Supplementary Information

DFT studies on the mechanism of palladium–catalyzed carbon–silicon cleavage for the synthesis of benzosilole derivatives

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Contents:

Complete Reference for Ref (19):

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*; Revision E. 01; Gaussian, Inc.: Wallingford, CT, 2004.

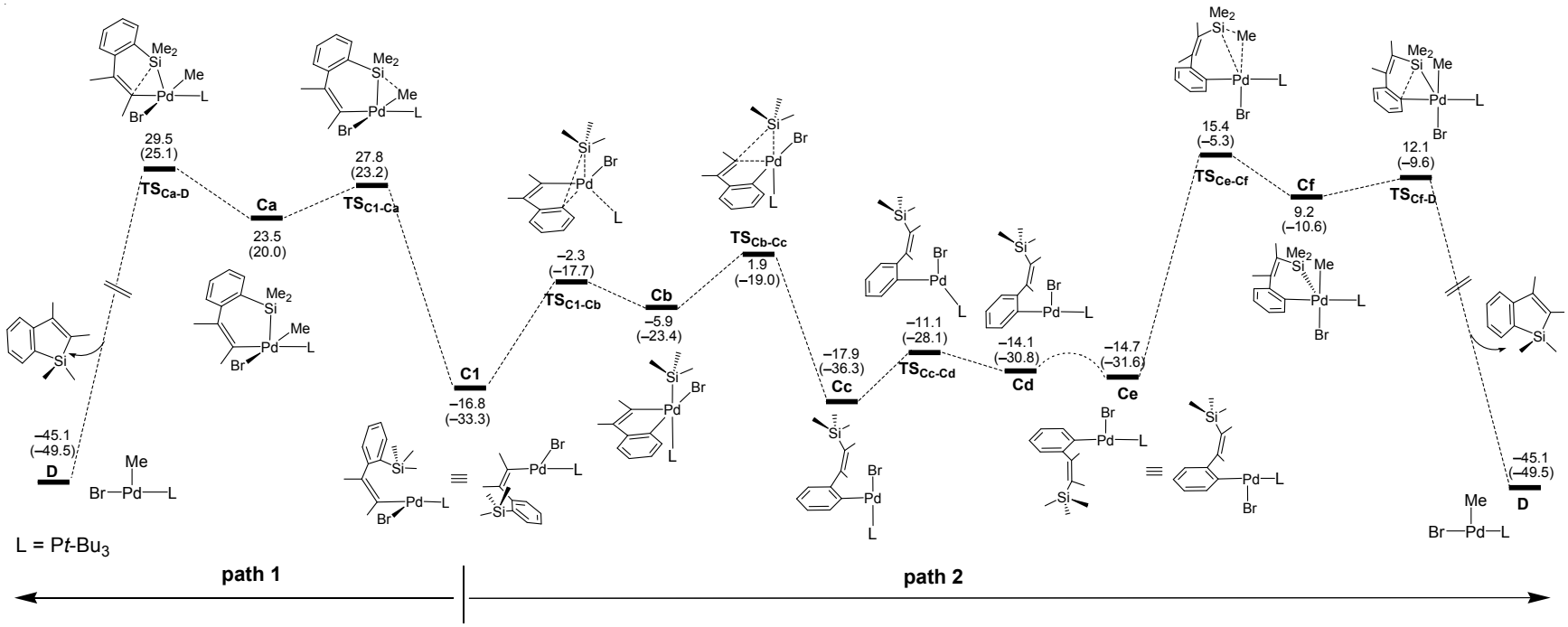

Figure S1. The energy profiles calculated for Paths 1 and 2 with an associative mechanism. The solvation-corrected relative free energies and electronic energies (in parentheses) are given in kcal/mol.

Figure S1 shows an associative mechanism, in which P*t*-Bu$_3$ ligand stays attached to the metal center from the complex **C1** to **D** in Paths 1 and 2. The overall barriers of the whole process were calculated to be 29.5 kcal/mol for Path 1 and 33.3 kcal/mol for Path 2, indicating that a dissociative mechanism shown in the text (Figure 2) is much more favorable. Therefore, we only discussed the free energy profiles calculated for Paths 1 and 2 involving a dissociative mechanism.

Cartesian coordinates and total energies, solvation energies and G_{sol} for all of the calculated structures

A

E_{gas}: -974.705650744
E_{sol}: -974.706940160
G_{sol}: -974.207844416

6	2.112823	-0.966787	0.542243
6	1.511708	-1.765182	1.553282
6	2.713857	0.297183	0.835287
6	1.540776	-1.320769	2.888999
6	2.691852	0.684939	2.187624
6	2.143992	-0.110103	3.204443
1	1.178264	-2.770421	1.320215
1	1.111438	-1.949438	3.664700
1	3.132620	1.638187	2.464040
1	2.186296	0.229086	4.235835
14	3.634788	1.416603	-0.404833
6	5.334019	0.680776	-0.788713
1	5.906893	1.356035	-1.436644
1	5.913239	0.529267	0.129619
1	5.252522	-0.285032	-1.296843
6	2.663782	1.703498	-1.997343
1	2.511917	0.777675	-2.558899
1	1.678690	2.132265	-1.782662
1	3.204055	2.407511	-2.643238
46	0.026845	-0.422064	0.240769
6	-2.603820	0.448239	-2.001794
15	-2.243030	0.163583	-0.093657
6	-2.699516	1.814593	0.870514
6	-3.430954	-1.265847	0.545469
35	2.549338	-1.911972	-1.138074
6	3.892976	3.102975	0.416438
1	2.945625	3.551211	0.737890
1	4.557145	3.054603	1.286903
1	4.354071	3.790825	-0.302986
6	-4.889326	-1.204771	0.052028
1	-4.970555	-1.322855	-1.031494
1	-5.455532	-2.029912	0.506654
1	-5.391336	-0.274982	0.331427
6	-3.429784	-1.266786	2.089020
1	-3.926990	-2.181588	2.438594
1	-2.410398	-1.268462	2.488931
1	-3.974490	-0.422420	2.517457
6	-2.808993	-2.619034	0.126604
1	-1.776595	-2.700246	0.482387
1	-3.395217	-3.430579	0.579820
1	-2.806396	-2.781505	-0.951496
6	-2.028600	1.746986	2.263708
1	-2.454948	0.980881	2.912103
1	-0.954805	1.552063	2.174870
1	-2.164255	2.714462	2.767220
6	-2.046889	3.016011	0.152698
1	-0.980388	2.846900	-0.029247
1	-2.529534	3.265918	-0.795084
1	-2.134855	3.898618	0.800336
6	-4.203213	2.103550	1.044254
1	-4.735297	2.154723	0.090817
1	-4.702236	1.360809	1.672266
1	-4.326535	3.076138	1.541032
6	-2.605785	-0.916837	-2.723427
1	-1.715731	-1.504440	-2.475726
1	-3.494026	-1.515611	-2.507907
1	-2.593698	-0.739086	-3.807146
6	-3.907993	1.192604	-2.347554
1	-4.012205	1.242661	-3.440522
1	-4.798740	0.691781	-1.959466
1	-3.911460	2.222489	-1.981270
6	-1.403473	1.227915	-2.588335
1	-0.461414	0.709404	-2.381336
1	-1.523769	1.296143	-3.678459
1	-1.319286	2.245772	-2.205654

TS_{A-B}

E_{gas}: -974.698228403
E_{sol}: -974.700110747
G_{sol}: -974.200119344
imaginary frequency: 119.3978*i* cm^{-1}

6	-2.067349	-1.090779	0.040397
6	-1.898428	-2.478511	-0.144583
6	-2.957138	-0.311840	-0.736807
6	-2.540758	-3.103561	-1.215024
6	-3.571534	-0.997832	-1.806853
6	-3.374369	-2.359392	-2.050239
1	-1.291325	-3.049164	0.549468
1	-2.399777	-4.169088	-1.378665
1	-4.240966	-0.449994	-2.464283
1	-3.889282	-2.839344	-2.878129
14	-3.503080	1.485477	-0.405800
6	-4.812424	1.483391	0.956300
1	-5.205143	2.495412	1.116213
1	-5.655790	0.835766	0.689626
1	-4.399915	1.124569	1.904046
6	-2.082734	2.641131	0.045813
1	-1.540272	2.291557	0.928517
1	-1.370524	2.727649	-0.782602
1	-2.472067	3.645266	0.258616
46	-0.151971	-0.391190	0.095906
6	3.001260	0.678143	1.556669
15	2.203798	0.138737	-0.152264
6	2.494718	1.577817	-1.454185
6	3.140269	-1.463260	-0.793576
35	-1.767527	-0.521834	2.231989
6	-4.295972	2.155375	-1.990807
1	-3.616445	2.094524	-2.849119
1	-5.222671	1.633761	-2.256173
1	-4.552383	3.212763	-1.850065
6	4.675196	-1.450373	-0.652893
1	5.000194	-1.433187	0.390866
1	5.082780	-2.368259	-1.099082
1	5.139346	-0.605087	-1.167127
6	2.781324	-1.699874	-2.276517
1	3.144384	-2.694109	-2.569219
1	1.698127	-1.685216	-2.437308
1	3.246391	-0.978508	-2.952117
6	2.572655	-2.681688	-0.027090
1	1.484783	-2.741693	-0.137239
1	3.009124	-3.597583	-0.448855
1	2.803002	-2.670586	1.038364
6	1.504249	1.354902	-2.622100
1	1.718957	0.461892	-3.209879
1	0.474183	1.276467	-2.257240
1	1.558608	2.215893	-3.302515
6	2.098018	2.927471	-0.817653
1	1.101290	2.889050	-0.367386
1	2.809660	3.269434	-0.062789
1	2.074630	3.691287	-1.606451
6	3.924028	1.705134	-2.017011
1	4.671488	1.869248	-1.236285
1	4.227003	0.831037	-2.598643
1	3.965156	2.569551	-2.694434
6	3.095297	-0.557142	2.478326
1	2.140022	-1.088583	2.541183
1	3.873420	-1.260899	2.173316
1	3.348533	-0.216931	3.491071
6	4.390179	1.339490	1.471952
1	4.749432	1.546775	2.489557

1	5.134375	0.701369	0.988491
1	4.367108	2.295793	0.942931
6	2.015578	1.646319	2.253205
1	1.022146	1.197825	2.352190
1	2.392187	1.861288	3.262612
1	1.908070	2.601728	1.738472

B

E_{gas}: -974.711410356
E_{sol}: -974.714571534
G_{sol}: -974.215170178

6	-2.168636	-1.016707	-0.402462
6	-2.188283	-2.375351	-0.743981
6	-3.260903	-0.162948	-0.645565
6	-3.264985	-2.889382	-1.472957
6	-4.326042	-0.720774	-1.387649
6	-4.331065	-2.053561	-1.803319
1	-1.371631	-3.029146	-0.449834
1	-3.273115	-3.938166	-1.759972
1	-5.183045	-0.099011	-1.633306
1	-5.179588	-2.442698	-2.360403
14	-3.461522	1.610967	0.017374
6	-3.853636	1.556929	1.859839
1	-3.996472	2.568172	2.261181
1	-4.773587	0.989766	2.044613
1	-3.045746	1.071858	2.417133
6	-1.912197	2.647985	-0.293211
1	-1.038555	2.204301	0.199687
1	-1.698414	2.732174	-1.365457
1	-2.037257	3.663328	0.103951
46	-0.327080	-0.396175	-0.038017
6	2.912860	1.213358	1.216946
15	2.149157	0.158583	-0.240277
6	2.336591	1.156432	-1.919527
6	3.131869	-1.527184	-0.399290
35	-0.788559	-0.932510	2.350981
6	-4.899758	2.439079	-0.894747
1	-4.759836	2.431962	-1.982147
1	-5.863001	1.964534	-0.675069
1	-4.978227	3.487247	-0.580552
6	4.666962	-1.414915	-0.324082
1	5.009376	-1.044228	0.645083
1	5.104306	-2.413913	-0.458206
1	5.083076	-0.769741	-1.101877
6	2.749004	-2.213182	-1.728758
1	3.168905	-3.227525	-1.729079
1	1.663346	-2.310899	-1.839960
1	3.145904	-1.701820	-2.608513
6	2.636982	-2.471192	0.722832
1	1.548716	-2.581123	0.709424
1	3.083108	-3.462504	0.564598
1	2.919945	-2.141178	1.721913
6	1.312443	0.556721	-2.913796
1	1.536697	-0.469456	-3.205470
1	0.294294	0.576765	-2.500092
1	1.299678	1.165041	-3.828320
6	1.909106	2.626459	-1.712846
1	0.916782	2.709239	-1.260027
1	2.616254	3.198331	-1.108653
1	1.860801	3.112260	-2.696694
6	3.738134	1.148087	-2.561255
1	4.500687	1.569004	-1.900102
1	4.062177	0.147887	-2.859383
1	3.719178	1.762954	-3.471832
6	3.106135	0.316646	2.459735
1	2.192416	-0.227413	2.716630
1	3.928911	-0.393838	2.348861
1	3.354800	0.964147	3.311033
6	4.252079	1.903988	0.893698
1	4.601570	2.435999	1.789147
1	5.033906	1.193458	0.612481
1	4.164734	2.644952	0.095384
6	1.860753	2.272904	1.620528
1	0.923616	1.798540	1.927265
1	2.247341	2.836993	2.480024
1	1.642652	2.993024	0.831123

