046	-0.12453528	8	-1.33908308	-0.49350601	2.02743101
6	-0.07352367	3.36439443	0.25563687	1	-4.59483910	-0.51392823	-0.04223174
1	0.37866825	2.37659359	0.39891607	1	-4.40595675	-2.26450682	-0.34701222
1	0.64148247	3.97407150	-0.31492537	1	2.98877192	-2.15193748	-0.57326055
1	-0.20773059	3.83442402	1.24258482	1	3.51601171	-1.74744046	1.09663963
6	-1.91464245	4.74148750	-0.65303147	8	4.82016563	-5.34869909	1.61822772
1	-1.20121038	5.35890102	-1.21645081	1	-3.20705318	-0.35884181	3.79018402
1	-2.89108133	4.79594707	-1.15492082	1	-3.97874880	0.61155111	2.50770736
1	-2.02647066	5.19293404	0.34413350	8	-6.19319153	-2.42735052	1.52493441
6	-0.18567824	-1.35997689	-4.82739210	12	0.26464933	-0.31264195	0.65472335
1	-1.17824316	-1.31479800	-5.29764891	8	1.86484516	0.02608617	1.57956815
1	0.51289368	-0.76742786	-5.43462563	6	2.50747299	0.90091866	2.41522264
1	0.15109032	-2.40668607	-4.86245298	6	3.58596849	0.21837625	3.26467752
6	1.22154391	-1.04042315	-2.82173419	8	4.16323566	1.10496759	4.11715174
1	1.31199646	-0.66656393	-1.79508078	6	5.22021961	0.56748486	4.94702864
1	1.53525233	-2.09614134	-2.84562635	1	3.03440762	1.72198665	1.87776995
1	1.91920829	-0.46223843	-3.44422388	1	1.83956480	1.41713977	3.14074540
6	-1.18600380	-1.85168111	-2.62051392	8	3.91532087	-0.95802283	3.20357442
1	-2.18503761	-1.80225122	-3.07955432	1	6.02848053	0.16235627	4.32533455
1	-0.82920444	-2.89016223	-2.70154834	1	5.57754803	1.41198766	5.54385948
1	-1.28095078	-1.59416234	-1.56137180	1	4.83233309	-0.22791760	5.59602261
8	1.67955530	-3.74118090	1.99710858	1	-1.61094439	3.20966530	-5.19749117

I-1c1m-si_DBP_Mg_MeG_GL_GL

E = -2074.461334   E0 = -2073.905829   ZPVE = 0.555505 a.u. = 348.5845 kcal/mol
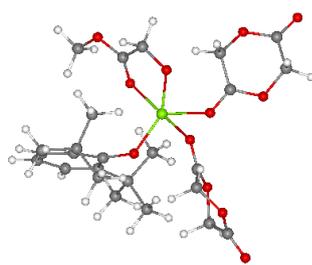
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	20.0437	44.7992	0.8887	1.4812	-11.8756
rotational	17.5039	37.7648	0.8887	0.8887	-10.3708
vibrational	48.6704	181.0845	373.7382	373.7382	319.7478
total	86.2179	263.6484	375.5156	376.1081	297.5014

8	-0.75878090	0.19014958	0.36203626		6	1.91859746	-3.01031733	-1.75521350
6	-0.67344934	1.04952121	1.38451242		6	3.21344471	-2.34926653	-2.16913891
6	-0.90309823	2.45535946	1.17739415		8	4.31111622	-3.27947402	-2.36216831
6	-0.63352400	3.34139132	2.22943974		6	4.04758787	-4.43596363	-3.02596307
1	-0.76327473	4.41173649	2.07774544		6	2.57604146	-4.72599173	-3.26904559
6	-0.21544831	2.89624643	3.48107791		8	1.08266151	-2.48611975	-1.02924716
6	-0.14173490	1.52552509	3.71913433		1	2.26332474	-4.27922773	-4.22657490
1	0.11205117	1.18852282	4.72277212		1	2.42848659	-5.80798769	-3.31364393
6	-0.39429936	0.58085471	2.71603441		6	-3.67838216	-2.68411708	-0.58387727
6	-1.48140836	3.00708365	-0.14792931		8	-2.32158041	-2.37050724	-1.00979328
6	-0.41203424	-0.92329991	3.07699108		6	-2.20084310	-1.44440413	-1.96916306
6	-2.77142644	2.23477840	-0.51330423		6	-3.47327447	-1.03659225	-2.67936730
1	-2.56268716	1.15922594	-0.55047548		8	-4.42618370	-2.11292005	-2.83382726
1	-3.15406418	2.57358885	-1.48972571		6	-4.64355850	-2.90022469	-1.73795450
1	-3.55232239	2.41568923	0.23964255		8	-1.11371875	-0.96281374	-2.25245047
6	-0.46873844	2.91637874	-1.31061566		1	-4.04045486	-1.87583244	0.07177750
1	-0.25223821	1.88355577	-1.60836077		1	-3.60341644	-3.60535455	-0.00111439
1	0.47608119	3.40998530	-1.03999913		1	3.53281283	-1.67055058	-1.37385547
1	-0.86752951	3.42458844	-2.20282054		1	3.02369952	-1.73975670	-3.06913495
6	-1.87616992	4.49425554	-0.03253600		8	4.93075323	-5.17329788	-3.39197516
1	-1.00391018	5.14691687	0.11579415		1	-3.22513771	-0.69183826	-3.68730235
1	-2.58231950	4.66843843	0.79115546		1	-3.92973685	-0.19806433	-2.12499666
1	-2.36441827	4.80822897	-0.96695352		8	-5.54192400	-3.70479417	-1.71468151
6	-0.29762715	-1.15505648	4.59765387		12	0.56747836	-0.39704326	-0.92160124
1	-1.08812392	-0.63214058	5.15399122		8	1.68312001	0.17542399	-2.42969656
1	0.67580128	-0.83455336	4.99627495		6	2.65806508	1.09569740	-2.13003731
1	-0.39793801	-2.23101878	4.80296612		6	2.88584328	1.19066131	-0.62132341
6	0.75651109	-1.69374025	2.42436481		8	3.76886535	2.10615492	-0.21857587
1	0.63601863	-1.76225507	1.33902621		6	3.92319632	2.23837590	1.22641587
1	0.79458165	-2.72329092	2.81433153		1	2.43278050	2.12905669	-2.47955990
1	1.71836722	-1.20767939	2.63809109		1	3.65483475	0.86246604	-2.57857633
6	-1.75510180	-1.54646444	2.62838864		8	2.26790833	0.46003187	0.16455694
1	-2.59388208	-1.07785213	3.16403937		1	2.95517516	2.46949911	1.68634987
1	-1.76632702	-2.62513161	2.85264516		1	4.63197803	3.05997705	1.36001611
1	-1.89375460	-1.40071118	1.55104947		1	4.31833124	1.30701733	1.64885712
8	1.68955362	-4.24747419	-2.21725321		1	0.00127261	3.60875988	4.27798510

TS-12ic1-si_DBP_Mg_MeG_GL

E =-1619.022378   E0 = -1618.548076   ZPVE =0.474302 a.u. = 297.6289 kcal/mol
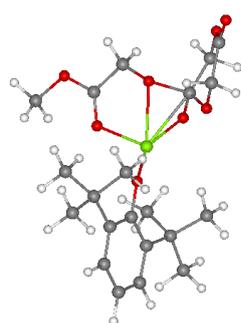
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	19.6885	44.0933	0.8887	1.4812	-11.6652
rotational	16.8392	36.4439	0.8887	0.8887	-9.9770
vibrational	32.2572	126.9104	316.3552	316.3552	278.5169
total	68.7849	207.4476	318.1327	318.7252	256.8747

8	-0.40644529	0.42498922	-0.33220348
6	-0.86530763	1.08784616	-1.39715970
6	-1.15737820	2.48571801	-1.28002369
6	-1.63257754	3.16201925	-2.41027927
1	-1.85943937	4.22473431	-2.34251404
6	-1.82951856	2.51813412	-3.63138723
6	-1.55385458	1.15723276	-3.73767233
1	-1.71839452	0.66286653	-4.69429255
6	-1.07655632	0.41896674	-2.64783335
6	-0.96021080	3.23224282	0.05657135
6	-0.80807042	-1.09238660	-2.77669907
6	-1.84503984	2.60172796	1.15838110
1	-1.61029112	1.54027164	1.29366219
1	-1.68951082	3.12653351	2.11419916
1	-2.90842795	2.69145679	0.89256757
6	0.52705985	3.19060397	0.48182148
1	0.87490731	2.15819573	0.59897131
1	1.15616083	3.68712139	-0.27179641
1	0.66132861	3.71958423	1.43857288
6	-1.35565948	4.71825886	-0.04234034
1	-0.74430102	5.26172018	-0.77721596
1	-2.41418386	4.84569263	-0.31050378
1	-1.20169330	5.19654465	0.93610746
6	-1.06355011	-1.62496972	-4.20027733
1	-2.11360288	-1.50229394	-4.49874878
1	-0.42992046	-1.12308300	-4.94517565
1	-0.83264875	-2.70041895	-4.23278713
6	0.68786305	-1.40521419	-2.45169139
1	1.18070698	-0.57870948	-1.91529894
1	0.80466086	-2.36119032	-1.91057885

1	1.27209473	-1.51318192	-3.37633586
6	-1.77073359	-1.87448859	-1.84635687
1	-2.80402088	-1.74709392	-2.19804001
1	-1.53771949	-2.95016384	-1.85488296
1	-1.74765253	-1.51747048	-0.80867410
6	-1.54718089	-1.85621440	3.34664607
8	-1.04692221	-2.23109722	2.04660654
6	0.27793789	-2.73018622	2.03841543
6	0.44314879	-3.85487032	3.04412746
8	-0.04053712	-3.55978918	4.37356901
6	-1.03728724	-2.64438081	4.54421282
8	0.70184845	-2.94963908	0.83497089
1	-2.63753748	-1.97388005	3.30914545
1	-1.31893802	-0.79873753	3.54622817
12	0.58972210	-1.02578449	0.27821857
8	1.04033852	-1.37096179	2.61012697
6	2.43595457	-1.47074068	2.74407005
6	3.16042399	-0.84700334	1.55827045
8	4.45408726	-0.65511292	1.77757978
6	5.21514559	-0.07685114	0.67232132
1	2.76865101	-0.96013105	3.66277170
1	2.79054952	-2.51580691	2.81292868
1	1.49590611	-4.14047003	3.15769315
1	-0.10478395	-4.71965504	2.64091468
8	-1.48213601	-2.44053769	5.65108633
8	2.60449576	-0.54589576	0.49504948
1	4.80403709	0.90538430	0.41481191
1	6.23650742	0.00827612	1.05070508
1	5.16869831	-0.74179983	-0.19730148
1	-2.20020747	3.07409239	-4.49325275

TS-12ic1m-si_DBP_Mg_MeG_GL_GL

E = -2074.456927   E0 = -2073.900406   ZPVE = 0.556521 a.u. = 349.2225 kcal/mol
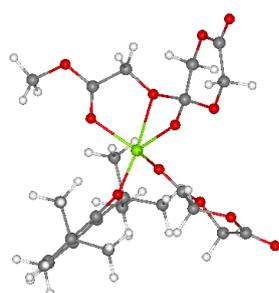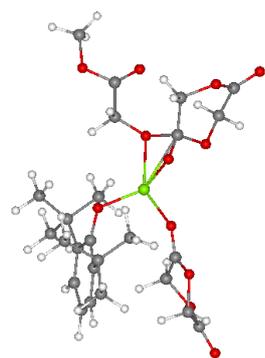

