Theoretical Investigation on Mechanism of Asymmetric Michael Addition of Malononitrile to Chalcones Catalyzed by Cinchona Alkaloid Aluminum (III) Complex

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Supporting Information:

XYZ Coordinates and Energies

Malononitrile (R1)

Energy+zep(gas) = -224.945627 au

Gibbs free energy (gas) = -224.973370 au

Energy(sol) = -224.9947037 au

Thermal correction to Gibbs Free Energy = 0.016818 au

Gibbs free energy (sol) = -224.9778857 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.835130	0.000003
2	6	0	1.225517	0.023856	-0.000082
3	6	0	-1.225517	0.023856	0.000068
4	1	0	-0.000075	1.484662	-0.883538
5	1	0	0.000076	1.484636	0.883563
6	7	0	-2.208851	-0.590454	-0.000028
7	7	0	2.208851	-0.590454	0.000034

R2

Energy+zep(gas) = -270.463699 au

Gibbs free energy (gas) = -270.494902 au

Energy(sol) = -270.5838654 au

Thermal correction to Gibbs Free Energy = 0.086297 au

Gibbs free energy (sol) = -270.4975684 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.311337	0.321045	-0.000381
2	6	0	-0.294274	-0.556938	0.000711

3	6	0	1.146917	-0.205962	0.000040
4	8	0	1.986221	-1.100458	-0.000557
5	1	0	-0.487207	-1.628293	0.001765
6	1	0	-1.092270	1.388616	-0.001605
7	6	0	-2.763334	-0.047907	-0.000097
8	1	0	-3.270127	0.369644	-0.879480
9	1	0	-2.906572	-1.131887	0.000259
10	1	0	-3.269813	0.370125	0.879253
11	6	0	1.572064	1.253891	0.000246
12	1	0	1.186368	1.775281	-0.882949
13	1	0	1.187880	1.774264	0.884735
14	1	0	2.661755	1.301134	-0.000640

CI

Energy+zep(gas) = -690.675867 au

Gibbs free energy(gas) = -690.716848 au

Energy(sol) = -690.9768067 au

Thermal correction to Gibbs Free Energy = 0.256091 au

Gibbs free energy (sol) = -690.7207157 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.862875	-0.419293	-1.073888
2	6	0	0.631701	-0.319470	-0.254092
3	6	0	2.651100	-1.558597	-0.559668
4	6	0	2.694838	0.802196	-0.974059
5	6	0	-0.470710	0.512490	-0.949820
6	6	0	0.965775	0.124770	1.203615
7	6	0	2.953691	-1.402103	0.965449
8	6	0	3.178486	1.048517	0.489661
9	1	0	2.097879	-2.482527	-0.762729
10	1	0	3.577039	-1.603933	-1.142950
11	1	0	3.542764	0.669791	-1.654913
12	1	0	2.107168	1.644576	-1.338850
13	8	0	-0.175854	1.907061	-0.811184
14	6	0	-1.852334	0.174963	-0.404039
15	6	0	2.493719	0.006205	1.396528
16	1	0	0.656271	1.160653	1.376317
17	1	0	0.432888	-0.503224	1.926783
18	1	0	4.024026	-1.529826	1.167294

19	1	0	4.268795	0.954052	0.568723
20	1	0	2.917977	2.061867	0.817329
21	1	0	-0.434959	0.230120	-2.011108
22	6	0	-2.461478	0.928188	0.604923
23	6	0	-2.562092	-0.927489	-0.897125
24	1	0	2.752250	0.185586	2.445931
25	6	0	-3.722762	0.546137	1.070078
26	6	0	-3.817002	-1.225803	-0.365064
27	1	0	-1.963135	1.798012	1.019305
28	7	0	-4.403372	-0.510025	0.605553
29	1	0	-4.210033	1.119080	1.856552
30	1	0	0.231010	-1.339558	-0.229633
31	1	0	-0.801619	2.409761	-1.349237
32	1	0	2.426056	-2.164679	1.551983
33	1	0	-4.382647	-2.076270	-0.740190
34	1	0	-2.149016	-1.544777	-1.691122

P

Energy+zep(gas) = -495.420901 au

Gibbs free energy(gas) = -495.460237 au

Energy(sol) = -495.5931204 au

Thermal correction to Gibbs Free Energy = 0.127232 au

Gibbs free energy (sol) = -495.4658884 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.445526	-0.917191	-0.682217
2	6	0	-0.506220	-1.150684	0.509758
3	6	0	-1.790339	-0.319155	0.591247
4	8	0	-2.090091	0.239436	1.630448
5	1	0	-0.134406	-0.862412	-1.610980
6	7	0	-0.333941	2.527006	-1.015605
7	6	0	0.357190	1.621727	-0.794908
8	6	0	1.225081	0.446608	-0.602794
9	6	0	2.018113	0.572201	0.633985
10	7	0	2.666819	0.628857	1.593971
11	1	0	1.941008	0.458888	-1.436476
12	1	0	-0.834539	-2.198530	0.456561
13	1	0	0.026008	-1.031414	1.458600
14	6	0	-2.698528	-0.273881	-0.624200

15	1	0	-2.719013	-1.230586	-1.157392
16	1	0	-3.706281	0.001158	-0.308248
17	1	0	-2.341167	0.492763	-1.321351
18	6	0	1.455527	-2.068680	-0.806784
19	1	0	0.927834	-3.013362	-0.966852
20	1	0	2.135174	-1.917997	-1.652457
21	1	0	2.057862	-2.170706	0.101922

B-TS

Energy+zep(gas) = -495.313559 au

Gibbs free energy(gas) = -495.354752 au

Energy(sol) = -495.4786419 au

Thermal correction to Gibbs Free Energy = 0.116445 au

Gibbs free energy (sol) = -495.3621969 au

Number of imaginary frequencies: 1 (-992.8832 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.895338	-0.390339	0.161671
2	7	0	3.825479	0.237018	-0.173875
3	6	0	1.734217	-1.052872	0.609179
4	6	0	0.852718	-1.671276	-0.277610
5	7	0	-0.027284	-2.019523	-0.981625
6	1	0	-0.025874	0.057725	-0.099082
7	1	0	1.696595	-1.352909	1.652551
8	6	0	-0.100038	1.328674	0.360157
9	6	0	-1.062256	0.753464	-0.489962
10	6	0	-2.349289	0.104621	-0.053943
11	8	0	-3.279865	0.153886	-0.838016
12	1	0	-0.975681	0.918658	-1.560562
13	1	0	-0.226225	1.210930	1.433602
14	6	0	0.972681	2.251651	-0.118516
15	1	0	1.946026	2.024383	0.322679
16	1	0	1.066537	2.240104	-1.206556
17	1	0	0.687094	3.265757	0.192833
18	6	0	-2.453598	-0.512464	1.320025
19	1	0	-1.642611	-1.227036	1.493689
20	1	0	-2.399019	0.262436	2.094879
21	1	0	-3.413927	-1.022364	1.402597

CI-TS

Energy+zep = -915.621102 au

Gibbs free energy = -915.669907 au

Energy(sol) = -915.968258 au

Thermal correction to Gibbs Free Energy = 0.291128 au

Gibbs free energy (sol) = -915.67713 au

Number of imaginary frequencies: 1 (-1031.3143 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.702952	-0.398936	0.143296
2	6	0	-0.210326	-0.597241	0.295105
3	6	0	-2.367465	-1.007618	1.339231
4	6	0	-2.241276	-1.057765	-1.094193
5	6	0	0.633023	0.417549	-0.516720
6	6	0	0.107893	-2.089054	0.024960
7	6	0	-1.885420	-2.472683	1.514320
8	6	0	-2.125193	-2.598444	-0.972067
9	1	0	-2.136698	-0.383813	2.206889
10	1	0	-3.446422	-0.950772	1.167122
11	1	0	-3.278628	-0.726548	-1.202778
12	1	0	-1.665711	-0.674190	-1.934029
13	8	0	0.422595	0.256026	-1.913308
14	6	0	2.107093	0.263413	-0.155447
15	6	0	-1.186289	-2.911010	0.209425
16	1	0	0.488934	-2.218530	-0.993604
17	1	0	0.891713	-2.424764	0.710399
18	1	0	-2.737122	-3.124992	1.733529
19	1	0	-3.106576	-3.058228	-0.808177
20	1	0	-1.724638	-3.014319	-1.902073
21	1	0	-1.194026	-2.554578	2.360164
22	1	0	0.325771	1.423603	-0.210471
23	6	0	3.027366	-0.289760	-1.048689
24	6	0	2.584395	0.675253	1.095377
25	1	0	-0.955707	-3.980119	0.242773
26	6	0	4.360143	-0.421077	-0.648816
27	6	0	3.936141	0.500699	1.396031
28	1	0	2.711429	-0.594472	-2.039809
29	1	0	1.927738	1.145996	1.823004
30	7	0	4.822706	-0.043309	0.550111
31	1	0	5.093006	-0.849727	-1.329383
32	1	0	4.326875	0.819744	2.359906

33	1	0	0.102442	1.101468	-2.276116
34	1	0	-0.012460	-0.369269	1.347262
35	1	0	-2.044015	0.832748	0.089275
36	7	0	-1.174020	2.817450	-2.191513
37	6	0	-1.772937	2.645989	-1.202471
38	6	0	-2.436957	2.234694	-0.000082
39	6	0	-1.940205	2.806055	1.223671
40	1	0	-3.525759	2.279533	-0.079089
41	7	0	-1.511565	3.150372	2.252943

CI-COM

Energy+zep(gas) = -915.630760 au

Gibbs free energy(gas)= -915.682560 au

Energy(sol) = -915.9787685 au

Thermal correction to Gibbs Free Energy = 0.291026 au

Gibbs free energy (sol) = -915.6877425 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.476008	0.870841	0.246618
2	6	0	-0.014125	0.810186	0.326753
3	6	0	1.938998	1.701724	1.386521
4	6	0	1.933051	1.525845	-1.010578
5	6	0	-0.611306	-0.408799	-0.410749
6	6	0	-0.630696	2.182961	-0.063796
7	6	0	1.204049	3.077618	1.410744
8	6	0	1.493966	3.018589	-1.072572
9	1	0	1.774810	1.144547	2.315185
10	1	0	3.020987	1.834729	1.276451
11	1	0	3.025416	1.436517	-1.045454
12	1	0	1.521005	0.961873	-1.846481
13	8	0	-0.415359	-0.273174	-1.817447
14	6	0	-2.085470	-0.589814	-0.061680
15	6	0	0.476645	3.252417	0.059965
16	1	0	-1.008419	2.161860	-1.092140
17	1	0	-1.479098	2.414231	0.589060
18	1	0	1.917235	3.894350	1.570795
19	1	0	2.351825	3.691466	-0.951808
20	1	0	1.042752	3.243648	-2.045504
21	1	0	0.481157	3.119856	2.234402

22	1	0	-0.069628	-1.291665	-0.047039
23	6	0	-3.103786	-0.237983	-0.951476
24	6	0	-2.468714	-1.111150	1.180557
25	1	0	0.044083	4.255675	-0.013063
26	6	0	-4.434497	-0.409361	-0.560485
27	6	0	-3.826364	-1.243144	1.474981
28	1	0	-2.860938	0.152838	-1.933338
29	1	0	-1.726509	-1.425051	1.910717
30	7	0	-4.808066	-0.898833	0.629182
31	1	0	-5.240779	-0.140052	-1.239821
32	1	0	-4.141263	-1.650480	2.433491
33	1	0	-0.276185	-1.151564	-2.199825
34	1	0	2.529873	-0.952647	0.092076
35	7	0	1.443782	-2.945998	-2.034813
36	6	0	2.154571	-2.538908	-1.212692
37	6	0	3.002351	-1.926275	-0.184150
38	6	0	3.143449	-2.758695	1.015065
39	1	0	3.993367	-1.718541	-0.604459
40	7	0	3.262416	-3.381724	1.986527
41	1	0	-0.228530	0.622541	1.385285

CI-IM1

Energy+zep(gas) = -915.625468 au

Gibbs free energy(gas) = -915.675517 au

Energy(sol) = -915.9786673 au

Thermal correction to Gibbs Free Energy = 0.29457 au

Gibbs free energy (sol) = -915.6840973 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.741309	-0.538870	0.511260
2	6	0	-0.267065	-0.872777	0.313699
3	6	0	-2.367447	-1.597205	1.379764
4	6	0	-2.497272	-0.443948	-0.793160
5	6	0	0.571044	0.339009	-0.163475
6	6	0	-0.188947	-2.118262	-0.603535
7	6	0	-2.133615	-2.986346	0.736544
8	6	0	-2.526852	-1.840003	-1.460106
9	1	0	-1.925300	-1.503494	2.373988
10	1	0	-3.426447	-1.341919	1.462334

11	1	0	-3.491102	-0.065613	-0.543762
12	1	0	-1.976456	0.293669	-1.400091
13	8	0	0.266040	0.622596	-1.514067
14	6	0	2.053612	0.031298	0.050789
15	6	0	-1.579208	-2.780740	-0.688275
16	1	0	0.139629	-1.819167	-1.602657
17	1	0	0.553725	-2.816033	-0.205822
18	1	0	-3.073574	-3.546344	0.707627
19	1	0	-3.543127	-2.249153	-1.464157
20	1	0	-2.207239	-1.753411	-2.502681
21	1	0	-1.428091	-3.573143	1.334230
22	1	0	0.313605	1.195611	0.472634
23	6	0	2.903219	-0.252244	-1.020127
24	6	0	2.608041	0.025453	1.336922
25	1	0	-1.504098	-3.742996	-1.203436
26	6	0	4.245202	-0.543056	-0.758316
27	6	0	3.961565	-0.277097	1.491262
28	1	0	2.526110	-0.228419	-2.036312
29	1	0	2.008465	0.273464	2.209765
30	7	0	4.780101	-0.566068	0.469456
31	1	0	4.924215	-0.766413	-1.578583
32	1	0	4.411877	-0.280945	2.481672
33	1	0	0.339306	1.596448	-1.655559
34	1	0	0.080279	-1.118556	1.320901
35	1	0	-1.856073	0.394253	1.025852
36	7	0	-2.064126	1.842898	1.803788
37	6	0	-1.992070	2.799404	1.106756
38	6	0	-1.809276	3.840273	0.217731
39	6	0	-0.735225	3.691903	-0.664338
40	1	0	-2.509787	4.660340	0.138372
41	7	0	0.174124	3.450196	-1.372303

A-COM

Energy+zep(gas) = -1658.314115 au

Gibbs free energy(gas) = -1658.387774 au

Energy(sol) = -1658.861127 au

Thermal correction to Gibbs Free Energy = 0.465026 au

Gibbs free energy (sol) = -1658.396101 au

Number of imaginary frequencies: 0

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	1	0	0.072653	-1.111771	0.274726
2	7	0	0.812645	-1.357103	0.983860
3	6	0	1.820469	-0.239979	1.218174
4	6	0	0.092682	-1.610526	2.285957
5	6	0	1.453891	-2.645899	0.523541
6	6	0	2.116336	0.620183	-0.043655
7	6	0	3.004583	-0.850871	1.996043
8	6	0	1.149040	-1.834824	3.394651
9	6	0	2.309795	-3.226936	1.671757
10	1	0	-0.547469	-0.746936	2.473496
11	1	0	-0.548117	-2.479670	2.124361
12	1	0	0.636582	-3.300142	0.214554
13	1	0	2.046321	-2.410241	-0.358272
14	8	0	0.923396	1.195910	-0.482263
15	6	0	2.817138	-0.086760	-1.200106
16	6	0	2.512221	-2.121628	2.727055
17	1	0	3.831928	-1.114177	1.328151
18	1	0	3.380762	-0.105828	2.704250
19	1	0	0.847478	-2.675315	4.027488
20	1	0	1.821556	-4.098064	2.121938
21	1	0	3.272459	-3.564973	1.276160
22	1	0	2.819937	1.380057	0.338653
23	13	0	0.021927	2.523287	0.263925
24	6	0	2.094991	-0.581868	-2.292247
25	6	0	4.208870	-0.237132	-1.233157
26	1	0	3.243088	-2.438566	3.476671
27	8	0	0.697817	2.730302	1.860346
28	6	0	2.781141	-1.219961	-3.327044
29	6	0	4.801162	-0.890935	-2.317009
30	1	0	1.018541	-0.459530	-2.331367
31	6	0	0.459186	3.744644	2.811400
32	7	0	4.112139	-1.387199	-3.352697
33	1	0	2.235138	-1.613639	-4.181840
34	1	0	1.321568	3.829417	3.486631
35	8	0	-0.300177	3.907012	-0.725773
36	6	0	0.545415	4.855626	-1.330090
37	1	0	1.165004	4.406010	-2.121208
38	6	0	-4.845673	0.379186	-0.400095
39	6	0	-3.786643	0.881445	0.283298
40	6	0	-2.572993	1.384357	-0.305825
41	8	0	-1.680824	1.804914	0.497430
42	1	0	-3.808305	0.911739	1.370207
43	1	0	-4.812201	0.335552	-1.485438

44	1	0	1.298904	0.466271	1.869677
45	6	0	-6.078551	-0.152941	0.239353
46	1	0	-6.118601	-1.246495	0.107692
47	1	0	-6.114746	0.065787	1.309901
48	1	0	-6.974252	0.254379	-0.244715
49	6	0	-2.349312	1.522273	-1.781379
50	1	0	-3.086747	0.987880	-2.377985
51	1	0	-2.373547	2.590359	-2.028428
52	1	0	-1.350345	1.154175	-2.025300
53	1	0	1.221824	-0.954062	4.041053
54	1	0	5.881800	-1.012829	-2.357841
55	1	0	4.835719	0.168583	-0.443404
56	1	0	1.220764	5.335403	-0.604490
57	1	0	-0.061469	5.646993	-1.789587
58	1	0	-0.426986	3.519073	3.424006
59	1	0	0.301671	4.727817	2.344040
60	7	0	-1.432125	-1.441445	-0.612203
61	6	0	-2.372584	-1.975823	-1.087909
62	6	0	-3.501038	-2.543441	-1.643637
63	6	0	-4.499552	-3.106011	-0.835257
64	7	0	-5.356973	-3.541604	-0.160963
65	1	0	-3.570922	-2.636694	-2.721613

A-TS1

Energy+zep(gas) = -1658.306530 au

Gibbs free energy(gas) = -1658.377998 au

Energy(sol) = -1658.854186 au

Thermal correction to Gibbs Free Energy = 0.468206 au

Gibbs free energy (sol) = -1658.38598 au

Number of imaginary frequencies: 1 (-194.0923 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.267192	-1.023288	-0.259732
2	7	0	-1.054443	-1.425326	-0.800626
3	6	0	-2.077087	-0.338182	-1.115850
4	6	0	-0.519862	-1.940746	-2.115715
5	6	0	-1.628940	-2.574011	-0.005822
6	6	0	-2.094485	0.762374	-0.013635
7	6	0	-3.368364	-1.044906	-1.564196
8	6	0	-1.731764	-2.341242	-2.994172

9	6	0	-2.640794	-3.337061	-0.889825
10	1	0	0.073238	-1.134832	-2.551376
11	1	0	0.136752	-2.781285	-1.881776
12	1	0	-0.780722	-3.180821	0.314282
13	1	0	-2.092618	-2.145650	0.881026
14	8	0	-0.770208	1.160181	0.192063
15	6	0	-2.767315	0.391921	1.304222
16	6	0	-2.987919	-2.447482	-2.099701
17	1	0	-4.085076	-1.149948	-0.742242
18	1	0	-3.849235	-0.441914	-2.341280
19	1	0	-1.531763	-3.299276	-3.484044
20	1	0	-2.222614	-4.291319	-1.227978
21	1	0	-3.537723	-3.565571	-0.306035
22	1	0	-2.703851	1.569360	-0.457695
23	13	0	0.156874	2.237688	-0.899881
24	6	0	-2.025913	-0.001131	2.424161
25	6	0	-4.158305	0.458359	1.452877
26	1	0	-3.819557	-2.879077	-2.664108
27	8	0	-0.089566	1.572177	-2.510058
28	6	0	-2.696687	-0.329566	3.603987
29	6	0	-4.734692	0.108414	2.676395
30	1	0	-0.943672	-0.037754	2.374524
31	6	0	0.244620	2.203959	-3.730187
32	7	0	-4.029744	-0.288160	3.744327
33	1	0	-2.134549	-0.637920	4.483215
34	1	0	-0.340775	1.761559	-4.548928
35	8	0	-0.241537	3.921291	-0.851282
36	6	0	0.052515	4.953200	0.052364
37	1	0	-0.567795	4.892470	0.961138
38	6	0	4.619352	0.130924	1.135819
39	6	0	3.779111	0.795022	0.236494
40	6	0	2.560704	1.403507	0.554344
41	8	0	1.876197	1.959412	-0.395799
42	1	0	4.046553	0.804326	-0.817671
43	1	0	4.406362	0.226383	2.195971
44	1	0	-1.631458	0.185341	-1.965519
45	7	0	1.448891	-1.650671	0.681238
46	6	0	2.549109	-1.915467	0.982651
47	6	0	3.907942	-2.079229	1.308533
48	6	0	4.704318	-2.826439	0.398687
49	7	0	5.400319	-3.385103	-0.355854
50	1	0	4.127733	-2.233602	2.362533
51	6	0	6.057665	-0.135613	0.790941
52	1	0	6.525186	-0.845322	1.477115