TS_{B-B1}

E_{gas}: -974.707863035
E_{sol}: -974.711573495
G_{sol}: -974.211526460
imaginary frequency: 60.6489*i* cm^{-1}

6	-1.964569	-0.282505	1.046846
6	-1.872327	-0.854208	2.319794
6	-2.994784	0.593236	0.669910
6	-2.767013	-0.449505	3.314273
6	-3.869470	0.980479	1.712478
6	-3.761100	0.480161	3.010063
1	-1.111797	-1.596689	2.538956
1	-2.689604	-0.873152	4.312615
1	-4.668822	1.683002	1.493616
1	-4.467113	0.797498	3.773095
14	-3.380053	1.218626	-1.090747
6	-1.835835	1.860027	-1.970171
1	-2.082039	2.180839	-2.990262
1	-1.403229	2.717832	-1.442404
1	-1.069067	1.079113	-2.040898
6	-4.178922	-0.161871	-2.093360
1	-3.507752	-1.022174	-2.179376
1	-5.103601	-0.505799	-1.615272
1	-4.431756	0.185665	-3.103090
46	-0.321555	-0.507005	-0.009838
6	2.876962	0.686918	-1.768706
15	2.170379	0.293408	0.015781
6	3.226660	-1.151311	0.814544
6	2.326423	1.892481	1.136633
35	-1.347870	-2.593479	-0.842758
6	-4.598495	2.662481	-0.955615
1	-5.572132	2.354138	-0.557920
1	-4.215759	3.472431	-0.323510
1	-4.778009	3.081410	-1.953484
6	3.661154	2.654621	1.027452
1	3.829539	3.068126	0.029963
1	3.646527	3.501973	1.726896
1	4.521678	2.033055	1.288597
6	2.098028	1.506449	2.613621
1	2.002819	2.428410	3.202145
1	1.172913	0.936344	2.749660
1	2.927734	0.938034	3.039090
6	1.159927	2.837233	0.763398
1	0.191891	2.337865	0.880947
1	1.172726	3.700161	1.442961
1	1.220227	3.222978	-0.254298
6	2.412360	-1.743987	1.989218
1	2.279590	-1.051405	2.820580
1	1.423763	-2.076959	1.656422
1	2.948521	-2.620777	2.376376
6	3.371950	-2.295691	-0.212320
1	2.404253	-2.601872	-0.623048
1	4.044065	-2.048057	-1.036782
1	3.800011	-3.166530	0.301083
6	4.626269	-0.748206	1.317668
1	5.251738	-0.320927	0.529773
1	4.585197	-0.033442	2.144204
1	5.140671	-1.643288	1.693582
6	2.313603	2.036915	-2.263498
1	1.222481	2.079030	-2.192663
1	2.734055	2.896899	-1.736814
1	2.575308	2.150289	-3.323615
6	4.413594	0.727362	-1.881356
1	4.687636	1.005694	-2.908309
1	4.865169	1.464632	-1.212291
1	4.875048	-0.242650	-1.680559
6	2.318282	-0.386963	-2.733166

1	1.224555	-0.426146	-2.701915
1	2.616828	-0.127565	-3.757820
1	2.691590	-1.390608	-2.529624

B1

E_{gas}: -974.720705642
E_{sol}: -974.725664146
G_{sol}: -974.225028504

6	1.334123	0.442958	-1.063792
6	1.067081	0.642382	-2.422626
6	2.369879	1.120399	-0.401352
6	1.791067	1.592259	-3.147803
6	3.065961	2.085446	-1.171280
6	2.786770	2.332134	-2.512662
1	0.306254	0.059821	-2.926738
1	1.573820	1.741724	-4.202739
1	3.872309	2.646511	-0.703780
1	3.356269	3.078423	-3.060383
14	3.145276	0.826034	1.320198
6	3.458515	2.523751	2.109478
1	3.930326	2.396099	3.091826
1	4.122206	3.158781	1.512415
1	2.522633	3.074724	2.262308
6	2.139829	-0.173835	2.560114
1	1.181289	0.299393	2.794031
1	1.952648	-1.192300	2.208861
1	2.709607	-0.237921	3.496779
46	0.195192	-0.924945	-0.158066
6	-2.571844	-0.371438	1.895395
15	-1.936102	0.229741	0.135925
6	-3.128212	-0.538821	-1.226926
6	-2.051708	2.181282	0.055508
35	1.881657	-2.716429	-0.465577
6	4.793244	-0.046968	1.027270
1	4.619885	-1.031452	0.578990
1	5.438106	0.523048	0.348584
1	5.337040	-0.189969	1.969247
6	-3.356213	2.771835	0.627925
1	-3.464286	2.594781	1.700488
1	-3.336162	3.860572	0.484415
1	-4.250522	2.394597	0.126619
6	-1.903484	2.646900	-1.409155
1	-1.822398	3.741780	-1.412127
1	-0.997822	2.251694	-1.876604
1	-2.766659	2.388416	-2.026563
6	-0.847701	2.770034	0.826754
1	0.102546	2.400864	0.434545
1	-0.860409	3.861173	0.702178
1	-0.881229	2.567246	1.897817
6	-2.414712	-0.466807	-2.596359
1	-2.156810	0.546617	-2.904004
1	-1.502301	-1.070495	-2.592061
1	-3.085969	-0.882807	-3.359530
6	-3.335901	-2.045326	-0.952508
1	-2.384903	-2.576711	-0.838635
1	-3.960650	-2.246905	-0.080367
1	-3.846792	-2.482494	-1.820293
6	-4.508577	0.138993	-1.342846
1	-5.058893	0.149716	-0.399347
1	-4.440616	1.165711	-1.711282
1	-5.114125	-0.421028	-2.068233
6	-1.940631	0.491238	3.008325
1	-0.854258	0.555886	2.911901
1	-2.350331	1.502698	3.051028
1	-2.154518	0.016430	3.974733
6	-4.101275	-0.356577	2.088589
1	-4.326653	-0.664725	3.118589
1	-4.533034	0.637046	1.944348
1	-4.619883	-1.053498	1.427272
6	-2.041310	-1.810079	2.114162
1	-0.945900	-1.851359	2.058900
1	-2.322563	-2.140637	3.123131
1	-2.445848	-2.538144	1.411014

TS_{B1-B2}

E_{gas}: -1130.681852480
E_{sol}: -1130.685016050
G_{sol}: -1130.104868570
imaginary frequency: 47.5037*i* cm^{-1}

6	-2.321787	0.532703	-0.661999
6	-2.615256	1.488155	-1.641818
6	-3.331952	-0.033174	0.140402
6	-3.908326	2.001152	-1.758441
6	-4.627497	0.521023	0.001680
6	-4.916343	1.527350	-0.918194
1	-1.837836	1.832738	-2.316708
1	-4.125478	2.755769	-2.511144
1	-5.436524	0.136136	0.617519
1	-5.928570	1.915559	-0.999291
14	-3.172340	-1.581688	1.233112
6	-1.605804	-1.568277	2.290132
1	-1.476640	-2.531385	2.799831
1	-0.719958	-1.401222	1.665014
1	-1.632744	-0.785415	3.056181
6	-4.652256	-1.665400	2.413702
1	-4.744695	-0.763441	3.030464
1	-5.601768	-1.810072	1.885946
1	-4.529830	-2.517267	3.094161
46	-0.372900	0.239592	-0.319554
6	2.741112	-1.942357	0.750891
15	2.290533	-0.102840	0.212053
6	2.953348	1.085605	1.634905
6	3.303225	0.305548	-1.425491
35	-0.603123	-1.287472	-2.290680
6	-1.118509	2.758650	1.518587
6	-0.653240	3.248173	0.509241
6	-1.777263	2.280441	2.733425
1	-2.175892	3.125778	3.307621
1	-1.091805	1.728750	3.386647
1	-2.613724	1.620117	2.479119
6	-0.208040	3.975403	-0.680778
1	-1.021683	4.036217	-1.412513
1	0.088931	4.998567	-0.419851
1	0.642454	3.492192	-1.170630
6	-3.185781	-3.115414	0.135575
1	-2.363745	-3.085843	-0.587102
1	-3.093913	-4.030811	0.733747
1	-4.121894	-3.177325	-0.431785
6	3.162995	-0.847060	-2.444401
1	3.595709	-0.511561	-3.396788
1	3.706696	-1.746928	-2.148881
1	2.117924	-1.107054	-2.629484
6	4.805067	0.597880	-1.234417
1	5.255347	0.768975	-2.222011
1	4.993864	1.494471	-0.639376
1	5.341247	-0.235756	-0.774808
6	2.628106	1.534921	-2.077572
1	2.716739	2.441663	-1.475680
1	3.112746	1.735488	-3.042715
1	1.567512	1.342895	-2.269708
6	4.228740	-2.328265	0.609843
1	4.895175	-1.680220	1.183659
1	4.361147	-3.350831	0.989921
1	4.565811	-2.330299	-0.428501
6	1.890907	-2.912134	-0.100056
1	2.118027	-3.939979	0.215553
1	0.820945	-2.742780	0.040957
1	2.088222	-2.842147	-1.168947
6	2.325289	-2.187945	2.217971
1	2.966099	-1.675430	2.938583
1	1.286735	-1.905396	2.408772
1	2.410946	-3.263655	2.421685
6	4.346230	0.757006	2.207821
1	4.378333	-0.210800	2.712481

1	5.130977	0.770749	1.448372
1	4.605748	1.517189	2.958095
6	2.974508	2.542925	1.126371
1	3.185765	3.204862	1.977006
1	3.748184	2.724950	0.378070
1	2.006941	2.843160	0.717583
6	1.918964	1.055207	2.783558
1	1.840001	0.084932	3.274195
1	2.217962	1.786094	3.547587
1	0.929322	1.342194	2.420491

B2

E_{gas}: -650.653410701
E_{sol}: -650.657844258
G_{sol}: -650.432599557

6	0.066784	-0.762382	-0.814281
6	-0.523457	-1.448827	-1.876403
6	1.433036	-0.830425	-0.520116
6	0.261475	-2.283454	-2.675213
6	2.185912	-1.696840	-1.351058
6	1.622708	-2.414272	-2.403493
1	-1.579369	-1.331355	-2.096560
1	-0.195089	-2.821376	-3.502208
1	3.254342	-1.795336	-1.173787
1	2.245953	-3.061619	-3.014669
14	2.482576	0.191112	0.712334
6	1.555737	1.044127	2.116383
1	2.293711	1.558339	2.746569
1	0.853022	1.796401	1.747434
1	1.014100	0.343794	2.760247
6	3.732912	-0.993339	1.507296
1	3.233695	-1.802798	2.053680
1	4.407441	-1.454392	0.777557
1	4.357811	-0.447896	2.225248
46	-1.206425	0.271879	0.306264
35	-0.714898	2.413559	-0.802257
6	-1.657644	-1.448516	1.666011
6	-2.595168	-1.353928	0.860808
6	-0.765329	-1.926694	2.733287
1	0.213481	-2.197013	2.323346
1	-1.197240	-2.814870	3.209903
1	-0.612208	-1.163425	3.502690
6	-3.840703	-1.544138	0.100202
1	-4.438795	-2.338418	0.563457
1	-4.441951	-0.629723	0.075048
1	-3.627668	-1.836929	-0.933582
6	3.396251	1.496904	-0.297641
1	2.680157	2.195098	-0.744294
1	4.086663	2.070772	0.332701
1	3.977782	1.044916	-1.109297

TS_{B2-C}

E_{gas}: -650.631503512
E_{sol}: -650.636611890
G_{sol}: -650.410669378
imaginary frequency: 224.0683*i* cm^{-1}

6	-0.865408	1.016396	-0.411484
6	-0.840821	2.219084	-1.131332
6	-1.990308	0.168118	-0.388461
6	-1.937198	2.576160	-1.917087
6	-3.074806	0.569986	-1.199099
6	-3.058619	1.746283	-1.949318
1	0.031770	2.862907	-1.085478
1	-1.913287	3.497367	-2.493234
1	-3.962644	-0.057115	-1.243833
1	-3.923247	2.017034	-2.549321
14	-2.201552	-1.521991	0.486901
6	-0.924680	-1.906000	1.820713
1	-1.187476	-2.866753	2.282471
1	0.088606	-2.001999	1.416017
1	-0.896156	-1.156758	2.618943
6	-3.916350	-1.531338	1.290077
1	-4.009285	-0.751427	2.055306
1	-4.723722	-1.380167	0.564999
1	-4.095404	-2.496463	1.779526
46	0.966404	0.146698	-0.125219
35	3.008304	-1.099462	-0.774660
6	0.117475	1.516855	1.466938
6	1.382240	1.469170	1.354956
6	-1.056585	1.949838	2.261958
1	-1.638178	2.713777	1.737018
1	-0.701973	2.363824	3.213851
1	-1.725543	1.112019	2.479201
6	2.739118	1.851695	1.801886
1	2.669797	2.516899	2.672610
1	3.320060	0.964146	2.068116
1	3.280421	2.370599	1.004497
6	-2.116048	-2.855571	-0.847676
1	-1.123094	-2.882794	-1.311437
1	-2.312306	-3.847346	-0.422364
1	-2.849873	-2.680879	-1.642734