	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	20.0437	44.7992	0.8887	1.4812	-11.8756
rotational	17.4562	37.6701	0.8887	0.8887	-10.3426
vibrational	44.9443	170.3449	373.3819	373.3819	322.5935
total	82.4443	252.8142	375.1593	375.7518	300.3753

8	-0.48068994	0.49302405	-0.67913795	6	1.85080123	-2.48054314	1.56589055
6	-0.78788650	1.19819927	-1.76723337	6	3.14493513	-3.27898669	1.47793519
6	-1.43657911	2.47733068	-1.63640451	8	3.78240943	-3.56438541	2.74837780
6	-1.72603655	3.21398211	-2.79177547	6	3.00585198	-3.67147374	3.86402965
1	-2.20519352	4.18759441	-2.70235205	6	1.51903689	-3.35322571	3.76800847
6	-1.42675686	2.73699069	-4.06480455	8	1.30628467	-2.19830632	0.43035716
6	-0.84012681	1.48097849	-4.19461489	1	1.35737801	-2.48146725	4.42271376
1	-0.63337928	1.10851514	-5.19644594	1	0.97456360	-4.20750427	4.19188833
6	-0.51626813	0.68826807	-3.08591104	6	-3.47798586	-2.24517107	1.16170144
6	-1.84459066	3.03655696	-0.25602403	8	-2.10411406	-1.76738155	1.23746252
6	0.12118801	-0.70085108	-3.30674648	6	-1.82216203	-0.88896501	2.19747114
6	-2.81847668	2.04600406	0.42730159	6	-2.87838364	-0.65537775	3.25137997
1	-2.37578988	1.04375839	0.44199115	8	-3.65591359	-1.83044648	3.56480670
1	-3.04095554	2.37501287	1.45632541	6	-4.08970594	-2.58668971	2.51053572
1	-3.76568842	2.00452757	-0.13040987	8	-0.74767447	-0.29590711	2.20679212
6	-0.60222608	3.28133535	0.63032067	1	-4.08709812	-1.48268235	0.65048313
1	-0.00995481	2.36966586	0.75453818	1	-3.44321299	-3.14686346	0.54522228
1	0.04395393	4.04361629	0.17104159	1	2.88664532	-4.22469378	0.97997659
1	-0.90323865	3.64532685	1.62559164	1	3.89451504	-2.76632595	0.86373711
6	-2.58396864	4.38548279	-0.35252842	8	3.51150036	-3.97060585	4.92331457
1	-1.95181394	5.17267561	-0.78728068	1	-2.39401031	-0.34342766	4.18145466
1	-3.50295663	4.31087732	-0.95067793	1	-3.53854918	0.16022171	2.90793157
1	-2.86971068	4.71217108	0.65876400	8	-4.90256739	-3.46306157	2.66412258
6	0.19683552	-1.08822930	-4.79807615	12	0.64723390	-0.33755133	0.60229087
1	-0.79790241	-1.11901259	-5.26481342	8	2.12023830	-1.04564583	2.35587382
1	0.83056504	-0.40192607	-5.37742472	6	3.36383700	-0.40071842	2.25859451
1	0.63650274	-2.09314823	-4.88319683	6	3.32866311	0.69061828	1.19916368
6	1.57828581	-0.70070124	-2.78830457	8	4.46137333	1.37485325	1.09521818
1	1.65096796	-0.34070688	-1.75681245	6	4.46866274	2.44647503	0.10025027
1	2.00723100	-1.71327662	-2.82689595	1	3.60762763	0.08317614	3.22217798
1	2.19716763	-0.03660625	-3.40980029	1	4.20775843	-1.07621181	2.04114699
6	-0.71847379	-1.80519950	-2.62097979	8	2.32858276	0.93071520	0.51544434
1	-1.71307266	-1.85979033	-3.08870482	1	3.70990610	3.19411397	0.35638750
1	-0.23021831	-2.78401637	-2.74184823	1	5.47504807	2.86863756	0.15209399
1	-0.85226214	-1.61474347	-1.55202079	1	4.26024961	2.03211617	-0.89217198
8	0.96184474	-3.10270143	2.47153378	1	-1.66204751	3.33170366	-4.94824028

TS-12om-si_DBP_Mg_MeG_GL_GL

E =-2074.444562　　E0 = -2073.887867　　　ZPVE = 0.556694 a.u. = 349.3311 kcal/mol

	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	20.0437	44.7992	0.8887	1.4812	-11.8756
rotational	17.5077	37.7724	0.8887	0.8887	-10.3731
vibrational	44.4773	169.2756	373.4484	373.4484	322.9788
total	82.0287	251.8472	375.2258	375.8183	300.7301

```
8   0.26793894   0.47212428  -0.92684197        6   2.27742982  -2.34850883   1.44366777
6  -0.91756964   0.91218102  -1.34548259        6   3.74024820  -2.77131057   1.70817208
6  -1.52221954   2.06784296  -0.73846883        8   3.87032557  -3.85102034   2.66806746
6  -2.83547068   2.39688420  -1.10029233        6   3.15980101  -3.72991443   3.83140588
1  -3.32281590   3.25230551  -0.63534534        6   2.02254796  -2.72665977   3.76401567
6  -3.54902053   1.66131771  -2.04934430        8   1.79686844  -2.54612613   0.25329369
6  -2.90801096   0.62330616  -2.72878671        1   2.38817024  -1.71050775   3.99178171
1  -3.44348526   0.12481555  -3.53598809        1   1.25249851  -3.01576543   4.48487902
6  -1.58934104   0.24721120  -2.43209839        6  -4.23314667  -2.33663821  -0.79370403
6  -0.73775029   2.96587729   0.24525735        8  -2.89655614  -2.40927792  -0.20654885
6  -0.83778429  -0.75295967  -3.34488583        6  -2.53265858  -1.37661886   0.55493122
6  -0.40445438   2.22917843   1.56222677        6  -3.60504246  -0.38795546   0.92249107
1   0.26177886   1.37512124   1.40007889        8  -4.90171909  -0.99994576   1.12768185
1   0.10227448   2.91535926   2.25775099        6  -5.30638933  -1.90469038   0.19135591
1  -1.31677032   1.86967456   2.06032300        8  -1.36760640  -1.27786183   0.94391078
6   0.56942594   3.44566560  -0.42952317        1  -4.19920635  -1.63598037  -1.64400101
1   1.18810344   2.59761500  -0.74427843        1  -4.45329714  -3.34542274  -1.15058625
1   0.34277496   4.05691290  -1.31481528        1   4.15011168  -3.16610384   0.77373552
1   1.14778101   4.06788540   0.27057222        1   4.35116577  -1.93307745   2.06309199
6  -1.53673613   4.22550726   0.63562030        8   3.42152190  -4.41871405   4.79037857
1  -1.81724286   4.82538700  -0.24130659        1  -3.34221721   0.10156204   1.86442113
1  -2.45008826   3.97904491   1.19688272        1  -3.66088629   0.38084760   0.12445004
1  -0.91354525   4.85685730   1.28480124        8  -6.43737841  -2.32304859   0.16308215
6  -1.75628018  -1.32064605  -4.44564199       12   0.52746260  -1.03827119   0.22069584
1  -2.58886242  -1.91157138  -4.03389359        8   2.13179064  -0.67142403   1.68068039
1  -2.17569661  -0.53108788  -5.08368206        6   3.16432953   0.17064856   1.20624602
1  -1.16972601  -1.98745954  -5.09277868        6   4.11864233   0.60231912   2.32209992
6   0.31025371   0.01221713  -4.04812813        8   4.94136667   1.58031428   1.86736155
1   1.00165272   0.43908796  -3.31118727        6   5.91762733   2.05404878   2.83143139
1   0.87468112  -0.67033970  -4.70213318        1   3.75835419  -0.29911703   0.39861172
1  -0.08912095   0.82638586  -4.66884613        1   2.72653818   1.08173895   0.76569843
6  -0.23084012  -1.96746719  -2.59713602        8   4.15233850   0.14042902   3.44604874
1  -0.92034650  -2.39810205  -1.85544813        1   6.56819391   1.23056233   3.15040398
1  -0.00281653  -2.77192140  -3.31205273        1   6.49121523   2.82249260   2.30560398
1   0.72754800  -1.71717823  -2.12441492        1   5.41123581   2.47540617   3.70816422
8   1.41221762  -2.76865935   2.45761037        1  -4.57411337   1.93522918  -2.30135584
```

I-2c1_DBP_Mg_MeG_GL

E = -1619.028324   E0 = -1618.553425   ZPVE = 0.474899 a.u. = 298.0039 kcal/mol
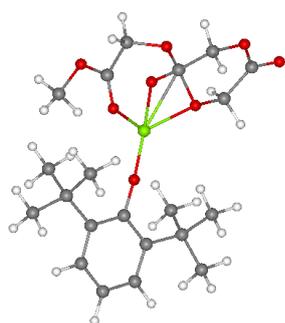
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	19.6885	44.0933	0.8887	1.4812	-11.6652
rotational	16.8555	36.4763	0.8887	0.8887	-9.9867
vibrational	34.0108	131.7164	317.1241	317.1241	277.8528
total	70.5548	212.2860	318.9015	319.4940	256.2010

```
12   0.22626884  -1.01265526   0.61398262        1   1.44828784  -1.71683180  -3.35904264
 8  -0.55294353   0.14549556  -0.57082188        1   1.73914778   0.03680797  -3.48050332
 6  -0.93953633   1.08928668  -1.43153751        6  -1.26063693  -1.67372525  -2.90188527
 6  -1.41932249   2.34979773  -0.94531107        1  -2.28711104  -1.55894268  -3.27866769
 6  -1.82365525   3.31325626  -1.87838960        1  -0.87065512  -2.63549924  -3.26976013
 1  -2.19324303   4.27631187  -1.53078401        1  -1.31167781  -1.71028554  -1.80833590
 6  -1.77107644   3.07791877  -3.24996376        8  -0.17686698  -1.30507112   2.62814021
 6  -1.30472445   1.85076773  -3.71480322        6   0.28117746  -2.75625467   2.39029527
 1  -1.27225351   1.68111384  -4.78957129        6  -0.62484282  -3.57956100   3.29674435
 6  -0.88404578   0.83910322  -2.84202051        8  -0.60620862  -3.17391872   4.69239759
 6  -1.49503899   2.65766549   0.56672132        6  -0.39619282  -1.87801254   5.04539156
 6  -0.37727225  -0.50734168  -3.40417528        6  -0.03353365  -0.84951186   3.97792816
 6  -2.43104243   1.65414894   1.28106666        8   0.16298206  -2.94955587   1.10392332
 1  -2.11710143   0.61630803   1.12401772        1   1.00233591  -0.53537518   4.18193340
 1  -2.45655179   1.86013448   2.36300325        1  -0.69354367   0.01744047   4.10865879
 1  -3.45624280   1.75210893   0.89635730        1  -1.65043712  -3.49738836   2.91303897
 6  -0.07992439   2.63132858   1.19233596        1  -0.30964437  -4.62968731   3.29002309
 1   0.43835449   1.68446195   0.99784863        8   1.63976943  -2.82154059   2.92704439
 1   0.53916985   3.43506050   0.76848537        6   2.67033625  -2.96993375   1.96793759
 1  -0.13714625   2.78586149   2.28142166        6   3.06973267  -1.67594504   1.26763833
 6  -2.06570315   4.06155872   0.85227358        8   4.38383675  -1.56165922   1.11679959
 1  -1.44533074   4.85718727   0.41624114        6   4.84684086  -0.39831552   0.36152804
 1  -3.09077954   4.17320681   0.47213265        1   3.54143715  -3.37346625   2.49751139
 1  -2.09604216   4.22332144   1.93998289        1   2.37344813  -3.67048812   1.16638327
 6  -0.42696106  -0.55626386  -4.94465828        8   2.28210402  -0.82183576   0.83678728
 1  -1.45061314  -0.43697852  -5.32595682        1   4.55454779   0.51943809   0.88316965
 1   0.20650591   0.21554571  -5.40446520        1   5.93349934  -0.50459874   0.32543096
 1  -0.05844317  -1.53513134  -5.28543711        1   4.41123629  -0.41069815  -0.64372784
 6   1.10376191  -0.72962427  -3.01313758        1  -2.09421921   3.84636211  -3.95314217
 1   1.25435042  -0.66464216  -1.92874694        8  -0.44856969  -1.55025637   6.21026611
```