53	1	0	6.168783	-0.517919	-0.227454
54	1	0	6.612158	0.810810	0.856610
55	6	0	2.022116	1.556689	1.954091
56	1	0	2.523659	0.924432	2.687040
57	1	0	2.141112	2.603701	2.260087
58	1	0	0.953067	1.333286	1.952654
59	1	0	-1.889851	-1.601662	-3.785784
60	1	0	-5.813957	0.157658	2.806394
61	1	0	-4.791966	0.801137	0.639009
62	1	0	-0.146954	5.925605	-0.418719
63	1	0	1.109141	4.948893	0.365899
64	1	0	1.310004	2.070934	-3.972454
65	1	0	0.032025	3.281895	-3.708027

A-IM1

Energy+zep(gas) = -1658.326503 au

Gibbs free energy(gas) = -1658.397962 au

Energy(sol) = -1658.876785 au

Thermal correction to Gibbs Free Energy = 0.471033 au

Gibbs free energy (sol) = -1658.405752 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.665793	2.003623	-1.865927
2	6	0	2.772671	1.691977	-1.711237
3	6	0	4.175731	1.285105	-1.529661
4	6	0	4.710024	1.910563	-0.306413
5	7	0	5.157346	2.402822	0.644534
6	1	0	4.748749	1.693694	-2.373951
7	1	0	-0.299786	0.878415	-0.128464
8	7	0	-0.978103	1.599305	0.173927
9	6	0	-1.955129	0.832004	1.054151
10	6	0	-0.300610	2.655998	1.010201
11	6	0	-1.642603	2.237277	-1.020233
12	6	0	-2.073480	-0.638748	0.516996
13	6	0	-3.182884	1.733812	1.275387
14	6	0	-1.409647	3.489289	1.699945
15	6	0	-2.569559	3.367709	-0.514743
16	1	0	0.348598	2.121011	1.704800
17	1	0	0.313235	3.247101	0.327747

18	1	0	-0.842034	2.588401	-1.671871
19	1	0	-2.191787	1.452401	-1.538435
20	8	0	-0.789376	-1.027968	0.127010
21	6	0	-3.087049	-0.882788	-0.598209
22	6	0	-2.760331	3.199134	1.006530
23	1	0	-4.009251	1.467951	0.608681
24	1	0	-3.539680	1.608503	2.302849
25	1	0	-1.168373	4.554619	1.631477
26	1	0	-2.138244	4.350178	-0.735340
27	1	0	-3.531733	3.313418	-1.033253
28	1	0	-2.426046	-1.218958	1.386560
29	13	0	0.434764	-1.637375	1.315795
30	6	0	-2.682286	-1.117536	-1.916451
31	6	0	-4.461925	-0.940444	-0.335117
32	1	0	-3.528798	3.887156	1.371008
33	8	0	0.834716	-0.141787	2.183248
34	6	0	-3.650399	-1.355046	-2.894946
35	6	0	-5.350857	-1.186207	-1.383741
36	1	0	-1.625829	-1.140088	-2.159183
37	6	0	1.647755	-0.084126	3.337824
38	7	0	-4.968745	-1.383671	-2.652946
39	1	0	-3.351143	-1.539905	-3.924778
40	1	0	1.539871	0.897873	3.822499
41	8	0	-0.220973	-2.822117	2.404625
42	6	0	-0.238646	-4.225809	2.329096
43	1	0	-1.201931	-4.592451	1.939591
44	6	0	4.327267	-0.294968	-1.533238
45	6	0	3.463527	-0.928909	-0.482578
46	6	0	2.454591	-1.811606	-0.681140
47	8	0	1.755460	-2.313660	0.345816
48	1	0	3.681010	-0.654892	0.548636
49	1	0	3.988102	-0.589438	-2.531280
50	1	0	-1.398101	0.717527	1.986422
51	6	0	5.818361	-0.654512	-1.400473
52	1	0	6.435037	-0.145588	-2.151943
53	1	0	6.200992	-0.395771	-0.408034
54	1	0	5.938470	-1.732969	-1.531458
55	6	0	2.021678	-2.380509	-2.012225
56	1	0	0.960890	-2.159370	-2.173748
57	1	0	2.593003	-2.008726	-2.865739
58	1	0	2.118040	-3.471623	-1.978794
59	1	0	-1.470221	3.241303	2.764841
60	1	0	-6.421106	-1.234945	-1.192959
61	1	0	-4.844278	-0.823070	0.675588

62	1	0	-0.102578	-4.656684	3.331729
63	1	0	0.557598	-4.623492	1.681884
64	1	0	2.713683	-0.212990	3.094511
65	1	0	1.371856	-0.852966	4.074000

A-IM2

Energy+zep(gas) = -1658.303597 au

Gibbs free energy(gas) = -1658.375969 au

Energy(sol) = -1658.857263 au

Thermal correction to Gibbs Free Energy = 0.469813 au

Gibbs free energy (sol) = -1658.38745 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.367109	1.433641	-0.149176
2	7	0	0.469357	2.029704	0.051742
3	6	0	1.747539	1.379047	-0.492589
4	6	0	0.306229	3.372397	-0.612788
5	6	0	0.510216	2.223630	1.561145
6	6	0	1.680644	-0.170401	-0.380056
7	6	0	2.927014	2.093998	0.197648
8	6	0	1.629485	4.160617	-0.444226
9	6	0	1.558481	3.302517	1.900992
10	1	0	0.046528	3.198955	-1.659612
11	1	0	-0.538528	3.866735	-0.126618
12	1	0	-0.503578	2.498106	1.859430
13	1	0	0.751537	1.245003	1.968711
14	8	0	1.323850	-0.548939	0.906040
15	6	0	3.023471	-0.748690	-0.829059
16	6	0	2.464983	3.490779	0.670105
17	1	0	3.278396	1.503357	1.049944
18	1	0	3.757576	2.167650	-0.509526
19	1	0	1.405415	5.200540	-0.187430
20	1	0	1.081864	4.251033	2.173964
21	1	0	2.144520	2.974415	2.764581
22	1	0	2.190929	4.174892	-1.384126
23	1	0	0.934015	-0.514876	-1.115775
24	13	0	-0.029440	-1.698703	1.221212
25	6	0	3.880929	-1.365286	0.083866
26	6	0	3.438238	-0.685708	-2.165339

27	1	0	3.327069	4.115814	0.919722
28	8	0	-0.321474	-2.442352	-0.326640
29	6	0	5.105122	-1.863278	-0.370389
30	6	0	4.681474	-1.212881	-2.517183
31	1	0	3.578466	-1.470444	1.120077
32	1	0	2.799752	-0.256800	-2.934654
33	6	0	-0.758404	-3.730952	-0.690243
34	7	0	5.518598	-1.789788	-1.643251
35	1	0	5.787014	-2.349745	0.324224
36	1	0	5.018724	-1.177601	-3.551362
37	1	0	-0.193849	-4.084189	-1.564576
38	1	0	-0.617782	-4.462761	0.118877
39	1	0	-1.823518	-3.724702	-0.964229
40	8	0	0.297631	-2.703730	2.586948
41	6	0	-0.281721	-2.837511	3.856523
42	1	0	-1.127649	-2.150030	4.011802
43	1	0	0.462837	-2.638179	4.643025
44	1	0	-0.651594	-3.863109	4.006200
45	6	0	-3.182466	1.047533	-1.272456
46	6	0	-2.234850	0.336891	-0.323295
47	6	0	-2.277379	0.168926	1.044054
48	6	0	-3.246563	0.813915	2.009797
49	8	0	-1.415484	-0.602354	1.678188
50	1	0	-3.911061	0.036059	2.400910
51	1	0	-3.862166	1.598759	1.577528
52	6	0	-3.848136	2.365656	-0.837027
53	1	0	-1.573338	-0.367921	-0.830309
54	1	0	-3.119969	3.023110	-0.353148
55	1	0	-4.248773	2.892942	-1.710206
56	1	0	-2.593955	1.280888	-2.169976
57	1	0	-4.676524	2.214299	-0.140880
58	1	0	-2.690480	1.214814	2.863845
59	7	0	-3.292785	-1.853727	-3.297532
60	6	0	-3.748608	-1.025698	-2.624584
61	6	0	-4.312407	0.086230	-1.842350
62	6	0	-5.209841	-0.406544	-0.784649
63	1	0	-4.934111	0.668321	-2.538626
64	7	0	-5.936318	-0.734674	0.058461
65	1	0	1.743219	1.631453	-1.557987

A-TS2

Energy+zep(gas) = -1658.297715 au

Gibbs free energy(gas) = -1658.367767 au

Energy(sol) = -1658.843113 au

Thermal correction to Gibbs Free Energy = 0.466784 au

Gibbs free energy (sol) = -1658.376329 au

Number of imaginary frequencies: 1 (-1249.7927 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.865112	1.261736	-0.031869
2	7	0	0.221001	2.029694	0.153691
3	6	0	1.501608	1.437052	-0.397293
4	6	0	0.048713	3.378797	-0.464345
5	6	0	0.283497	2.192691	1.647001
6	6	0	1.511333	-0.118276	-0.349781
7	6	0	2.690050	2.156184	0.287717
8	6	0	1.349095	4.210499	-0.282606
9	6	0	1.311677	3.284110	2.032276
10	1	0	-0.205416	3.243697	-1.519803
11	1	0	-0.804790	3.856113	0.027485
12	1	0	-0.727659	2.443436	1.983368
13	1	0	0.552632	1.217325	2.046610
14	8	0	1.194634	-0.590359	0.925069
15	6	0	2.866115	-0.622631	-0.845551
16	6	0	2.207781	3.529037	0.804765
17	1	0	3.070802	1.554892	1.120398
18	1	0	3.508991	2.266606	-0.429227
19	1	0	1.100759	5.237056	0.007532
20	1	0	0.815959	4.214363	2.335047
21	1	0	1.907367	2.943414	2.885324
22	1	0	1.906133	4.269120	-1.224247
23	1	0	0.771085	-0.462837	-1.088722
24	13	0	-0.021937	-1.860559	1.207813
25	6	0	3.798126	-1.186475	0.028498
26	6	0	3.222327	-0.536415	-2.197315
27	1	0	3.060303	4.162669	1.067974
28	8	0	-0.404199	-2.573559	-0.324030
29	6	0	5.030051	-1.610631	-0.476443
30	6	0	4.478799	-0.988953	-2.601878
31	1	0	3.551766	-1.305518	1.077873
32	1	0	2.528638	-0.144284	-2.937596
33	6	0	-0.750997	-3.883281	-0.712882
34	7	0	5.385057	-1.515165	-1.765393
35	1	0	5.768555	-2.053313	0.189138

36	1	0	4.769350	-0.933968	-3.649262
37	1	0	-0.201242	-4.159869	-1.622623
38	1	0	-0.518012	-4.623886	0.065162
39	1	0	-1.825362	-3.953124	-0.937560
40	8	0	0.295171	-2.906258	2.537434
41	6	0	0.158744	-2.819655	3.929119
42	1	0	-0.768375	-2.305130	4.228096
43	1	0	1.005067	-2.282629	4.386866
44	1	0	0.134179	-3.828934	4.362654
45	6	0	-2.942927	1.130037	-1.171612
46	6	0	-1.987587	0.415270	-0.208928
47	6	0	-2.265815	0.011240	1.134987
48	6	0	-3.344984	0.591808	2.020988
49	8	0	-1.518583	-0.844868	1.723231
50	1	0	-4.317457	0.175257	1.737981
51	1	0	-3.411240	1.678732	1.943399
52	6	0	-3.796891	2.288875	-0.631702
53	1	0	-1.438175	-0.377558	-0.727753
54	1	0	-3.181282	2.986802	-0.057398
55	1	0	-4.241668	2.848744	-1.461609
56	1	0	-2.307403	1.551083	-1.961937
57	1	0	-4.611589	1.949027	0.011738
58	1	0	-3.137129	0.310733	3.054419
59	7	0	-2.492002	-1.387356	-3.607362
60	6	0	-3.111519	-0.752395	-2.859703
61	6	0	-3.879618	0.136313	-1.971598
62	6	0	-4.775803	-0.630003	-1.090031
63	1	0	-4.523998	0.740788	-2.626304
64	7	0	-5.503122	-1.178343	-0.371352
65	1	0	1.496137	1.706083	-1.459528

A-IM3

Energy+zep(gas) = -1658.309281 au

Gibbs free energy(gas) = -1658.381595 au

Energy(sol) = -1658.856534 au

Thermal correction to Gibbs Free Energy = 0.467904 au

Gibbs free energy (sol) = -1658.38863 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	-1.295097	1.102927	-0.490555
2	7	0	0.703572	2.280431	-0.381760
3	6	0	1.887792	1.396377	-0.600848
4	6	0	0.965081	3.545659	-1.106952
5	6	0	0.534565	2.607169	1.058811
6	6	0	1.558922	-0.108877	-0.424778
7	6	0	3.098637	1.919307	0.218951
8	6	0	2.354537	4.139567	-0.714211
9	6	0	1.714699	3.465313	1.602449
10	1	0	0.905423	3.352593	-2.183864
11	1	0	0.156287	4.242986	-0.857773
12	1	0	-0.418297	3.141390	1.167314
13	1	0	0.465117	1.664022	1.598622
14	8	0	1.142039	-0.412283	0.882377
15	6	0	2.762609	-0.950720	-0.848599
16	6	0	2.841486	3.405514	0.554637
17	1	0	3.213843	1.344185	1.144969
18	1	0	4.023635	1.798156	-0.354970
19	1	0	2.276841	5.217233	-0.527570
20	1	0	1.410040	4.506073	1.770971
21	1	0	2.061337	3.070793	2.564487
22	1	0	3.080124	4.007824	-1.526074
23	1	0	0.753987	-0.325258	-1.145394
24	13	0	-0.106279	-1.566823	1.328352
25	6	0	3.564457	-1.613816	0.083999
26	6	0	3.111061	-1.085952	-2.198964
27	1	0	3.752862	3.874242	0.940687
28	8	0	-0.830065	-2.385844	-0.014906
29	6	0	4.662348	-2.352825	-0.364323
30	6	0	4.226737	-1.848357	-2.545655
31	1	0	3.324909	-1.561195	1.140156
32	1	0	2.515663	-0.618640	-2.979854
33	6	0	-0.841176	-3.743530	-0.411877
34	7	0	5.006087	-2.477187	-1.653457
35	1	0	5.296608	-2.874084	0.350227
36	1	0	4.505663	-1.966268	-3.591048
37	1	0	0.115358	-4.031952	-0.870508
38	1	0	-1.028333	-4.414710	0.437465
39	1	0	-1.632630	-3.895455	-1.155111
40	8	0	0.158421	-2.455024	2.771341
41	6	0	0.910807	-2.264039	3.941156
42	1	0	0.342557	-1.693643	4.691996
43	1	0	1.853289	-1.727126	3.753097
44	1	0	1.161250	-3.238043	4.382168

45	6	0	-3.270823	0.961064	-1.329908
46	6	0	-2.185112	0.447936	-0.358556
47	6	0	-2.330099	0.388700	1.140756
48	6	0	-3.265516	1.241090	1.945840
49	8	0	-1.554223	-0.347618	1.778491
50	1	0	-4.304598	0.977268	1.728942
51	1	0	-3.130181	2.295990	1.688091
52	6	0	-3.874008	2.344336	-1.040936
53	1	0	-1.843160	-0.548791	-0.670850
54	1	0	-3.079886	3.060897	-0.811655
55	1	0	-4.407919	2.716476	-1.921592
56	1	0	-2.741992	1.041686	-2.286961
57	1	0	-4.580379	2.337054	-0.207322
58	1	0	-3.067015	1.088444	3.007021
59	7	0	-3.496555	-2.246461	-2.814812
60	6	0	-3.901767	-1.306905	-2.268603
61	6	0	-4.412729	-0.076490	-1.638405
62	6	0	-5.246560	-0.400361	-0.467732
63	1	0	-5.081229	0.393289	-2.373819
64	7	0	-5.908764	-0.603876	0.463026
65	1	0	2.122090	1.505184	-1.666786

N-COM

Energy+zep(gas) = -1186.091948 au

Gibbs free energy(gas) = -1186.155803 au

Energy(sol) = -1186.564515 au

Thermal correction to Gibbs Free Energy = 0.399624 au

Gibbs free energy (sol) = -1186.164891 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.356275	0.056669	1.039918
2	7	0	0.904462	0.959420	0.821584
3	6	0	1.249336	1.167482	-0.642093
4	6	0	-0.004092	2.090084	1.241990
5	6	0	2.114973	0.950633	1.721477
6	6	0	1.579842	-0.125012	-1.440801
7	6	0	2.279625	2.317517	-0.713135
8	6	0	0.668754	3.434165	0.871395
9	6	0	2.752138	2.359225	1.739309

10	1	0	-0.960132	1.935577	0.739155
11	1	0	-0.164694	1.971637	2.314985
12	1	0	1.760739	0.619316	2.699526
13	1	0	2.796212	0.193668	1.338411
14	8	0	0.468195	-0.989271	-1.454832
15	6	0	2.787962	-0.929424	-0.987386
16	6	0	2.159627	3.170508	0.570170
17	1	0	3.300842	1.930859	-0.798525
18	1	0	2.082728	2.917234	-1.607660
19	1	0	0.565139	4.142092	1.699691
20	1	0	2.555605	2.866971	2.689924
21	1	0	3.838578	2.273321	1.638702
22	1	0	1.801333	0.252253	-2.454950
23	6	0	2.644466	-2.028185	-0.131308
24	6	0	4.078712	-0.624694	-1.434792
25	1	0	2.697223	4.115575	0.449399
26	6	0	3.785565	-2.734835	0.254269
27	6	0	5.155417	-1.394252	-0.986391
28	1	0	1.661590	-2.326946	0.216429
29	7	0	5.028637	-2.431818	-0.149560
30	1	0	3.695780	-3.590753	0.919504
31	1	0	0.309251	1.511418	-1.081637
32	1	0	-0.346732	-0.490891	-1.691382
33	6	0	-5.239544	0.549353	-0.827651
34	6	0	-4.041539	0.965498	-1.282563
35	6	0	-2.938402	0.068166	-1.650847
36	8	0	-1.799360	0.547261	-1.799593
37	1	0	-3.804279	2.026923	-1.336994
38	1	0	-5.432119	-0.515654	-0.716584
39	7	0	-0.547687	-0.943066	1.975368
40	6	0	-1.431336	-1.724736	2.063987
41	6	0	-2.466609	-2.627568	2.174606
42	1	0	-2.281857	-3.605645	2.602399
43	6	0	-3.740118	-2.305064	1.690970
44	7	0	-4.798621	-2.028147	1.258921
45	6	0	-6.339258	1.454366	-0.377149
46	1	0	-7.256942	1.253387	-0.944563
47	1	0	-6.577331	1.250788	0.674280
48	1	0	-6.081779	2.511804	-0.487166
49	6	0	-3.187427	-1.405752	-1.855706
50	1	0	-3.664354	-1.848648	-0.974420
51	1	0	-3.868383	-1.550148	-2.702506
52	1	0	-2.247139	-1.919715	-2.059329
53	1	0	0.179565	3.884439	0.000929