C

E_{gas}: -650.689730939
E_{sol}: -650.694015144
G_{sol}: -650.462948205

6	-1.155603	1.251601	0.499566
6	-1.279092	2.629475	0.176393
6	-1.552545	0.252632	-0.452008
6	-1.738829	3.038098	-1.060920
6	-1.967838	0.729426	-1.734144
6	-2.064146	2.076515	-2.035276
1	-0.978201	3.366137	0.916433
1	-1.821972	4.096912	-1.289704
1	-2.255443	0.006534	-2.494059
1	-2.401679	2.391237	-3.018963
14	-2.021686	-1.585460	-0.124945
6	-1.570433	-2.288827	1.562966
1	-2.022471	-3.285458	1.649306
1	-0.490380	-2.399291	1.691243
1	-1.951964	-1.682347	2.390507
6	-3.909656	-1.632133	-0.283827
1	-4.389294	-1.019596	0.488930
1	-4.249230	-1.259992	-1.256969
1	-4.281838	-2.657873	-0.172137
6	0.617411	0.240259	1.642343
6	-0.545806	0.871690	1.823576
6	1.642023	-0.311193	2.572987
1	2.592608	0.220548	2.468033
1	1.295557	-0.221637	3.612045
1	1.844203	-1.366440	2.363111
6	-1.201501	1.262159	3.123855
1	-0.603007	0.958276	3.986858
1	-1.346172	2.349111	3.181127
1	-2.195213	0.803511	3.216386
46	0.843237	0.223431	-0.323634
35	3.197355	-0.356459	-0.628814
6	-1.251602	-2.658017	-1.473785
1	-0.160147	-2.685873	-1.380092
1	-1.622229	-3.687558	-1.395140
1	-1.490168	-2.301627	-2.482390

TS_{C-CD}

E_{gas}: -650.661240416
E_{sol}: -650.665560678
G_{sol}: -650.431601262
imaginary frequency: 124.7380*i* cm^{-1}

6	1.462145	-1.106837	0.612616
6	2.080427	-2.363765	0.515716
6	1.759894	-0.117022	-0.358194
6	2.943518	-2.668746	-0.535803
6	2.625743	-0.449431	-1.413651
6	3.215211	-1.710964	-1.510327
1	1.859240	-3.129304	1.252683

1	3.391464	-3.657014	-0.595918
1	2.858830	0.289087	-2.175535
1	3.881980	-1.938534	-2.337686
14	1.156699	1.677127	-0.218182
6	-0.643827	2.695773	0.552869
1	-0.238752	3.585965	0.062970
1	-1.731315	2.763377	0.401451
1	-0.444168	2.742022	1.623509
6	2.234771	2.487607	1.105201
1	2.074576	2.022381	2.083777
1	3.287801	2.338295	0.838234
1	2.055639	3.563533	1.202642
6	-0.632578	-0.154709	1.567923
6	0.498621	-0.860824	1.722720
6	-1.753567	0.093728	2.531897
1	-2.615796	-0.533703	2.276365
1	-1.455048	-0.139101	3.561691
1	-2.093072	1.135207	2.512997
6	0.822096	-1.529747	3.054696
1	0.301718	-1.060980	3.892241
1	0.535988	-2.589377	3.046472
1	1.897867	-1.480870	3.254066
46	-1.097193	0.646991	-0.206950
35	-2.275810	-1.326898	-1.068588
6	1.390331	2.539399	-1.883445
1	0.839150	2.032730	-2.683314
1	1.057171	3.582204	-1.851794
1	2.450478	2.547383	-2.163322

CD

E_{gas}: -650.667878525
E_{sol}: -650.672491686
G_{sol}: -650.439890161

6	-1.908671	-0.221802	0.703787
6	-3.058895	0.413566	1.202904
6	-1.709513	-0.251092	-0.698004
6	-3.976107	1.026591	0.350694
6	-2.641790	0.373357	-1.540905
6	-3.773291	1.007800	-1.028580
1	-3.230038	0.458687	2.273363
1	-4.845887	1.525918	0.769245
1	-2.487623	0.363493	-2.617219
1	-4.484466	1.483757	-1.697992
14	-0.219255	-1.110673	-1.415829
6	2.447812	-1.785038	-0.403039
1	2.709118	-1.815607	-1.466465
1	3.346329	-1.581402	0.191542
1	2.003156	-2.730633	-0.096124
6	-0.402104	-2.984434	-1.372303
1	-0.531386	-3.354344	-0.351114
1	-1.300241	-3.253874	-1.943032
1	0.449788	-3.499370	-1.827018
6	0.393155	-0.901381	1.499004
6	-0.943260	-0.832160	1.662506
6	1.396226	-1.425075	2.495342
1	2.284616	-0.786161	2.539729
1	0.973775	-1.441078	3.505161
1	1.735122	-2.438473	2.247420
6	-1.561684	-1.367209	2.955932
1	-0.964769	-2.166665	3.398063
1	-1.672097	-0.577511	3.710727
1	-2.557835	-1.773801	2.756469
46	1.375100	-0.050611	-0.044119
35	1.164712	2.444471	0.142949
6	0.200695	-0.527592	-3.157272
1	0.271355	0.563103	-3.204994
1	1.151287	-0.950675	-3.499370
1	-0.575596	-0.857501	-3.860926

TS_{CD-CD1}

E_{gas}: -650.669756866
E_{sol}: -650.672640492
G_{sol}: -650.438104626
imaginary frequency: 23.7068*i* cm^{-1}

6	-2.015045	0.334537	-0.505444
6	-3.131761	-0.131377	-1.221843
6	-1.697716	-0.288254	0.727060
6	-3.901717	-1.194623	-0.753685
6	-2.481901	-1.361031	1.180681
6	-3.582113	-1.814498	0.453982
1	-3.390792	0.321551	-2.173152
1	-4.747954	-1.542621	-1.340048
1	-2.233677	-1.851894	2.118587
1	-4.178428	-2.643911	0.823838
14	-0.237742	0.297996	1.721464
6	2.306668	1.678731	0.993802
1	2.684135	1.201681	1.904310
1	3.135437	1.888036	0.308820
1	1.769486	2.594551	1.234013
6	-0.559272	1.938692	2.583848
1	-0.848497	2.719796	1.875133
1	-1.388903	1.799664	3.289361
1	0.306702	2.287318	3.155653
6	0.124120	1.621445	-0.912238
6	-1.207522	1.455645	-1.066868
6	0.954413	2.715098	-1.538674
1	1.923169	2.337727	-1.881183
1	0.455170	3.135177	-2.417543
1	1.154913	3.534509	-0.836697
6	-1.990151	2.451321	-1.925512
1	-1.535202	3.443283	-1.922128
1	-2.062064	2.122007	-2.970605
1	-3.009954	2.557939	-1.543667
46	1.299063	0.218197	-0.055388
35	1.565514	-2.083561	-1.045590
6	0.384499	-0.982358	2.949417
1	0.550911	-1.946853	2.461095
1	1.325650	-0.665376	3.411703
1	-0.346591	-1.116951	3.758359

CD1

E_{gas}: -650.675503438
E_{sol}: -650.680068833
G_{sol}: -650.447513395

6	-2.187961	-0.203658	-0.493723
6	-3.105389	-0.954460	-1.248938
6	-1.617191	-0.793004	0.666545
6	-3.423017	-2.264353	-0.893892
6	-1.936067	-2.120531	0.996417
6	-2.839135	-2.854637	0.229668
1	-3.560333	-0.523818	-2.135113
1	-4.123298	-2.829822	-1.502961
1	-1.484116	-2.582597	1.870509
1	-3.086346	-3.876244	0.504296
14	-0.382563	0.214623	1.640828
6	2.250376	1.730867	0.479087
1	3.003421	1.129464	0.985335
1	2.664879	2.229628	-0.400234
1	1.762013	2.439587	1.147103
6	-1.058264	1.691673	2.595942
1	-1.868583	2.193861	2.062970
1	-1.436386	1.345923	3.566235
1	-0.272134	2.427812	2.800026
6	-0.635422	1.742877	-0.557827
6	-1.845712	1.203153	-0.856978
6	-0.266331	3.195187	-0.694651
1	0.529105	3.342229	-1.435304
1	-1.111824	3.826607	-0.986402
1	0.114644	3.590277	0.254741
6	-2.950231	1.973284	-1.562987
1	-2.762123	3.046918	-1.596542
1	-3.058386	1.635712	-2.602188
1	-3.916017	1.810357	-1.070109
46	0.916694	0.409178	-0.317274

35	2.652469	-1.343683	-0.793473
6	0.666461	-0.828924	2.804058
1	1.119044	-1.676481	2.282737
1	1.474464	-0.230373	3.238830
1	0.050837	-1.201912	3.634338

TS_{CD1-D}

E_{gas}: -650.674819426
E_{sol}: -650.679513780
G_{sol}: -650.447758354
imaginary frequency: 74.3290*i* cm^{-1}

6	-2.111894	-0.419778	-0.561110
6	-2.876824	-1.382410	-1.239058
6	-1.651021	-0.696116	0.753055
6	-3.142945	-2.613788	-0.641951
6	-1.912837	-1.947358	1.328184
6	-2.661560	-2.901717	0.639288
1	-3.245038	-1.183768	-2.241012
1	-3.721683	-3.357952	-1.182554
1	-1.542351	-2.174982	2.324597
1	-2.872026	-3.864480	1.096548
14	-0.623595	0.675699	1.501156
6	2.280974	1.804505	0.132914
1	3.141954	1.321380	0.590498
1	2.528821	2.234699	-0.839986
1	1.820638	2.541630	0.791693
6	-1.559874	2.187567	2.139855
1	-2.430259	2.429118	1.524940
1	-1.894603	1.993939	3.166312
1	-0.910787	3.070703	2.172834
6	-0.681803	1.583740	-0.699436
6	-1.792609	0.916794	-1.126452
6	-0.390104	3.030850	-1.008925
1	0.303179	3.128388	-1.854113
1	-1.293884	3.601254	-1.250741
1	0.085345	3.530411	-0.158924
6	-2.780275	1.479763	-2.126885
1	-2.594012	2.529379	-2.358574
1	-2.715325	0.926520	-3.073429
1	-3.811477	1.378356	-1.767408
46	0.944392	0.324752	-0.290514
35	2.722437	-1.404065	-0.496933
6	0.465427	0.080707	2.928136
1	1.026227	-0.821039	2.668699
1	1.185342	0.852948	3.221092
1	-0.165020	-0.129167	3.803940

D

E_{gas}: -659.926219199
E_{sol}: -659.932106388
G_{sol}: -659.573342189

6	-1.431164	-2.207872	-0.053488
1	-2.296355	-2.434989	0.569277
1	-1.624107	-2.463753	-1.098084
1	-0.528667	-2.686109	0.323053
46	-1.250433	-0.184947	-0.017788
15	1.110363	0.010697	0.002138
6	2.137904	-1.054991	-1.281241
35	-3.708302	0.167156	-0.002722
6	1.836906	-0.254908	1.797767
6	1.257965	1.907215	-0.481678
6	3.375537	-0.222108	1.889439
1	3.801266	0.718659	1.531332
1	3.668253	-0.332392	2.942262
1	3.847238	-1.040191	1.339766
6	1.259341	0.816126	2.748719
1	1.651229	1.817971	2.559265
1	0.165697	0.848635	2.707469
1	1.540968	0.550677	3.775929
6	1.317130	-1.611228	2.329855
1	0.223810	-1.633724	2.347756
1	1.670305	-2.470124	1.757715
1	1.673205	-1.738868	3.360590
6	0.088981	2.651433	0.212916
1	0.124758	3.709249	-0.080536
1	-0.894149	2.278811	-0.110898
1	0.124055	2.611890	1.300830
6	2.587536	2.586984	-0.104489
1	3.453080	2.104735	-0.565914
1	2.565013	3.626394	-0.459245
1	2.751007	2.621966	0.975360
6	1.022823	2.082090	-1.998462
1	0.098070	1.598766	-2.329545
1	0.923526	3.155095	-2.208005
1	1.850343	1.712558	-2.607322
6	3.515882	-0.461844	-1.639324
1	4.020565	-1.144500	-2.336361
1	3.443568	0.506546	-2.138512
1	4.165548	-0.349769	-0.767456
6	2.360162	-2.485655	-0.741766
1	2.825694	-3.080545	-1.538279
1	3.032186	-2.521978	0.118196
1	1.422589	-2.980516	-0.476455
6	1.288459	-1.199763	-2.564811
1	0.304556	-1.623376	-2.347319
1	1.139125	-0.257082	-3.091555
1	1.807888	-1.880311	-3.252521

TS_{C-E}

E_{gas}: -650.680015248
E_{sol}: -650.684245224
G_{sol}: -650.451766976
imaginary frequency: 97.9168*i* cm^{-1}