I-2c1m-si_DBP_Mg_MeG_GL_GL

E = -2074.467571   E0 = -2073.909424   ZPVE = 0.558147 a.u. = 350.2426 kcal/mol
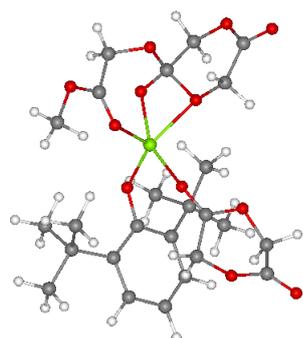
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	20.0437	44.7992	0.8887	1.4812	-11.8756
rotational	17.3582	37.4752	0.8887	0.8887	-10.2845
vibrational	42.0129	164.2225	374.3134	374.3134	325.3505
total	79.4147	246.4969	376.0909	376.6834	303.1903

12	0.99780178	-0.78094423	0.52712512
8	0.72443962	0.51472712	-0.88021696
6	-0.34408277	1.15797257	-1.32047713
6	-0.53196037	2.55945277	-1.03561771
6	-1.76553583	3.14401269	-1.34780478
1	-1.93976688	4.19170189	-1.10757816
6	-2.79244041	2.42564011	-1.96491230
6	-2.54059911	1.12040734	-2.39419961
1	-3.30567050	0.61339474	-2.98109770
6	-1.32227182	0.47565973	-2.13633537
6	0.60532689	3.42556596	-0.44841576
6	-0.98386419	-0.85599989	-2.85174727
6	0.89109159	3.05711126	1.02347767
1	1.20355487	2.01386642	1.12655485
1	1.69507360	3.69923806	1.41868842
1	0.00082594	3.21846008	1.64983058
6	1.89082325	3.24388981	-1.29025352
1	2.21094418	2.19649339	-1.30661643
1	1.72021723	3.57219696	-2.32570076
1	2.70203996	3.85952210	-0.87144339
6	0.25848210	4.92773771	-0.47650468
1	0.02590829	5.27612448	-1.49260628
1	-0.58979845	5.17631006	0.17788300
1	1.12581587	5.50100183	-0.11814778
6	-2.16107321	-1.35387087	-3.71425796
1	-3.04635429	-1.60617828	-3.11025429
1	-2.45958710	-0.61926949	-4.47449589
1	-1.85449278	-2.26718664	-4.24312544
6	0.20815814	-0.58936769	-3.80399966
1	1.08324921	-0.24125533	-3.24193382
1	0.48206571	-1.51490450	-4.33374786
1	-0.05550063	0.16858983	-4.55504274
6	-0.59689295	-2.01692653	-1.90288746
1	-1.26201081	-2.09028292	-1.03084409
1	-0.66900778	-2.97367930	-2.44252634
1	0.44703019	-1.93471694	-1.57538128

8	0.82373047	-2.78422642	1.27596998
6	2.26452827	-2.98232555	0.83917332
6	2.32054615	-4.42284727	0.34126225
8	1.82590842	-5.41228914	1.28864181
6	0.86985898	-5.09626102	2.19994617
6	0.39968881	-3.65043378	2.33000779
8	2.49912763	-2.04779625	-0.03611260
1	0.75560248	-3.28975701	3.30866718
1	-0.69763136	-3.65519524	2.33842206
6	-4.10139894	-0.91138738	0.37675136
8	-2.74605036	-1.18741250	0.84193146
6	-2.02967763	-0.11702081	1.22128499
6	-2.78652501	1.17712903	1.35791731
8	-4.12714624	0.99342805	1.88465893
6	-4.87373734	0.01130657	1.30528033
8	-0.83238566	-0.23511398	1.47063351
1	-4.04268551	-0.46813387	-0.63118118
1	-4.60323763	-1.88062191	0.32823840
1	1.72296441	-4.48708534	-0.57779640
1	3.35724115	-4.71039486	0.12995082
1	-2.26672530	1.83117032	2.06296611
1	-2.82937121	1.67950749	0.36995357
8	-6.05401802	-0.10342361	1.53100336
8	3.05931544	-2.91346693	2.07935262
6	3.90862465	-1.78914213	2.17897558
6	3.20394135	-0.51077020	2.61437893
8	3.92423916	0.18857858	3.49142671
6	3.37605214	1.48108482	3.88784838
1	4.68616056	-2.03611684	2.91203284
1	4.38196945	-1.55542827	1.20757520
8	2.10789800	-0.11743385	2.20061564
1	2.39265275	1.34204555	4.35045624
1	4.09643888	1.88290977	4.60470533
1	3.28417635	2.13142991	3.01067281
1	-3.74965978	2.90269351	-2.17787838
8	0.42764562	-5.95170879	2.93687701

I-2om-si_DBP_Mg_MeG_GL_GL

E = -2074.450803   E0 = -2073.893358   ZPVE = 0.557445 a.u. = 349.8019 kcal/mol
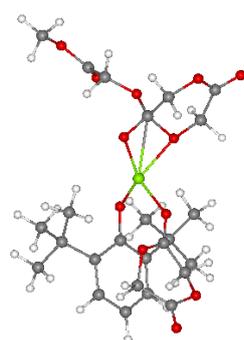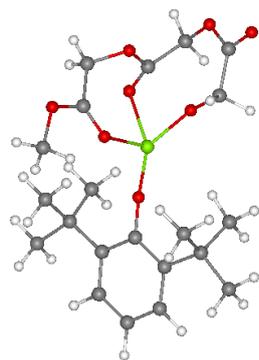

	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	20.0437	44.7992	0.8887	1.4812	-11.8756
rotational	17.5438	37.8441	0.8887	0.8887	-10.3945
vibrational	46.7836	175.0646	374.2787	374.2787	322.0832
total	84.3711	257.7078	376.0562	376.6487	299.8131

12	-0.23775415	-1.01943064	-0.39304432
8	0.30518359	0.54226786	0.55702937
6	0.13475311	1.79765451	0.15373421
6	-0.93986952	2.59306240	0.68462360
6	-1.17661774	3.85097313	0.11525500
1	-2.00070262	4.46102524	0.48152781
6	-0.38159645	4.35910130	-0.91557169
6	0.74131197	3.63867903	-1.32911539
1	1.40875578	4.09445858	-2.05969763
6	1.05063915	2.37922812	-0.79407716
6	-1.77413797	2.11256766	1.89393723
6	2.41260219	1.70923769	-1.10211754
6	-2.60442924	0.85011941	1.56677091
1	-1.95773792	-0.01703494	1.39202285
1	-3.26001859	0.60495406	2.41599703
1	-3.24479842	1.00478017	0.68572485
6	-0.82756436	1.80818939	3.07990789
1	-0.09821942	1.03354847	2.81833553
1	-0.28470606	2.71569920	3.38023853
1	-1.41153646	1.46165311	3.94606018
6	-2.77030659	3.18947291	2.36691093
1	-2.26409888	4.12462282	2.64420176
1	-3.53205609	3.41956758	1.60710061
1	-3.29684806	2.82145548	3.25879478
6	3.23197055	2.52852678	-2.11936355
1	2.74027467	2.58999276	-3.10252190
1	3.42737675	3.55022883	-1.76675308
1	4.20577097	2.04206753	-2.26971960
6	3.22639203	1.65660799	0.21441692
1	2.69335103	1.07909787	0.97953236
1	4.20308304	1.18090928	0.03559077
1	3.40673089	2.66972780	0.60005522
6	2.30518627	0.27073970	-1.66864657
1	1.54123878	0.17984039	-2.45482183
1	3.26254654	-0.02072890	-2.12590551
1	2.12016058	-0.46628192	-0.87648803

8	-1.41622519	-2.58359766	0.35902107
6	-0.28881449	-3.50910187	-0.02167439
6	-0.96941435	-4.65463686	-0.77186155
8	-2.04532933	-5.29552841	-0.03228849
6	-2.77437925	-4.60421562	0.88417077
6	-2.38586092	-3.17306972	1.24042511
8	0.54047769	-2.78727365	-0.75208348
1	-2.00627422	-3.18588400	2.27301311
1	-3.29081202	-2.55499172	1.19715559
6	-0.59347904	2.01276255	-4.46409178
8	-0.62782258	0.77269655	-3.69108963
6	-1.44985819	0.76104450	-2.63983727
6	-2.41242695	1.91007578	-2.51772261
8	-2.90459037	2.37571406	-3.79931498
6	-1.97425246	2.56447816	-4.77776527
8	-1.41585732	-0.18177617	-1.84559941
1	-0.00954163	2.75720668	-3.89855194
1	-0.08040696	1.76569939	-5.39636135
1	-1.37248206	-4.26216316	-1.71525657
1	-0.24731071	-5.45096207	-0.99323392
1	-3.29048347	1.59364367	-1.94798160
1	-1.91266966	2.73736405	-1.97199512
8	-2.24599886	3.12528396	-5.81060886
8	0.20339635	-3.93685031	1.26162755
6	1.50419450	-4.50010729	1.22463059
6	2.14471912	-4.35285234	2.59848547
8	3.27997088	-5.10629654	2.63706970
6	4.01757193	-5.01577425	3.88091278
1	1.48398304	-5.57084608	0.95517671
1	2.13529944	-3.97053599	0.49085021
8	1.74085236	-3.66866660	3.51252985
1	3.40109968	-5.37031364	4.71614122
1	4.89307404	-5.65735960	3.74467802
1	4.31960869	-3.97851205	4.07214165
1	-0.59858012	5.33713198	-1.34651041
8	-3.70570898	-5.13836718	1.44587004

TS-23c23-si_DBP_Mg_MeG_GL

E = -1619.021509   E0 = -1618.547969   ZPVE = 0.473540 a.u. = 297.1511 kcal/mol
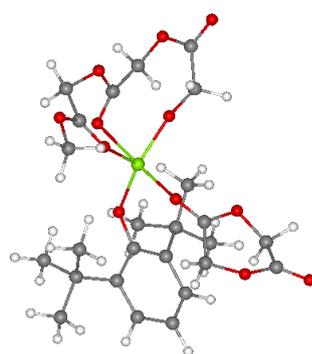
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	19.6885	44.0933	0.8887	1.4812	-11.6652
rotational	16.8413	36.4481	0.8887	0.8887	-9.9783
vibrational	34.0787	131.7520	316.2418	316.2418	276.9599
total	70.6084	212.2934	318.0193	318.6117	255.3165