54	1	0	6.165327	-1.170804	-1.324418
55	1	0	4.252793	0.181779	-2.142015

N-TS1

Energy+zep(gas) = -1186.067434 au

Gibbs free energy(gas) = -1186.126485 au

Energy(sol) = -1186.541139 au

Thermal correction to Gibbs Free Energy = 0.406244 au

Gibbs free energy (sol) = -1186.134895 au

Number of imaginary frequencies: 1 (-302.0140 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.028281	-0.081870	0.346672
2	7	0	0.436991	0.805120	0.012018
3	6	0	1.319481	0.529111	-1.200199
4	6	0	-0.697255	1.710510	-0.424232
5	6	0	1.185307	1.453407	1.152547
6	6	0	2.064560	-0.841190	-1.096778
7	6	0	2.132515	1.810424	-1.476985
8	6	0	-0.088804	2.947605	-1.123923
9	6	0	1.602828	2.879092	0.721834
10	1	0	-1.337343	1.111099	-1.071342
11	1	0	-1.252647	1.967079	0.478301
12	1	0	0.511002	1.436619	2.010146
13	1	0	2.040641	0.818463	1.377749
14	8	0	1.155667	-1.829168	-0.688164
15	6	0	3.293250	-0.907351	-0.199102
16	6	0	1.419344	3.006084	-0.804948
17	1	0	3.150693	1.730472	-1.084508
18	1	0	2.209758	1.957342	-2.559100
19	1	0	-0.592624	3.852399	-0.771184
20	1	0	0.997711	3.632062	1.237617
21	1	0	2.646071	3.055057	1.001339
22	1	0	2.417483	-1.019977	-2.127639
23	6	0	3.238378	-1.491475	1.071939
24	6	0	4.539113	-0.437525	-0.632928
25	1	0	1.848249	3.947734	-1.159602
26	6	0	4.399847	-1.541444	1.846367
27	6	0	5.641509	-0.532193	0.219707
28	1	0	2.311279	-1.920776	1.434721

29	7	0	5.588136	-1.065749	1.447081
30	1	0	4.375203	-1.992828	2.835967
31	6	0	-4.391330	-1.183273	-0.209981
32	6	0	-3.304617	-0.971198	-1.094892
33	6	0	-2.121073	-1.726088	-1.154800
34	8	0	-1.106177	-1.328683	-1.835042
35	1	0	-3.328804	-0.078266	-1.718680
36	1	0	-4.422726	-2.152633	0.283419
37	1	0	0.588572	0.370223	-1.996345
38	7	0	-1.545630	-0.466595	1.882709
39	6	0	-2.706581	-0.343646	1.834730
40	6	0	-4.100478	-0.197157	1.576165
41	6	0	-4.491350	1.171864	1.401459
42	7	0	-4.803835	2.273351	1.174199
43	1	0	-4.745421	-0.755780	2.254199
44	6	0	-5.761683	-0.664787	-0.593079
45	1	0	-6.474716	-0.711223	0.235921
46	1	0	-5.716955	0.368433	-0.949365
47	1	0	-6.152594	-1.284054	-1.409640
48	6	0	-1.976672	-3.078300	-0.471036
49	1	0	-2.856181	-3.393198	0.092875
50	1	0	-1.776532	-3.828400	-1.244529
51	1	0	-1.116138	-3.068553	0.204308
52	1	0	-0.245154	2.893553	-2.206422
53	1	0	6.615268	-0.170197	-0.103868
54	1	0	4.666952	-0.024463	-1.629900
55	1	0	0.307377	-1.773208	-1.238708

N-IM1

Energy+zep(gas) = -1186.100915 au

Gibbs free energy(gas) = -1186.162454 au

Energy(sol) = -1186.573018 au

Thermal correction to Gibbs Free Energy = 0.404541 au

Gibbs free energy (sol) = -1186.168477 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.496813	-0.635797	0.158294
2	7	0	-0.302979	0.889452	0.146360
3	6	0	-1.777852	0.682534	0.326437

4	6	0	0.104869	1.959381	1.096973
5	6	0	0.022851	1.364448	-1.236405
6	6	0	-2.232643	-0.750205	-0.069291
7	6	0	-2.547474	1.861036	-0.321033
8	6	0	-0.821810	3.203214	0.942631
9	6	0	-0.554355	2.781253	-1.500949
10	1	0	0.070304	1.555412	2.114464
11	1	0	1.147419	2.213365	0.880565
12	1	0	1.112619	1.348312	-1.335156
13	1	0	-0.386863	0.640599	-1.939120
14	8	0	-1.867757	-1.104654	-1.400241
15	6	0	-3.733528	-0.910554	0.105573
16	6	0	-1.584666	3.069336	-0.394666
17	1	0	-2.891353	1.598340	-1.328696
18	1	0	-3.438137	2.096408	0.270762
19	1	0	-0.228465	4.124155	0.953770
20	1	0	0.235886	3.541291	-1.491207
21	1	0	-1.026784	2.819177	-2.488881
22	1	0	-1.738377	-1.440296	0.627106
23	6	0	-4.589225	-1.085457	-0.985241
24	6	0	-4.314572	-0.886303	1.380369
25	1	0	-2.140257	3.987697	-0.610413
26	6	0	-5.961839	-1.213251	-0.755250
27	6	0	-5.697345	-1.024487	1.502688
28	1	0	-4.187765	-1.136102	-1.990533
29	7	0	-6.525069	-1.183117	0.459891
30	1	0	-6.643002	-1.349991	-1.592793
31	1	0	-1.936855	0.729030	1.410574
32	1	0	-1.530353	3.269918	1.777132
33	1	0	-6.163035	-1.012740	2.486094
34	1	0	-3.705745	-0.775264	2.274191
35	1	0	-0.991831	-1.519408	-1.355527
36	6	0	4.383873	-1.174296	0.895507
37	6	0	2.907893	-1.001562	0.671223
38	6	0	2.067895	-1.862510	0.058195
39	8	0	0.744311	-1.586555	-0.095013
40	1	0	2.485121	-0.075505	1.058458
41	1	0	4.708154	-2.163252	0.558399
42	6	0	4.773730	-1.008650	2.374923
43	1	0	5.853239	-1.124238	2.526931
44	1	0	4.477641	-0.025386	2.755779
45	1	0	4.261082	-1.766126	2.973657
46	6	0	2.400266	-3.206787	-0.522601
47	1	0	3.431326	-3.509893	-0.338124

48	1	0	1.731659	-3.962203	-0.095504
49	1	0	2.233511	-3.196047	-1.605352
50	7	0	4.998248	-0.741094	-2.541617
51	6	0	5.093113	-0.455837	-1.420857
52	6	0	5.229212	-0.163444	0.015802
53	6	0	4.869889	1.238816	0.292491
54	7	0	4.577058	2.332062	0.549058
55	1	0	6.291122	-0.282966	0.272201

N-IM2

Energy+zep(gas) = -1186.093894 au

Gibbs free energy(gas) = -1186.156237 au

Energy(sol) = -1186.565316 au

Thermal correction to Gibbs Free Energy = 0.403326 au

Gibbs free energy (sol) = -1186.16199 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.104603	-1.074391	1.463234
2	6	0	2.790764	-0.016675	0.472901
3	6	0	4.547316	-1.375897	1.348826
4	6	0	2.351045	-2.322102	1.200710
5	6	0	1.491108	0.745913	0.812284
6	6	0	2.893326	-0.567313	-0.982613
7	6	0	4.933936	-1.759037	-0.115745
8	6	0	2.722325	-2.934911	-0.186526
9	1	0	5.113240	-0.503586	1.694574
10	1	0	4.765346	-2.195071	2.042350
11	1	0	2.582870	-3.016329	2.015613
12	1	0	1.286072	-2.096573	1.261151
13	8	0	0.329206	-0.034561	0.471259
14	6	0	1.455235	2.110292	0.136356
15	6	0	3.627821	-1.925302	-0.920817
16	1	0	1.905213	-0.709795	-1.433067
17	1	0	3.434095	0.140758	-1.620617
18	1	0	5.513056	-2.689852	-0.137040
19	1	0	3.251464	-3.888584	-0.067302
20	1	0	1.821038	-3.137768	-0.775614
21	1	0	1.504667	0.890400	1.899148
22	6	0	0.839293	2.320824	-1.101336

23	6	0	2.073125	3.212955	0.738655
24	1	0	3.846992	-2.276562	-1.934847
25	6	0	0.876992	3.595661	-1.671411
26	6	0	2.054941	4.447231	0.087341
27	1	0	0.332839	1.510332	-1.613903
28	7	0	1.471287	4.652515	-1.101793
29	1	0	0.404893	3.775708	-2.635223
30	1	0	3.577787	0.733647	0.612346
31	1	0	5.561204	-0.983461	-0.573008
32	1	0	2.525640	5.314618	0.545460
33	1	0	2.555911	3.119622	1.708202
34	1	0	-0.416174	0.285766	1.005117
35	1	0	-0.284735	-1.314177	-0.849485
36	6	0	-4.092895	-0.418020	-0.678010
37	6	0	-2.644727	-0.718845	-0.949395
38	6	0	-2.081490	-1.907793	-1.243648
39	8	0	-0.726144	-2.057718	-1.308765
40	1	0	-1.972703	0.126274	-0.816482
41	1	0	-4.741838	-1.209712	-1.066117
42	6	0	-4.523753	0.924629	-1.285047
43	1	0	-5.575034	1.146992	-1.080649
44	1	0	-3.915655	1.748708	-0.895292
45	1	0	-4.383707	0.892513	-2.369100
46	6	0	-2.777028	-3.199786	-1.554464
47	1	0	-3.861629	-3.091146	-1.605399
48	1	0	-2.420426	-3.578929	-2.518549
49	1	0	-2.529488	-3.956596	-0.801543
50	7	0	-2.387194	0.890016	2.069372
51	6	0	-3.284132	0.329012	1.591913
52	6	0	-4.322196	-0.454192	0.897803
53	6	0	-5.676752	-0.046239	1.303295
54	7	0	-6.766755	0.239436	1.581055
55	1	0	-4.184549	-1.494426	1.219829

N-TS2

Energy+zep(gas) = -1186.053041 au

Gibbs free energy(gas) = -1186.110924 au

Energy(sol) = -1186.517192 au

Thermal correction to Gibbs Free Energy = 0.400691 au

Gibbs free energy (sol) = -1186.116501 au

Number of imaginary frequencies: 1 (-653.2829 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.076861	1.880883	0.000136
2	6	0	-1.248501	1.226145	0.215287
3	6	0	-0.015995	3.235181	0.601347
4	6	0	0.379148	2.054503	-1.448623
5	6	0	-1.153765	-0.322420	0.246400
6	6	0	-2.301902	1.834193	-0.747909
7	6	0	-1.274764	3.991058	0.070816
8	6	0	-0.616745	3.032623	-2.137176
9	1	0	-0.040112	3.134113	1.691457
10	1	0	0.903776	3.773115	0.347005
11	1	0	1.408100	2.425162	-1.525384
12	1	0	0.340507	1.072747	-1.918803
13	8	0	-0.544629	-0.826046	-0.931350
14	6	0	-2.514414	-0.954781	0.494223
15	6	0	-1.797907	3.233586	-1.170390
16	1	0	-2.430697	1.205873	-1.637261
17	1	0	-3.276505	1.894797	-0.252045
18	1	0	-1.022000	5.024587	-0.192531
19	1	0	-0.141391	3.995672	-2.360063
20	1	0	-0.964676	2.616745	-3.089946
21	1	0	-0.516227	-0.564153	1.113593
22	6	0	-3.265295	-1.531864	-0.534259
23	6	0	-3.071340	-0.966573	1.779324
24	1	0	-2.601989	3.798968	-1.652868
25	6	0	-4.517278	-2.076504	-0.237253
26	6	0	-4.332193	-1.532887	1.971428
27	1	0	-2.879611	-1.563441	-1.547559
28	7	0	-5.058931	-2.082808	0.987929
29	1	0	-5.114150	-2.531414	-1.025213
30	1	0	-1.533278	1.495075	1.239671
31	1	0	-2.055448	4.040303	0.839646
32	1	0	-4.777177	-1.553044	2.964112
33	1	0	-2.530030	-0.553936	2.627071
34	1	0	0.710735	-0.895888	-0.671847
35	1	0	-0.326578	-2.097829	-1.116272
36	6	0	3.162005	-0.971278	-0.093645
37	6	0	1.808581	-1.640146	-0.295856
38	6	0	1.546146	-2.606479	-1.310564
39	8	0	0.320443	-2.980644	-1.483239
40	1	0	1.320878	-1.909580	0.648222
41	1	0	3.511265	-0.567693	-1.052056

42	6	0	4.252411	-1.888060	0.486515
43	1	0	5.190651	-1.345425	0.643476
44	1	0	3.936752	-2.313514	1.444696
45	1	0	4.458434	-2.717577	-0.194916
46	6	0	2.546397	-3.149741	-2.287056
47	1	0	3.389411	-2.470278	-2.431228
48	1	0	2.946705	-4.091986	-1.891502
49	1	0	2.063408	-3.362716	-3.242829
50	7	0	2.283643	-0.373571	3.273053
51	6	0	2.602729	-0.063851	2.200824
52	6	0	2.943146	0.298969	0.813285
53	6	0	4.111162	1.193162	0.782537
54	7	0	5.027554	1.900969	0.699806
55	1	0	2.069080	0.867495	0.438082

N-IM3

Energy+zep(gas) = -1186.112729 au

Gibbs free energy(gas) = -12.06387014 au

Energy(sol) = -1186.583675 au

Thermal correction to Gibbs Free Energy = 0.403123 au

Gibbs free energy (sol) = -1186.180552 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.081265	1.906271	0.312355
2	6	0	-1.393821	1.198040	0.306060
3	6	0	-0.226320	3.074471	1.215739
4	6	0	0.271719	2.422978	-1.040913
5	6	0	-1.269449	-0.282916	-0.109106
6	6	0	-2.453445	2.020463	-0.478926
7	6	0	-1.463805	3.939864	0.821075
8	6	0	-0.744029	3.497843	-1.531828
9	1	0	-0.306533	2.712563	2.246847
10	1	0	0.698669	3.657057	1.149038
11	1	0	1.280849	2.841088	-0.977723
12	1	0	0.298504	1.573660	-1.722270
13	8	0	-0.867511	-0.386287	-1.467198
14	6	0	-2.564114	-1.044199	0.165958
15	6	0	-1.946320	3.476617	-0.570339
16	1	0	-2.592126	1.615182	-1.487571

17	1	0	-3.422862	1.969294	0.028827
18	1	0	-1.199801	5.003480	0.798061
19	1	0	-0.289421	4.495982	-1.545958
20	1	0	-1.069490	3.277332	-2.554948
21	1	0	-0.491076	-0.707239	0.541529
22	6	0	-3.416226	-1.448283	-0.865005
23	6	0	-2.945820	-1.364632	1.475596
24	1	0	-2.743489	4.132992	-0.935227
25	6	0	-4.591889	-2.132811	-0.544794
26	6	0	-4.141015	-2.051557	1.690555
27	1	0	-3.159252	-1.239396	-1.897557
28	7	0	-4.965271	-2.436676	0.705492
29	1	0	-5.267179	-2.454667	-1.335098
30	1	0	-1.697779	1.162022	1.359074
31	1	0	-2.270973	3.828007	1.555573
32	1	0	-4.450010	-2.309822	2.701511
33	1	0	-2.321941	-1.093012	2.324131
34	1	0	1.382463	-1.650273	0.967881
35	1	0	-0.372405	-1.217316	-1.582660
36	6	0	2.896874	-0.875107	-0.396761
37	6	0	2.217458	-2.034191	0.367783
38	6	0	1.616959	-3.081495	-0.568924
39	8	0	0.798529	-2.759662	-1.420895
40	1	0	2.925079	-2.496620	1.062772
41	1	0	2.241078	-0.582351	-1.223329
42	6	0	4.261761	-1.295465	-0.955576
43	1	0	4.721684	-0.491284	-1.536147
44	1	0	4.952025	-1.575786	-0.151814
45	1	0	4.149224	-2.157144	-1.621581
46	6	0	2.040702	-4.517114	-0.388573
47	1	0	3.127712	-4.604963	-0.505129
48	1	0	1.810117	-4.844587	0.632930
49	1	0	1.531787	-5.159741	-1.107946
50	7	0	4.053775	-0.169542	2.859761
51	6	0	3.596782	0.103918	1.828348
52	6	0	2.976586	0.395290	0.523318
53	6	0	3.689904	1.502563	-0.135973
54	7	0	4.231285	2.372028	-0.681692
55	1	0	1.942389	0.752905	0.703822

IM2

Energy+zep(gas) = -495.409554 au

Gibbs free energy(gas) = -495.448675 au

Energy(sol) = -495.5819418 au
Thermal correction to Gibbs Free Energy = 0.127766 au
Gibbs free energy (sol) = -495.4541758 au
Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.311752	-0.919659	2.063549
2	6	0	0.303908	-0.596891	-0.857822
3	6	0	-0.692800	-0.732322	0.260151
4	6	0	-1.942363	-0.232457	0.295360
5	8	0	-2.772746	-0.427371	1.369407
6	1	0	-0.348902	-1.307282	1.121466
7	1	0	-0.161467	-0.107076	-1.718262
8	6	0	0.855687	-1.959881	-1.311004
9	1	0	1.583266	-1.852181	-2.123561
10	1	0	1.342570	-2.487177	-0.483938
11	1	0	0.034233	-2.585869	-1.669457
12	6	0	-2.650669	0.579321	-0.746402
13	1	0	-2.050504	0.727323	-1.644091
14	1	0	-3.587753	0.084802	-1.024074
15	1	0	-2.906367	1.561961	-0.336284
16	7	0	0.668415	2.829769	-0.147944
17	6	0	1.049588	1.739285	-0.256426
18	6	0	1.505368	0.354902	-0.464842
19	6	0	2.238533	-0.136497	0.715374
20	7	0	2.812716	-0.566916	1.627231
21	1	0	2.217225	0.371403	-1.301951

TS2

Energy+zep(gas) = -495.329057 au
Gibbs free energy(gas) = -495.368218 au
Energy(sol) = -495.4938952 au
Thermal correction to Gibbs Free Energy = 0.121174 au
Gibbs free energy (sol) = -495.3727212 au
Number of imaginary frequencies: 1 (-2089.8244 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.268864	0.816551	-0.837053
2	6	0	0.351278	1.010299	0.665248
3	6	0	1.345430	0.420614	1.522645
4	8	0	0.828029	0.311488	2.697074
5	1	0	1.266453	0.596041	-1.246584
6	6	0	-0.286963	2.053243	-1.557247
7	1	0	-0.377273	1.891070	-2.636746
8	1	0	-1.274292	2.323949	-1.168952
9	1	0	0.382479	2.904000	-1.399751
10	6	0	2.726103	-0.074611	1.260746
11	1	0	3.191092	0.422268	0.406180
12	1	0	3.330924	0.062338	2.161640
13	1	0	2.683486	-1.151231	1.056604
14	7	0	0.574995	-2.623030	-0.304864
15	6	0	0.021870	-1.682314	-0.699689
16	6	0	-0.591199	-0.450992	-1.223984
17	6	0	-1.992403	-0.332913	-0.784317
18	7	0	-3.103862	-0.205806	-0.477015
19	1	0	-0.602392	-0.540375	-2.319540
20	1	0	0.181331	2.044935	0.980318
21	1	0	-0.198481	0.616176	1.996355

A-COM-*Re*-1

Energy+zep = -2521.641752 au

Gibbs free energy = -2521.738970 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.047581	0.569905	-1.472523
2	7	0	-0.866152	0.912689	-2.007967
3	6	0	-2.058483	1.079643	-1.078548
4	6	0	-0.508894	2.270052	-2.561708
5	6	0	-1.122222	-0.051814	-3.138346
6	6	0	-2.057257	0.007271	0.057334
7	6	0	-3.299570	1.286535	-1.967071
8	6	0	-1.762090	2.879528	-3.270091
9	6	0	-2.192227	0.549990	-4.076002
10	1	0	-0.165842	2.859914	-1.709979
11	1	0	0.331076	2.117010	-3.240551