6	-1.906137	1.036110	-0.240623
6	-3.137099	1.410742	-0.789724
6	-1.316541	-0.201739	-0.623591
6	-3.762088	0.593552	-1.736395
6	-1.921851	-0.972435	-1.625401
6	-3.151268	-0.584773	-2.169715
1	-3.596210	2.353890	-0.507874
1	-4.720867	0.891050	-2.152623
1	-1.451712	-1.888710	-1.969854
1	-3.627544	-1.202298	-2.926147
14	-0.701324	-1.557730	1.095542
6	-2.406582	-1.420410	1.897145
1	-3.216988	-1.585563	1.181452
1	-2.483947	-2.174409	2.691550
1	-2.552885	-0.438181	2.358501
6	-0.487201	-3.238767	0.255531
1	-0.341499	-3.992341	1.040085
1	-1.362789	-3.531693	-0.330996
1	0.394416	-3.278207	-0.394340
6	0.191062	1.486998	0.801348
6	-1.097452	1.867629	0.658898
6	1.304256	2.109577	1.581003
1	1.864987	1.361198	2.148902
1	2.020378	2.601193	0.913766
1	0.912153	2.854434	2.286292
6	-1.708277	3.084892	1.315020
1	-1.036304	3.547249	2.040328
1	-1.958309	3.847316	0.565454
1	-2.639367	2.822650	1.833260
46	0.736740	-0.076552	-0.335691
35	3.159277	0.147932	-0.809054
6	0.536668	-1.454023	2.531016
1	0.449627	-0.504995	3.069156
1	0.300744	-2.261809	3.238636
1	1.574993	-1.572890	2.208484

E

E_{gas}: -650.685487508
E_{sol}: -650.689141736
G_{sol}: -650.458405228

6	-2.354812	0.552200	-0.263480

6	-3.719799	0.349446	-0.483664
6	-1.435954	-0.433946	-0.680897
6	-4.158448	-0.826287	-1.107605
6	-1.863963	-1.589055	-1.319082
6	-3.241598	-1.787590	-1.527724
1	-4.443585	1.103188	-0.184425
1	-5.221263	-0.983656	-1.270269
1	-1.153553	-2.341027	-1.655805
1	-3.586144	-2.695892	-2.015139
14	0.400801	-1.147253	1.553018
6	-1.235597	-1.226307	2.476645
1	-2.010640	-1.741378	1.903724
1	-1.074173	-1.777081	3.413543
1	-1.602141	-0.228292	2.733403
6	0.926724	-2.849799	0.938446
1	1.050601	-3.511693	1.807390
1	0.176534	-3.299922	0.281342
1	1.880598	-2.802832	0.404972
6	-0.373284	1.693510	0.384341
6	-1.721961	1.734594	0.334395
6	0.626031	2.712879	0.830239
1	1.337729	2.300779	1.552735
1	1.215986	3.084854	-0.015602
1	0.121569	3.568768	1.297447
6	-2.566272	2.893988	0.804828
1	-1.971874	3.694282	1.249751
1	-3.134214	3.322465	-0.031116
1	-3.297604	2.560344	1.552559
46	0.502484	0.090235	-0.494610
35	2.954396	0.211247	-1.056847
6	1.721532	-0.388748	2.659700
1	1.405027	0.572237	3.077293
1	1.901655	-1.071642	3.502050
1	2.660589	-0.245727	2.118750

TS_{E-F}

E_{gas}: -650.676585105
E_{sol}: -650.680958845
G_{sol}: -650.449540740
imaginary frequency: 122.9489*i* cm^{-1}

6	1.816328	1.153238	-0.329578
6	2.728082	2.190304	-0.079630
6	0.488004	1.303137	0.117772
6	2.316555	3.329589	0.614889
6	0.056071	2.441527	0.783073
6	0.994521	3.453356	1.045620
1	3.750305	2.115307	-0.440857
1	3.028172	4.126146	0.813524
1	-0.976080	2.547958	1.095283
1	0.679271	4.340028	1.589372
14	0.529813	-1.683167	1.159200
6	2.329754	-2.165681	1.476944
1	2.957189	-1.274796	1.586478
1	2.384235	-2.730090	2.417442
1	2.754022	-2.787803	0.683217
6	-0.046395	-0.780894	2.719722
1	0.112134	-1.444338	3.581830
1	0.528522	0.134724	2.886220
1	-1.106314	-0.514990	2.675809
6	1.087345	-1.018098	-1.031352
6	2.079284	-0.078561	-1.077199
6	1.026603	-2.243346	-1.916583
1	-0.002091	-2.607986	-2.014432
1	1.383695	-2.019985	-2.928683
1	1.624443	-3.080590	-1.529205
6	3.351985	-0.218167	-1.870468
1	4.225351	-0.179306	-1.205476
1	3.397821	-1.159697	-2.421213
1	3.461672	0.606033	-2.586941
46	-0.714035	-0.195597	-0.400679
35	-3.051329	0.639712	-0.364944
6	-0.522005	-3.234378	0.902668
1	-0.161467	-3.871077	0.090287
1	-0.477349	-3.821686	1.830003
1	-1.575589	-2.998126	0.717582

F

E_{gas}: -650.692492072
E_{sol}: -650.696643826
G_{sol}: -650.465214754

6	-0.694616	1.688988	0.556790
6	-1.169107	3.003117	0.501230
6	0.428704	1.323141	-0.178638
6	-0.522251	3.902758	-0.350864
6	1.108134	2.205134	-1.010235
6	0.594408	3.506966	-1.098604
1	-2.024585	3.317973	1.094201
1	-0.885725	4.923500	-0.430775
1	1.993086	1.906605	-1.559451
1	1.082808	4.224545	-1.753058
14	-2.226195	-0.947641	-0.933272
6	-4.037728	-1.404450	-0.597320
1	-4.570177	-0.594156	-0.085048
1	-4.555385	-1.588994	-1.546673
1	-4.138264	-2.309818	0.011071
6	-2.221726	0.533468	-2.094710
1	-2.815112	0.272702	-2.980682
1	-2.672714	1.422362	-1.643091
1	-1.216636	0.800891	-2.431139
6	-1.480117	-0.679874	0.824438
6	-1.129460	0.538180	1.411291
6	-1.760733	-1.875771	1.736787
1	-1.739820	-2.815314	1.176088
1	-1.032493	-1.968765	2.550374
1	-2.756765	-1.799494	2.193549
6	-1.173886	0.818686	2.896920
1	-1.996289	1.521663	3.093713
1	-1.346401	-0.071228	3.503661
1	-0.253680	1.306654	3.233720
46	0.786025	-0.506865	0.428485
35	3.090051	-0.877613	-0.290014
6	-1.375941	-2.410416	-1.771364
1	-1.364836	-3.308895	-1.143819
1	-1.904455	-2.667333	-2.698059
1	-0.338871	-2.173209	-2.032904

TS_{F-F1}

E_{gas}: -650.672738898
E_{sol}: -650.674101166
G_{sol}: -650.443903268
imaginary frequency: 40.8625*i* cm^{-1}

6	-0.424924	1.302530	0.735784
6	-0.879868	2.615925	0.942822
6	0.610118	1.120261	-0.185159
6	-0.314968	3.685869	0.246631
6	1.216241	2.171255	-0.868655
6	0.730337	3.466442	-0.653743
1	-1.681563	2.788389	1.657493
1	-0.682974	4.693919	0.416578
1	2.042747	1.992063	-1.547267
1	1.180880	4.300927	-1.184454
14	-2.829582	-0.481034	-0.568341
6	-3.905062	1.071048	-0.561042
1	-3.301815	1.979541	-0.466416
1	-4.482574	1.145189	-1.490898
1	-4.619858	1.053861	0.270189
6	-1.642589	-0.415385	-2.049247
1	-1.199622	0.572612	-2.197482
1	-0.820381	-1.153795	-1.948384
1	-2.159512	-0.691041	-2.977809
6	-1.910972	-0.699046	1.093234
6	-0.941590	0.139476	1.544251
6	-2.422207	-1.859057	1.934443
1	-2.358802	-2.804785	1.382434

1	-1.880187	-1.994131	2.872381
1	-3.483139	-1.724773	2.186272
6	-0.249226	0.070672	2.892997
1	-0.591188	-0.748101	3.527439
1	0.833866	-0.032053	2.752920
1	-0.406286	1.011354	3.437413
46	0.981993	-0.748535	-0.580166
35	3.290222	-0.757445	0.151513
6	-3.952076	-1.977387	-0.840899
1	-3.387394	-2.914030	-0.917920
1	-4.689989	-2.099437	-0.040343
1	-4.506790	-1.853669	-1.779192

F1

E_{gas}: -650.670820628
E_{sol}: -650.674381645
G_{sol}: -650.445211017

6	-0.404984	1.281057	0.735091
6	-0.840584	2.598971	0.966160
6	0.607128	1.105821	-0.213405
6	-0.283980	3.676204	0.276108
6	1.205097	2.165924	-0.892544
6	0.739163	3.462710	-0.650018
1	-1.625839	2.766890	1.699803
1	-0.640241	4.683906	0.471375
1	2.016635	1.991025	-1.590584
1	1.188015	4.300291	-1.177171
14	-2.831608	-0.472193	-0.532703
6	-3.780396	1.154172	-0.688899
1	-3.115946	2.021734	-0.634259
1	-4.315868	1.196198	-1.645470
1	-4.524898	1.250077	0.110268
6	-1.580880	-0.620308	-1.962400
1	-1.060107	0.320325	-2.163442
1	-0.842689	-1.420299	-1.737691
1	-2.056350	-0.935036	-2.899999
6	-1.954187	-0.657803	1.152346
6	-0.937153	0.139411	1.563137
6	-2.502958	-1.779042	2.021093
1	-2.416831	-2.750568	1.517495
1	-2.003175	-1.869841	2.987524
1	-3.573141	-1.633760	2.220081
6	-0.197711	0.045576	2.884630
1	-0.553301	-0.753458	3.536691
1	0.871767	-0.115083	2.698277
1	-0.281606	0.994878	3.430029
46	1.017603	-0.734679	-0.719207
35	3.220455	-0.776188	0.271083
6	-4.063059	-1.891762	-0.748936
1	-3.573128	-2.872220	-0.742051
1	-4.832584	-1.899154	0.031010
1	-4.576819	-1.788972	-1.712627

TS_{F1-G}

E_{gas}: -650.656251744
E_{sol}: -650.660338999
G_{sol}: -650.428340255
imaginary frequency: 144.2165*i* cm^{-1}

6	0.288348	1.776105	0.504464
6	0.706979	3.124839	0.519109
6	0.811524	0.976789	-0.522226
6	1.581277	3.635868	-0.435941
6	1.691120	1.463736	-1.485319
6	2.080058	2.806283	-1.440696
1	0.327939	3.781559	1.296713
1	1.875769	4.680735	-0.392644
1	2.096323	0.807399	-2.249053
1	2.776777	3.188835	-2.181643
14	-2.062610	-0.195783	-0.484349
6	-3.142063	1.185940	-1.193165
1	-2.564914	2.109218	-1.314549
1	-3.588500	0.928280	-2.159511
1	-3.955538	1.398191	-0.488698
6	-1.005897	-0.421913	-2.397433
1	-0.954352	0.612051	-2.738136
1	-0.181146	-0.972279	-2.875145
1	-1.916252	-0.902978	-2.766761
6	-1.613629	0.370637	1.280407
6	-0.630561	1.262193	1.560213
6	-2.546325	-0.197203	2.335448
1	-2.441673	-1.287627	2.404964
1	-2.372957	0.213185	3.332629
1	-3.599118	-0.000307	2.088923
6	-0.364305	1.825354	2.945731
1	-0.736955	1.176225	3.739305
1	0.711036	1.955898	3.103561
1	-0.834630	2.809297	3.082205
46	0.301763	-0.935994	-0.658853
35	2.035334	-1.835417	0.819341
6	-3.042724	-1.811504	-0.395413
1	-2.456988	-2.622350	0.052362
1	-3.943862	-1.681610	0.214988
1	-3.365006	-2.140208	-1.389391

G

E_{gas}: -650.676949110
E_{sol}: -650.681288751
G_{sol}: -650.449894641

6	-2.133107	0.309953	-0.591704
6	-3.503629	0.201671	-0.895614
6	-1.450273	-0.821750	-0.080514
6	-4.196479	-0.982700	-0.658179
6	-2.162422	-1.998272	0.171410
6	-3.526470	-2.083684	-0.119866
1	-4.035474	1.060882	-1.295118
1	-5.256826	-1.044732	-0.887147
1	-1.655902	-2.872762	0.567885
1	-4.060024	-3.013547	0.060352
14	-0.008335	0.847357	1.527158
6	-1.357237	0.490080	2.790376
1	-2.354190	0.470452	2.345589
1	-1.183826	-0.474195	3.281615
1	-1.329691	1.263770	3.568429
6	0.929766	-2.372422	0.881976
1	0.219966	-2.466135	1.704145
1	0.798122	-3.165843	0.141590
1	1.961958	-2.315862	1.224119
6	-0.429863	1.982484	0.095771
6	-1.419512	1.601766	-0.771080
6	0.350695	3.269591	-0.104499
1	0.838418	3.300047	-1.086764
1	-0.306575	4.146979	-0.036918
1	1.136194	3.395305	0.645083
6	-1.861552	2.489431	-1.914305
1	-1.031755	3.090203	-2.295990
1	-2.268035	1.901233	-2.741934
1	-2.643264	3.192189	-1.591954
46	0.583161	-0.662231	-0.171423
35	2.968233	-0.350890	-0.926908
6	1.574953	1.292723	2.435817
1	2.411919	1.428601	1.746468
1	1.429322	2.212700	3.018975
1	1.843555	0.498246	3.141059

TS_{G-D}

E_{gas}: -650.676019848
E_{sol}: -650.680554768
G_{sol}: -650.448321920
imaginary frequency: 71.9287*i* cm^{-1}

6	-2.025302	0.260025	-0.763240
6	-3.304665	0.020731	-1.292630
6	-1.392212	-0.751828	0.006708
6	-3.969372	-1.173922	-1.021903
6	-2.087393	-1.933284	0.294738