12	0.07761248	-0.79359305	0.93177074
8	-0.57846171	0.13373411	-0.51785445
6	-0.92260945	1.07299721	-1.39984310
6	-1.36623991	2.36474276	-0.96004212
6	-1.72223711	3.31366229	-1.92737329
1	-2.06390786	4.29851580	-1.61355615
6	-1.65558064	3.03709006	-3.29038739
6	-1.22305715	1.78155649	-3.71120000
1	-1.17817318	1.57964230	-4.77998829
6	-0.85270023	0.78215301	-2.80284524
6	-1.45545745	2.72091007	0.53994906
6	-0.38433868	-0.59725285	-3.31626678
6	-2.43891239	1.77391362	1.26826680
1	-2.18470597	0.71718431	1.12835157
1	-2.45578361	1.99295700	2.34725285
1	-3.45645666	1.91731560	0.87743407
6	-0.04832336	2.67533731	1.18417859
1	0.48432228	1.74219811	0.96062076
1	0.57264811	3.49324775	0.79088902
1	-0.11408874	2.79335022	2.27684975
6	-1.98483407	4.14994240	0.77773589
1	-1.33513200	4.91284418	0.32648692
1	-3.00129938	4.28130341	0.38126886
1	-2.02292776	4.34416533	1.85997283
6	-0.40234444	-0.68625116	-4.85522079
1	-1.41250134	-0.54074746	-5.26320124
1	0.26893368	0.04910987	-5.32151842
1	-0.06294123	-1.68705165	-5.16082048
6	1.07549274	-0.86640227	-2.87797236
1	1.17958188	-0.81013465	-1.78848064

1	1.39582610	-1.86541939	-3.21377921
1	1.75126112	-0.12264071	-3.32580614
6	-1.31970751	-1.71433640	-2.79687834
1	-2.33864236	-1.56465209	-3.18228531
1	-0.96736294	-2.69802451	-3.14504004
1	-1.36810303	-1.72548187	-1.70318103
8	-0.27379361	-1.14585125	2.77932024
6	0.38956127	-3.05710316	2.16848993
6	-0.59546709	-3.63361335	3.16195321
8	-0.27789804	-3.37628484	4.54024220
6	-0.17164773	-2.10091782	5.05720425
6	-0.18319586	-0.87409306	4.13618422
8	0.13256174	-2.90573525	0.95198661
1	0.73328561	-0.31516987	4.41220045
1	-1.03396046	-0.25681764	4.48533392
1	-1.59174550	-3.26585698	2.89231968
1	-0.57955581	-4.73273897	3.07393289
8	1.68316364	-3.12439561	2.62006211
6	2.71090984	-3.01212883	1.62625206
6	3.00665545	-1.58662760	1.18279171
8	4.30453205	-1.40544164	0.96493006
6	4.68198538	-0.10705821	0.40580109
1	3.60751677	-3.45247817	2.07382512
1	2.43123174	-3.57495117	0.72012752
8	2.16669321	-0.70654196	0.98712361
1	4.41313601	0.68801117	1.10998750
1	5.76412773	-0.16672462	0.26894119
1	4.16721249	0.04826034	-0.54958802
1	-1.93968761	3.79548049	-4.02086926
8	-0.03446769	-1.98710108	6.25396061

TS-23c23m-si_DBP_Mg_MeG_GL_GL

E = -2074.455884   E0 = -2073.898942   ZPVE = 0.556942 a.u. = 349.4867 kcal/mol
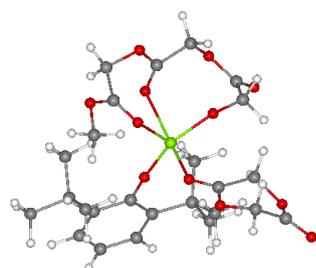
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	20.0437	44.7992	0.8887	1.4812	-11.8756
rotational	17.3519	37.4627	0.8887	0.8887	-10.2808
vibrational	41.4237	162.4905	373.3902	373.3902	324.9436
total	78.8192	244.7524	375.1676	375.7601	302.7872

|							
12	0.83551347	-0.89909369	0.62835258	8	0.73612601	-2.75475359	1.17179430
8	0.64887792	0.36156011	-0.83053857	6	2.81516314	-2.77641940	0.58763993
6	-0.36997384	1.06174600	-1.30002737	6	2.56405568	-4.20602989	0.15900892
6	-0.46502340	2.48051882	-1.05659246	8	2.29347944	-5.12967491	1.22882819
6	-1.65831614	3.13556719	-1.38563418	6	1.25976646	-4.96805286	2.12893772
1	-1.76418674	4.19839239	-1.17331004	6	0.42061478	-3.68266225	2.14467645
6	-2.72838759	2.46968603	-1.98792887	8	2.74875927	-1.79967415	-0.17721522
6	-2.55731249	1.14251935	-2.38935804	1	0.53248453	-3.29939866	3.18177652
1	-3.35037947	0.67255378	-2.96997976	1	-0.63007522	-4.02881527	2.06750870
6	-1.38338578	0.42762399	-2.11151505	6	-4.16288853	-0.76858532	0.43639034
6	0.73231816	3.28759217	-0.50528538	8	-2.82282853	-1.04615414	0.94035381
6	-1.11998832	-0.93030870	-2.80834270	6	-2.10336471	0.02641964	1.30766582
6	1.01385570	2.94793630	0.97410160	6	-2.84808135	1.33297563	1.38764179
1	1.26214540	1.89040577	1.10057080	8	-4.20430183	1.18312061	1.88369942
1	1.86174536	3.55073404	1.33913755	6	-4.94706535	0.19122523	1.31577575
1	0.14236876	3.17884254	1.60498238	8	-0.91200018	-0.08983690	1.58048642
6	1.99297702	2.99320769	-1.35318649	1	-4.07637501	-0.35748008	-0.58336323
1	2.24216413	1.92652738	-1.33637726	1	-4.67580986	-1.73278236	0.40554625
1	1.83197308	3.29736757	-2.39748454	1	1.75793052	-4.19209242	-0.58219135
1	2.84820437	3.56709528	-0.96348387	1	3.48303723	-4.59468317	-0.31172696
6	0.48480049	4.80762100	-0.57903230	1	-2.33808827	2.00254607	2.08521533
1	0.26492858	5.13804245	-1.60389400	1	-2.85775638	1.80414164	0.38357121
1	-0.33888376	5.13188457	0.07373443	8	-6.13459682	0.09884191	1.51322746
1	1.39155185	5.33366871	-0.24657169	8	3.49321651	-2.71495366	1.78408837
6	-2.32371640	-1.37656355	-3.66219592	6	4.10261345	-1.45478225	2.08877039
1	-3.22060585	-1.56917727	-3.05338287	6	3.13524199	-0.44335559	2.68244743
1	-2.58264327	-0.63935280	-4.43434858	8	3.68081713	0.21386111	3.70540309
1	-2.06893659	-2.31416655	-4.17590809	6	2.86084247	1.26960456	4.29403019
6	0.08311971	-0.73854488	-3.76508927	1	4.90083408	-1.67074406	2.80577087
1	0.97635698	-0.43122411	-3.20727658	1	4.52338886	-1.00082457	1.17617977
1	0.30654347	-1.68364668	-4.28429699	8	2.00088978	-0.21050559	2.26824617
1	-0.13978945	0.02367565	-4.52493906	1	1.92855394	0.84045422	4.67728519
6	-0.79017377	-2.09588456	-1.84640527	1	3.47127295	1.67783725	5.10301399
1	-1.45514798	-2.13283491	-0.97253996	1	2.63706565	2.03165054	3.53903675
1	-0.89789236	-3.05521679	-2.37552452	1	-3.65360188	3.00091863	-2.21373630
1	0.25158101	-2.04824495	-1.50906777	8	1.06439912	-5.86184311	2.92285299

I-3c23m_DBP_Mg_MeG_GL

E = -2074.452682   E0 = -2073.896542   ZPVE = 0.556140 a.u. = 348.9832 kcal/mol

	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	20.0437	44.7992	0.8887	1.4812	-11.8756
rotational	17.4318	37.6216	0.8887	0.8887	-10.3281
vibrational	45.6768	174.4800	373.9415	373.9415	321.9202
total	83.1523	256.9008	375.7189	376.3114	299.7164

12	0.28829071	-0.72608209	0.63392234	8	0.55778772	-2.61344385	0.83314496
8	0.15174985	0.74207330	-0.52802473	6	2.97920418	-1.44618690	1.70484149
6	0.14079237	1.61431551	-1.53277421	6	3.36053324	-2.89715505	1.47758079
6	0.18505290	3.02529621	-1.25521970	8	3.41207695	-3.23695898	0.10226715
6	0.16413271	3.92833161	-2.32517242	6	2.29575157	-3.77003670	-0.53297007
1	0.19734889	4.99821854	-2.12648869	6	0.95285034	-3.78644037	0.22315462
6	0.09937227	3.50249863	-3.64892220	8	3.03790712	-1.16560996	3.03952765
6	0.05412340	2.13734746	-3.91817164	6	2.72635698	0.19400725	3.40249372
1	0.00369716	1.81593382	-4.95700407	6	1.22285914	0.41122574	3.46349120
6	0.07377946	1.17482531	-2.90114665	8	0.87728429	1.16634202	4.50267315
6	0.24419323	3.55935407	0.19167428	6	-0.54535437	1.49010491	4.60775137
6	0.03394866	-0.32252938	-3.27065039	1	3.18089867	0.36167598	4.38312960
6	-1.01703537	3.11797166	0.96981388	1	3.14025927	0.89601052	2.66155338
1	-1.11071002	2.02710009	1.00153565	8	0.41756004	-0.04161507	2.65549231
1	-0.98365915	3.51612329	1.99838829	1	-1.11406171	0.57058311	4.78551435
1	-1.91955101	3.52219582	0.48918021	1	-0.61331069	2.16830969	5.46163511
6	1.52719235	3.05522370	0.89345163	1	-0.88724422	1.96976185	3.68442726
1	1.60574400	1.96466017	0.83012074	1	0.08439058	4.22772408	-4.46336699
1	2.41741776	3.48526073	0.41201031	8	2.45131254	-4.21317482	-1.64611161
1	1.53360605	3.37063098	1.95126081	1	4.37384272	-3.05550742	1.87863374
6	0.28379446	5.09897614	0.25532311	1	2.66503191	-3.52297020	2.05488658
1	1.16379762	5.51120996	-0.25816032	1	1.04075837	-4.62029028	0.96403164
1	-0.61650515	5.55355167	-0.18174092	1	0.24184614	-4.15401554	-0.54524767
1	0.33694482	5.41364336	1.30873954	8	2.68939161	-0.61959422	0.85782254
6	-0.05773014	-0.56003177	-4.79168415	6	-4.70421553	-2.76116896	1.80006754
1	-0.96588886	-0.11798763	-5.22574997	8	-3.83975697	-1.59445667	1.71468568
1	0.81477910	-0.15662915	-5.32428837	6	-2.66230774	-1.75913382	1.08736515
1	-0.08854169	-1.64293432	-4.98278666	6	-2.46019554	-3.06885433	0.35677177
6	1.32905769	-1.02299702	-2.80205417	8	-3.67127180	-3.59069490	-0.24349819
1	1.52293968	-0.87461710	-1.73350775	6	-4.80150652	-3.56526423	0.51330900
1	1.28831744	-2.10283804	-3.00659800	8	-1.83450043	-0.86259663	1.14109182
1	2.19411182	-0.61135733	-3.34128475	1	-4.34940481	-3.41214228	2.61586952
6	-1.22054684	-0.98936021	-2.65660930	1	-5.69617844	-2.37962127	2.05562353
1	-2.13123131	-0.58983910	-3.12621593	1	-1.74978507	-2.92068529	-0.46016061
1	-1.19903052	-2.07746434	-2.83025408	1	-2.02651358	-3.80391312	1.05489576
1	-1.29223847	-0.78665757	-1.58128726	8	-5.80380440	-4.14763117	0.17798688