12	1	0	-0.157954	-0.218952	-3.618722
13	1	0	-1.444639	-0.989016	-2.687364
14	8	0	-0.749149	-0.067625	0.552939
15	6	0	-2.560859	-1.424504	-0.298319
16	6	0	-2.839693	1.755537	-3.366632
17	1	0	-3.875568	0.360823	-2.075469
18	1	0	-3.961507	2.020675	-1.499402
19	1	0	-1.478497	3.131624	-4.298578
20	1	0	-1.745462	0.862592	-5.025847
21	1	0	-2.947495	-0.207125	-4.309442
22	6	0	-2.266083	4.168919	-2.603092
23	1	0	-2.743176	0.421528	0.814091
24	13	0	-0.020892	1.109660	1.676308
25	6	0	-1.652538	-2.385617	-0.594837
26	6	0	-3.953828	-1.800895	-0.265258
27	1	0	-3.695807	2.117509	-3.943711
28	8	0	-0.151181	2.665316	0.860424
29	6	0	-2.074056	-3.711496	-0.903745
30	6	0	-4.275023	-3.131120	-0.584776
31	1	0	-0.596830	-2.151653	-0.585329
32	6	0	-5.013297	-0.905774	0.093480
33	6	0	-0.001139	3.957227	1.413102
34	7	0	-3.330279	-4.105595	-0.919623
35	1	0	-1.322432	-4.458341	-1.149083
36	6	0	-5.648757	-3.546639	-0.565804
37	1	0	0.023995	4.673395	0.573352
38	6	0	-1.221855	4.310218	2.325956
39	6	0	1.352504	4.099731	2.187308
40	8	0	-0.695762	1.206314	3.264981
41	6	0	-0.866392	0.434826	4.423610
42	1	0	-0.834507	-0.643303	4.182088
43	6	0	-2.270884	0.738195	5.039004
44	6	0	0.278986	0.736365	5.447808
45	6	0	4.840576	-0.556606	0.323768
46	6	0	3.795566	0.221774	0.774794
47	6	0	2.522921	-0.254269	1.186797
48	6	0	2.097151	-1.701826	1.214987
49	8	0	1.725677	0.616993	1.710616
50	6	0	1.467597	-2.164564	2.371233
51	6	0	2.307518	-2.578325	0.152597
52	6	0	6.216692	-0.113191	0.030748
53	1	0	3.911785	1.295140	0.866584
54	6	0	6.617682	1.224229	0.122321
55	1	0	4.687081	-1.629316	0.260913

56	6	0	7.161959	-1.076392	-0.339694
57	1	0	-1.819119	2.002661	-0.546915
58	6	0	7.925709	1.583204	-0.145691
59	6	0	8.853888	0.616270	-0.510406
60	6	0	8.470255	-0.713730	-0.607846
61	1	0	6.858552	-2.113252	-0.425585
62	1	0	5.903452	1.986541	0.403655
63	1	0	8.225249	2.620512	-0.071644
64	1	0	9.877742	0.901715	-0.720370
65	1	0	9.190709	-1.468158	-0.896069
66	6	0	1.072138	-3.486239	2.472470
67	6	0	1.288808	-4.356278	1.412305
68	6	0	1.899573	-3.899749	0.253769
69	1	0	0.978094	-5.391299	1.489790
70	1	0	2.065734	-4.572399	-0.578327
71	1	0	2.766081	-2.230836	-0.763611
72	1	0	1.307819	-1.487109	3.200418
73	1	0	0.595438	-3.838613	3.378107
74	6	0	-6.628302	-2.684131	-0.231663
75	6	0	-6.306679	-1.327902	0.116496
76	1	0	-4.767389	0.106773	0.359109
77	1	0	-7.668721	-2.980240	-0.207191
78	1	0	-5.865808	-4.576013	-0.823538
79	1	0	-2.139189	4.269752	1.746761
80	1	0	-1.126186	5.306065	2.747979
81	1	0	2.178594	3.824977	1.538460
82	1	0	1.505269	5.120007	2.525519
83	1	0	1.363752	3.447620	3.056126
84	1	0	-2.439185	0.146748	5.934269
85	1	0	-2.347628	1.789622	5.297248
86	1	0	0.168047	0.140508	6.348945
87	1	0	0.264463	1.786164	5.722935
88	1	0	1.245849	0.513832	5.006210
89	1	0	-3.048432	0.503951	4.318573
90	1	0	-1.293849	3.588369	3.134503
91	6	0	-2.451150	5.291268	-3.249404
92	1	0	-2.467854	4.110417	-1.540100
93	1	0	-2.811135	6.182261	-2.752580
94	1	0	-2.253743	5.387871	-4.309059
95	7	0	1.922523	0.164606	-2.042400
96	6	0	2.997671	-0.204888	-2.355168
97	6	0	4.274789	-0.650716	-2.658042
98	1	0	5.027006	0.069912	-2.955844
99	6	0	4.548454	-2.023134	-2.791958

100	7	0	4.793125	-3.167448	-2.870237
101	8	0	-7.427639	-0.565274	0.449012
102	6	0	-7.143567	0.775184	0.867742
103	1	0	-6.683437	1.368400	0.072157
104	1	0	-8.103314	1.226597	1.125322
105	1	0	-6.495547	0.806101	1.748402

A-COM-*Si*-1

Energy+zep = -2521.641686 au

Gibbs free energy = -2521.737287 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.232356	1.333083	-1.555584
2	7	0	-1.150732	1.731770	-1.823076
3	6	0	-2.172384	1.455033	-0.732225
4	6	0	-0.977780	3.225071	-1.945306
5	6	0	-1.544870	1.151854	-3.159879
6	6	0	-1.903428	0.088881	-0.025394
7	6	0	-3.558662	1.782222	-1.321024
8	6	0	-2.371081	3.877959	-2.174142
9	6	0	-2.777405	1.916832	-3.687276
10	1	0	-0.477306	3.543368	-1.032911
11	1	0	-0.296092	3.386498	-2.781133
12	1	0	-0.663213	1.233255	-3.795111
13	1	0	-1.749149	0.094693	-2.997119
14	8	0	-0.547418	0.050098	0.279739
15	6	0	-2.291452	-1.214057	-0.791002
16	6	0	-3.373595	2.734370	-2.525977
17	1	0	-4.076131	0.876789	-1.655849
18	1	0	-4.178199	2.242785	-0.546070
19	1	0	-2.294465	4.508241	-3.072466
20	1	0	-2.500528	2.578775	-4.514946
21	1	0	-3.514984	1.207229	-4.075621
22	6	0	-2.922341	4.791059	-1.060719
23	1	0	-2.521440	0.133694	0.886611
24	13	0	0.436583	0.824810	1.536265
25	6	0	-1.327552	-1.886816	-1.466028
26	6	0	-3.616940	-1.783702	-0.760141
27	1	0	-4.335504	3.164912	-2.819491

28	8	0	0.488331	2.528060	1.113564
29	6	0	-1.634825	-3.095589	-2.157373
30	6	0	-3.826863	-2.975738	-1.473728
31	1	0	-0.311432	-1.514630	-1.475847
32	6	0	-4.712796	-1.218375	-0.030464
33	6	0	1.352510	3.604641	1.392207
34	7	0	-2.831740	-3.643898	-2.193547
35	1	0	-0.840610	-3.606638	-2.697504
36	6	0	-5.131408	-3.574255	-1.473355
37	1	0	0.934557	4.499305	0.897935
38	6	0	1.433361	3.919394	2.923851
39	6	0	2.777406	3.367861	0.788969
40	8	0	-0.007655	0.414761	3.174204
41	6	0	-0.901545	0.657678	4.229612
42	1	0	-1.455247	-0.276221	4.429197
43	6	0	-1.955294	1.759718	3.870410
44	6	0	-0.106660	1.021169	5.525517
45	6	0	4.563661	-0.223328	0.084085
46	6	0	3.867076	-1.276675	0.632268
47	6	0	2.542601	-1.134781	1.141201
48	6	0	1.757550	-2.347129	1.543947
49	8	0	2.054234	0.053520	1.279041
50	6	0	0.823062	-2.265422	2.578365
51	6	0	1.964242	-3.560802	0.881927
52	6	0	5.957524	-0.228005	-0.400098
53	1	0	4.291915	-2.268862	0.649302
54	6	0	6.714626	-1.399453	-0.503999
55	1	0	4.056332	0.735843	0.069558
56	6	0	6.545906	0.988555	-0.761225
57	1	0	-1.919741	2.192500	0.032484
58	7	0	1.562112	1.196163	-2.628429
59	6	0	2.454922	0.432862	-2.701582
60	6	0	3.509856	-0.476770	-2.770731
61	6	0	3.298490	-1.819008	-2.441721
62	1	0	4.434433	-0.180279	-3.250861
63	7	0	3.127814	-2.935594	-2.117022
64	6	0	8.022905	-1.349961	-0.951223
65	6	0	8.596110	-0.134216	-1.299602
66	6	0	7.855622	1.035635	-1.204235
67	1	0	5.964717	1.900024	-0.691297
68	1	0	6.274625	-2.353288	-0.244132
69	1	0	8.598655	-2.262881	-1.031510
70	1	0	9.620972	-0.099618	-1.649010
71	1	0	8.299677	1.983656	-1.478562

72	6	0	0.131123	-3.401683	2.964531
73	6	0	0.348972	-4.609022	2.317065
74	6	0	1.254513	-4.684484	1.266982
75	1	0	-0.199319	-5.492903	2.621663
76	1	0	1.404777	-5.619767	0.743947
77	1	0	2.638585	-3.609571	0.031681
78	1	0	0.612073	-1.303123	3.057009
79	1	0	-0.587490	-3.343690	3.771491
80	6	0	-6.148744	-3.018716	-0.786486
81	6	0	-5.936532	-1.813045	-0.035450
82	1	0	-4.548042	-0.319884	0.536714
83	1	0	-7.137240	-3.458262	-0.770833
84	1	0	-5.264364	-4.488388	-2.038968
85	1	0	0.444327	4.137396	3.313122
86	1	0	2.071302	4.778139	3.109676
87	1	0	2.692307	3.087437	-0.256820
88	1	0	3.384591	4.265148	0.859969
89	1	0	3.285318	2.569840	1.320992
90	1	0	-2.651015	1.917431	4.688932
91	1	0	-1.462462	2.701560	3.652207
92	1	0	-0.775590	1.114255	6.375987
93	1	0	0.424056	1.959283	5.398774
94	1	0	0.618138	0.241950	5.738983
95	1	0	-2.523807	1.458590	2.995821
96	1	0	1.837010	3.070163	3.467167
97	6	0	-2.414365	5.029385	0.120409
98	1	0	-3.847501	5.276079	-1.352318
99	1	0	-2.904276	5.704782	0.808419
100	1	0	-1.497668	4.585344	0.481985
101	8	0	-7.081662	-1.372071	0.631748
102	6	0	-6.895844	-0.206435	1.443336
103	1	0	-6.611387	0.668851	0.852015
104	1	0	-7.857915	-0.005613	1.918137
105	1	0	-6.146353	-0.360113	2.225107

A-COM-*Re*-2

Energy+zep = -2521.638355 au

Gibbs free energy = -2521.736444 au

Number of imaginary frequencies: 0

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	1	0	1.004990	-2.115054	1.446766
2	7	0	2.053958	-2.240242	1.447966
3	6	0	2.794080	-0.938556	1.184300
4	6	0	2.445517	-2.738259	2.814936
5	6	0	2.360881	-3.310293	0.430334
6	6	0	2.018337	0.027877	0.252362
7	6	0	4.254452	-1.308324	0.860446
8	6	0	3.997390	-2.808525	2.909673
9	6	0	3.830382	-3.754096	0.592282
10	1	0	1.990147	-2.064120	3.538034
11	1	0	1.977959	-3.716764	2.938466
12	1	0	1.638264	-4.110086	0.599634
13	1	0	2.161685	-2.881093	-0.549538
14	8	0	0.778537	0.220655	0.861356
15	6	0	1.849888	-0.402812	-1.242388
16	6	0	4.554527	-2.703837	1.456056
17	1	0	4.430713	-1.330169	-0.220795
18	1	0	4.918033	-0.546466	1.279860
19	1	0	4.259371	-3.814300	3.272063
20	1	0	3.893537	-4.742016	1.061319
21	1	0	4.302739	-3.834156	-0.391809
22	6	0	4.697096	-1.816970	3.861355
23	1	0	2.613171	0.953814	0.262173
24	13	0	-0.274651	1.635450	0.643964
25	6	0	2.782217	-0.048506	-2.285738
26	6	0	0.739441	-1.095887	-1.596681
27	1	0	5.631837	-2.893082	1.460575
28	8	0	-0.715907	2.362456	2.182088
29	6	0	2.490392	-0.476257	-3.592419
30	6	0	0.526974	-1.483419	-2.951018
31	6	0	3.970428	0.720483	-2.064875
32	1	0	0.006928	-1.362594	-0.845856
33	6	0	-0.206750	2.483022	3.487920
34	7	0	1.352762	-1.210796	-3.939542
35	6	0	3.394721	-0.149683	-4.657970
36	1	0	-0.367952	-2.047613	-3.203272
37	1	0	-0.813117	3.237827	4.013446
38	8	0	0.539371	2.605708	-0.537414
39	6	0	0.448606	3.823503	-1.221046
40	1	0	1.369209	3.935307	-1.819648
41	6	0	-3.556597	-1.068484	-0.803512
42	6	0	-3.999756	0.204892	-0.486541
43	6	0	-3.128497	1.245963	-0.069083

44	8	0	-1.867225	1.001201	0.050712
45	1	0	-5.055444	0.433751	-0.518458
46	1	0	-2.482209	-1.219900	-0.777146
47	1	0	2.760735	-0.428284	2.150073
48	6	0	-4.360903	-2.180035	-1.340271
49	6	0	-5.758011	-2.138898	-1.399405
50	6	0	-3.700356	-3.316426	-1.820320
51	6	0	-6.468647	-3.200731	-1.928540
52	1	0	-6.291377	-1.276184	-1.022945
53	6	0	-4.412751	-4.375219	-2.353517
54	1	0	-2.619479	-3.362850	-1.767406
55	6	0	-5.798607	-4.318816	-2.407599
56	1	0	-7.549531	-3.160418	-1.964811
57	1	0	-3.889703	-5.248380	-2.721112
58	1	0	-6.358771	-5.149747	-2.819560
59	6	0	-3.682584	2.612521	0.238557
60	6	0	-3.086150	3.400245	1.222825
61	6	0	-4.799704	3.089486	-0.454315
62	6	0	-3.622674	4.648461	1.510838
63	1	0	-2.191201	3.032073	1.759704
64	6	0	-5.314317	4.338681	-0.169347
65	1	0	-5.254770	2.491221	-1.232866
66	6	0	-4.728472	5.118055	0.822152
67	1	0	-3.168723	5.260312	2.279844
68	1	0	-6.172015	4.707745	-0.716087
69	1	0	-5.137443	6.095110	1.051222
70	6	0	1.274142	2.990720	3.471336
71	1	0	1.649291	3.141551	4.479177
72	1	0	1.916019	2.271781	2.970668
73	1	0	1.333269	3.933681	2.937065
74	6	0	-0.351653	1.125592	4.252387
75	1	0	-0.005890	1.210866	5.278424
76	1	0	-1.393289	0.820624	4.262684
77	1	0	0.224120	0.351716	3.753872
78	6	0	0.380546	5.036514	-0.231654
79	1	0	-0.515130	4.981748	0.379755
80	1	0	1.244610	5.021612	0.425004
81	1	0	0.372612	5.980560	-0.768139
82	6	0	-0.757587	3.826480	-2.221794
83	1	0	-0.761867	4.727445	-2.827552
84	1	0	-0.685740	2.967995	-2.882485
85	1	0	-1.700944	3.772080	-1.686974
86	6	0	4.805082	1.027871	-3.094569
87	6	0	4.509054	0.570341	-4.423650

88	1	0	4.183684	1.068277	-1.070026
89	1	0	5.200180	0.829904	-5.214697
90	1	0	3.146023	-0.498291	-5.652780
91	6	0	4.151233	-0.981866	4.706725
92	1	0	4.762020	-0.352102	5.338951
93	1	0	3.084370	-0.866736	4.835015
94	1	0	5.777981	-1.881449	3.799157
95	7	0	-0.643118	-2.695408	1.536769
96	6	0	-1.811887	-2.612094	1.643704
97	6	0	-3.189955	-2.483529	1.745959
98	6	0	-4.028724	-3.613078	1.693993
99	7	0	-4.742447	-4.540860	1.638837
100	1	0	-3.591008	-1.547169	2.113422
101	8	0	5.986586	1.768295	-3.018185
102	6	0	6.271926	2.315842	-1.725407
103	1	0	6.439770	1.538036	-0.974666
104	1	0	7.189773	2.896589	-1.833243
105	1	0	5.477665	2.979469	-1.371577

A-COM-*Si*-2

Energy+zep = -2521.636370 au

Gibbs free energy = -2521.735804 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.265772	-1.876416	1.057776
2	7	0	1.176015	-2.393254	1.133727
3	6	0	2.354261	-1.435940	1.200500
4	6	0	1.130649	-3.189274	2.412992
5	6	0	1.255262	-3.343022	-0.034686
6	6	0	2.105491	-0.148195	0.363943
7	6	0	3.631069	-2.272672	0.987846
8	6	0	2.517381	-3.850608	2.655243
9	6	0	2.433672	-4.315267	0.190753
10	1	0	0.825634	-2.501517	3.199351
11	1	0	0.332244	-3.923287	2.294997
12	1	0	0.283287	-3.834547	-0.095417
13	1	0	1.383647	-2.735597	-0.928514
14	8	0	0.835475	0.280254	0.737397
15	6	0	2.242290	-0.265862	-1.191275

16	6	0	3.316547	-3.749350	1.319475
17	1	0	3.986897	-2.201560	-0.045695
18	1	0	4.427212	-1.885012	1.629988
19	1	0	2.344109	-4.922456	2.835439
20	1	0	2.071974	-5.314501	0.456297
21	1	0	3.011254	-4.416894	-0.733402
22	6	0	3.345649	-3.344720	3.853846
23	1	0	2.878455	0.558731	0.703285
24	13	0	0.108841	1.891806	0.558252
25	6	0	3.491221	-0.091504	-1.894190
26	6	0	1.127603	-0.479656	-1.932462
27	1	0	4.242802	-4.325554	1.400153
28	8	0	-0.602999	2.438520	2.071582
29	6	0	3.470063	-0.193611	-3.295698
30	6	0	1.202985	-0.563669	-3.352880
31	6	0	4.736021	0.193272	-1.245376
32	1	0	0.166916	-0.584400	-1.446914
33	6	0	-0.215746	2.501645	3.424475
34	7	0	2.315886	-0.441574	-4.045052
35	6	0	4.691623	-0.031377	-4.031199
36	1	0	0.291985	-0.745996	-3.918338
37	1	0	-0.947952	3.135751	3.949008
38	8	0	1.317831	2.884035	-0.187650
39	6	0	1.409049	4.250608	-0.504953
40	1	0	0.918319	4.858684	0.277108
41	6	0	-4.364401	-0.181717	-0.997370
42	6	0	-3.089530	0.333257	-1.162098
43	6	0	-2.611902	1.505904	-0.526624
44	8	0	-1.333080	1.694487	-0.511307
45	1	0	-2.342648	-0.231413	-1.705388
46	1	0	-5.043998	0.359166	-0.345278
47	1	0	2.327738	-1.077054	2.232585
48	6	0	-4.950280	-1.342393	-1.690107
49	6	0	-4.234272	-2.106188	-2.619577
50	6	0	-6.283206	-1.677701	-1.428631
51	6	0	-4.836377	-3.168797	-3.265529
52	1	0	-3.202510	-1.865360	-2.837549
53	6	0	-6.884601	-2.742400	-2.077803
54	1	0	-6.845066	-1.098501	-0.705711
55	6	0	-6.161580	-3.489355	-2.996036
56	1	0	-4.273689	-3.752588	-3.982222
57	1	0	-7.914655	-2.993918	-1.861166
58	1	0	-6.629450	-4.324818	-3.502958
59	6	0	-3.503351	2.567533	0.054839