6	-3.367568	-2.147109	-0.218360
1	-3.793109	0.779521	-1.897034
1	-4.962561	-1.342330	-1.429291
1	-1.619403	-2.711282	0.890302
1	-3.886957	-3.078521	-0.008644
14	-0.407744	0.763768	1.541443
6	-1.944337	0.632354	2.629636
1	-2.871360	0.695393	2.055199
1	-1.949530	-0.315404	3.180417
1	-1.927973	1.442498	3.369643
6	1.071862	-2.375618	0.812204
1	0.447579	-2.472896	1.702366
1	0.826569	-3.131374	0.062338
1	2.133423	-2.378082	1.052856
6	-0.504476	1.966323	0.095058
6	-1.331547	1.566054	-0.920265
6	0.323747	3.228992	0.102117
1	1.375559	2.996713	0.307798
1	0.289423	3.775128	-0.844462
1	-0.011100	3.915023	0.892064
6	-1.637562	2.371633	-2.159894
1	-0.928525	3.186828	-2.311688
1	-1.622515	1.733727	-3.050683
1	-2.639688	2.817627	-2.099282
46	0.679356	-0.593642	-0.097546
35	3.036730	-0.256335	-0.841243
6	1.050710	1.056837	2.703981
1	1.991173	1.190859	2.163607
1	0.857915	1.947267	3.318677
1	1.172232	0.208687	3.387334

TS_{D-A}

E_{gas}: -659.878333079
E_{sol}: -659.880350714
G_{sol}: -659.525203635
imaginary frequency: 297.18*i* cm^{-1}

6	2.808395	-1.816516	-0.000393
1	2.100379	-2.073723	0.782959
1	2.481244	-2.052408	-1.007930
1	3.807132	-2.175399	0.217317
46	1.210585	0.146924	0.003882
6	-1.814638	-0.436833	1.787049
15	-1.131451	0.008237	-0.000901
6	-1.787393	-1.347329	-1.262087
6	-1.879736	1.747260	-0.527648
35	3.674373	0.340409	-0.002788
6	-3.373229	1.963879	-0.216543
1	-3.581059	1.971479	0.856786
1	-3.680971	2.943527	-0.608027
1	-4.016097	1.212103	-0.681817
6	-1.653269	1.950291	-2.041361
1	-1.868690	2.997999	-2.289959
1	-0.614101	1.751490	-2.323572
1	-2.310225	1.333814	-2.659756
6	-1.048662	2.848605	0.173004
1	0.018151	2.739901	-0.050544
1	-1.377601	3.828169	-0.200511
1	-1.165455	2.856879	1.256923
6	-0.935408	-1.251049	-2.550142
1	-1.113094	-0.338122	-3.118814
1	0.134292	-1.298246	-2.320989
1	-1.186416	-2.098010	-3.203284
6	-1.512331	-2.750687	-0.680254
1	-0.470986	-2.858745	-0.359759
1	-2.163707	-3.001596	0.159810
1	-1.696180	-3.497464	-1.464057
6	-3.279275	-1.256640	-1.639183
1	-3.940101	-1.322014	-0.771145
1	-3.518507	-0.337251	-2.179432
1	-3.531273	-2.093501	-2.305581
6	-1.632309	0.783315	2.715972
1	-0.609170	1.171380	2.677426
1	-2.325892	1.597481	2.493922
1	-1.827577	0.466967	3.749379
6	-3.285100	-0.892789	1.857655
1	-3.560094	-1.051073	2.909762
1	-3.977101	-0.151874	1.449477
1	-3.456070	-1.839475	1.339173
6	-0.909786	-1.545389	2.375677
1	0.138615	-1.228771	2.377323
1	-1.211608	-1.732618	3.415360
1	-0.979596	-2.493993	1.841614

C1

E_{gas}: -1130.733700380
E_{sol}: -1130.736540810
G_{sol}: -1130.154920430

6	-2.533569	-0.730664	0.838615
6	-1.885199	-1.153492	2.015506
6	-3.235702	0.507905	0.828078
6	-1.915700	-0.387523	3.180970
6	-3.247580	1.252035	2.025412
6	-2.606716	0.822623	3.188198
1	-1.356999	-2.101649	2.003619
1	-1.410436	-0.743095	4.075206
1	-3.769459	2.205086	2.055298
1	-2.650072	1.429722	4.089063
14	-4.166898	1.309631	-0.633861
6	-3.429156	0.907474	-2.328265
1	-3.974389	1.463743	-3.101326
1	-2.379146	1.217565	-2.379253
1	-3.471782	-0.153724	-2.585574
6	-6.009034	0.864245	-0.585621
1	-6.207402	-0.197209	-0.764737
1	-6.438054	1.116964	0.391348
1	-6.556680	1.436178	-1.345151
46	0.243653	-0.895919	-0.382537
6	3.408517	0.488561	1.327734
15	2.118969	0.837497	-0.103323
6	1.286165	2.580111	0.223330
6	3.074273	0.912295	-1.811687
35	1.227125	-3.050455	0.471836
6	-2.491444	-1.671836	-0.338605
6	-1.326633	-1.999387	-0.923421
6	-3.819657	-2.307659	-0.714215
1	-3.731003	-2.997244	-1.556782
1	-4.583459	-1.565692	-0.965321
1	-4.203016	-2.874570	0.145612
6	-1.076938	-2.971717	-2.041457
1	-0.326431	-2.589459	-2.743326
1	-0.689533	-3.918037	-1.649145
1	-1.989583	-3.172956	-2.617377
6	-4.072779	3.193856	-0.441422
1	-3.039249	3.546675	-0.353733
1	-4.512706	3.673724	-1.324548
1	-4.626395	3.559548	0.430675
6	2.149148	1.512232	-2.892810
1	1.969366	2.581859	-2.763509
1	2.628680	1.382225	-3.871805
1	1.183119	0.996613	-2.935195
6	3.351585	-0.543238	-2.260134
1	4.031434	-1.081207	-1.599926
1	2.426517	-1.124893	-2.325854
1	3.809257	-0.519419	-3.258673
6	4.398473	1.701450	-1.807097

1	4.270963	2.739751	-1.490119
1	5.155256	1.240824	-1.167558
1	4.807210	1.717635	-2.826926
6	0.844205	2.681915	1.699798
1	0.241255	1.823770	2.012185
1	1.682844	2.791210	2.390164
1	0.217189	3.576727	1.810501
6	-0.019832	2.620384	-0.604178
1	0.139532	2.566418	-1.681511
1	-0.697087	1.808315	-0.310965
1	-0.541960	3.564902	-0.398526
6	2.143629	3.814537	-0.118295
1	1.592588	4.722155	0.165116
1	3.093065	3.828790	0.423006
1	2.360412	3.893559	-1.186389
6	2.614492	-0.007403	2.559311
1	3.332109	-0.297797	3.338713
1	1.960661	0.752753	2.987838
1	2.012494	-0.886720	2.312898
6	4.336452	-0.676284	0.918096
1	4.928221	-0.964477	1.797210
1	3.770410	-1.556657	0.601289
1	5.045809	-0.399989	0.133725
6	4.283625	1.692799	1.728264
1	3.702581	2.520306	2.142704
1	4.985440	1.371868	2.510471
1	4.879304	2.077508	0.896284

$TS_{C1\text{-}Ca}$

E_{gas}: -1130.69651987
E_{sol}: -1130.69962148
G_{sol}: -1130.11067361
imaginary frequency: 132.8779*i* cm^{-1}

6	-3.606214	-0.056376	0.456471
6	-4.494603	-0.584014	1.405825
6	-2.836193	1.082733	0.793187
6	-4.588412	-0.036713	2.685323
6	-2.937209	1.613619	2.088349
6	-3.803369	1.061430	3.034373
1	-5.093942	-1.454535	1.157490
1	-5.268014	-0.476721	3.410656
1	-2.346092	2.481870	2.366924
1	-3.869082	1.491386	4.030510
14	-1.808042	1.938233	-0.541103
6	-0.404603	1.392765	-2.252106
1	-0.081846	2.434644	-2.195307
1	0.480455	0.819319	-2.546870
1	-1.160186	1.282451	-3.028718
6	-3.026406	2.683300	-1.783210
1	-3.567903	1.910450	-2.335383
1	-3.762200	3.276844	-1.227250
1	-2.533777	3.345186	-2.503649
6	-2.281137	-0.794889	-1.502880
6	-3.469446	-0.694311	-0.878471
6	-1.994245	-1.511462	-2.793256
1	-1.603747	-2.513979	-2.576193
1	-2.891882	-1.625841	-3.414026
1	-1.240871	-0.996422	-3.398784
6	-4.735206	-1.308982	-1.459806
1	-4.677777	-1.436245	-2.543034
1	-4.923943	-2.301562	-1.028832
1	-5.607400	-0.684016	-1.238669
46	-0.514144	-0.171979	-0.684793
6	3.415217	1.574477	-0.711532
15	2.414741	0.092498	0.139021
6	3.278361	-1.574520	-0.468341
6	2.695298	0.247392	2.079404
35	-0.722422	-2.369238	0.569332
6	-0.895221	3.385388	0.264305
1	-0.173217	3.066443	1.020838
1	-0.369106	4.005278	-0.468560
1	-1.636152	4.027436	0.756831
6	1.649111	-0.650834	2.775928
1	0.628123	-0.380807	2.494656
1	1.772688	-1.710288	2.555254
1	1.750062	-0.521397	3.862649
6	4.100938	-0.129738	2.592264
1	4.128785	0.022562	3.680487
1	4.347669	-1.178254	2.413260
1	4.893598	0.484859	2.159896
6	2.390181	1.689712	2.536259
1	3.160392	2.406980	2.242432
1	1.422038	2.040976	2.165023
1	2.340752	1.702586	3.632975
6	2.951870	-2.750562	0.478017
1	1.879822	-2.858230	0.649537
1	3.304692	-3.674443	-0.000856
1	3.464386	-2.677355	1.440099
6	2.635310	-1.925732	-1.831320
1	2.803174	-1.168089	-2.600074
1	3.069875	-2.865591	-2.198626
1	1.556809	-2.079700	-1.724288
6	4.812781	-1.524669	-0.619099
1	5.317259	-1.275951	0.318717
1	5.162748	-2.522089	-0.919202
1	5.154070	-0.827047	-1.386075
6	2.582491	2.866529	-0.562906
1	3.066910	3.668591	-1.136818
1	1.573610	2.740151	-0.955224
1	2.500080	3.211535	0.467424
6	4.825712	1.856956	-0.155967
1	5.494597	0.997064	-0.217942
1	5.280264	2.667562	-0.743498
1	4.799199	2.195122	0.882551
6	3.531776	1.322643	-2.232351
1	3.940705	2.226423	-2.704094
1	4.200474	0.499121	-2.486464
1	2.560063	1.130476	-2.696548

Ca

E_{gas}: -1130.70109727
E_{sol}: -1130.70472267
G_{sol}: -1130.11742840

6	3.917870	-0.019851	-0.107297
6	5.047536	-0.163325	-0.931561
6	3.238983	1.220272	-0.104518
6	5.480901	0.876206	-1.753140
6	3.685555	2.254974	-0.939508
6	4.801234	2.093611	-1.761812
1	5.579438	-1.108663	-0.959353
1	6.347143	0.728802	-2.393056
1	3.162240	3.208229	-0.946742
1	5.134054	2.907977	-2.399866
14	1.802736	1.480229	1.053546
6	0.044587	-0.252185	2.590869
1	-0.433116	0.687788	2.869602
1	-0.669443	-1.073122	2.706336
1	0.908896	-0.427637	3.230038
6	2.445345	1.748436	2.807576
1	3.028857	0.892017	3.158125
1	3.111370	2.620874	2.786339
1	1.650664	1.950197	3.531972
6	2.177328	-1.435182	1.046982
6	3.456908	-1.168238	0.715170
6	1.761390	-2.702894	1.766093
1	2.253417	-3.571351	1.311785
1	2.026307	-2.681504	2.832864
1	0.685874	-2.886865	1.704029
6	4.538712	-2.161563	1.135499
1	4.278495	-2.681190	2.060695
1	4.707871	-2.928321	0.366490
1	5.490266	-1.647379	1.303061
46	0.477462	-0.419605	0.554027
6	-3.638193	0.844065	1.409194

15	-2.558217	0.130681	-0.087518
6	-3.213766	-1.690230	-0.454617
6	-2.978785	1.242462	-1.658690
35	0.899379	-1.147177	-1.880165
6	0.773346	2.978551	0.548754
1	0.453074	2.915533	-0.495137
1	-0.113273	3.092193	1.179487
1	1.379375	3.887222	0.667777
6	-1.890294	0.990783	-2.724916
1	-0.890688	1.225798	-2.351829
1	-1.859491	-0.037400	-3.082027
1	-2.095255	1.639651	-3.588112
6	-4.363384	1.004833	-2.296917
1	-4.492481	1.716194	-3.124853
1	-4.462041	0.003767	-2.721493
1	-5.190168	1.162552	-1.601058
6	-2.869985	2.738092	-1.289347
1	-3.701886	3.093781	-0.677017
1	-1.932249	2.968090	-0.774903
1	-2.884051	3.323138	-2.218333
6	-2.772240	-2.152537	-1.861170
1	-1.699684	-2.019211	-2.023731
1	-2.990457	-3.225919	-1.948786
1	-3.317687	-1.652084	-2.664496
6	-2.496823	-2.629156	0.543912
1	-2.718021	-2.406533	1.589667
1	-2.814381	-3.663230	0.352702
1	-1.410844	-2.591726	0.402575
6	-4.737948	-1.898890	-0.343737
1	-5.297855	-1.254465	-1.026196
1	-4.969060	-2.938300	-0.615641
1	-5.122911	-1.742211	0.666582
6	-2.921917	2.099754	1.960493
1	-3.444470	2.434975	2.866782
1	-1.886578	1.887781	2.236841
1	-2.919605	2.935484	1.260816
6	-5.095068	1.231372	1.080144
1	-5.681162	0.396248	0.690716
1	-5.585891	1.570656	2.003599
1	-5.159011	2.055259	0.366412
6	-3.672416	-0.174351	2.571070
1	-4.136588	0.308354	3.441943
1	-4.265844	-1.062018	2.345000
1	-2.672944	-0.493865	2.872875