I-3c3_si_DBP_Mg_MeG_GL

E = -1619.002159   E0 = -1618.528474   ZPVE = 0.473685 a.u. = 297.2416 kcal/mol
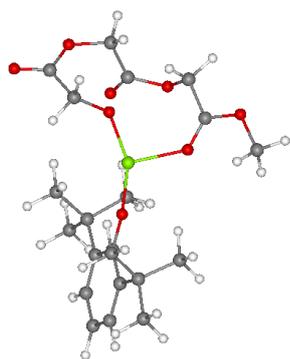
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	19.6885	44.0933	0.8887	1.4812	-11.6652
rotational	16.8348	36.4351	0.8887	0.8887	-9.9744
vibrational	33.7259	132.4373	316.7456	316.7456	277.2594
total	70.2492	212.9657	318.5230	319.1155	255.6198

12	0.52659476	-0.47383034	0.72530800
8	-0.49680376	-0.00377695	-0.77653742
6	-1.31929684	0.97303075	-1.17141414
6	-1.84629154	1.92163217	-0.23319134
6	-2.70264459	2.92909455	-0.69313657
1	-3.11001873	3.65483546	0.00981016
6	-3.05147600	3.02757788	-2.03762484
6	-2.53717852	2.10348701	-2.94729137
1	-2.82088184	2.19525433	-3.99449635
6	-1.67533028	1.07206130	-2.55552292
6	-1.47871900	1.81703961	1.25816619
6	-1.12618446	0.06761651	-3.59048939
6	-2.01511049	0.48148724	1.84405863
1	-1.81018651	-0.39010110	1.20302916
1	-1.62183988	0.29811066	2.85555458
1	-3.11012363	0.52832270	1.91558874
6	0.06885296	1.95448041	1.43658137
1	0.62827730	1.73394883	0.51093948
1	0.33795786	2.99811220	1.64943254
1	0.45416701	1.38904130	2.30846214
6	-2.10645866	2.93204570	2.11655998
1	-1.78839636	3.92964435	1.78286684
1	-3.20377779	2.89174247	2.09380460
1	-1.78975940	2.80904031	3.16283751
6	-1.63592625	0.36148831	-5.01429462
1	-2.73109961	0.29365522	-5.08206987
1	-1.32815337	1.35641432	-5.36731577
1	-1.21486223	-0.38175994	-5.70726681
6	0.41941774	0.13960056	-3.63953781
1	0.85173738	-0.08642692	-2.65810919

1	0.80571568	-0.58263731	-4.37653875
1	0.74778950	1.14413679	-3.94533348
6	-1.57653069	-1.36861169	-3.23301077
1	-2.67357349	-1.44240344	-3.25474215
1	-1.17484999	-2.08465743	-3.96743584
1	-1.22957158	-1.65355694	-2.23377371
8	0.73518968	-1.98914087	1.84012663
6	1.95602858	-0.92764252	3.71630478
6	1.94758618	-2.36715436	4.21748590
8	0.65249610	-2.72972107	4.69963598
6	-0.36411563	-3.05301595	3.81882668
6	-0.11608893	-2.99380374	2.30109787
1	-1.13164520	-2.94568682	1.86932790
1	0.27272326	-4.00323963	2.03482580
8	2.99564219	-0.51497108	2.87782955
6	3.67488384	-1.40298474	1.99302280
6	3.53423738	-0.85929173	0.58075160
8	4.62119436	-1.05372608	-0.15342090
6	4.52586985	-0.64680248	-1.55666733
1	4.73581553	-1.47605562	2.26749516
1	3.21825600	-2.40359163	1.97219133
8	2.51405334	-0.32362428	0.13983229
1	4.34815264	0.43233100	-1.61443496
1	5.49242163	-0.91423613	-1.98949921
1	3.70596361	-1.18576431	-2.04413176
1	-3.72110891	3.81874132	-2.37634945
8	-1.41303635	-3.42811632	4.28970957
8	1.23055863	-0.06495764	4.14722586
1	2.31200743	-3.08633876	3.47557974
1	2.60744810	-2.41634250	5.09936857

I-3c3m-si_DBP_Mg_MeG_GL_GL

E = -2074.454378   E0 = -2073.898030   ZPVE = 0.556348 a.u. = 349.1138 kcal/mol
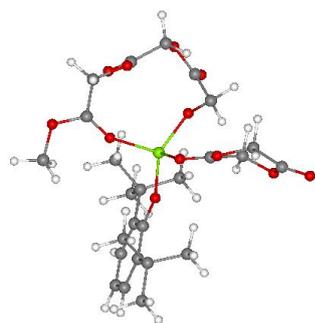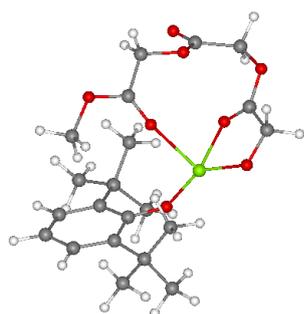
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	20.0437	44.7992	0.8887	1.4812	-11.8756
rotational	17.4588	37.6752	0.8887	0.8887	-10.3441
vibrational	47.7518	179.0016	374.1907	374.1907	320.8214
total	85.2543	261.4760	375.9682	376.5607	298.6016

12	0.37494645	-0.74208182	0.34736183	8	1.81339192	-1.88474274	-0.12691680
8	-0.41905272	0.72939098	-0.48773047	6	2.99745512	-1.91061378	2.53333664
6	-0.77545702	1.98617315	-0.75838697	6	3.80961132	-2.79233313	1.59937501
6	0.21385798	3.00724626	-0.97002304	8	4.67125893	-2.00536013	0.78250861
6	-0.21753049	4.31381989	-1.23381305	6	4.26689959	-1.56057620	-0.46514413
1	0.51994920	5.09856892	-1.39348388	6	2.88328505	-1.96808243	-1.00690269
6	-1.56746590	4.64696980	-1.30857360	8	3.21937656	-0.75672442	2.82216597
6	-2.52358055	3.65071440	-1.12839806	8	1.96220040	-2.63320327	3.09149599
1	-3.57538748	3.92117953	-1.20518804	6	1.25117397	-1.90145993	4.09487772
6	-2.16914797	2.32256007	-0.85970366	6	0.54951757	-0.66905397	3.54292202
6	1.72532380	2.69498158	-0.92375958	8	0.26442963	0.19504029	4.50675964
6	-3.27103472	1.25480926	-0.68317485	6	-0.45937651	1.39901400	4.09166336
6	2.14078808	2.25353980	0.49925262	1	0.48751494	-2.59175515	4.47916985
1	1.50744653	1.44556046	0.88579154	1	1.91320586	-1.59509468	4.91517687
1	3.18580294	1.91141367	0.51904094	8	0.21206290	-0.50755197	2.37222338
1	2.04455376	3.09702325	1.19921196	1	-1.41646552	1.11983526	3.63760042
6	2.08507776	1.61559749	-1.97189355	1	-0.60482657	1.96512985	5.01436901
1	1.47314405	0.71464443	-1.85060549	1	0.14706686	1.95976877	3.37225103
1	1.90570331	2.00391722	-2.98498464	1	-1.87200129	5.67327881	-1.51732814
1	3.14762449	1.34015703	-1.89530182	8	5.06165457	-0.91106099	-1.10564303
6	2.59702682	3.92283916	-1.25802124	1	4.46948910	-3.42160773	2.21911669
1	2.39189529	4.30774975	-2.26678133	1	3.12876177	-3.43487382	1.03069746
1	2.45565128	4.74179173	-0.53829408	1	3.02709436	-3.01505494	-1.37425828
1	3.65614748	3.62867618	-1.22254050	1	2.76968241	-1.34677410	-1.91396666
6	-4.68695211	1.82456636	-0.89953530	6	-2.01809883	-5.36254930	-1.09363103
1	-4.93495989	2.60831809	-0.16957617	8	-2.05259514	-4.20192480	-0.21430603
1	-4.81318474	2.23968744	-1.90937257	6	-1.21653879	-3.19800067	-0.50421596
1	-5.42166138	1.01455808	-0.77833927	6	-0.48424399	-3.27612281	-1.82695103
6	-3.09004879	0.12140238	-1.72093177	8	-1.25629079	-3.89308429	-2.88364220
1	-2.08667326	-0.31191272	-1.65065610	6	-1.94403422	-5.02715921	-2.57453442
1	-3.84303522	-0.66681439	-1.55995679	8	-1.08538365	-2.28603888	0.30247939
1	-3.22361851	0.51383078	-2.73927140	1	-1.16102982	-5.99574089	-0.81302404
6	-3.24025822	0.68505269	0.75445557	1	-2.94423676	-5.90954685	-0.89928377
1	-3.47119141	1.47977149	1.47987914	1	-0.24654520	-2.26646948	-2.17538071
1	-3.99446440	-0.10934198	0.87042105	1	0.46661052	-3.81308436	-1.67251670
1	-2.25755501	0.26896435	0.99933565	8	-2.45275736	-5.71176052	-3.42699170