60	6	0	-3.103017	3.230887	1.214785
61	6	0	-4.692796	2.928202	-0.584775
62	6	0	-3.917500	4.223699	1.741657
63	1	0	-2.142365	2.953212	1.691109
64	6	0	-5.486471	3.929303	-0.058939
65	1	0	-4.981257	2.444058	-1.508872
66	6	0	-5.102640	4.571071	1.112921
67	1	0	-3.620944	4.735480	2.648242
68	1	0	-6.402045	4.213515	-0.560575
69	1	0	-5.729059	5.351823	1.528284
70	6	0	1.191125	3.169872	3.577892
71	1	0	1.461566	3.279686	4.623825
72	1	0	1.953165	2.570479	3.088015
73	1	0	1.182363	4.153536	3.118895
74	6	0	-0.261425	1.077051	4.069919
75	1	0	-0.028984	1.117179	5.130057
76	1	0	-1.252433	0.651137	3.947518
77	1	0	0.454498	0.422811	3.582127
78	6	0	0.695886	4.550783	-1.866647
79	1	0	1.151463	3.969895	-2.662473
80	1	0	-0.354679	4.282068	-1.805713
81	1	0	0.764734	5.603619	-2.123504
82	6	0	2.917080	4.655650	-0.550844
83	1	0	3.029853	5.712103	-0.776273
84	1	0	3.382037	4.454883	0.409341
85	1	0	3.436286	4.080552	-1.311122
86	6	0	5.878392	0.356268	-1.966682
87	6	0	5.851324	0.230661	-3.397350
88	1	0	4.750079	0.293071	-0.174818
89	1	0	6.781197	0.360942	-3.935117
90	1	0	4.644871	-0.121740	-5.109480
91	6	0	2.989065	-2.500955	4.787042
92	1	0	3.663279	-2.246051	5.593165
93	1	0	2.023589	-2.016770	4.823438
94	1	0	4.329919	-3.798553	3.893691
95	7	0	-1.579366	-2.057851	1.013699
96	6	0	-2.728494	-1.967433	1.252459
97	6	0	-4.082874	-1.811396	1.515041
98	8	0	7.149787	0.638440	-1.463419
99	6	0	7.203047	0.857912	-0.048646
100	1	0	6.925215	-0.034983	0.519062
101	1	0	8.239535	1.107892	0.184838
102	1	0	6.563670	1.687538	0.266569
103	6	0	-4.981326	-2.887820	1.413844

104	7	0	-5.755897	-3.763009	1.319618
105	1	0	-4.401139	-0.914044	2.033721

A-TS1-*Re*-1

Energy+zep = -2521.635245 au

Gibbs free energy = -2521.730602 au

Number of imaginary frequencies: 1 (-261.6718 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.189032	0.857724	-1.292617
2	7	0	-0.989006	1.295220	-1.778406
3	6	0	-2.163100	1.256911	-0.811572
4	6	0	-0.660916	2.735907	-2.076060
5	6	0	-1.253656	0.547054	-3.059178
6	6	0	-2.086408	-0.026439	0.083537
7	6	0	-3.427084	1.604276	-1.619362
8	6	0	-1.941963	3.442127	-2.628711
9	6	0	-2.352162	1.293837	-3.848618
10	1	0	-0.301100	3.160370	-1.137328
11	1	0	0.160448	2.726448	-2.793367
12	1	0	-0.299881	0.486690	-3.583238
13	1	0	-1.556651	-0.460767	-2.778464
14	8	0	-0.740283	-0.198484	0.430572
15	6	0	-2.649161	-1.354958	-0.509245
16	6	0	-3.003271	2.334364	-2.915606
17	1	0	-3.991888	0.704775	-1.887653
18	1	0	-4.088385	2.226858	-1.010635
19	1	0	-1.686966	3.890656	-3.596030
20	1	0	-1.929673	1.786390	-4.730835
21	1	0	-3.100953	0.579886	-4.206061
22	6	0	-2.450903	4.570549	-1.718266
23	1	0	-2.693885	0.222365	0.968703
24	13	0	0.040823	0.696175	1.776679
25	6	0	-1.785518	-2.262910	-1.024877
26	6	0	-4.049845	-1.701842	-0.476154
27	1	0	-3.876970	2.780788	-3.399652
28	8	0	-0.057551	2.381215	1.256209
29	6	0	-2.261998	-3.495625	-1.558378
30	6	0	-4.427421	-2.937676	-1.027822
31	1	0	-0.723403	-2.059769	-1.016860

32	6	0	-5.061168	-0.870965	0.105871
33	6	0	0.125272	3.541450	2.041888
34	7	0	-3.529624	-3.850150	-1.590203
35	1	0	-1.545606	-4.199535	-1.975765
36	6	0	-5.811271	-3.318107	-1.017446
37	1	0	0.139256	4.406453	1.355290
38	6	0	-1.066962	3.722554	3.039789
39	6	0	1.500797	3.520442	2.790480
40	8	0	-0.706661	0.502257	3.330117
41	6	0	-0.739090	-0.514594	4.299360
42	1	0	-0.653436	-1.508189	3.821916
43	6	0	-2.112363	-0.462620	5.043583
44	6	0	0.457504	-0.354172	5.296460
45	6	0	4.747558	-0.486166	-0.232056
46	6	0	3.717295	0.084431	0.562223
47	6	0	2.539563	-0.541367	0.946949
48	6	0	2.158655	-1.983663	0.640074
49	8	0	1.730419	0.086495	1.767244
50	6	0	1.702982	-2.767111	1.700400
51	6	0	2.225295	-2.549038	-0.630175
52	6	0	6.191962	-0.084692	-0.093922
53	1	0	3.838416	1.089660	0.952438
54	6	0	6.576203	1.181623	0.350653
55	1	0	4.620673	-1.531935	-0.497722
56	6	0	7.185025	-1.010727	-0.416584
57	1	0	-1.922498	2.062699	-0.115106
58	6	0	7.915570	1.507606	0.471780
59	6	0	8.893930	0.576426	0.152673
60	6	0	8.525144	-0.683801	-0.291805
61	1	0	6.901980	-1.995616	-0.766517
62	1	0	5.824567	1.917806	0.600859
63	1	0	8.199048	2.493357	0.817812
64	1	0	9.941083	0.833901	0.250318
65	1	0	9.282836	-1.414926	-0.543134
66	6	0	1.342187	-4.088221	1.500355
67	6	0	1.420141	-4.644302	0.231330
68	6	0	1.856498	-3.870678	-0.832161
69	1	0	1.137162	-5.677265	0.072280
70	1	0	1.912679	-4.296125	-1.826105
71	1	0	2.548023	-1.955139	-1.473112
72	1	0	1.642071	-2.331563	2.689695
73	1	0	0.998740	-4.686084	2.334990
74	6	0	-6.745566	-2.515809	-0.470845
75	6	0	-6.364585	-1.261628	0.117202

76	1	0	-4.769039	0.063635	0.550517
77	1	0	-7.792451	-2.788398	-0.448529
78	1	0	-6.073546	-4.272588	-1.457069
79	1	0	-1.997239	3.822608	2.489038
80	1	0	-0.938496	4.605924	3.658064
81	1	0	2.305363	3.370143	2.077228
82	1	0	1.676376	4.453940	3.316607
83	1	0	1.527717	2.710610	3.513902
84	1	0	-2.179022	-1.243577	5.795574
85	1	0	-2.238516	0.499499	5.530046
86	1	0	0.454407	-1.138487	6.047782
87	1	0	0.396844	0.606006	5.798951
88	1	0	1.398881	-0.397862	4.756737
89	1	0	-2.922869	-0.596569	4.333887
90	1	0	-1.140735	2.847997	3.680264
91	6	0	-2.674387	5.789826	-2.136654
92	1	0	-2.621835	4.308163	-0.680986
93	1	0	-3.036744	6.562601	-1.471920
94	1	0	-2.508348	6.088870	-3.163421
95	7	0	1.942659	0.735999	-2.288584
96	6	0	3.079577	0.480608	-2.376377
97	6	0	4.455587	0.154830	-2.323015
98	1	0	5.116556	1.017984	-2.342134
99	6	0	4.900268	-0.954040	-3.102437
100	7	0	5.295507	-1.893301	-3.671636
101	8	0	-7.443021	-0.555004	0.652483
102	6	0	-7.093900	0.663635	1.320385
103	1	0	-8.024324	1.074638	1.716196
104	1	0	-6.403358	0.497775	2.152291
105	1	0	-6.652852	1.396879	0.638859

A-TS2-*Re*-1

Energy+zep = -2521.628434 au

Gibbs free energy = -2521.723352 au

Number of imaginary frequencies: 1 (-1305.0295 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.669390	-0.933908	0.844153
2	7	0	-0.210855	-0.989167	1.885435
3	6	0	-1.619269	-0.559697	1.527251

4	6	0	-0.286197	-2.369838	2.453653
5	6	0	0.401092	-0.079405	2.911663
6	6	0	-1.656979	0.549870	0.435458
7	6	0	-2.370748	-0.251357	2.845525
8	6	0	-1.292502	-2.427058	3.658124
9	6	0	-0.333034	-0.211508	4.268259
10	1	0	-0.583655	-3.047213	1.652530
11	1	0	0.723928	-2.643024	2.775478
12	1	0	1.457716	-0.352056	2.994483
13	1	0	0.330395	0.928043	2.510628
14	8	0	-0.807888	1.615728	0.743599
15	6	0	-3.121469	1.071927	0.245349
16	6	0	-1.655990	-0.955931	4.017577
17	1	0	-2.388269	0.828335	3.030676
18	1	0	-3.411416	-0.578178	2.755934
19	1	0	-0.765089	-2.847191	4.523528
20	1	0	0.275824	-0.752929	5.001848
21	1	0	-0.524479	0.784825	4.680307
22	1	0	-1.351231	0.076428	-0.509974
23	13	0	0.422028	2.326888	-0.321614
24	6	0	-3.455046	2.276511	0.757565
25	6	0	-4.142135	0.339550	-0.472979
26	1	0	-2.282712	-0.938758	4.914909
27	8	0	0.308621	1.676552	-1.939720
28	6	0	-4.780665	2.791361	0.607944
29	6	0	-5.418547	0.924606	-0.570519
30	1	0	-2.709478	2.860472	1.279284
31	6	0	0.098945	2.321160	-3.179048
32	7	0	-5.754410	2.169777	-0.017147
33	1	0	-5.016910	3.762208	1.038289
34	1	0	0.144486	1.546004	-3.962394
35	8	0	0.586766	4.036716	-0.205013
36	6	0	0.441467	5.016044	0.790824
37	1	0	-0.391749	4.750110	1.466599
38	6	0	2.255880	-1.970344	-0.793666
39	6	0	1.601894	-0.699827	-0.199866
40	6	0	2.397241	0.344731	0.372372
41	8	0	1.981791	1.561652	0.372242
42	1	0	0.907553	-0.252257	-0.917202
43	1	0	2.405433	-2.750151	-0.040224
44	7	0	-1.047650	-3.239231	-0.753555
45	6	0	-0.038339	-2.955017	-1.249897
46	6	0	1.255234	-2.591381	-1.850249
47	1	0	-2.063746	-1.444289	1.065286

48	6	0	3.610924	-1.730083	-1.512794
49	6	0	3.759235	-0.684265	-2.420211
50	6	0	4.688769	-2.575434	-1.279826
51	6	0	4.962669	-0.487445	-3.075616
52	1	0	2.928997	-0.017267	-2.616016
53	6	0	5.895430	-2.378673	-1.935073
54	1	0	4.587163	-3.396376	-0.581500
55	6	0	6.035333	-1.334197	-2.834005
56	1	0	5.064596	0.329684	-3.778737
57	1	0	6.726642	-3.045189	-1.742469
58	1	0	6.976141	-1.179466	-3.346669
59	6	0	3.708977	0.151702	1.104982
60	6	0	4.605083	1.218708	1.133066
61	6	0	4.028979	-1.023928	1.780951
62	6	0	5.809986	1.105816	1.807244
63	1	0	4.346809	2.136422	0.618620
64	6	0	5.227420	-1.131118	2.465823
65	1	0	3.335721	-1.853410	1.789293
66	6	0	6.121923	-0.069757	2.474431
67	1	0	6.503565	1.936901	1.816294
68	1	0	5.465227	-2.045047	2.994804
69	1	0	7.061475	-0.158606	3.006387
70	6	0	1.226509	3.368677	-3.460814
71	1	0	1.216470	4.138411	-2.694040
72	1	0	2.195692	2.879467	-3.445641
73	1	0	1.095687	3.840503	-4.429911
74	6	0	-1.321229	2.976040	-3.238109
75	1	0	-2.079770	2.228404	-3.027397
76	1	0	-1.402698	3.768183	-2.499308
77	1	0	-1.518266	3.400137	-4.218030
78	6	0	0.094582	6.379193	0.112577
79	1	0	-0.819717	6.281528	-0.464265
80	1	0	-0.045158	7.158820	0.855853
81	1	0	0.893477	6.677520	-0.558920
82	6	0	1.746247	5.121654	1.651465
83	1	0	1.960845	4.167172	2.123255
84	1	0	2.588345	5.387259	1.020141
85	1	0	1.646330	5.873322	2.428927
86	6	0	-6.448669	0.233897	-1.274256
87	6	0	-3.929486	-0.920461	-1.095992
88	6	0	-2.510084	-3.323850	3.384831
89	1	0	-3.074652	-3.103007	2.486410
90	6	0	-2.876204	-4.308567	4.164705
91	1	0	-2.336075	-4.562388	5.067035

92	1	0	-3.740363	-4.920354	3.944612
93	6	0	-6.225344	-0.967977	-1.858487
94	6	0	-4.929974	-1.562769	-1.772734
95	1	0	-7.422194	0.705316	-1.331119
96	1	0	-7.022531	-1.466792	-2.387231
97	1	0	-2.961933	-1.396664	-1.054012
98	6	0	1.825498	-3.775091	-2.518229
99	7	0	2.287734	-4.702425	-3.040358
100	1	0	1.059826	-1.832808	-2.619716
101	8	0	-4.573413	-2.792178	-2.341375
102	6	0	-5.619741	-3.458120	-3.058341
103	1	0	-5.982916	-2.872040	-3.907521
104	1	0	-5.186287	-4.384991	-3.438558
105	1	0	-6.469529	-3.711201	-2.417790

A-TS1-*Si*-1

Energy+zep = -2521.634862 au

Gibbs free energy = -2521.729564 au

Number of imaginary frequencies: 1 (-244.1638 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.248588	1.432669	-1.204533
2	7	0	-1.113294	1.924591	-1.487783
3	6	0	-2.208213	1.557954	-0.501102
4	6	0	-0.866794	3.409738	-1.404893
5	6	0	-1.443429	1.535402	-2.905864
6	6	0	-2.037563	0.079358	-0.009337
7	6	0	-3.541283	2.048946	-1.100465
8	6	0	-2.209572	4.159209	-1.639361
9	6	0	-2.620622	2.407627	-3.395186
10	1	0	-0.416936	3.582750	-0.429218
11	1	0	-0.122268	3.639915	-2.167706
12	1	0	-0.526525	1.668171	-3.479885
13	1	0	-1.688304	0.474462	-2.893019
14	8	0	-0.677567	-0.133723	0.188850
15	6	0	-2.608836	-1.055323	-0.918006
16	6	0	-3.240281	3.117808	-2.176498
17	1	0	-4.102088	1.227245	-1.558107
18	1	0	-4.165525	2.462195	-0.303104
19	1	0	-2.044594	4.880846	-2.453161

20	1	0	-2.280520	3.144443	-4.130887
21	1	0	-3.366799	1.778589	-3.890978
22	6	0	-2.788934	4.969937	-0.463085
23	1	0	-2.596404	0.046625	0.940374
24	13	0	0.404268	0.328491	1.532546
25	6	0	-1.757277	-1.746312	-1.714204
26	6	0	-3.993673	-1.460949	-0.901068
27	1	0	-4.162668	3.629229	-2.467213
28	8	0	0.393629	2.091790	1.496246
29	6	0	-2.234337	-2.804106	-2.541837
30	6	0	-4.373324	-2.512216	-1.752587
31	1	0	-0.703141	-1.503687	-1.709972
32	6	0	-4.986248	-0.871078	-0.052908
33	6	0	1.164111	3.065454	2.162192
34	7	0	-3.491381	-3.192299	-2.597714
35	1	0	-1.528872	-3.332413	-3.179267
36	6	0	-5.742201	-2.943574	-1.769024
37	1	0	0.851830	4.053658	1.779542
38	6	0	0.901936	3.061774	3.705428
39	6	0	2.690050	2.915607	1.844484
40	8	0	0.050393	-0.437324	3.060791
41	6	0	-1.019290	-0.749395	3.912933
42	1	0	-1.653525	-1.516904	3.431505
43	6	0	-1.927664	0.492727	4.214700
44	6	0	-0.455242	-1.357698	5.236964
45	6	0	4.572523	-0.076104	-0.195868
46	6	0	3.862677	-1.287824	-0.024854
47	6	0	2.588555	-1.349159	0.539657
48	6	0	1.882137	-2.684735	0.671702
49	8	0	2.013483	-0.269029	1.000884
50	6	0	1.011179	-2.912334	1.735779
51	6	0	2.094613	-3.700820	-0.261229
52	6	0	6.068925	-0.000492	-0.266511
53	1	0	4.320180	-2.220251	-0.323327
54	6	0	6.846743	-1.059088	-0.739206
55	1	0	4.090756	0.800037	0.227372
56	6	0	6.710260	1.162581	0.164564
57	1	0	-1.952320	2.155764	0.376116
58	7	0	1.716768	1.537495	-2.194193
59	6	0	2.816956	1.148767	-2.261381
60	6	0	4.151298	0.674631	-2.289478
61	6	0	4.403570	-0.483832	-3.075700
62	1	0	4.907379	1.453347	-2.349536
63	7	0	4.628195	-1.471374	-3.656804

64	6	0	8.226889	-0.953520	-0.775869
65	6	0	8.852353	0.204895	-0.338188
66	6	0	8.090223	1.263421	0.133363
67	1	0	6.117683	1.990829	0.532416
68	1	0	6.371291	-1.965480	-1.089077
69	1	0	8.818027	-1.780427	-1.148108
70	1	0	9.932008	0.282579	-0.365380
71	1	0	8.572669	2.169507	0.476663
72	6	0	0.380336	-4.139646	1.868612
73	6	0	0.601658	-5.145645	0.941555
74	6	0	1.455855	-4.921146	-0.128896
75	1	0	0.104909	-6.102189	1.047324
76	1	0	1.623492	-5.699004	-0.862535
77	1	0	2.750925	-3.531380	-1.104905
78	1	0	0.808816	-2.115721	2.451145
79	1	0	-0.290554	-4.310216	2.700790
80	6	0	-6.659460	-2.367249	-0.967938
81	6	0	-6.274469	-1.308452	-0.076601
82	1	0	-4.691320	-0.083445	0.617208
83	1	0	-7.694425	-2.682744	-0.962543
84	1	0	-6.006710	-3.750335	-2.441581
85	1	0	-0.150864	3.236691	3.901342
86	1	0	1.476716	3.838555	4.200821
87	1	0	2.842617	2.927137	0.769774
88	1	0	3.262492	3.727438	2.283157
89	1	0	3.069920	1.976836	2.235971
90	1	0	-2.793814	0.206016	4.803707
91	1	0	-1.372469	1.244136	4.765517
92	1	0	-1.261855	-1.645703	5.904941
93	1	0	0.174631	-0.633776	5.744306
94	1	0	0.142172	-2.236351	5.016021
95	1	0	-2.278398	0.938527	3.288647
96	1	0	1.176220	2.102980	4.135353
97	6	0	-2.343435	5.053193	0.763389
98	1	0	-3.673906	5.527348	-0.749752
99	1	0	-2.845473	5.671743	1.494809
100	1	0	-1.468966	4.529649	1.122901
101	8	0	-7.333684	-0.827482	0.695567
102	6	0	-6.976378	0.180440	1.648955
103	1	0	-6.602879	1.089864	1.169247
104	1	0	-7.889865	0.426323	2.193377
105	1	0	-6.227612	-0.171832	2.364302