TS_{Ca-D}

E_{gas}: -1130.69328562
E_{sol}: -1130.69653353
G_{sol}: -1130.10793691
imaginary frequency: 96.2764*i* cm^{-1}

6	-3.525048	-0.376103	0.489298
6	-4.260914	-1.335314	1.200698
6	-2.962916	0.722964	1.171131
6	-4.400974	-1.218464	2.582720
6	-3.103416	0.821984	2.560068
6	-3.825293	-0.142611	3.266489
1	-4.691440	-2.189130	0.686976
1	-4.955417	-1.974828	3.132268
1	-2.666028	1.660973	3.096618
1	-3.944605	-0.055402	4.343379
14	-2.047046	1.872568	0.024960
6	0.180944	2.013333	-1.799570
1	0.834183	2.685254	-1.252016
1	0.711409	1.579107	-2.654211
1	-0.673621	2.577330	-2.177390
6	-3.197064	3.021125	-0.959192
1	-4.124363	2.507593	-1.227098
1	-3.444690	3.896472	-0.345930
1	-2.738360	3.390242	-1.882959
6	-2.271929	0.224594	-1.565454
6	-3.331349	-0.403900	-0.973050
6	-2.186414	0.344337	-3.074087
1	-1.872244	-0.615133	-3.506698
1	-3.152124	0.610830	-3.523024
1	-1.466873	1.094056	-3.402326
6	-4.393873	-1.123164	-1.775697
1	-4.428228	-0.809265	-2.819797
1	-4.168425	-2.199273	-1.770728
1	-5.389550	-0.988943	-1.339706
46	-0.287740	0.259137	-0.757860
6	3.434690	1.643475	0.093285
15	2.313044	0.004052	0.191202
6	3.212035	-1.356387	-0.926753
6	2.372500	-0.587885	2.068148
35	-0.739652	-2.330623	-0.454556
6	-1.018270	3.071049	1.078492
1	-0.293697	2.574951	1.727925
1	-0.491475	3.810138	0.467907
1	-1.723514	3.621476	1.717510
6	1.259178	-1.627152	2.309552
1	0.264963	-1.215265	2.123355
1	1.355162	-2.517660	1.690906
1	1.309220	-1.938503	3.362390
6	3.719334	-1.204067	2.504798
1	3.662158	-1.428579	3.578888
1	3.934662	-2.145424	1.996059
1	4.569280	-0.535910	2.358997
6	2.063166	0.602230	3.000668
1	2.895277	1.303659	3.086830
1	1.168844	1.151398	2.690345
1	1.869249	0.208544	4.006766
6	2.816742	-2.791319	-0.514723
1	1.736341	-2.929586	-0.464668
1	3.204307	-3.474507	-1.283052
1	3.263639	-3.096537	0.434112
6	2.683880	-1.143216	-2.364787
1	2.894260	-0.145379	-2.757420
1	3.168324	-1.868857	-3.032096
1	1.604403	-1.317948	-2.412437
6	4.754496	-1.307516	-0.930740
1	5.179016	-1.459812	0.065403
1	5.115696	-2.130214	-1.562436
1	5.167697	-0.386907	-1.345466
6	2.669203	2.835532	0.718862
1	3.128517	3.770465	0.371291
1	1.617037	2.860411	0.444008
1	2.723349	2.842005	1.807981
6	4.803769	1.577953	0.807158
1	5.444236	0.769066	0.454950
1	5.334382	2.521207	0.614252
1	4.704054	1.491262	1.891418
6	3.695118	1.995399	-1.391160
1	4.205510	2.966990	-1.430018
1	4.343960	1.276049	-1.892440
1	2.776804	2.087087	-1.971944

TS_{C1-Cb}

E_{gas}: -1130.71220588
E_{sol}: -1130.71162241
G_{sol}: -1130.13173953
imaginary frequency: 97.8900*i* cm^{-1}

6	-1.840090	1.946475	0.901362
6	-1.332824	3.243815	1.032040
6	-1.879779	1.335797	-0.384075
6	-0.831763	3.918359	-0.085365
6	-1.305035	1.998517	-1.477662
6	-0.798136	3.294637	-1.334298
1	-1.296147	3.720583	2.007291
1	-0.446717	4.928452	0.026128
1	-1.269951	1.518795	-2.451370
1	-0.383035	3.812591	-2.194420
14	-3.885298	0.487251	-0.995270
6	-4.766163	2.110329	-0.602862
1	-4.261213	2.974463	-1.044400

1	-5.789544	2.065315	-0.998163
1	-4.836387	2.272601	0.477881
6	-3.708578	0.251828	-2.861918
1	-4.696244	-0.006873	-3.265186
1	-3.366690	1.156531	-3.373156
1	-3.031737	-0.569735	-3.123174
6	-2.387038	-0.220014	1.731751
6	-2.268833	1.095275	2.017350
6	-2.737276	-1.373008	2.616515
1	-3.469032	-2.034356	2.143654
1	-1.853272	-1.983347	2.830565
1	-3.155775	-1.016564	3.567102
6	-2.495622	1.699686	3.384541
1	-2.918185	0.982775	4.090939
1	-1.551816	2.064451	3.810863
1	-3.176888	2.557838	3.323447
46	-1.857694	-0.727847	-0.137974
15	3.054749	0.097518	-0.020072
6	3.956038	1.346834	1.198606
35	-1.158227	-3.114346	-0.101499
6	3.659484	0.520231	-1.839375
6	3.698321	-1.706073	0.404365
6	-5.030729	-0.874579	-0.337911
1	-5.181309	-0.787802	0.742768
1	-6.011366	-0.754891	-0.821067
1	-4.662900	-1.881860	-0.554034
6	3.325004	-2.668436	-0.745674
1	3.928177	-2.519729	-1.644988
1	3.501581	-3.698858	-0.408506
1	2.265297	-2.594926	-1.011842
6	2.871532	-2.190928	1.621810
1	3.068120	-1.624525	2.533099
1	1.797864	-2.145403	1.412271
1	3.125192	-3.239897	1.829322
6	5.199770	-1.866439	0.709276
1	5.832050	-1.541605	-0.121782
1	5.506262	-1.313963	1.601758
1	5.422735	-2.926929	0.897207
6	3.148090	2.667612	1.149212
1	3.517230	3.345555	1.932049
1	3.238851	3.192755	0.197742
1	2.083096	2.488072	1.332103
6	5.443494	1.653919	0.941157
1	5.609385	2.127693	-0.029865
1	5.812478	2.353113	1.706318
1	6.067756	0.757800	0.990382
6	3.810274	0.833504	2.647967
1	4.436255	-0.036521	2.857995
1	4.122032	1.629521	3.338473
1	2.771836	0.579491	2.887447
6	2.638637	-0.141765	-2.798374
1	2.655021	-1.231330	-2.765134
1	1.618159	0.183714	-2.568396
1	2.865450	0.159272	-3.831128
6	5.083431	0.088128	-2.236982
1	5.850402	0.543535	-1.604499
1	5.215846	-0.995866	-2.197457
1	5.285660	0.399376	-3.272566
6	3.524373	2.038961	-2.085346
1	3.647634	2.235846	-3.159498
1	2.535396	2.411068	-1.795079
1	4.283764	2.626564	-1.563615

Cb

E_{gas}: -1130.72202450
E_{sol}: -1130.72070990
G_{sol}: -1130.13756240

6	-1.828796	2.271572	0.466855
6	-2.132970	3.610878	0.201945
6	-1.452885	1.421920	-0.595811
6	-2.081957	4.091422	-1.112117
6	-1.402719	1.897357	-1.899506
6	-1.722931	3.242543	-2.158488
1	-2.410179	4.281958	1.011043
1	-2.327506	5.130244	-1.315882
1	-1.126564	1.244179	-2.724634
1	-1.691772	3.615953	-3.179003
14	-3.332987	-0.909746	-0.472540
6	-4.520948	0.552942	-0.386078
1	-4.301695	1.324733	-1.127903
1	-5.530888	0.166126	-0.583267
1	-4.533575	1.020300	0.602638
6	-3.266653	-1.542344	-2.248740
1	-4.287255	-1.785831	-2.576712
1	-2.873516	-0.784440	-2.935059
1	-2.649509	-2.440925	-2.326898
6	-1.510248	0.298427	1.747877
6	-1.835550	1.609519	1.774859
6	-1.335900	-0.690174	2.856168
1	-1.955481	-1.580032	2.710061
1	-0.297749	-1.035741	2.918761
1	-1.599631	-0.238531	3.821536
6	-2.165957	2.391899	3.023593
1	-2.144590	1.775720	3.924590
1	-1.455804	3.217383	3.163330
1	-3.165843	2.838877	2.946241
46	-0.977433	-0.466479	-0.054299
15	2.261036	0.136954	-0.026520
6	2.811069	1.742903	0.962238
35	-0.522201	-3.013996	-0.099386
6	2.802348	0.376028	-1.895854
6	3.297539	-1.367406	0.697899
6	-3.981405	-2.216974	0.716967
1	-4.104574	-1.814909	1.728455
1	-4.974220	-2.535893	0.369327
1	-3.326980	-3.089931	0.758991
6	3.248544	-2.563839	-0.279647
1	3.839034	-2.401676	-1.183873
1	3.677462	-3.437755	0.229497
1	2.223821	-2.821477	-0.557868
6	2.574966	-1.845401	1.980814
1	2.562031	-1.097598	2.775351
1	1.547534	-2.148366	1.760790
1	3.102215	-2.726208	2.372643
6	4.776629	-1.081991	1.029781
1	5.345808	-0.733088	0.163762
1	4.898394	-0.352969	1.834612
1	5.245249	-2.015334	1.372421
6	1.768889	2.850781	0.684482
1	2.007255	3.722132	1.310761
1	1.757574	3.190854	-0.351007
1	0.759817	2.521315	0.939257
6	4.215884	2.298230	0.654541
1	4.306599	2.648677	-0.376715
1	4.407113	3.164626	1.304102
1	5.010742	1.572254	0.837686
6	2.713835	1.457252	2.477626
1	3.499028	0.791534	2.841553
1	2.818508	2.406716	3.019892
1	1.741668	1.031219	2.748938
6	1.991447	-0.648781	-2.724699
1	2.215780	-1.685838	-2.475466
1	0.913741	-0.504762	-2.588502
1	2.215301	-0.504538	-3.790877
6	4.303468	0.210053	-2.207893
1	4.925779	0.911169	-1.646013
1	4.669429	-0.799799	-2.011637
1	4.469925	0.409624	-3.276201
6	2.367524	1.770065	-2.398490
1	2.481312	1.795693	-3.490954
1	1.319499	1.984725	-2.172470
1	2.982552	2.578338	-1.995608

TS_{Cb-Cc}

E_{gas}: -1130.71451582
E_{sol}: -1130.71370167
G_{sol}: -1130.12513285
imaginary frequency: 135.4834*i* cm^{-1}