I-3c13_DBP_Mg_MeG_GL

E = -1619.039243   E0 = -1618.565016   ZPVE = 0.474227 a.u. = 297.5820 kcal/mol

	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	19.6885	44.0933	0.8887	1.4812	-11.6652
rotational	16.6518	36.0715	0.8887	0.8887	-9.8660
vibrational	32.7105	130.0903	316.9878	316.9878	278.2014
total	69.0508	210.2551	318.7653	319.3578	256.6702

```
12  -0.57096636  -0.85076404   1.56551373          1   0.16803674  -2.48524451  -2.60304856
 8  -1.41524279   0.01422696   0.12186085          1   1.24211836  -1.11952686  -2.23093534
 6  -1.09186101   1.05681419  -0.64850861          6  -2.24034405  -1.11496997  -2.52627873
 6  -1.14028502   2.38975024  -0.11724652          1  -2.97698760  -0.46811128  -3.02461028
 6  -0.68515706   3.44720531  -0.91600591          1  -2.29661989  -2.11138082  -2.99164748
 1  -0.68910843   4.46190691  -0.52172369          1  -2.51262617  -1.19979668  -1.46897149
 6  -0.23955782   3.24435830  -2.22134542          8  -0.75367564  -1.35079789   3.40517783
 6  -0.29134369   1.96245933  -2.76586843          6   2.55390668  -3.91078353   0.61004251
 1   0.01026778   1.82770133  -3.80318928          6   1.70438957  -4.87154675   1.43778896
 6  -0.72273266   0.85450172  -2.02262664          8   1.14111805  -4.31607246   2.64882994
 6  -1.73918486   2.67200780   1.27957010          6   0.31645340  -3.27289987   2.46272731
 6  -0.81625605  -0.53462774  -2.69392705          6  -0.16354437  -2.54970264   3.71518540
 6  -3.22904563   2.25287628   1.28489292          8   2.88124228  -4.16626501  -0.52695960
 1  -3.33808446   1.19473457   1.01828706          1   0.72622710  -2.46086216   4.37895536
 1  -3.66647506   2.41143441   2.28304625          1  -0.84427994  -3.26483870   4.23725271
 1  -3.79955268   2.85506272   0.56372744          1   0.91485602  -5.25016689   0.77715605
 6  -0.98850739   1.92111278   2.41670847          1   2.33338976  -5.70643616   1.77091634
 1  -1.48782325   0.98269606   2.70051551          8   2.91635966  -2.79430985   1.30795097
 1   0.06681769   1.73484755   2.16464043          6   3.57871318  -1.77241182   0.54912847
 1  -0.98574525   2.51794147   3.34079480          6   2.75067544  -0.49085957   0.55117041
 6  -1.68823028   4.17348671   1.62889671          8   3.38168263   0.44813770  -0.15154620
 1  -0.65660703   4.54989052   1.69761968          6   2.68806052   1.73428488  -0.27696651
 1  -2.23139143   4.78545046   0.89586705          1   4.55334663  -1.57242227   1.01490676
 1  -2.16525936   4.32882786   2.60722160          1   3.74078059  -2.10938501  -0.48463178
 6  -0.53500122  -0.46728063  -4.20865583          8   1.67984080  -0.32929790   1.12078798
 1  -1.23057008   0.20858756  -4.72567940          1   2.53168774   2.16435623   0.71840304
 1   0.49240011  -0.14171903  -4.42772865          1   3.36522889   2.35278177  -0.87047046
 1  -0.66134238  -1.47099161  -4.63969231          1   1.72823381   1.59398556  -0.78812307
 6   0.22186141  -1.51028538  -2.09491515          1   0.11028330   4.08501482  -2.82178140
 1   0.04454426  -1.68166518  -1.02859139          8   0.01088624  -2.88100934   1.32613313
```

I-3c13m-si_DBP_Mg_MeG_GL_GL

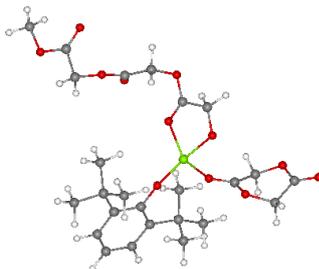E = -2074.473036   E0 = -2073.916647   ZPVE = 0.556390 a.u. = 349.1399 kcal/mol
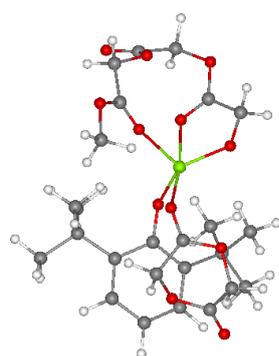
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	20.0437	44.7992	0.8887	1.4812	-11.8756
rotational	17.3475	37.4540	0.8887	0.8887	-10.2782
vibrational	44.0846	170.3712	373.8164	373.8164	323.0203
total	81.4757	252.6243	375.5939	376.1864	300.8664

12	0.33753309	-1.31576419	0.62718111
8	0.35876343	0.01685992	-0.77925193
6	-0.44045085	0.96164227	-1.23696482
6	-0.19081113	2.35039902	-0.92618746
6	-1.18776333	3.28933120	-1.21595526
1	-1.03842437	4.33404160	-0.94670826
6	-2.37816596	2.93195605	-1.85434246
6	-2.51603031	1.62942433	-2.34018373
1	-3.38371515	1.39768672	-2.95719457
6	-1.55200756	0.63867670	-2.10465813
6	1.16393673	2.81709051	-0.34573728
6	-1.63410354	-0.71196693	-2.86201715
6	1.34707868	2.36347699	1.11852598
1	1.32391620	1.27321076	1.20007205
1	2.31559968	2.72110248	1.50423443
1	0.55387044	2.78029490	1.75834131
6	2.32049060	2.25557828	-1.20684052
1	2.29989576	1.16077733	-1.23443532
1	2.24747634	2.63245082	-2.23717833
1	3.28760648	2.58329678	-0.79510194
6	1.29722488	4.35316944	-0.35925919
1	1.16801488	4.76628256	-1.36939824
1	0.57551515	4.84421301	0.31002405
1	2.30424404	4.62725449	-0.01233443
6	-2.66098595	-0.64444274	-4.01340437
1	-3.69465089	-0.54096705	-3.65167332
1	-2.45083213	0.18471012	-4.70353174
1	-2.61250663	-1.58104944	-4.58730841
6	-0.26445723	-1.02293301	-3.51287270
1	0.52686715	-1.10998225	-2.76103997
1	-0.32897678	-1.96797824	-4.07362938
1	0.01484023	-0.22855017	-4.22042942
6	-2.06044364	-1.89403868	-1.96594322
1	-3.05339694	-1.72173333	-1.52666450
1	-2.12887168	-2.80992413	-2.57379222
1	-1.36407232	-2.11096334	-1.14697874
8	-0.32251704	-3.11816359	0.86507201
6	4.53877449	-2.71995378	1.08518898
6	4.24290371	-3.82164478	0.07037397
8	2.95605350	-4.45199203	0.23858547
6	1.91332483	-3.59242082	0.17462739
6	0.55650067	-4.13525724	0.60720849
8	5.41360474	-1.89821792	0.93283421
1	0.75413561	-4.79894972	1.47990465
1	0.22938463	-4.82590866	-0.21004191
6	-4.48359919	-0.05576971	0.52915132
8	-3.23920178	-0.63704240	1.01471150
6	-2.29726291	0.23806033	1.39386821
6	-2.73110843	1.67885303	1.48826241
8	-4.07941008	1.82643723	2.00908566
6	-5.02947998	1.03131533	1.43995273
8	-1.16232395	-0.14617456	1.66436887
1	-4.31329966	0.35148382	-0.48178554
1	-5.19853354	-0.88045514	0.47903624
1	4.34316015	-3.37464166	-0.92625576
1	4.97966623	-4.62667799	0.18801434
1	-2.07611680	2.21666384	2.17855072
1	-2.65417600	2.15115547	0.48793057
8	3.73317695	-2.81425595	2.18960309
6	3.81845784	-1.73571682	3.12574673
6	2.47500658	-1.02565885	3.22594333
8	2.36346221	-0.41871324	4.41168594
6	1.14457965	0.36075923	4.60941029
1	4.10133600	-2.13846922	4.10592699
1	4.58404446	-1.01237798	2.79913807
8	1.61955237	-0.97883838	2.35385776
1	0.26780143	-0.27807614	4.45644855
1	1.20475578	0.71620065	5.64094019
1	1.12228620	1.19735718	3.90193033
1	-3.14739728	3.67995882	-2.04941726
8	2.07556868	-2.41003776	-0.13996962
8	-6.20531130	1.19454479	1.66276360

I-3c1_DBP_Mg_MeG_GL_GL

E = -2074.472588   E0 = -2073.916513   ZPVE = 0.556075 a.u. = 348.9425 kcal/mol

	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	20.0437	44.7992	0.8887	1.4812	-11.8756
rotational	17.8375	38.4278	0.8887	0.8887	-10.5685
vibrational	49.5755	182.6490	374.0263	374.0263	319.5695
total	87.4567	265.8759	375.8038	376.3963	297.1254

```
8 -0.93335915  0.74380970 -0.24062280        8 -4.18555403 -1.83940899  2.98891258
6 -1.29038525  1.47743070 -1.29192340        6 -3.10064244 -1.06553304  2.88784170
6 -1.75473762  2.82514763 -1.11580193        6 -2.77696013 -0.15933764  4.04964209
6 -2.11816669  3.56254792 -2.24992752        8 -3.14240670 -0.72212201  5.33326769
1 -2.47088289  4.58607721 -2.13493490        6 -4.35652399 -1.32950675  5.42795706
6 -2.04061103  3.02808166 -3.53343558        8 -2.41853309 -1.13815558  1.86655545
6 -1.58796120  1.72141695 -3.70012450        1 -5.68562460 -0.66968483  3.85769844
1 -1.53159916  1.31734240 -4.70947647        1 -5.72890139 -2.42477298  4.19676161
6 -1.20686233  0.92341650 -2.61427236       12 -0.62344074 -0.19903678  1.32153952
6 -1.85499513  3.46829700  0.28468239        8  0.05911194  0.17981187  3.10105968
6 -0.71049422 -0.51937753 -2.85353732        6  1.21727300 -0.50210977  3.40698814
6 -2.86649871  2.68675971  1.15851009        6  1.56606615 -1.52539277  2.33424115
1 -2.63089728  1.61585212  1.18030608        1  2.11279106  0.15396759  3.49215388
1 -2.86661839  3.08028507  2.18785310        1  1.17158151 -1.05622482  4.37132072
1 -3.88205600  2.79191184  0.74956858        1 -1.68139684  0.01591989  4.05351591
6 -0.46477517  3.52115202  0.96069866        1 -3.28458881  0.80996013  3.90052152
1  0.00103912  2.53266239  1.03261578        8 -4.81787395 -1.66479409  6.49150610
1  0.21013914  4.16593838  0.37972793        8  0.88144010 -1.65481889  1.30535042
1 -0.54642117  3.94072199  1.97535229        1 -2.33009315  3.62619805 -4.39832163
6 -2.36736202  4.92174673  0.23209772        8  2.64986753 -2.27085805  2.56901908
1 -1.69397628  5.57282639 -0.34261364        6  3.05792069 -3.13981247  1.49055517
1 -3.37359285  4.99125242 -0.20507883        1  2.21694469 -3.74644709  1.13318229
1 -2.42020750  5.32147980  1.25581658        6  3.65149879 -2.32978344  0.34100080
6 -0.69901568 -0.89624512 -4.34863424        1  3.83412218 -3.78807688  1.91427553
1 -1.70314872 -0.85313356 -4.79388237        8  3.82937121 -3.15431595 -0.72661757
1 -0.03268913 -0.24576357 -4.93290091        8  3.92185259 -1.15233278  0.37837911
1 -0.33318830 -1.92850220 -4.45499516        6  4.50527573 -2.55475163 -1.84448183
6  0.74411309 -0.67846692 -2.35032988        6  6.01473761 -2.53251863 -1.61172402
1  0.84456921 -0.39805341 -1.29698861        1  4.14202118 -1.53283298 -2.01710939
1  1.07286322 -1.72364342 -2.47114015        1  4.26765251 -3.17951488 -2.71329045
1  1.41816008 -0.03710853 -2.93723512        8  6.57831573 -2.92724848 -0.61393565
6 -1.64693022 -1.53379416 -2.15585089        8  6.62156677 -2.00501132 -2.70092940
1 -2.65462685 -1.48227894 -2.59311962        6  8.06805038 -1.91406322 -2.60598660
1 -1.27093148 -2.56009936 -2.29039001        1  8.38969326 -1.46869981 -3.55136466
1 -1.73982966 -1.33353817 -1.08325016        1  8.50272179 -2.91241717 -2.47508001
6 -5.07609320 -1.55308783  4.10652590        1  8.35068321 -1.27933216 -1.75770009
```