A-TS2-*Si*-1

Energy+zep = -2521.615267 au

Gibbs free energy = -2521.708576 au

Number of imaginary frequencies: 1 (-1375.3301 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.822931	1.080695	-0.885262
2	7	0	-0.295084	1.868635	-0.674031
3	6	0	-1.375196	1.390557	0.281124
4	6	0	0.242497	3.144347	-0.093683
5	6	0	-0.832800	2.143732	-2.042030
6	6	0	-1.718727	-0.132298	0.243397
7	6	0	-2.590426	2.348975	0.174212
8	6	0	-0.875074	4.223637	0.096561
9	6	0	-1.865903	3.301701	-2.007720
10	1	0	0.712267	2.880300	0.856160
11	1	0	1.005553	3.514841	-0.776462
12	1	0	0.018466	2.385679	-2.683222
13	1	0	-1.276234	1.218469	-2.409090
14	8	0	-0.545109	-0.878035	0.208483
15	6	0	-2.678468	-0.643188	-0.882235
16	6	0	-2.169237	3.647100	-0.537079
17	1	0	-3.400922	1.887582	-0.399278
18	1	0	-2.987542	2.554970	1.172853
19	1	0	-0.595661	5.111782	-0.483265
20	1	0	-1.476798	4.181435	-2.531809
21	1	0	-2.785603	3.000350	-2.520718
22	6	0	-1.040775	4.661343	1.560247
23	1	0	-2.250815	-0.285371	1.197588
24	13	0	0.714961	-1.103645	1.447750
25	6	0	-2.148488	-1.140417	-2.026517
26	6	0	-4.116145	-0.691514	-0.740480
27	1	0	-2.973638	4.387675	-0.483009
28	8	0	0.913605	0.378999	2.363942
29	6	0	-2.985619	-1.644733	-3.061980
30	6	0	-4.862269	-1.206248	-1.815088
31	1	0	-1.077016	-1.172576	-2.153081
32	6	0	-4.817007	-0.266723	0.435466
33	6	0	1.017191	0.568753	3.761393
34	7	0	-4.300203	-1.682895	-3.002822
35	1	0	-2.526003	-2.024744	-3.971556

36	6	0	-6.292649	-1.269233	-1.713617
37	1	0	1.373514	1.600177	3.925983
38	6	0	-0.389013	0.436131	4.439699
39	6	0	2.045062	-0.417007	4.406703
40	8	0	0.603111	-2.484975	2.478629
41	6	0	0.320080	-3.854655	2.342990
42	1	0	-0.119704	-4.062832	1.350691
43	6	0	-0.728055	-4.271439	3.424911
44	6	0	1.638612	-4.686959	2.475287
45	6	0	3.189765	1.352446	-0.501924
46	6	0	2.101378	0.557899	-1.271919
47	6	0	1.922084	-0.830126	-1.009301
48	6	0	1.570415	-1.837978	-2.075526
49	8	0	2.053019	-1.291713	0.194237
50	6	0	1.356906	-3.159152	-1.678458
51	6	0	1.480312	-1.521129	-3.432580
52	6	0	4.219688	0.551791	0.339937
53	1	0	2.117143	0.782432	-2.336767
54	6	0	4.913391	-0.542037	-0.174229
55	1	0	2.730136	2.066068	0.186128
56	6	0	4.513793	0.981644	1.628428
57	1	0	-0.894754	1.502914	1.255421
58	6	0	5.870769	-1.190885	0.585973
59	6	0	6.155545	-0.754362	1.872106
60	6	0	5.474774	0.333798	2.391184
61	1	0	3.985451	1.830101	2.044055
62	1	0	4.707227	-0.894991	-1.175789
63	1	0	6.398889	-2.040512	0.171984
64	1	0	6.905176	-1.262271	2.465398
65	1	0	5.690276	0.682912	3.393067
66	6	0	1.052928	-4.138990	-2.607277
67	6	0	0.957831	-3.808778	-3.951729
68	6	0	1.172660	-2.500007	-4.361787
69	1	0	0.719214	-4.572523	-4.682564
70	1	0	1.104326	-2.242209	-5.410673
71	1	0	1.651431	-0.510361	-3.776364
72	1	0	1.438933	-3.407384	-0.628007
73	1	0	0.889998	-5.158927	-2.283844
74	6	0	-6.927502	-0.856838	-0.599450
75	6	0	-6.172762	-0.347618	0.511302
76	1	0	-4.249393	0.110987	1.266712
77	1	0	-8.004325	-0.900959	-0.503705
78	1	0	-6.838845	-1.664247	-2.561265
79	1	0	-1.089154	1.128612	3.982320

80	1	0	-0.335483	0.655338	5.501836
81	1	0	3.021517	-0.280687	3.953728
82	1	0	2.134861	-0.249476	5.475555
83	1	0	1.723087	-1.440185	4.234450
84	1	0	-0.972193	-5.326852	3.345957
85	1	0	-0.335902	-4.078569	4.418469
86	1	0	1.445730	-5.749846	2.362358
87	1	0	2.088550	-4.518031	3.448397
88	1	0	2.350744	-4.383181	1.713904
89	1	0	-1.639485	-3.695465	3.298019
90	1	0	-0.771327	-0.572992	4.316537
91	6	0	-0.997743	5.907217	1.957404
92	1	0	-1.196636	3.865702	2.279725
93	1	0	-1.119087	6.180384	2.996762
94	1	0	-0.838324	6.726970	1.269686
95	7	0	5.305506	0.914266	-3.365706
96	6	0	4.733275	1.504851	-2.547126
97	6	0	4.010984	2.266911	-1.511477
98	6	0	3.183593	3.289092	-2.177402
99	7	0	2.525655	4.100387	-2.683393
100	1	0	4.764286	2.806092	-0.921810
101	8	0	-6.972005	0.026681	1.594033
102	6	0	-6.252510	0.500590	2.738653
103	1	0	-7.001230	0.730526	3.498836
104	1	0	-5.568199	-0.252656	3.139706
105	1	0	-5.684975	1.410629	2.523401

A-TS1-*Re*-2

Energy+zep = -2521.633843 au

Gibbs free energy = -2521.729200 au

Number of imaginary frequencies: 1 (-221.7403 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.765032	-2.113322	1.092241
2	7	0	1.738328	-2.467177	1.064792
3	6	0	2.670910	-1.266546	1.048247
4	6	0	2.003856	-3.277493	2.307525
5	6	0	1.894146	-3.352326	-0.148687
6	6	0	2.013928	-0.072233	0.297623
7	6	0	4.068976	-1.786776	0.666148

8	6	0	3.523564	-3.605895	2.376447
9	6	0	3.276943	-4.034914	-0.084020
10	1	0	1.641987	-2.691894	3.150593
11	1	0	1.382536	-4.170817	2.234704
12	1	0	1.053993	-4.046218	-0.127198
13	1	0	1.786692	-2.710915	-1.021546
14	8	0	0.716804	0.000586	0.810916
15	6	0	2.011690	-0.122699	-1.266779
16	6	0	4.129189	-3.302429	0.970044
17	1	0	4.281289	-1.621740	-0.395427
18	1	0	4.825087	-1.239189	1.235865
19	1	0	3.616836	-4.691899	2.527828
20	1	0	3.178141	-5.094222	0.176393
21	1	0	3.757817	-3.988031	-1.066048
22	6	0	4.342339	-2.944927	3.503712
23	1	0	2.607342	0.807187	0.588143
24	13	0	-0.289291	1.490181	0.787950
25	6	0	3.113931	0.340218	-2.076148
26	6	0	0.902253	-0.564230	-1.908581
27	1	0	5.163746	-3.655172	0.932402
28	8	0	-0.748138	2.016896	2.397035
29	6	0	2.977438	0.257866	-3.472236
30	6	0	0.852406	-0.604999	-3.332164
31	6	0	4.320293	0.891214	-1.535223
32	1	0	0.038466	-0.881356	-1.340283
33	6	0	-0.220848	2.026352	3.696044
34	7	0	1.838169	-0.230090	-4.119832
35	6	0	4.053788	0.702048	-4.311089
36	1	0	-0.048909	-0.973940	-3.816491
37	1	0	-0.891776	2.631498	4.327279
38	8	0	0.643775	2.561281	-0.204883
39	6	0	0.615959	3.819161	-0.817707
40	1	0	1.585723	3.959529	-1.326294
41	6	0	-3.594721	-1.067464	-0.743738
42	6	0	-4.020415	0.256833	-0.466546
43	6	0	-3.125026	1.241075	-0.049603
44	8	0	-1.859148	0.948741	0.088654
45	1	0	-5.070564	0.513473	-0.509554
46	1	0	-2.521842	-1.176587	-0.871802
47	1	0	2.680436	-0.941239	2.091839
48	6	0	-4.423202	-2.072731	-1.479081
49	6	0	-5.818577	-2.052730	-1.442810
50	6	0	-3.786402	-3.064978	-2.227768
51	6	0	-6.553017	-2.994966	-2.143454

52	1	0	-6.332516	-1.301269	-0.858403
53	6	0	-4.521427	-4.002510	-2.931227
54	1	0	-2.704597	-3.094199	-2.259575
55	6	0	-5.907816	-3.969502	-2.890345
56	1	0	-7.634463	-2.970120	-2.103943
57	1	0	-4.013507	-4.761716	-3.511841
58	1	0	-6.484672	-4.704152	-3.438132
59	6	0	-3.613967	2.638719	0.276383
60	6	0	-3.053300	3.340433	1.342715
61	6	0	-4.636866	3.224784	-0.469317
62	6	0	-3.523572	4.607617	1.654810
63	1	0	-2.242528	2.886721	1.925528
64	6	0	-5.092698	4.493479	-0.158425
65	1	0	-5.068397	2.690013	-1.305474
66	6	0	-4.538694	5.185852	0.909358
67	1	0	-3.092591	5.148779	2.487536
68	1	0	-5.880868	4.943684	-0.747801
69	1	0	-4.898459	6.176990	1.156593
70	6	0	1.195985	2.694407	3.737245
71	1	0	1.577419	2.748873	4.752636
72	1	0	1.901928	2.128505	3.136163
73	1	0	1.137347	3.701344	3.336899
74	6	0	-0.193818	0.574477	4.285361
75	1	0	0.158281	0.567984	5.312870
76	1	0	-1.193411	0.152073	4.259906
77	1	0	0.459093	-0.058453	3.691848
78	6	0	0.467485	4.971077	0.233941
79	1	0	-0.477286	4.886889	0.762128
80	1	0	1.272466	4.910255	0.959376
81	1	0	0.507955	5.945714	-0.243224
82	6	0	-0.500010	3.892441	-1.915482
83	1	0	-0.456003	4.831559	-2.458725
84	1	0	-0.369567	3.079347	-2.622860
85	1	0	-1.484807	3.803443	-1.467233
86	6	0	5.319868	1.320515	-2.352646
87	6	0	5.181929	1.210760	-3.778127
88	1	0	4.414810	0.979237	-0.467684
89	1	0	6.001350	1.556202	-4.394575
90	1	0	3.922641	0.619478	-5.383022
91	6	0	3.912498	-2.204583	4.492183
92	1	0	4.596779	-1.817415	5.234702
93	1	0	2.875523	-1.937568	4.638591
94	1	0	5.399209	-3.177348	3.431923
95	7	0	-1.068179	-3.167990	1.120810

96	6	0	-2.133126	-2.694912	1.226373
97	6	0	-3.383598	-2.037674	1.276520
98	6	0	-4.544207	-2.825194	1.516913
99	7	0	-5.528576	-3.434570	1.668492
100	1	0	-3.355234	-1.082987	1.793463
101	8	0	6.538232	1.877916	-1.958900
102	6	0	6.671240	2.101073	-0.550011
103	1	0	6.659445	1.167138	0.019582
104	1	0	7.640123	2.582295	-0.404938
105	1	0	5.891059	2.760493	-0.158960

A-TS2-*Re*-2

Energy+zep = -2521.623160 au

Gibbs free energy = -2521.715878 au

Number of imaginary frequencies: 1 (-1306.2278 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.246036	2.292723	-0.499185
2	6	0	-1.478100	1.482878	-0.850058
3	6	0	-0.726967	3.588301	0.072224
4	6	0	0.592018	2.569209	-1.718320
5	6	0	-1.221952	-0.051921	-0.890996
6	6	0	-2.111875	2.096899	-2.122492
7	6	0	-1.708806	4.314421	-0.915618
8	6	0	-0.156157	3.508044	-2.696753
9	1	0	-1.210553	3.369958	1.029794
10	1	0	0.148308	4.207154	0.269550
11	1	0	1.521663	3.022687	-1.375260
12	1	0	0.813436	1.601240	-2.160793
13	8	0	-0.064393	-0.352039	-1.600321
14	6	0	-2.456270	-0.803375	-1.492504
15	6	0	-1.634828	3.554327	-2.273447
16	1	0	-1.813727	1.525488	-3.008379
17	1	0	-3.202303	2.031356	-2.052535
18	1	0	-1.319929	5.325022	-1.089374
19	1	0	0.276459	4.514893	-2.684707
20	1	0	-0.063029	3.127160	-3.719369
21	1	0	-1.134720	-0.379863	0.157328
22	6	0	-2.373079	-1.309187	-2.741950
23	6	0	-3.691930	-1.000129	-0.766588

24	1	0	-2.234468	4.079562	-3.023667
25	6	0	-3.483812	-1.997264	-3.324440
26	6	0	-4.732714	-1.683883	-1.420960
27	1	0	-1.456681	-1.198437	-3.305420
28	6	0	-3.913302	-0.555656	0.565857
29	7	0	-4.637144	-2.191070	-2.725883
30	1	0	-3.385173	-2.389109	-4.334578
31	6	0	-5.967314	-1.890824	-0.736902
32	1	0	-2.163174	1.648801	-0.013394
33	13	0	1.213911	-1.460820	-1.072373
34	6	0	2.998785	1.224398	0.827600
35	6	0	1.543214	1.193617	1.369918
36	6	0	0.982497	-0.109244	1.542231
37	8	0	1.283529	-1.069007	0.742881
38	1	0	1.403025	1.835465	2.240832
39	1	0	3.008301	1.084192	-0.256335
40	7	0	2.453625	4.787094	0.372141
41	6	0	2.993055	3.809747	0.688238
42	6	0	3.697671	2.600411	1.145881
43	8	0	2.729054	-0.985288	-1.816585
44	8	0	0.735719	-3.114625	-1.190989
45	6	0	3.162924	-1.248087	-3.140446
46	6	0	1.151330	-4.342079	-0.652485
47	1	0	2.818185	-2.249859	-3.450201
48	1	0	1.325529	-4.238903	0.435220
49	6	0	0.011174	-5.389607	-0.858704
50	1	0	-0.182857	-5.527402	-1.917644
51	1	0	0.280967	-6.348755	-0.426161
52	1	0	-0.901423	-5.039542	-0.386545
53	6	0	2.491931	-4.822275	-1.304928
54	1	0	2.363700	-4.943763	-2.375871
55	1	0	3.274438	-4.088689	-1.134916
56	1	0	2.814625	-5.770635	-0.885740
57	6	0	2.554533	-0.202054	-4.133572
58	1	0	2.887718	0.798327	-3.875537
59	1	0	2.855870	-0.412003	-5.155488
60	1	0	1.469858	-0.227005	-4.083192
61	6	0	4.722302	-1.238262	-3.190855
62	1	0	5.073861	-1.436519	-4.199047
63	1	0	5.105642	-0.273192	-2.874328
64	1	0	5.122415	-2.001315	-2.530854
65	6	0	-0.030722	-0.442648	2.613945
66	6	0	-0.414747	-1.775872	2.758321
67	6	0	-0.590481	0.519209	3.455361

68	6	0	-1.335323	-2.143950	3.724715
69	1	0	0.021910	-2.518765	2.101861
70	6	0	-1.517152	0.152151	4.415599
71	1	0	-0.314117	1.560484	3.361089
72	6	0	-1.888865	-1.178699	4.553584
73	1	0	-1.623280	-3.182093	3.829405
74	1	0	-1.951714	0.905651	5.059632
75	1	0	-2.612760	-1.462143	5.308376
76	6	0	3.890525	0.101414	1.439838
77	6	0	4.371149	-0.912613	0.621485
78	6	0	4.204653	0.085436	2.796628
79	6	0	5.171202	-1.915950	1.150222
80	1	0	4.066376	-0.930050	-0.424517
81	6	0	5.004083	-0.914736	3.321389
82	1	0	3.822408	0.853427	3.455971
83	6	0	5.495989	-1.916241	2.496554
84	1	0	5.539636	-2.704152	0.505600
85	1	0	5.244004	-0.914084	4.376999
86	1	0	6.122661	-2.697883	2.906824
87	6	0	-3.134588	4.463465	-0.361793
88	1	0	-3.635770	3.546355	-0.074616
89	6	0	-3.746769	5.612089	-0.227790
90	1	0	-3.280749	6.549490	-0.500572
91	1	0	-4.752644	5.681901	0.163374
92	6	0	-6.159719	-1.450761	0.530131
93	6	0	-5.103233	-0.767238	1.205154
94	1	0	-6.752941	-2.416943	-1.265608
95	1	0	-7.103819	-1.622096	1.023220
96	1	0	-3.131823	-0.046728	1.108003
97	1	0	0.617587	1.701945	0.437568
98	6	0	5.075431	2.626042	0.618521
99	7	0	6.161562	2.640819	0.211407
100	1	0	3.772424	2.700431	2.236002
101	8	0	-5.174210	-0.272289	2.514625
102	6	0	-6.419825	-0.501682	3.184448
103	1	0	-6.644751	-1.566402	3.294586
104	1	0	-6.316249	-0.065902	4.179937
105	1	0	-7.260449	-0.016006	2.680633

A-TS1-*Si*-2

Energy+zep = -2521.626616 au

Gibbs free energy = -2521.724098 au

Number of imaginary frequencies: 1 (-270.4761 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.517362	-0.748734	1.692019
2	7	0	1.330220	-1.317029	1.999255
3	6	0	2.558836	-0.562232	1.514039
4	6	0	1.370876	-1.408132	3.499760
5	6	0	1.221480	-2.701839	1.408709
6	6	0	2.217565	0.172970	0.176234
7	6	0	3.762920	-1.511850	1.649070
8	6	0	2.719663	-2.075435	3.932245
9	6	0	2.381331	-3.565951	1.951903
10	1	0	1.260642	-0.392524	3.884265
11	1	0	0.493619	-1.979882	3.804642
12	1	0	0.233514	-3.073252	1.679295
13	1	0	1.259511	-2.585424	0.327173
14	8	0	0.939937	0.677032	0.388750
15	6	0	2.310731	-0.661907	-1.144773
16	6	0	3.398738	-2.638267	2.644571
17	1	0	4.024785	-1.959875	0.685022
18	1	0	4.637196	-0.948392	1.985938
19	1	0	2.477163	-2.937359	4.564059
20	1	0	2.008953	-4.316934	2.656626
21	1	0	2.856393	-4.106563	1.127386
22	6	0	3.620251	-1.141593	4.755201
23	1	0	2.960148	0.981652	0.096025
24	13	0	0.083484	2.020763	-0.448631
25	6	0	3.550844	-0.882411	-1.850404
26	6	0	1.175320	-1.152389	-1.698947
27	1	0	4.295324	-3.200394	2.921363
28	8	0	-0.368236	3.267316	0.674976
29	6	0	3.501984	-1.632989	-3.036849
30	6	0	1.223013	-1.898491	-2.912954
31	6	0	4.813554	-0.362483	-1.417942
32	1	0	0.217203	-0.968055	-1.231429
33	6	0	0.299345	4.324517	1.304841
34	7	0	2.327034	-2.163477	-3.578985
35	6	0	4.714797	-1.878395	-3.763581
36	1	0	0.295318	-2.287708	-3.326434
37	1	0	0.127402	5.255504	0.734781
38	8	0	1.102352	2.424550	-1.798032
39	6	0	0.947492	3.114071	-3.009004