6	-2.024051	2.061710	0.578826
6	-2.462341	3.392294	0.494824
6	-1.269396	1.502724	-0.477482
6	-2.227757	4.128325	-0.668095
6	-1.069063	2.231233	-1.647269
6	-1.562957	3.540083	-1.747837
1	-3.005271	3.845009	1.320688
1	-2.582569	5.152832	-0.741493
1	-0.540201	1.796651	-2.491457
1	-1.419209	4.100362	-2.668595
14	-3.095445	-0.845602	-0.688932
6	-4.404359	0.512786	-0.818576
1	-4.041994	1.419812	-1.308101
1	-5.216337	0.104050	-1.436269
1	-4.831308	0.788098	0.150384
6	-2.586551	-1.232154	-2.478152
1	-3.504313	-1.453363	-3.042863
1	-2.097993	-0.381612	-2.964794
1	-1.925811	-2.100495	-2.531447
6	-2.076241	-0.202355	1.377172
6	-2.332441	1.115706	1.647349
6	-2.156680	-1.305330	2.408289
1	-1.986635	-2.286435	1.967780
1	-1.394166	-1.160889	3.185244
1	-3.137729	-1.317364	2.901608
6	-2.916055	1.605048	2.949901
1	-3.057081	0.800315	3.673274
1	-2.263284	2.360823	3.406213
1	-3.889983	2.085941	2.785417
46	-0.635889	-0.383226	-0.127715
15	2.124591	0.220833	0.016935
6	2.534182	1.981261	0.808674
35	-0.296291	-3.003141	-0.165161
6	2.963004	0.146481	-1.752088
6	3.017711	-1.116593	1.165481
6	-3.948692	-2.377631	0.004241
1	-4.466038	-2.186354	0.949341
1	-4.704110	-2.683412	-0.732473
1	-3.252693	-3.208917	0.136913
6	3.213690	-2.456543	0.420862
1	3.979468	-2.403809	-0.355705
1	3.556462	-3.197157	1.156083
1	2.285231	-2.834586	-0.007777
6	2.072224	-1.408310	2.355384
1	1.863361	-0.530010	2.968739
1	1.126816	-1.832042	2.008971
1	2.552252	-2.153581	3.004115
6	4.400376	-0.702443	1.714014
1	5.122800	-0.482373	0.923293
1	4.361563	0.150134	2.394269
1	4.800779	-1.548385	2.288991
6	1.632610	3.074816	0.194304
1	1.938775	4.041324	0.617962
1	1.713599	3.156102	-0.888874
1	0.583402	2.922648	0.444043
6	3.997131	2.446940	0.640893
1	4.234283	2.677603	-0.401192
1	4.131663	3.377243	1.209955
1	4.734048	1.733007	1.007780
6	2.174004	1.955550	2.311214
1	2.856782	1.356038	2.915219
1	2.220399	2.983394	2.694992
1	1.153973	1.592470	2.474350
6	2.311666	-1.035803	-2.505661
1	2.481524	-2.001076	-2.029279
1	1.228039	-0.904533	-2.595186
1	2.729921	-1.081883	-3.520602
6	4.497299	-0.018780	-1.764094
1	5.010843	0.794082	-1.245650
1	4.828424	-0.963127	-1.329632
1	4.840419	-0.008501	-2.807989
6	2.626616	1.418972	-2.558268
1	2.931843	1.257398	-3.600584
1	1.556155	1.637027	-2.561546
1	3.158711	2.303887	-2.201047

Cc

E_{gas}: -1130.74134454
E_{sol}: -1130.74137612
G_{sol}: -1130.15668458

6	-1.723267	1.314036	0.192245
6	-2.311889	2.566686	-0.086853
6	-0.676825	0.904440	-0.660707
6	-1.960033	3.331782	-1.196988
6	-0.371832	1.625900	-1.817144
6	-1.006097	2.843041	-2.086842
1	-3.079495	2.924022	0.594188
1	-2.446150	4.287132	-1.375666
1	0.356928	1.243522	-2.522708
1	-0.746076	3.397065	-2.985383
14	-4.848843	0.112035	0.078285
6	-6.155633	1.427998	0.481988
1	-5.750570	2.441156	0.372963
1	-7.013560	1.342137	-0.196773
1	-6.536949	1.333661	1.505827
6	-4.277608	0.333248	-1.703066
1	-5.119668	0.099424	-2.368210
1	-3.941489	1.347664	-1.931722
1	-3.462793	-0.358524	-1.939394
6	-3.531308	0.140293	1.455540
6	-2.246577	0.561396	1.379710
6	-4.061943	-0.487127	2.743548
1	-3.876274	-1.569662	2.770716
1	-3.619098	-0.050060	3.644341
1	-5.146600	-0.356975	2.834021
6	-1.236372	0.382603	2.492826
1	-0.355240	-0.139239	2.096656
1	-0.890585	1.353295	2.876190
1	-1.614689	-0.204233	3.331245
46	0.406698	-0.742977	-0.338248
15	2.633100	0.121985	0.182607
6	2.899259	1.608195	1.422780
35	-1.338619	-2.341200	-1.035473
6	3.603963	0.511238	-1.476924
6	3.385012	-1.510009	0.971271
6	-5.668860	-1.594223	0.166576
1	-6.138038	-1.801249	1.134494
1	-6.448404	-1.676659	-0.601127
1	-4.930848	-2.381754	-0.026108
6	3.476658	-2.607292	-0.114547
1	4.271974	-2.424815	-0.839974
1	3.701756	-3.561879	0.378112
1	2.534244	-2.740387	-0.658506
6	2.387922	-2.044984	2.030333
1	2.227104	-1.360786	2.863137
1	1.409256	-2.279757	1.594508
1	2.790914	-2.978978	2.443807
6	4.770751	-1.354114	1.629891
1	5.528671	-0.974175	0.941406
1	4.748554	-0.703062	2.507127
1	5.107173	-2.341749	1.973248
6	1.931893	2.746944	1.023126
1	2.026532	3.553954	1.761852
1	2.148078	3.176071	0.044418
1	0.892238	2.411781	1.019984
6	4.340712	2.156336	1.475368
1	4.657115	2.612182	0.535104
1	4.384765	2.941700	2.241865
1	5.073198	1.393030	1.749503
6	2.504781	1.183127	2.854062

1	3.210281	0.478073	3.299020
1	2.505002	2.079938	3.487058
1	1.501174	0.755347	2.899308
6	3.044961	-0.405108	-2.592286
1	3.281575	-1.458886	-2.442368
1	1.958373	-0.320855	-2.686679
1	3.493174	-0.103561	-3.548253
6	5.132220	0.318808	-1.398355
1	5.598968	0.931305	-0.623379
1	5.414920	-0.722414	-1.229740
1	5.571361	0.618413	-2.359512
6	3.325426	1.965494	-1.921720
1	3.725109	2.094488	-2.936015
1	2.258887	2.196775	-1.956959
1	3.818144	2.705946	-1.288762

$TS_{Cc\text{-}Cd}$

E_{gas}: -1130.72927937
E_{sol}: -1130.72825188
G_{sol}: -1130.14575851
imaginary frequency: 66.9629*i* cm^{-1}

6	-2.195040	1.289875	0.555445
6	-2.949037	2.473673	0.679372
6	-1.151510	1.311689	-0.388322
6	-2.735342	3.581679	-0.140822
6	-0.968723	2.382588	-1.265993
6	-1.750096	3.534477	-1.126523
1	-3.726068	2.502787	1.439081
1	-3.349757	4.470006	-0.021021
1	-0.221805	2.325496	-2.052581
1	-1.590970	4.377297	-1.794223
14	-4.993101	-0.534603	0.141590
6	-6.578919	0.085590	0.980408
1	-6.493399	1.142257	1.261732
1	-7.436046	-0.005584	0.301340
1	-6.819776	-0.478563	1.889156
6	-4.703684	0.473620	-1.422617
1	-5.517706	0.258605	-2.127712
1	-4.688658	1.552598	-1.246920
1	-3.761130	0.193516	-1.903349
6	-3.617713	-0.568946	1.457135
6	-2.477740	0.156796	1.493799
6	-3.876656	-1.634169	2.523460
1	-3.290542	-2.544212	2.335670
1	-3.631310	-1.284635	3.532761
1	-4.927784	-1.940114	2.545365
6	-1.382330	-0.043575	2.523992
1	-0.434774	-0.267179	2.009295
1	-1.214291	0.873878	3.105417
1	-1.583051	-0.862600	3.216902
46	0.345125	0.029630	-0.402221
15	2.883087	-0.078431	0.208654
6	3.303963	0.880119	1.858696
35	-1.076149	-1.337393	-1.871361
6	3.897241	0.714700	-1.262156
6	3.400664	-1.952931	0.407039
6	-5.253871	-2.330000	-0.403772
1	-5.493658	-3.003011	0.426946
1	-6.077925	-2.392561	-1.125575
1	-4.351841	-2.711591	-0.896433
6	3.388035	-2.630975	-0.980827
1	4.219076	-2.315315	-1.615403
1	3.488017	-3.714354	-0.834971
1	2.447954	-2.459677	-1.515448
6	2.299878	-2.661926	1.233187
1	2.232653	-2.308502	2.262490
1	1.314907	-2.548825	0.767634
1	2.529569	-3.735145	1.270519
6	4.773311	-2.195676	1.064175
1	5.590696	-1.711348	0.523502
1	4.806380	-1.860073	2.103833
1	4.978355	-3.274878	1.069622
6	2.479886	2.191261	1.863822
1	2.623840	2.693965	2.829640
1	2.776242	2.894229	1.085155
1	1.408404	1.993797	1.749729
6	4.794135	1.213770	2.071434
1	5.182852	1.901968	1.317058
1	4.913112	1.706350	3.046228
1	5.426226	0.321979	2.076271
6	2.809987	0.065866	3.074489
1	3.402785	-0.833154	3.255546
1	2.897351	0.695691	3.969411
1	1.758147	-0.220640	2.979859
6	3.244117	0.262062	-2.590849
1	3.362090	-0.802486	-2.791939
1	2.172967	0.487581	-2.610794
1	3.721846	0.805812	-3.416816
6	5.400520	0.375369	-1.298109
1	5.923646	0.669948	-0.384779
1	5.582116	-0.689088	-1.467114
1	5.867703	0.916379	-2.132341
6	3.736112	2.250340	-1.215587
1	4.142570	2.669773	-2.145003
1	2.684275	2.549851	-1.155032
1	4.280147	2.714796	-0.390225

Cd

E_{gas}: -1130.73420330
E_{sol}: -1130.73250130
G_{sol}: -1130.150674000

6	-2.435368	1.224738	0.754311
6	-3.388312	2.238282	0.966314
6	-1.342768	1.537543	-0.080370
6	-3.305802	3.475756	0.324477
6	-1.291468	2.745936	-0.783628
6	-2.259851	3.731359	-0.561382
1	-4.210770	2.035704	1.648106
1	-4.068298	4.229202	0.504320
1	-0.499590	2.922008	-1.507863
1	-2.200705	4.679031	-1.090774
14	-4.848147	-0.914523	-0.145503
6	-6.557434	-0.580610	0.606986
1	-6.627274	0.441364	0.998631
1	-7.342857	-0.697221	-0.150349
1	-6.791568	-1.266144	1.430128
6	-4.557971	0.288140	-1.565651
1	-5.259047	0.044468	-2.375074
1	-4.718122	1.333126	-1.287040
1	-3.542068	0.195522	-1.963295
6	-3.574147	-0.948963	1.269582
6	-2.575738	-0.066600	1.500813
6	-3.730994	-2.194219	2.140024
1	-3.108088	-3.022199	1.774690
1	-3.467146	-2.018583	3.188178
1	-4.764199	-2.559694	2.134482
6	-1.509764	-0.243165	2.566427
1	-0.519294	-0.284396	2.082797
1	-1.487816	0.615718	3.251014
1	-1.623329	-1.155757	3.154505
46	0.389280	0.568700	-0.090618
15	2.798328	-0.170939	0.150174
6	3.360823	0.457230	1.915248
35	-0.586564	-0.751794	-1.957069
6	3.882572	0.722076	-1.206336
6	3.081378	-2.094744	0.039201
6	-4.848174	-2.653488	-0.899353
1	-5.072989	-3.439253	-0.169922
1	-5.598319	-2.720613	-1.697219
1	-3.871381	-2.877232	-1.344644
6	2.984285	-2.543845	-1.436035
1	3.850101	-2.240698	-2.029436
1	2.950198	-3.641184	-1.457111
1	2.071827	-2.176360	-1.914684

6	1.901204	-2.781658	0.768305
1	1.869782	-2.573367	1.838510
1	0.943299	-2.488988	0.328145
1	2.006264	-3.868580	0.651320
6	4.416255	-2.602362	0.620497
1	5.286308	-2.155293	0.131808
1	4.504415	-2.428929	1.695881
1	4.477494	-3.688113	0.465102
6	2.675246	1.826264	2.152071
1	2.886069	2.160201	3.176961
1	3.016125	2.610703	1.476236
1	1.582624	1.748946	2.058025
6	4.880294	0.604818	2.128343
1	5.326442	1.355948	1.472050
1	5.068600	0.927828	3.161602
1	5.414741	-0.337241	1.978821
6	2.808887	-0.478892	3.013730
1	3.294452	-1.456567	3.028985
1	2.994013	-0.011782	3.990080
1	1.728433	-0.629099	2.925867
6	3.172330	0.559435	-2.572385
1	3.169789	-0.466539	-2.938896
1	2.133038	0.897879	-2.534358
1	3.704895	1.170808	-3.313380
6	5.335824	0.224253	-1.332109
1	5.900700	0.324260	-0.401853
1	5.390186	-0.818437	-1.654328
1	5.852152	0.823093	-2.094918
6	3.901230	2.240117	-0.920464
1	4.356352	2.749242	-1.779832
1	2.890084	2.645149	-0.801638
1	4.491278	2.507664	-0.041050