I-1c1_DBP_Mg_rMeL_sLA

E = -1736.863821   E0 = -1736.309919   ZPVE = 0.553902 a.u. = 347.5787 kcal/mol
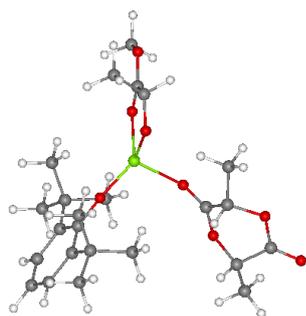
	ln(Q)	S,	U,	H,	G,
		cal/mol·K	kcal/mol	kcal/mol	kcal/mol
translational	19.8271	44.3688	0.8887	1.4812	-11.7473
rotational	17.1996	37.1602	0.8887	0.8887	-10.1906
vibrational	43.0115	161.8321	370.3452	370.3452	322.0949
total	80.0382	243.3611	372.1227	372.7151	300.1570

```
8   0.31023988   0.59688902  -0.77640468          6  -3.60213232  -1.86546707   2.34541368
6  -0.43081856   1.15982473  -1.72637010          8  -2.38425565  -2.08101583   1.54299951
6  -1.21246231   2.32919598  -1.43101501          6  -1.23749375  -1.61590600   2.03834248
6  -1.98669767   2.89547849  -2.45159411          6  -1.27025890  -1.10682881   3.47582126
1  -2.58385730   3.78190851  -2.24442577          8  -2.13591170  -1.96083474   4.28918266
6  -2.01543927   2.36266494  -3.73794794          6  -3.36010981  -2.29711795   3.79233098
6  -1.24805629   1.23620307  -4.02431059          8  -0.23606041  -1.62354290   1.32794476
1  -1.27380252   0.83515656  -5.03613663          1  -3.79956222  -0.77878571   2.33658099
6  -0.44931018   0.61497939  -3.05612969          6  -4.72786760  -2.61883879   1.67264247
6  -1.20720887   2.96905422  -0.02550384         12   1.22330511  -0.36476228   0.52738971
6   0.39259556  -0.62351120  -3.43194675          8   2.27224684   0.24496427   2.02143025
6  -1.76417530   1.96770585   1.01555634          6   3.55186653  -0.26201287   2.07468867
1  -1.19449937   1.03177750   0.98564488          6   3.75057173  -1.33396864   0.99040347
1  -1.70565712   2.39631176   2.02905464          8   4.91802740  -1.97295713   1.00504708
1  -2.81811070   1.73905361   0.79492015          6   5.11082792  -2.98227668  -0.02860525
6   0.22075263   3.41615272   0.36639243          6   4.63727856   0.82803190   1.92084479
1   0.93080699   2.58290839   0.35161060          1   3.75618958  -0.79413867   3.03481579
1   0.57983673   4.18273306  -0.33527440          6   0.09021442  -1.06406796   4.14081287
1   0.21987081   3.85500979   1.37641883          1  -1.71431983  -0.09375793   3.44464302
6  -2.10052276   4.22276974   0.05603486          8  -4.16512299  -2.88932061   4.47002554
1  -1.76133192   5.01192093  -0.62938946          8   2.86867976  -1.59437633   0.15048665
1  -3.15341306   3.99885869  -0.16803816          1   5.04046631  -2.52105355  -1.02032244
1  -2.05605984   4.63003826   1.07711768          1   6.11292267  -3.38132524   0.14912456
6   0.24033901  -1.01217031  -4.91647196          1   4.35145187  -3.76692867   0.06743777
1  -0.79621744  -1.27526605  -5.17097616          1  -2.62681985   2.82565331  -4.51346493
1   0.56952548  -0.20747322  -5.58896637          1   5.65318060   0.41707987   2.00205922
1   0.86602318  -1.89356375  -5.12207842          1   4.48328495   1.56795168   2.71572399
6   1.89669669  -0.33488700  -3.21136832          1   4.52266645   1.33773637   0.95390373
1   2.10264611   0.00194831  -2.18992591          1  -0.01691484  -0.64980853   5.15042400
1   2.49360442  -1.23821688  -3.41327262          1   0.78981233  -0.43972710   3.56038880
1   2.23294425   0.45594418  -3.89758444          1   0.50522459  -2.07747984   4.21526766
6  -0.06424774  -1.85445285  -2.61381578          1  -5.65650845  -2.45017743   2.22993279
1  -1.09201610  -2.13153076  -2.89040375          1  -4.52242756  -3.69586110   1.66525531
1   0.58731627  -2.71782708  -2.82043576          1  -4.85443640  -2.26240206   0.64357561
1  -0.05730541  -1.66227221  -1.53551602
```

TS-12ic2_si_DBP_Mg_rMeL_rLA

E = -1736.845347   E0 = -1736.290342   ZPVE = 0.555004 a.u. = 348.2705 kcal/mol
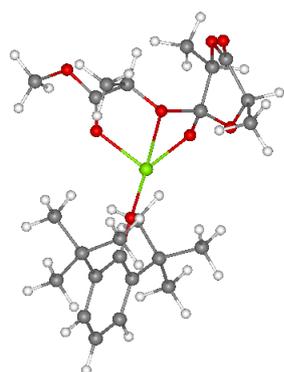
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	19.8271	44.3688	0.8887	1.4812	-11.7473
rotational	17.0428	36.8486	0.8887	0.8887	-10.0977
vibrational	37.4837	147.1877	369.9459	369.9459	326.0619
total	74.3536	228.4050	371.7233	372.3158	304.2168

8	-0.93156445	0.49693319	-0.73663205
6	-1.72725749	0.99681240	-1.68546689
6	-2.45942187	2.20067048	-1.42429137
6	-3.28705573	2.70722818	-2.43382144
1	-3.85231328	3.62047505	-2.25511718
6	-3.41655207	2.07833385	-3.67170572
6	-2.70648217	0.90626234	-3.91963243
1	-2.81856203	0.42099410	-4.88843632
6	-1.86212075	0.34352922	-2.95486736
6	-2.34378767	2.92540073	-0.06628369
6	-1.10919547	-0.97043198	-3.23568153
6	-2.79751110	1.99284828	1.08187830
1	-2.19672728	1.07748294	1.11062288
1	-2.70354652	2.51176214	2.04904366
1	-3.85274005	1.71177351	0.95135975
6	-0.88611853	3.38782239	0.17080668
1	-0.19702107	2.53591585	0.15546496
1	-0.57613283	4.09964609	-0.60852665
1	-0.80407941	3.89462495	1.14556479
6	-3.22898316	4.18493319	-0.00075694
1	-2.94862461	4.92885351	-0.76045120
1	-4.29457855	3.94579101	-0.12680699
1	-3.10968900	4.65662527	0.98574811
6	-1.35245240	-1.50591588	-4.66036272
1	-2.41019797	-1.74973369	-4.82927036
1	-1.03524470	-0.78628254	-5.42828274
1	-0.77194905	-2.42950106	-4.80546522
6	0.43230113	-0.74818712	-3.10899520
1	0.67897153	0.17316683	-2.55654860
1	0.94483697	-1.62574065	-2.67670345
1	0.88460219	-0.59513706	-4.09883022
6	-1.61111605	-2.07560802	-2.27089524
1	-2.66037917	-2.31001925	-2.49834657
1	-1.02161050	-2.99754310	-2.38646913
1	-1.58168447	-1.76985979	-1.21701562

8	0.17585689	-2.91805458	1.79905558
6	1.36629820	-2.42203641	1.26667213
6	2.56324506	-3.16255736	1.89209390
8	2.63472557	-2.86982560	3.31508994
6	1.43985713	-2.77111101	3.97674727
6	0.18654187	-3.23205900	3.21720791
8	1.33606040	-2.31536746	-0.02454162
6	-1.09124100	-2.69687963	3.84084129
6	3.92424560	-2.91534114	1.26896393
8	1.42854357	-2.42310214	5.13635826
12	0.57479000	-0.53820485	-0.36751798
8	1.25136125	-0.85212266	1.90838444
6	2.35458875	-0.00874101	2.17812729
6	2.89405346	0.62163734	0.89275295
8	4.06533003	1.22954226	1.04882145
6	4.60028362	1.90984941	-0.12701179
6	1.88704598	1.10985398	3.12752604
8	2.29672456	0.60541230	-0.19313496
1	3.90437436	2.69107199	-0.45263332
1	5.54872990	2.33913183	0.20479621
1	4.75424719	1.18729270	-0.93629241
1	-4.06948328	2.49924946	-4.43710995
1	2.31664395	-4.23281431	1.76935446
1	0.20212111	-4.33768654	3.29327273
1	-1.15313661	-2.99690843	4.89326382
1	-1.95620966	-3.09676814	3.29739952
1	-1.10828543	-1.60186434	3.78203797
1	4.66222668	-3.59139562	1.71936798
1	4.27563763	-1.88694632	1.41106474
1	3.86358333	-3.12157011	0.19373007
1	3.18023252	-0.55104172	2.66534901
1	2.70941162	1.79955053	3.35796332
1	1.53992295	0.64652902	4.05852747
1	1.05565858	1.66935086	2.67864537