40	1	0	1.952560	3.259750	-3.440794
41	6	0	-4.430136	-0.757069	-0.181172
42	6	0	-3.174832	-0.320913	-0.696511
43	6	0	-2.575277	0.892966	-0.397343
44	8	0	-1.444523	1.204483	-0.978105
45	1	0	-2.635703	-0.945611	-1.401167
46	1	0	-4.932729	-0.029946	0.453623
47	1	0	2.649674	0.251726	2.238066
48	6	0	-5.389704	-1.590419	-0.991130
49	6	0	-4.958112	-2.469880	-1.984272
50	6	0	-6.759525	-1.472993	-0.750723
51	6	0	-5.873425	-3.205840	-2.718261
52	1	0	-3.901374	-2.581877	-2.185216
53	6	0	-7.673760	-2.206049	-1.487074
54	1	0	-7.108689	-0.794448	0.017393
55	6	0	-7.232292	-3.075567	-2.473384
56	1	0	-5.523885	-3.885314	-3.485037
57	1	0	-8.733043	-2.099166	-1.291637
58	1	0	-7.945778	-3.650898	-3.049814
59	6	0	-3.222300	1.975896	0.464577
60	6	0	-3.540095	1.784822	1.804653
61	6	0	-3.490277	3.210698	-0.124381
62	6	0	-4.122138	2.806057	2.540803
63	1	0	-3.320186	0.839251	2.280964
64	6	0	-4.079209	4.226809	0.608528
65	1	0	-3.239082	3.370288	-1.165723
66	6	0	-4.397457	4.025567	1.944159
67	1	0	-4.361392	2.646889	3.584539
68	1	0	-4.289057	5.179058	0.138181
69	1	0	-4.856116	4.820355	2.518644
70	6	0	1.852176	4.098234	1.365438
71	1	0	2.358358	4.939898	1.828540
72	1	0	2.080482	3.204897	1.939289
73	1	0	2.246778	3.972025	0.361053
74	6	0	-0.297834	4.529209	2.735987
75	1	0	0.149072	5.388721	3.227513
76	1	0	-1.368866	4.687474	2.663912
77	1	0	-0.123428	3.650398	3.349217
78	6	0	0.320485	4.535394	-2.794866
79	1	0	-0.682170	4.452743	-2.385184
80	1	0	0.927583	5.104137	-2.097522
81	1	0	0.263082	5.086094	-3.729031
82	6	0	0.110938	2.266865	-4.027978
83	1	0	0.034556	2.765638	-4.989705

84	1	0	0.586430	1.302609	-4.176747
85	1	0	-0.891732	2.097187	-3.646612
86	6	0	5.946968	-0.595509	-2.133852
87	6	0	5.892123	-1.384358	-3.332715
88	1	0	4.847600	0.234083	-0.523879
89	1	0	6.815546	-1.553749	-3.870561
90	1	0	4.647109	-2.466655	-4.670483
91	6	0	4.078152	-1.442035	5.943383
92	1	0	4.715673	-0.764989	6.496442
93	1	0	3.844489	-2.378281	6.433618
94	1	0	3.872416	-0.192744	4.297000
95	7	0	-1.691912	-1.453882	2.196355
96	6	0	-2.784941	-1.771738	1.934213
97	6	0	-4.098540	-2.086130	1.496675
98	6	0	-4.278031	-3.442396	1.076892
99	7	0	-4.435478	-4.530380	0.686037
100	1	0	-4.887535	-1.719040	2.150549
101	8	0	7.233991	-0.146703	-1.828549
102	6	0	7.314537	0.726180	-0.695558
103	1	0	8.359904	1.029496	-0.614460
104	1	0	6.699015	1.622162	-0.817238
105	1	0	7.025977	0.225836	0.233529

A-TS2-*Si*-2

Energy+zep = -2521.599225 au

Gibbs free energy = -2521.692404 au

Number of imaginary frequencies: 1 (-1422.7800 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.087609	-1.272901	0.010485
2	7	0	-0.007013	-2.109933	0.282815
3	6	0	1.239869	-1.601379	0.995763
4	6	0	-0.646164	-3.115652	1.196405
5	6	0	0.351148	-2.796199	-1.001644
6	6	0	1.881450	-0.233315	0.599908
7	6	0	2.287031	-2.748429	1.009587
8	6	0	0.349027	-4.220075	1.654522
9	6	0	1.127042	-4.108105	-0.725508
10	1	0	-1.084603	-2.569815	2.030171
11	1	0	-1.463887	-3.570429	0.637709

12	1	0	-0.572936	-2.987643	-1.547934
13	1	0	0.945739	-2.097663	-1.586516
14	8	0	1.038443	0.802493	0.964463
15	6	0	2.436780	-0.093533	-0.862808
16	6	0	1.596970	-4.094469	0.740217
17	1	0	3.052955	-2.578103	0.244192
18	1	0	2.798694	-2.753937	1.977473
19	1	0	-0.115037	-5.195101	1.437926
20	1	0	0.494023	-4.982225	-0.915389
21	1	0	1.986377	-4.180738	-1.400755
22	6	0	0.737937	-4.261507	3.146701
23	1	0	2.754121	-0.214648	1.270719
24	13	0	0.383191	2.322619	0.371373
25	6	0	3.838986	-0.229089	-1.193559
26	6	0	1.592228	0.234217	-1.873511
27	1	0	2.285391	-4.924489	0.928427
28	8	0	-0.247958	3.294504	1.662816
29	6	0	4.217314	-0.042231	-2.535140
30	6	0	2.069870	0.409224	-3.203883
31	6	0	4.863017	-0.532060	-0.236955
32	1	0	0.536998	0.374325	-1.689746
33	6	0	0.220797	3.660787	2.934868
34	7	0	3.327743	0.275112	-3.565556
35	6	0	5.597347	-0.174397	-2.905907
36	1	0	1.358728	0.665031	-3.985960
37	1	0	-0.514298	4.358375	3.370290
38	8	0	1.318746	3.071120	-0.868336
39	6	0	1.311424	4.260333	-1.611791
40	1	0	1.341268	3.993941	-2.683106
41	6	0	-3.672935	-0.959057	-0.618989
42	6	0	-2.183850	-0.534130	-0.559808
43	6	0	-1.974432	0.764288	0.030691
44	8	0	-1.104874	1.547098	-0.478548
45	1	0	-1.735749	-0.545762	-1.556715
46	1	0	-4.189716	-0.500979	0.227487
47	1	0	0.893973	-1.412248	2.016156
48	6	0	-4.365512	-0.403311	-1.897244
49	6	0	-3.934881	-0.752886	-3.174790
50	6	0	-5.443176	0.465082	-1.769944
51	6	0	-4.569920	-0.245695	-4.295703
52	1	0	-3.097084	-1.425509	-3.301029
53	6	0	-6.078401	0.976962	-2.891875
54	1	0	-5.791173	0.748364	-0.784763
55	6	0	-5.644012	0.622100	-4.158005

56	1	0	-4.224046	-0.527761	-5.282257
57	1	0	-6.914736	1.654422	-2.773773
58	1	0	-6.138059	1.019715	-5.035307
59	6	0	-2.706980	1.241932	1.270146
60	6	0	-2.994258	0.388290	2.333100
61	6	0	-3.083194	2.580942	1.346524
62	6	0	-3.650139	0.866530	3.454089
63	1	0	-2.693869	-0.650027	2.290396
64	6	0	-3.753970	3.054895	2.463327
65	1	0	-2.856945	3.249102	0.524326
66	6	0	-4.035278	2.199112	3.517552
67	1	0	-3.862912	0.198688	4.278932
68	1	0	-4.050555	4.094748	2.511620
69	1	0	-4.553607	2.570648	4.393237
70	6	0	1.589594	4.419144	2.845942
71	1	0	1.915037	4.758843	3.824606
72	1	0	2.359162	3.771259	2.435749
73	1	0	1.488537	5.283933	2.197893
74	6	0	0.318478	2.414868	3.880093
75	1	0	0.656804	2.697445	4.872567
76	1	0	-0.655977	1.945723	3.969240
77	1	0	1.011760	1.686925	3.469057
78	6	0	2.600003	5.089529	-1.297098
79	1	0	2.604911	5.408871	-0.259636
80	1	0	3.477538	4.475075	-1.471321
81	1	0	2.661723	5.969899	-1.930158
82	6	0	0.010598	5.100630	-1.369413
83	1	0	0.010272	6.010017	-1.962523
84	1	0	-0.862426	4.515611	-1.644097
85	1	0	-0.074089	5.372097	-0.321103
86	6	0	6.165786	-0.643358	-0.612314
87	6	0	6.538378	-0.464988	-1.987008
88	1	0	4.588104	-0.660431	0.794043
89	1	0	7.583581	-0.565211	-2.247819
90	1	0	5.851718	-0.028214	-3.948397
91	6	0	0.260672	-3.545668	4.131496
92	1	0	0.607835	-3.689944	5.145169
93	1	0	-0.495730	-2.784606	4.007584
94	1	0	1.491393	-5.013684	3.355953
95	7	0	-2.776890	-4.135489	-2.059596
96	6	0	-3.334940	-3.411997	-1.344021
97	6	0	-4.061050	-2.487867	-0.460405
98	6	0	-3.998496	-2.939604	0.940334
99	1	0	-5.119643	-2.564184	-0.746276

100	7	0	-4.003390	-3.249858	2.058468
101	8	0	7.251342	-0.931359	0.219230
102	6	0	6.927596	-1.065487	1.608103
103	1	0	7.868493	-1.261194	2.125594
104	1	0	6.485372	-0.154277	2.021180
105	1	0	6.247413	-1.901332	1.796337

N-COM-*Re*-1

Energy+zep = -1895.218940 au

Gibbs free energy = -1895.301520 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.399353	0.674256	1.557496
2	7	0	0.989832	1.453693	1.092304
3	6	0	1.602199	1.078417	-0.245702
4	6	0	0.037960	2.598515	0.856015
5	6	0	2.016469	1.862433	2.116527
6	6	0	2.060853	-0.403749	-0.380315
7	6	0	2.634624	2.172334	-0.595772
8	6	0	0.789064	3.782319	0.164220
9	6	0	2.686271	3.184298	1.679509
10	1	0	-0.778762	2.203555	0.249440
11	1	0	-0.369925	2.872964	1.830624
12	1	0	1.486826	1.934751	3.067875
13	1	0	2.727773	1.042606	2.196806
14	8	0	0.958842	-1.265220	-0.193814
15	6	0	3.172239	-0.915446	0.570589
16	6	0	2.311837	3.451259	0.208489
17	1	0	3.651186	1.847272	-0.347874
18	1	0	2.613222	2.358960	-1.673250
19	1	0	0.642151	4.679016	0.777485
20	1	0	2.359578	4.016888	2.311793
21	1	0	3.772472	3.104180	1.789857
22	6	0	0.258848	4.097306	-1.243240
23	1	0	2.420554	-0.462600	-1.419783
24	6	0	2.809253	-1.466154	1.756586
25	6	0	4.573531	-0.886591	0.231081
26	1	0	2.884366	4.298222	-0.180975
27	6	0	3.801917	-1.965462	2.649756

28	6	0	5.476643	-1.397483	1.179309
29	1	0	1.764531	-1.531176	2.036381
30	6	0	5.090146	-0.389221	-1.009356
31	7	0	5.096690	-1.938931	2.410095
32	1	0	3.485647	-2.393853	3.598014
33	6	0	6.882756	-1.383612	0.890567
34	1	0	0.759372	1.153174	-0.936890
35	6	0	7.344954	-0.902366	-0.279620
36	6	0	6.427016	-0.398723	-1.263377
37	1	0	4.401734	-0.021451	-1.748626
38	1	0	8.400488	-0.887489	-0.516866
39	1	0	7.553464	-1.777724	1.644312
40	6	0	-0.149054	5.284149	-1.612986
41	1	0	0.233726	3.269816	-1.942282
42	1	0	-0.514443	5.475407	-2.613182
43	1	0	-0.144249	6.132652	-0.941207
44	8	0	7.058399	0.049958	-2.424468
45	6	0	6.174662	0.501936	-3.457542
46	1	0	5.591036	1.374698	-3.150303
47	1	0	6.807285	0.787340	-4.299937
48	1	0	5.487061	-0.282234	-3.787346
49	1	0	0.206575	-0.987328	-0.758001
50	6	0	-4.803043	-0.428207	-0.884581
51	6	0	-3.558787	0.066556	-1.108974
52	6	0	-2.353018	-0.740116	-1.257016
53	6	0	-2.364939	-2.271328	-1.246588
54	8	0	-1.259115	-0.168925	-1.435485
55	6	0	-1.740208	-2.935783	-2.299777
56	6	0	-2.914470	-3.009363	-0.202877
57	6	0	-6.055608	0.359314	-0.717041
58	1	0	-3.381824	1.135717	-1.168878
59	6	0	-6.149481	1.709045	-1.062666
60	1	0	-4.924526	-1.502688	-0.787943
61	6	0	-7.184144	-0.278369	-0.196526
62	6	0	-7.336120	2.399638	-0.890026
63	6	0	-8.448048	1.755966	-0.366214
64	6	0	-8.369088	0.415657	-0.018644
65	1	0	-7.119002	-1.322510	0.083971
66	1	0	-5.292021	2.221224	-1.477789
67	1	0	-7.395636	3.444593	-1.165698
68	1	0	-9.375057	2.298905	-0.230508
69	1	0	-9.233092	-0.090216	0.392662
70	6	0	-1.683060	-4.318468	-2.323405
71	6	0	-2.237959	-5.050838	-1.283758

72	6	0	-2.846966	-4.395185	-0.225360
73	1	0	-2.191240	-6.132576	-1.297975
74	1	0	-3.273183	-4.962689	0.592214
75	1	0	-3.388682	-2.509756	0.634550
76	1	0	-1.301235	-2.362675	-3.106961
77	1	0	-1.202830	-4.825767	-3.150206
78	7	0	-0.546539	-0.080351	2.650051
79	6	0	-1.671469	-0.116408	3.018589
80	6	0	-2.976963	-0.160253	3.460911
81	1	0	-3.242064	0.337498	4.386356
82	6	0	-3.960180	-0.846513	2.737668
83	7	0	-4.779622	-1.419340	2.117845

N-COM-*Si*-1

Energy+zep = -1895.222705 au

Gibbs free energy = -1895.304180 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.529260	1.815392	1.502628
2	7	0	1.523720	2.139768	1.254470
3	6	0	1.978759	1.774125	-0.148121
4	6	0	1.520191	3.641541	1.362678
5	6	0	2.417328	1.570810	2.328974
6	6	0	1.427068	0.434212	-0.690420
7	6	0	3.502358	2.003265	-0.206441
8	6	0	2.930259	4.203979	0.983524
9	6	0	3.808038	2.238183	2.253193
10	1	0	0.727120	4.005565	0.707007
11	1	0	1.236585	3.880443	2.389306
12	1	0	1.899132	1.738620	3.274242
13	1	0	2.462233	0.495803	2.165827
14	8	0	0.038468	0.665345	-0.805139
15	6	0	1.734556	-0.865373	0.106975
16	6	0	3.907265	2.990422	0.911821
17	1	0	4.048185	1.063462	-0.065297
18	1	0	3.772236	2.382563	-1.196246
19	1	0	3.271343	4.836863	1.810906
20	1	0	3.958005	2.929186	3.089724
21	1	0	4.589246	1.474601	2.323531

22	6	0	2.919882	5.075037	-0.282266
23	1	0	1.877931	0.352866	-1.691577
24	6	0	0.890607	-1.241479	1.100199
25	6	0	2.850300	-1.727393	-0.200699
26	1	0	4.927963	3.348954	0.750385
27	6	0	1.126658	-2.443265	1.830882
28	6	0	3.002920	-2.887906	0.577147
29	1	0	0.033387	-0.632359	1.361631
30	6	0	3.794203	-1.475796	-1.248549
31	7	0	2.138769	-3.256496	1.612140
32	1	0	0.437008	-2.715720	2.626603
33	6	0	4.101679	-3.772888	0.313420
34	1	0	1.476566	2.510500	-0.780085
35	6	0	4.979775	-3.511641	-0.674342
36	6	0	4.821758	-2.336417	-1.484945
37	1	0	3.671811	-0.600226	-1.860082
38	1	0	5.811931	-4.168469	-0.890615
39	1	0	4.194180	-4.656154	0.933598
40	6	0	3.365120	6.304823	-0.316408
41	1	0	2.516696	4.616959	-1.177459
42	1	0	3.348051	6.892380	-1.224748
43	1	0	3.770782	6.797497	0.557702
44	8	0	5.803737	-2.212059	-2.469014
45	6	0	5.644858	-1.088722	-3.343834
46	1	0	5.720748	-0.135867	-2.811796
47	1	0	6.458769	-1.146348	-4.068767
48	1	0	4.693952	-1.114954	-3.883815
49	1	0	-0.434920	-0.139532	-1.114494
50	7	0	-0.793961	1.512253	2.431015
51	6	0	-1.849290	1.246114	2.892713
52	6	0	-3.074739	0.926625	3.439297
53	1	0	-3.275657	1.167941	4.476350
54	6	0	-4.052333	0.286019	2.671292
55	7	0	-4.866183	-0.254834	2.015647
56	6	0	-3.353079	0.453936	-1.721569
57	6	0	-3.473847	-0.631746	-0.919950
58	6	0	-2.483514	-1.718534	-0.946193
59	6	0	-2.844796	-3.076631	-0.351076
60	8	0	-1.356035	-1.580906	-1.450114
61	6	0	-2.181135	-4.201659	-0.837035
62	6	0	-3.779752	-3.223538	0.670874
63	6	0	-4.294036	1.607461	-1.789136
64	1	0	-4.318949	-0.736689	-0.255351
65	6	0	-5.267937	1.829571	-0.811824

66	1	0	-2.504383	0.485116	-2.405365
67	6	0	-4.199846	2.500923	-2.858307
68	6	0	-6.124841	2.912818	-0.914323
69	6	0	-6.026778	3.787634	-1.986715
70	6	0	-5.060203	3.579952	-2.959257
71	1	0	-3.445009	2.341807	-3.618019
72	1	0	-5.345199	1.163514	0.040370
73	1	0	-6.872696	3.076784	-0.148990
74	1	0	-6.699830	4.632412	-2.062043
75	1	0	-4.977045	4.260802	-3.796484
76	6	0	-2.455669	-5.457576	-0.325821
77	6	0	-3.391840	-5.599155	0.688944
78	6	0	-4.045844	-4.483173	1.187619
79	1	0	-3.607542	-6.580234	1.093649
80	1	0	-4.768122	-4.590709	1.986693
81	1	0	-4.287177	-2.359334	1.086692
82	1	0	-1.447091	-4.078659	-1.623695
83	1	0	-1.939905	-6.326009	-0.714619

N-COM-*Re*-2

Energy+zep = -1895.216190 au

Gibbs free energy = -1895.299357 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.110082	0.542781	1.722684
2	7	0	-0.635395	-0.174141	1.995821
3	6	0	-1.115036	-1.028442	0.832869
4	6	0	0.023033	-1.079873	3.005878
5	6	0	-1.755164	0.586132	2.663752
6	6	0	-1.207434	-0.270664	-0.526357
7	6	0	-2.364634	-1.794840	1.317765
8	6	0	-0.950061	-2.228116	3.392261
9	6	0	-2.689444	-0.417228	3.374653
10	1	0	0.954075	-1.422472	2.557549
11	1	0	0.281987	-0.451711	3.859788
12	1	0	-1.286677	1.303023	3.339249
13	1	0	-2.264350	1.152563	1.886306
14	8	0	0.021246	0.379217	-0.781147
15	6	0	-2.319022	0.792160	-0.706721