Ce

E_{gas}: -1130.73076910
E_{sol}: -1130.73379184
G_{sol}: -1130.15151574

6	2.662467	-1.235058	0.149966
6	3.912264	-1.723303	-0.271933
6	1.515170	-1.726684	-0.502628
6	4.020749	-2.659646	-1.301511
6	1.613815	-2.685061	-1.515342
6	2.871061	-3.135023	-1.932751
1	4.805261	-1.362885	0.233370
1	5.000067	-3.027187	-1.597065
1	0.716075	-3.090867	-1.971812
1	2.943907	-3.874640	-2.726296
14	3.895154	1.871915	-0.259845
6	5.780861	1.880506	-0.062254
1	6.197680	0.872343	-0.168209
1	6.250065	2.515772	-0.823771
1	6.084812	2.262449	0.919425
6	3.465528	1.212226	-1.978404
1	3.899046	0.229054	-2.176927
1	2.384035	1.132949	-2.132185
1	3.852571	1.912332	-2.730313
6	3.131510	0.983047	1.237576
6	2.600799	-0.264402	1.293404
6	3.172203	1.827819	2.510491
1	2.220623	2.350902	2.685649
1	3.379195	1.224651	3.401066
1	3.945434	2.602728	2.462191
6	2.022209	-0.848840	2.574438
1	1.484116	-0.104964	3.170072
1	1.337356	-1.671782	2.357708
1	2.828697	-1.253753	3.204408
46	-0.218766	-0.802772	-0.209422
15	-2.288234	0.683816	-0.155491
6	-1.615924	2.482452	-0.535450
35	-0.933413	-2.922860	0.875807
6	-3.222353	0.704633	1.560763
6	-3.540242	0.168632	-1.567674
6	3.299788	3.674952	-0.211945
1	2.209623	3.737835	-0.309493
1	3.579626	4.190865	0.712826
1	3.737454	4.237249	-1.046132
6	-4.141867	1.919726	1.792370
1	-4.932741	1.998561	1.041164
1	-4.630967	1.810296	2.769975
1	-3.596496	2.866412	1.812189
6	-4.061708	-0.583265	1.710600
1	-4.942132	-0.595703	1.063498
1	-3.466368	-1.482039	1.526018
1	-4.425078	-0.633476	2.745661
6	-2.149002	0.642749	2.674211
1	-1.515533	-0.242150	2.561451
1	-1.508060	1.524551	2.711328
1	-2.658528	0.569577	3.644454
6	-3.724287	-1.366074	-1.501623
1	-4.334643	-1.679190	-2.359625
1	-2.765845	-1.890071	-1.555248
1	-4.232554	-1.703518	-0.598895
6	-4.921243	0.850100	-1.510274
1	-4.858345	1.940626	-1.549092
1	-5.514090	0.525147	-2.376460
1	-5.485415	0.572669	-0.616531
6	-2.903338	0.458261	-2.944399
1	-1.902318	0.021542	-3.031761
1	-3.528744	-0.004803	-3.718650
1	-2.843826	1.524030	-3.177376
6	-2.653271	3.514167	-1.018356
1	-2.155278	4.483242	-1.161671
1	-3.103141	3.241743	-1.976404
1	-3.459322	3.666772	-0.295729
6	-0.909556	3.046177	0.717261
1	-0.388411	3.970666	0.434915
1	-1.601941	3.301390	1.522114
1	-0.156309	2.354296	1.109012
6	-0.508913	2.330825	-1.605240
1	0.279550	1.644623	-1.265945
1	-0.873226	1.975617	-2.568953
1	-0.032145	3.306182	-1.771352

$TS_{Ce\text{-}Cf}$

E_{gas}: -1130.68860306
E_{sol}: -1130.69184944
G_{sol}: -1130.10366638
imaginary frequency: 174.5686*i* cm^{-1}

6	3.482123	-0.415970	0.000290
6	4.733758	-0.922924	-0.402155
6	2.381976	-0.642830	-0.847609
6	4.891215	-1.611193	-1.602591
6	2.537993	-1.322535	-2.057817
6	3.790929	-1.813157	-2.436632
1	5.601809	-0.758338	0.229835
1	5.871068	-1.985438	-1.886969
1	1.680745	-1.503758	-2.700903
1	3.898404	-2.359367	-3.370503
14	1.769388	2.084844	-0.319037
6	3.193748	2.667911	-1.422375
1	3.786076	1.834290	-1.809325
1	2.836938	3.264257	-2.269718
1	3.859244	3.300543	-0.822323
6	0.601743	1.330222	-2.086733
1	1.484893	1.323935	-2.724045
1	-0.053290	0.537088	-2.468363
1	0.046247	2.264653	-2.183342
6	2.525012	1.435949	1.302125
6	3.335170	0.348748	1.269039
6	2.227462	2.234136	2.555767
1	1.146119	2.344475	2.703657
1	2.627874	1.773483	3.462357
1	2.637508	3.252224	2.499057
6	4.104941	-0.203475	2.447723

1	3.918342	0.343113	3.373108
1	3.831250	-1.253467	2.607120
1	5.187419	-0.175120	2.269163
46	0.478018	-0.103765	-0.378855
15	-2.378025	-0.037707	-0.062457
6	-3.333046	1.387450	-1.057709
35	0.632292	-2.038038	1.269364
6	-2.822506	0.204762	1.852159
6	-3.026788	-1.755719	-0.806803
6	0.773188	3.637043	0.109720
1	-0.049541	3.448873	0.804310
1	1.452191	4.350934	0.592679
1	0.367825	4.129597	-0.780136
6	-4.199341	0.821612	2.158835
1	-5.021966	0.256705	1.709592
1	-4.348926	0.804813	3.247091
1	-4.278676	1.865604	1.846536
6	-2.736468	-1.111829	2.650334
1	-3.610208	-1.746763	2.486257
1	-1.828650	-1.677651	2.438976
1	-2.724409	-0.852889	3.718014
6	-1.719525	1.137068	2.403822
1	-0.734869	0.665816	2.330576
1	-1.683415	2.102280	1.890609
1	-1.921450	1.336835	3.465195
6	-2.782450	-2.954992	0.134027
1	-2.893839	-3.870385	-0.463136
1	-1.778713	-2.960745	0.561622
1	-3.517670	-3.010201	0.938539
6	-4.515924	-1.789752	-1.199451
1	-4.761341	-1.120291	-2.026730
1	-4.765176	-2.807889	-1.528647
1	-5.171791	-1.554841	-0.354073
6	-2.152624	-2.014127	-2.058596
1	-1.101521	-2.137440	-1.777388
1	-2.482669	-2.948881	-2.531633
1	-2.218634	-1.226374	-2.811720
6	-4.868134	1.516700	-0.906881
1	-5.216846	2.253184	-1.644562
1	-5.405580	0.589636	-1.100824
1	-5.171461	1.884905	0.071551
6	-2.711397	2.728617	-0.619713
1	-3.098043	3.533212	-1.260252
1	-2.966843	2.988601	0.411290
1	-1.624038	2.721332	-0.707813
6	-3.051621	1.218895	-2.569109
1	-1.992598	1.087497	-2.795351
1	-3.603124	0.383041	-3.006347
1	-3.385348	2.127576	-3.088039

Cf

E_{gas}: -1130.69695326
E_{sol}: -1130.70031396
G_{sol}: -1130.11346770

6	3.528582	-0.520785	0.066003
6	4.675411	-1.337914	-0.017789
6	2.368877	-0.949916	-0.622706
6	4.693410	-2.522148	-0.747358
6	2.401230	-2.128316	-1.378610
6	3.548278	-2.924056	-1.431174
1	5.579771	-1.025133	0.494680
1	5.598947	-3.121716	-0.785272
1	1.516542	-2.462601	-1.909998
1	3.535583	-3.851655	-1.997816
14	1.845596	1.660941	-1.085500
6	2.888106	1.594363	-2.660741
1	3.546268	0.723080	-2.697742
1	2.273593	1.610701	-3.566418
1	3.516931	2.494461	-2.673123
6	0.223392	-0.240088	-2.496353
1	1.165462	-0.371772	-3.026085
1	-0.379823	-1.143633	-2.616223
1	-0.318067	0.621016	-2.893208
6	2.903673	1.831812	0.443257
6	3.612021	0.747298	0.841313
6	2.858158	3.152800	1.180538
1	1.852101	3.340922	1.580785
1	3.556616	3.203557	2.019682
1	3.091572	3.995533	0.516040
6	4.514187	0.719397	2.057510
1	4.289824	1.529913	2.752291
1	4.390395	-0.224928	2.596903
1	5.574523	0.808139	1.783569
46	0.458754	-0.201431	-0.424051
15	-2.419650	-0.083949	-0.005753
6	-3.505327	0.611652	-1.521127
35	0.736756	-0.630485	2.138633
6	-2.876284	1.042998	1.567494
6	-2.939676	-1.975253	0.244702
6	0.694025	3.146907	-1.280393
1	0.012192	3.277258	-0.437402
1	1.313724	4.050896	-1.357391
1	0.103489	3.078914	-2.198430
6	-4.285418	1.664461	1.567208
1	-5.078438	0.917782	1.464323
1	-4.433468	2.165953	2.533123
1	-4.414341	2.425936	0.795462
6	-2.735872	0.289394	2.905857
1	-3.572409	-0.393111	3.078850
1	-1.792824	-0.248800	2.993768
1	-2.763338	1.038297	3.709206
6	-1.836414	2.185392	1.570173
1	-0.823147	1.794858	1.696887
1	-1.874266	2.787358	0.657717
1	-2.050983	2.855664	2.413812
6	-2.485773	-2.533772	1.611010
1	-2.518451	-3.630055	1.549287
1	-1.464211	-2.243884	1.867685
1	-3.150041	-2.240894	2.424120
6	-4.446406	-2.258398	0.099184
1	-4.818384	-2.093958	-0.915133
1	-4.630884	-3.314067	0.341694
1	-5.047349	-1.658303	0.791222
6	-2.152696	-2.783651	-0.814825
1	-1.074336	-2.723190	-0.631033
1	-2.438595	-3.840769	-0.731062
1	-2.345017	-2.474290	-1.842577
6	-5.038001	0.757461	-1.343654
1	-5.476675	0.918668	-2.338094
1	-5.514484	-0.127883	-0.923115
1	-5.320075	1.614564	-0.735840
6	-2.935573	2.004583	-1.859574
1	-3.415339	2.379430	-2.774148
1	-3.128824	2.737258	-1.071071
1	-1.857963	1.971763	-2.033549
6	-3.307931	-0.290855	-2.760759
1	-2.263267	-0.507611	-2.975576
1	-3.849492	-1.236562	-2.673671
1	-3.719633	0.231570	-3.634798

$TS_{Cf\text{-}D}$

E_{gas}: -1130.69543409
E_{sol}: -1130.69876604
G_{sol}: -1130.10880995
imaginary frequency: 89.5916*i* cm^{-1}

6	3.462110	-0.561893	-0.029655
6	4.520779	-1.441468	-0.319713
6	2.363256	-0.504002	-0.933399
6	4.527420	-2.234925	-1.463270
6	2.415216	-1.269821	-2.110696
6	3.473629	-2.143081	-2.369853
1	5.366759	-1.489388	0.358597
1	5.360834	-2.906574	-1.651667
1	1.602627	-1.231489	-2.826009

1	3.460798	-2.753216	-3.269322
14	2.018809	1.812700	-0.558754
6	3.170063	2.269315	-1.993823
1	4.023407	1.591264	-2.067908
1	2.658887	2.290144	-2.961836
1	3.548474	3.282815	-1.805639
6	0.064763	0.687228	-2.432179
1	1.002621	0.877607	-2.954191
1	-0.441816	-0.146409	-2.926092
1	-0.558909	1.578734	-2.463525
6	2.953114	1.555811	1.034687
6	3.569857	0.353670	1.132576
6	2.914420	2.612177	2.112579
1	1.886727	2.769499	2.468177
1	3.525911	2.360552	2.983706
1	3.265255	3.583775	1.738862
6	4.383479	-0.117137	2.315055
1	4.205553	0.493882	3.201705
1	4.123881	-1.151357	2.563540
1	5.461794	-0.084768	2.106883
46	0.343624	-0.027692	-0.492977
15	-2.371014	-0.060911	-0.018910
6	-3.497209	1.119450	-1.163668
35	0.725203	-1.348444	1.752323
6	-2.761352	0.476817	1.858308
6	-2.922022	-1.920848	-0.414620
6	0.847269	3.295924	-0.393587
1	0.099385	3.171247	0.392461
1	1.457192	4.175608	-0.145062
1	0.333212	3.509625	-1.335386
6	-4.143565	1.110622	2.105795
1	-4.971787	0.469346	1.791751
1	-4.246717	1.266475	3.187916
1	-4.254913	2.089558	1.636362
6	-2.649304	-0.699913	2.848426
1	-3.511607	-1.369930	2.780008
1	-1.727638	-1.267355	2.730833
1	-2.650620	-0.278259	3.862932
6	-1.681777	1.517968	2.228427
1	-0.682175	1.078180	2.202902
1	-1.703043	2.393966	1.572282
1	-1.871897	1.871402	3.251309
6	-2.437828	-2.924367	0.655024
1	-2.515679	-3.930543	0.221085
1	-1.397575	-2.764673	0.946647
1	-3.060155	-2.914777	1.549898
6	-4.439551	-2.119120	-0.582704
1	-4.845904	-1.615403	-1.462743
1	-4.638629	-3.192253	-0.707093
1	-4.998005	-1.787514	0.299231
6	-2.194262	-2.318667	-1.720149
1	-1.108680	-2.320597	-1.575917
1	-2.492280	-3.341673	-1.986484
1	-2.428836	-1.678733	-2.571303
6	-5.021079	1.192486	-0.875084
1	-5.505344	1.633274	-1.757022
1	-5.486706	0.221890	-0.707358
1	-5.266241	1.835619	-0.032642
6	-2.935799	2.551014	-1.024473
1	-3.472661	3.213855	-1.716873
1	-3.078044	2.953926	-0.018105
1	-1.872029	2.611656	-1.261526
6	-3.377280	0.693611	-2.645769
1	-2.353578	0.533047	-2.973544
1	-3.956933	-0.208036	-2.860908
1	-3.797921	1.496137	-3.266473