TS-12ic2_si_DBP_Mg_rMeL_sLA

E = -1736.849131   E0 = -1736.293564   ZPVE = 0.555568 a.u. = 348.6240 kcal/mol
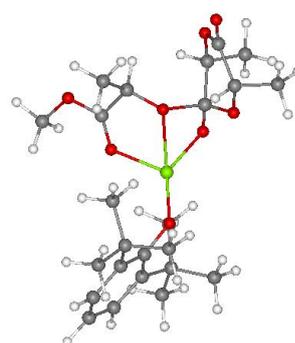
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	19.8271	44.3688	0.8887	1.4812	-11.7473
rotational	17.0564	36.8755	0.8887	0.8887	-10.1057
vibrational	37.7763	147.4299	370.1982	370.1982	326.2419
total	74.6598	228.6743	371.9756	372.5681	304.3889

```
8 -1.32798898  0.01378261 -0.78016531        8  0.25697574 -2.49734116  2.32515001
6 -1.67743587  0.93651932 -1.69020462        6  1.37600756 -2.15707850  1.56549406
6 -2.17093444  2.21362400 -1.26715505        6  2.65315270 -2.77275038  2.13589478
6 -2.45921302  3.17105556 -2.24866319        8  2.84525275 -2.43246770  3.53984189
1 -2.82023382  4.15406132 -1.95097923        6  1.76430905 -2.18363667  4.33300829
6 -2.30346370  2.90553260 -3.60773778        6  0.35192651 -2.23199821  3.74546432
6 -1.88859260  1.63924694 -4.01346636        8  1.19261420 -2.31040335  0.29110587
1 -1.80599916  1.43714952 -5.08000708        8  1.93900752 -1.89950264  5.49904013
6 -1.58729768  0.63226014 -3.08695078       12  0.35929576 -0.62763864 -0.28381529
6 -2.40877438  2.53346086  0.22536021        8  1.40317893 -0.48427543  1.87251389
6 -1.23146129 -0.79231077 -3.56882119        6  2.59464073  0.26542377  1.77726460
6 -3.38985443  1.50601947  0.83784717        6  2.80884695  0.76322007  0.34262383
1 -3.00977468  0.48424953  0.72917247        8  3.94494438  1.42782104  0.17246431
1 -3.54093885  1.71887779  1.90789998        6  4.19083929  1.95303702 -1.16828871
1 -4.36814642  1.56949794  0.33992457        6  2.52924323  1.45577264  2.74977970
6 -1.08069181  2.52182293  1.01795053        8  2.00416994  0.58507216 -0.58306003
1 -0.64990938  1.51461196  1.05978966        1  3.39139795  2.64834666 -1.44685781
1 -0.34839141  3.20581484  0.56321758        1  5.15339422  2.46495104 -1.09572542
1 -1.25590158  2.84909725  2.05482817        1  4.23461866  1.12761152 -1.88757181
6 -3.02992058  3.92987156  0.42652509        1 -2.52785087  3.67441034 -4.34799767
1 -2.36539102  4.73590946  0.08244239        6  2.67182779 -4.28515720  1.94277811
1 -3.99219370  4.02872944 -0.09506898        6 -0.50571769 -3.26557994  4.47076654
1 -3.21569753  4.08845949  1.49885476        1 -0.05491770 -1.22337294  3.92118907
6 -1.14903784 -0.87261426 -5.10671759        1  3.52243447 -2.33643579  1.62398708
1 -2.09943414 -0.59454554 -5.58140135        1  3.59396935 -4.69773769  2.37098908
1 -0.35744503 -0.22668065 -5.51446819        1  2.63575363 -4.51743507  0.87136662
1 -0.92417133 -1.90779567 -5.40199661        1  1.80858362 -4.75558186  2.43030620
6  0.14396800 -1.28160810 -3.02452469        1 -0.51427525 -3.04740238  5.54490280
1  0.02437253 -1.92171919 -2.13442206        1 -0.11557566 -4.27993679  4.31402779
1  0.64756233 -1.92977977 -3.75707269        1 -1.53143728 -3.22064114  4.08422184
1  0.83291012 -0.44279116 -2.83369446        1  3.48413992 -0.33621985  2.03651357
6 -2.33689475 -1.77499449 -3.11378312        1  3.44299841  2.06068230  2.69402218
1 -3.29718781 -1.50761557 -3.57614446        1  2.42334008  1.06527960  3.76884007
1 -2.08725071 -2.80381155 -3.41843891        1  1.66035378  2.08646226  2.52162266
1 -2.45661640 -1.74888194 -2.02379751
```

TS-12ic2_si_DBP_Mg_sMeL_rLA

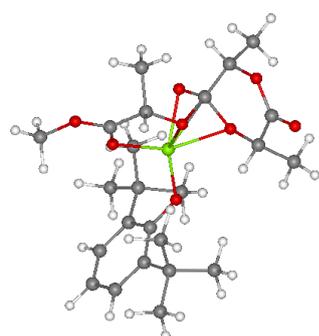E = -1736.833817   E0 = -1736.278601   ZPVE = 0.555216 a.u. = 348.4035 kcal/mol
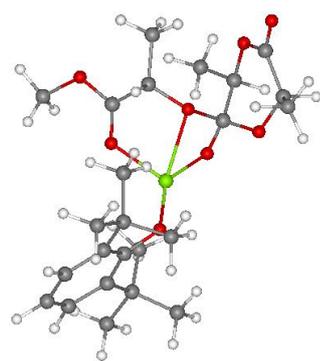
	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	19.8271	44.3688	0.8887	1.4812	-11.7473
rotational	17.0200	36.8032	0.8887	0.8887	-10.0842
vibrational	37.7800	147.3304	369.9459	369.9459	326.0193
total	74.6271	228.5025	371.7234	372.3159	304.1878

8	-1.48998439	-0.08292271	-0.70372081		8	0.18644360	-2.62157655	2.40038705
6	-1.80586255	0.84115374	-1.62491512		6	1.27609885	-2.28392339	1.59827054
6	-2.19424605	2.15913939	-1.21801209		6	2.54761314	-2.95877051	2.12862420
6	-2.44924545	3.11221743	-2.21290040		8	2.85252810	-2.51331186	3.47726774
1	-2.73028755	4.12476349	-1.92830157		6	1.80283689	-2.26048017	4.31128883
6	-2.35944390	2.80541468	-3.56918979		6	0.39757165	-2.65309048	3.83582067
6	-2.04690504	1.50432193	-3.95641828		8	1.03120315	-2.44690681	0.33687061
1	-2.01460075	1.27315998	-5.01975155		6	-0.68477166	-1.82366025	4.51098299
6	-1.78422177	0.49957180	-3.01576853		6	3.78930569	-2.82591867	1.26797915
6	-2.35996628	2.52767301	0.27312416		8	2.01795721	-1.81391060	5.41736937
6	-1.54085302	-0.95631242	-3.47370243		12	0.18229309	-0.78580272	-0.23634030
6	-3.39548683	1.59042645	0.93816817		8	1.23500931	-0.61283553	1.91351366
1	-3.09571910	0.54095602	0.84236747		6	2.21821642	0.41315246	1.77827668
1	-3.49723601	1.83619225	2.00700665		6	2.62756300	0.60537088	0.31423223
1	-4.38103151	1.71681106	0.46745715		8	3.79568958	1.20885384	0.13238610
6	-1.01333070	2.43081856	1.02880800		6	4.14679527	1.52475417	-1.25020683
1	-0.67265445	1.39011502	1.09382772		1	1.63617504	1.34360623	1.96102703
1	-0.24098688	3.03588367	0.53018606		6	3.36572075	0.44175261	2.78888965
1	-1.12910771	2.80421662	2.05821323		8	1.89050961	0.30310833	-0.63732880
6	-2.86632013	3.97152495	0.46009895		1	3.38868189	2.18661928	-1.68350136
1	-2.15399384	4.71681976	0.07682464		1	5.11733675	2.02242351	-1.18499506
1	-3.83430839	4.13248491	-0.03453508		1	4.21304750	0.60119051	-1.83577037
1	-3.00579500	4.16664505	1.53338993		1	-2.55515933	3.57111192	-4.32078505
6	-1.51894557	-1.07638240	-5.01106977		1	3.89317727	1.40129900	2.71188354
1	-2.46399593	-0.74311393	-5.46023989		1	4.09011841	-0.36554110	2.65014648
1	-0.69916606	-0.49702942	-5.46100616		1	2.95057774	0.35656330	3.79976320
1	-1.37686181	-2.13111544	-5.28793335		1	2.27377582	-4.02832079	2.17554045
6	-0.18175539	-1.52213442	-2.96560812		1	0.28882429	-3.71341944	4.13654423
1	-0.30508789	-2.10980320	-2.04092169		1	-0.59539509	-1.90190029	5.60049868
1	0.23769815	-2.23862433	-3.68749189		1	-1.67013431	-2.19127703	4.19895506
1	0.57292366	-0.72829145	-2.84525251		1	-0.58815134	-0.77131850	4.21762037
6	-2.69083309	-1.85311830	-2.95646644		1	4.61385727	-3.38907385	1.72341406
1	-3.64765263	-1.53497744	-3.39332080		1	4.11185265	-1.78521991	1.14778352
1	-2.51878595	-2.90304327	-3.24223757		1	3.57711363	-3.24376583	0.27702540
1	-2.77023602	-1.79323030	-1.86413825					

TS-12ic2_si_DBP_Mg_sMeL_sLA

E = -1736.843187   E0 = -1736.287456   ZPVE = 0.555731 a.u. = 348.7264 kcal/mol

	ln(Q)	S, cal/mol·K	U, kcal/mol	H, kcal/mol	G, kcal/mol
translational	19.8271	44.3688	0.8887	1.4812	-11.7473
rotational	16.9710	36.7058	0.8887	0.8887	-10.0551
vibrational	36.4824	144.4691	370.1845	370.1845	327.1110
total	73.2805	225.5437	371.9619	372.5544	305.3086

8	-1.17593253	-0.05031443	-0.48351628
6	-1.63435817	0.84890014	-1.36625659
6	-2.09925985	2.12881231	-0.91765600
6	-2.50631070	3.06199145	-1.88048780
1	-2.84865975	4.04603243	-1.56456447
6	-2.49281931	2.77064681	-3.24302506
6	-2.10421062	1.50150013	-3.66630244
1	-2.13273501	1.27874863	-4.73155451
6	-1.69066453	0.51741087	-2.75898433
6	-2.17662239	2.48048902	0.58515871
6	-1.36661673	-0.91187215	-3.24997807
6	-3.04438233	1.44028080	1.33244526
1	-2.64889860	0.42803597	1.19241047
1	-3.07116723	1.67225385	2.40890789
1	-4.07743359	1.46373069	0.95661336
6	-0.76721323	2.53769732	1.21906781
1	-0.28396848	1.55342507	1.21823418
1	-0.12322132	3.24445081	0.67511272
1	-0.83370179	2.87188458	2.26611114
6	-2.82102013	3.86036706	0.82564187
1	-2.22615576	4.67925119	0.39550713
1	-3.83663940	3.91521287	0.40945572
1	-2.89458442	4.03833675	1.90847445
6	-1.44763517	-1.02150714	-4.78623486
1	-2.44647932	-0.76270092	-5.16234493
1	-0.71157205	-0.37597674	-5.28783941
1	-1.24251544	-2.05989385	-5.08452892
6	0.06354221	-1.37367141	-2.84659076
1	0.05373444	-1.95165122	-1.90811253
1	0.47497100	-2.06915450	-3.59329534
1	0.76721632	-0.52916521	-2.78250027
6	-2.40289974	-1.89905572	-2.66144729
1	-3.41131449	-1.65504456	-3.02370811
1	-2.17052007	-2.93066454	-2.97069359
1	-2.40505791	-1.85067320	-1.56554401

8	0.32286686	-1.95369935	1.71322846
6	1.74707425	-1.93693888	1.46992552
6	2.46423054	-2.80803752	2.49344969
8	2.10699439	-2.46840048	3.86313200
6	0.88237113	-1.95987630	4.16966248
6	-0.12151220	-1.62495530	3.06377244
8	1.97376668	-2.09285116	0.21858880
8	0.60428607	-1.73957098	5.32865572
12	0.57525212	-0.60451859	-0.08787648
8	1.93764079	-0.29289344	1.85829973
6	3.10248566	0.42255506	1.49147618
6	2.94203663	1.02005744	0.08512995
8	3.91173100	1.86922443	-0.23985927
6	3.78445530	2.51789713	-1.54209018
1	3.13288689	1.30475080	2.15966988
6	4.44979334	-0.30110240	1.63301885
8	1.98930418	0.79024494	-0.66910517
1	2.84252262	3.07554126	-1.58861518
1	4.64566422	3.18737316	-1.60673916
1	3.80939960	1.76327085	-2.33604646
1	-2.80707312	3.52090716	-3.96959591
1	5.26618433	0.39571497	1.40656185
1	4.52085543	-1.15787888	0.95180714
1	4.57105780	-0.64068848	2.66895819
6	2.19728112	-4.28733158	2.22913909
6	-1.45719028	-2.32319856	3.28996825
1	-0.25166085	-0.53348863	3.12280226
1	3.54074192	-2.61334777	2.43768930
1	2.71076012	-4.88935184	2.98908353
1	2.57712245	-4.55904198	1.23645651
1	1.12294626	-4.50875187	2.26411533
1	-1.83687830	-2.06593275	4.28527975
1	-1.34537029	-3.41322923	3.22031116
1	-2.17691422	-1.99057019	2.53176570