16	6	0	-2.361912	-1.833036	2.861756
17	1	0	-3.283591	-1.309366	0.973304
18	1	0	-2.355671	-2.804229	0.895955
19	1	0	-1.021786	-2.244649	4.490233
20	1	0	-2.561878	-0.367545	4.461509
21	1	0	-3.733003	-0.164449	3.162516
22	1	0	-1.371940	-1.077665	-1.257295
23	6	0	-2.050334	2.090232	-0.437106
24	6	0	-3.630570	0.460786	-1.219982
25	1	0	-3.105735	-2.548634	3.223863
26	6	0	-3.055450	3.096300	-0.615217
27	6	0	-4.550436	1.514996	-1.368395
28	1	0	-1.072489	2.394069	-0.085580
29	6	0	-4.041591	-0.846951	-1.598808
30	7	0	-4.270673	2.853395	-1.053259
31	1	0	-2.803585	4.125117	-0.358709
32	6	0	-5.855214	1.234017	-1.873179
33	1	0	0.761135	-0.259899	-0.735156
34	6	0	3.506796	0.991860	-0.712535
35	6	0	3.941597	-0.230611	-1.117585
36	6	0	3.238478	-1.468163	-0.765315
37	8	0	2.050539	-1.497498	-0.408376
38	1	0	4.849536	-0.337613	-1.699078
39	1	0	2.628219	1.040511	-0.068312
40	1	0	-0.296663	-1.739332	0.689329
41	6	0	3.989466	-2.798381	-0.849937
42	6	0	5.374709	-2.880195	-0.741487
43	6	0	3.252706	-3.969472	-1.009406
44	6	0	6.009764	-4.110934	-0.797496
45	1	0	5.962831	-1.983071	-0.599225
46	6	0	3.886455	-5.198749	-1.072876
47	1	0	2.174559	-3.904359	-1.086730
48	6	0	5.268167	-5.270552	-0.967260
49	1	0	7.087213	-4.165273	-0.707440
50	1	0	3.304777	-6.102216	-1.204273
51	1	0	5.766753	-6.230739	-1.015024
52	6	0	4.133505	2.307997	-1.012038
53	6	0	5.212950	2.452209	-1.887861
54	6	0	3.613743	3.447750	-0.394669
55	6	0	5.755803	3.699818	-2.134759
56	1	0	5.628698	1.585564	-2.383767
57	6	0	4.159774	4.696775	-0.642288
58	1	0	2.777135	3.345787	0.286350
59	6	0	5.231409	4.825018	-1.512490

60	1	0	6.590606	3.798157	-2.816570
61	1	0	3.745162	5.570374	-0.155537
62	1	0	5.658444	5.800707	-1.708815
63	6	0	-0.563594	-3.660053	2.969978
64	1	0	-1.301359	-4.391204	3.282242
65	6	0	0.506207	-4.058953	2.332474
66	1	0	1.288278	-3.394893	1.992838
67	1	0	0.662747	-5.105843	2.111573
68	7	0	1.255001	1.801193	1.908431
69	6	0	0.876581	2.868191	2.271315
70	6	0	0.408790	4.098994	2.668955
71	6	0	-5.294991	-1.093382	-2.086680
72	6	0	-6.228152	-0.020863	-2.221992
73	1	0	-3.362264	-1.680679	-1.518480
74	1	0	-7.220815	-0.203616	-2.602950
75	1	0	-6.543117	2.065171	-1.972150
76	6	0	-0.480478	4.813786	1.846240
77	7	0	-1.236020	5.391822	1.158486
78	1	0	0.725361	4.518386	3.616555
79	8	0	-5.555333	-2.431065	-2.409240
80	6	0	-6.839131	-2.676906	-2.996883
81	1	0	-6.871552	-3.744233	-3.223444
82	1	0	-7.661216	-2.443327	-2.314181
83	1	0	-6.985620	-2.120249	-3.926829

N-COM-*Si*-2

Energy+zep = -1895.219120 au

Gibbs free energy = -1895.300726 au

Number of imaginary frequencies: 0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.585793	-1.976626	-1.141933
2	7	0	2.639338	-1.751056	-1.092157
3	6	0	3.085648	-1.065873	0.188596
4	6	0	3.357364	-3.072397	-1.182990
5	6	0	2.948169	-0.940198	-2.325548
6	6	0	2.042298	-0.113728	0.817879
7	6	0	4.506288	-0.519965	-0.059293
8	6	0	4.888927	-2.847335	-1.027703
9	6	0	4.477124	-0.879339	-2.527939

10	1	0	2.925562	-3.717147	-0.419474
11	1	0	3.100551	-3.500083	-2.153754
12	1	0	2.412694	-1.418037	-3.147372
13	1	0	2.509770	0.044827	-2.176140
14	8	0	0.982615	-0.969652	1.186249
15	6	0	1.546206	1.093583	-0.029049
16	6	0	5.149703	-1.320705	-1.213921
17	1	0	4.484746	0.543149	-0.324541
18	1	0	5.089283	-0.611347	0.862050
19	1	0	5.383852	-3.353532	-1.870584
20	1	0	4.791749	-1.528082	-3.352710
21	1	0	4.775941	0.140710	-2.789658
22	6	0	5.562262	-3.389979	0.249388
23	1	0	2.547081	0.267943	1.718966
24	1	0	0.224103	-0.474006	1.566157
25	6	0	2.136027	2.407616	0.061214
26	6	0	0.478857	0.927384	-0.849515
27	1	0	6.226401	-1.132464	-1.254723
28	6	0	1.578466	3.421778	-0.736033
29	6	0	-0.019825	2.021556	-1.616372
30	6	0	3.238125	2.735552	0.915675
31	1	0	-0.005973	-0.036860	-0.942356
32	7	0	0.490120	3.235232	-1.593128
33	6	0	2.135521	4.743576	-0.685243
34	1	0	-0.873026	1.856175	-2.270495
35	1	0	3.138677	-1.881997	0.913522
36	6	0	3.741457	3.999513	0.952917
37	6	0	3.176073	5.026116	0.122497
38	1	0	3.656721	1.968973	1.542354
39	1	0	3.607165	6.017002	0.177159
40	1	0	1.686365	5.501610	-1.315306
41	6	0	5.034752	-4.123086	1.195077
42	1	0	5.628202	-4.459855	2.034009
43	1	0	4.001666	-4.440222	1.204784
44	1	0	6.611541	-3.121393	0.306371
45	6	0	-4.512577	0.498449	0.541283
46	6	0	-3.440432	0.887988	1.275816
47	6	0	-2.428119	-0.067984	1.735085
48	8	0	-1.270151	0.323588	1.946328
49	1	0	-3.187937	1.933544	1.424953
50	1	0	-4.634095	-0.561681	0.323054
51	6	0	-5.512745	1.384115	-0.118395
52	6	0	-5.685620	2.724151	0.232931
53	6	0	-6.306389	0.845524	-1.133705

54	6	0	-6.626513	3.504642	-0.415647
55	1	0	-5.086852	3.156381	1.023694
56	6	0	-7.242627	1.630932	-1.785466
57	1	0	-6.165612	-0.192926	-1.413306
58	6	0	-7.405686	2.960805	-1.426886
59	1	0	-6.754373	4.541311	-0.131987
60	1	0	-7.847787	1.204470	-2.575146
61	1	0	-8.140223	3.574037	-1.933694
62	6	0	-2.794916	-1.533617	1.976746
63	6	0	-1.953614	-2.551813	1.538616
64	6	0	-3.947247	-1.861297	2.687253
65	6	0	-2.268908	-3.877214	1.795430
66	1	0	-1.056529	-2.312464	0.981546
67	6	0	-4.254331	-3.184839	2.953677
68	1	0	-4.603086	-1.075019	3.038758
69	6	0	-3.417016	-4.195450	2.504071
70	1	0	-1.616570	-4.663336	1.437534
71	1	0	-5.150185	-3.429171	3.509918
72	1	0	-3.661282	-5.231032	2.705073
73	7	0	0.163120	-2.473223	-1.762764
74	6	0	-0.922271	-2.713164	-2.167469
75	6	0	-2.179546	-2.999595	-2.650076
76	8	0	4.804396	4.450744	1.737046
77	6	0	5.353967	3.474916	2.630452
78	1	0	6.142331	3.980776	3.190713
79	1	0	4.611109	3.095673	3.338140
80	1	0	5.795768	2.627997	2.097261
81	6	0	-3.333756	-2.490021	-2.039046
82	7	0	-4.310081	-2.066129	-1.540622
83	1	0	-2.276478	-3.632080	-3.524970

N-TS1-*Re*-1

Energy+zep = -1895.209492 au

Gibbs free energy = -1895.288321 au

Number of imaginary frequencies: 1 (-248.2782 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.003067	-0.175195	-0.643212
2	7	0	0.641613	-0.663501	-1.360121
3	6	0	2.091383	-0.382407	-0.990998

4	6	0	0.441910	-2.155613	-1.386806
5	6	0	0.251948	-0.092132	-2.711552
6	6	0	2.260469	0.996156	-0.280290
7	6	0	2.938900	-0.672782	-2.244480
8	6	0	1.495069	-2.798831	-2.353170
9	6	0	1.022920	-0.834775	-3.823638
10	1	0	0.545789	-2.516624	-0.360497
11	1	0	-0.583745	-2.331448	-1.716421
12	1	0	-0.828213	-0.221276	-2.791122
13	1	0	0.490363	0.968069	-2.676042
14	8	0	1.600938	2.044338	-0.970179
15	6	0	3.759375	1.354080	-0.124572
16	6	0	2.157175	-1.640452	-3.163795
17	1	0	3.150208	0.253905	-2.789607
18	1	0	3.902480	-1.091872	-1.939569
19	1	0	0.942499	-3.413817	-3.072365
20	1	0	0.354984	-1.499100	-4.381598
21	1	0	1.431634	-0.110095	-4.534991
22	1	0	1.801807	0.895119	0.711027
23	6	0	4.318608	2.256949	-0.964691
24	6	0	4.589827	0.758022	0.891370
25	1	0	2.821291	-2.060476	-3.925029
26	6	0	5.701794	2.584399	-0.847009
27	6	0	5.941575	1.137604	0.924826
28	1	0	3.720788	2.741478	-1.724708
29	7	0	6.516086	2.059072	0.044043
30	1	0	6.129695	3.309931	-1.534966
31	1	0	2.324131	-1.134009	-0.231714
32	6	0	2.500800	-3.719301	-1.644026
33	6	0	6.806152	0.564349	1.916561
34	6	0	4.110170	-0.177674	1.862903
35	1	0	0.694250	2.076111	-0.601465
36	6	0	6.334429	-0.319899	2.817301
37	6	0	4.948465	-0.698784	2.800318
38	1	0	7.845109	0.870712	1.915958
39	1	0	6.969688	-0.759949	3.574679
40	8	0	4.616161	-1.610462	3.802717
41	1	0	3.069398	-0.448758	1.853260
42	6	0	2.661391	-4.982328	-1.945453
43	1	0	3.096904	-3.268661	-0.859513
44	1	0	3.382153	-5.604466	-1.431562
45	1	0	2.084180	-5.469119	-2.720799
46	6	0	3.228941	-1.964319	3.863236
47	1	0	3.122825	-2.648242	4.707161

48	1	0	2.893350	-2.476880	2.956963
49	1	0	2.586430	-1.095814	4.034535
50	6	0	-4.160418	-0.094747	0.582469
51	6	0	-2.741517	-0.064054	0.586467
52	6	0	-1.956732	1.076140	0.379424
53	8	0	-0.684358	0.998739	0.159561
54	1	0	-2.195763	-1.001356	0.647233
55	1	0	-4.655579	0.872682	0.578267
56	6	0	-4.943182	-1.167655	1.300844
57	6	0	-2.520843	2.495937	0.450170
58	7	0	-2.840829	-1.849741	-2.334626
59	6	0	-3.785034	-1.251045	-1.993244
60	6	0	-4.855172	-0.490320	-1.451856
61	6	0	-4.470614	-2.474415	1.430447
62	6	0	-5.209882	-3.427549	2.109165
63	6	0	-6.177842	-0.847693	1.865908
64	6	0	-6.914603	-1.800672	2.549840
65	6	0	-6.432667	-3.094165	2.673636
66	6	0	-2.230941	3.403583	-0.565261
67	6	0	-2.691761	4.708270	-0.499447
68	6	0	-3.435398	5.127531	0.593605
69	6	0	-3.715931	4.236436	1.617888
70	6	0	-3.263532	2.928456	1.545468
71	1	0	-6.560856	0.160419	1.770081
72	1	0	-7.868448	-1.532648	2.986081
73	1	0	-3.522115	-2.749233	0.990073
74	1	0	-4.830915	-4.437639	2.198793
75	1	0	-7.007692	-3.840997	3.205954
76	1	0	-1.649551	3.081227	-1.419585
77	1	0	-2.470077	5.400215	-1.302023
78	1	0	-3.793410	6.147734	0.647717
79	1	0	-4.289133	4.561509	2.476865
80	1	0	-3.478534	2.239276	2.351981
81	7	0	-5.197606	1.906930	-2.379145
82	6	0	-5.047118	0.811893	-2.002639
83	1	0	-5.774445	-1.050126	-1.291216

N-TS2-*Re*-1

Energy+zep = -1895.180937 au

Gibbs free energy = -1895.257019 au

Number of imaginary frequencies: 1 (-1292.5561 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.970252	2.282875	-0.098137
2	6	0	-1.923673	1.241642	-0.585181
3	6	0	-1.775159	3.323084	0.581387
4	6	0	-0.231641	2.930841	-1.217167
5	6	0	-1.252731	-0.150410	-0.747231
6	6	0	-2.704675	1.782013	-1.810712
7	6	0	-2.906015	3.893021	-0.361925
8	6	0	-1.186177	3.718441	-2.161209
9	1	0	-2.203469	2.891074	1.491583
10	1	0	-1.095953	4.124247	0.891762
11	1	0	0.516371	3.596846	-0.770812
12	1	0	0.291189	2.147258	-1.763912
13	8	0	-0.111653	-0.088879	-1.573087
14	6	0	-2.266666	-1.203011	-1.293217
15	6	0	-2.627345	3.325821	-1.788986
16	1	0	-2.263384	1.415568	-2.745156
17	1	0	-3.741904	1.430229	-1.786537
18	1	0	-2.794272	4.983400	-0.422410
19	1	0	-1.049035	4.801573	-2.056324
20	1	0	-0.981903	3.467112	-3.208605
21	1	0	-0.954057	-0.461643	0.269628
22	6	0	-2.229779	-1.554443	-2.597870
23	6	0	-3.263077	-1.837716	-0.456072
24	1	0	-3.339423	3.753754	-2.502575
25	6	0	-3.152361	-2.513557	-3.121701
26	6	0	-4.130604	-2.767266	-1.058522
27	1	0	-1.498953	-1.112355	-3.260513
28	7	0	-4.082280	-3.116425	-2.417106
29	1	0	-3.094891	-2.771026	-4.177146
30	1	0	-2.635555	1.106832	0.236494
31	6	0	-5.125411	-3.407924	-0.262467
32	6	0	-3.410421	-1.581837	0.934462
33	6	0	-4.327126	3.610196	0.149857
34	1	0	-4.571726	2.569292	0.328845
35	6	0	-5.222537	4.537464	0.375431
36	1	0	-5.018743	5.587130	0.213284
37	1	0	-6.213692	4.301096	0.737061
38	1	0	0.688090	-1.202478	-1.915412
39	6	0	2.734606	0.455533	0.805060
40	6	0	2.003153	-0.498358	-0.140726
41	6	0	2.529337	-1.060127	-1.359307

42	8	0	1.651941	-1.653094	-2.124862
43	1	0	1.393436	-1.238934	0.386343
44	1	0	3.244046	1.221916	0.210008
45	7	0	0.384620	-0.294639	3.342747
46	6	0	0.947078	0.405794	2.607358
47	6	0	1.631045	1.257573	1.620671
48	6	0	2.197941	2.448804	2.270411
49	7	0	2.651811	3.414911	2.726882
50	1	0	0.831150	1.612672	0.934967
51	6	0	3.765375	-0.154945	1.794294
52	6	0	4.875975	0.595841	2.172993
53	6	0	3.596337	-1.421360	2.344874
54	6	0	5.795129	0.093811	3.079605
55	1	0	5.024858	1.582333	1.752754
56	6	0	4.515972	-1.925147	3.251766
57	1	0	2.742446	-2.024835	2.069002
58	6	0	5.617130	-1.169619	3.622471
59	1	0	6.652553	0.691323	3.362488
60	1	0	4.369234	-2.912595	3.670913
61	1	0	6.334418	-1.563860	4.330977
62	6	0	3.880786	-0.942243	-1.983360
63	6	0	5.050819	-0.779029	-1.242511
64	6	0	3.962825	-1.035459	-3.376436
65	6	0	6.276273	-0.702545	-1.883200
66	1	0	5.008574	-0.731086	-0.164119
67	6	0	5.186469	-0.949764	-4.014807
68	1	0	3.051587	-1.170800	-3.946595
69	6	0	6.345111	-0.782487	-3.266936
70	1	0	7.180370	-0.582278	-1.300619
71	1	0	5.240017	-1.015011	-5.093755
72	1	0	7.305623	-0.717963	-3.765060
73	1	0	0.963270	0.007389	-0.756735
74	6	0	-5.253217	-3.144062	1.060427
75	6	0	-4.371626	-2.207135	1.680422
76	1	0	-5.781243	-4.117628	-0.751758
77	1	0	-6.015421	-3.642939	1.638565
78	1	0	-2.754742	-0.885762	1.434816
79	8	0	-4.404131	-1.848549	3.033668
80	6	0	-5.374075	-2.544486	3.825744
81	1	0	-5.255243	-2.175517	4.846167
82	1	0	-6.399328	-2.342560	3.502161
83	1	0	-5.213113	-3.626351	3.827626

N-TS1-*Si*-1

Energy+zep = -1895.202543 au

Gibbs free energy = -1895.281152 au

Number of imaginary frequencies: 1 (-283.8998 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.088938	-1.547060	0.618152
2	7	0	-0.493034	-1.899838	-0.161103
3	6	0	-1.361489	-0.766382	-0.689206
4	6	0	0.431841	-2.348622	-1.267359
5	6	0	-1.297458	-3.071679	0.338731
6	6	0	-1.790385	0.208839	0.454583
7	6	0	-2.420249	-1.401499	-1.610897
8	6	0	-0.413441	-2.682716	-2.527302
9	6	0	-1.977879	-3.747636	-0.872269
10	1	0	1.143224	-1.537188	-1.405362
11	1	0	0.969624	-3.216572	-0.883376
12	1	0	-0.600981	-3.718488	0.873226
13	1	0	-2.017601	-2.679965	1.056081
14	8	0	-0.671340	0.428264	1.284791
15	6	0	-2.970485	-0.202192	1.372431
16	6	0	-1.903130	-2.783138	-2.073796
17	1	0	-3.378434	-1.529080	-1.096130
18	1	0	-2.597465	-0.741019	-2.464381
19	1	0	-0.121121	-3.689257	-2.861937
20	1	0	-1.486864	-4.695871	-1.115713
21	1	0	-3.020109	-3.977355	-0.629296
22	6	0	-0.245937	-1.757367	-3.749472
23	1	0	-2.070276	1.135326	-0.070922
24	1	0	0.101086	0.716379	0.727772
25	6	0	-2.715627	-0.748830	2.583283
26	6	0	-4.351003	0.040387	1.013767
27	1	0	-2.516305	-3.159096	-2.897858
28	6	0	-3.790540	-1.109295	3.456399
29	6	0	-5.339886	-0.347965	1.936497
30	1	0	-1.696191	-0.905095	2.910485
31	6	0	-4.766758	0.661008	-0.195843
32	7	0	-5.063022	-0.942613	3.176160
33	1	0	-3.552939	-1.556079	4.419207
34	6	0	-6.713493	-0.124454	1.621238
35	1	0	-0.659122	-0.181311	-1.284975

36	6	0	-7.087851	0.462614	0.459283
37	6	0	-6.088662	0.873397	-0.476058
38	1	0	-4.038742	0.990790	-0.920158
39	1	0	-8.133714	0.622537	0.247442
40	1	0	-7.452841	-0.437625	2.348542
41	6	0	0.500584	-0.688981	-3.858474
42	1	0	-0.832898	-2.090305	-4.598236
43	1	0	0.538288	-0.132927	-4.785498
44	1	0	1.114514	-0.295926	-3.059172
45	6	0	4.105571	-0.203259	0.099368
46	6	0	3.695632	1.153547	-0.033934
47	6	0	2.359284	1.504955	-0.265148
48	6	0	1.983859	2.985902	-0.421537
49	8	0	1.397212	0.657823	-0.376919
50	6	0	0.938365	3.326466	-1.276504
51	6	0	2.624655	4.002905	0.282240
52	6	0	5.558563	-0.585410	-0.090395
53	1	0	4.423972	1.946744	0.072227
54	6	0	6.594034	0.202432	0.415236
55	1	0	3.404456	-0.924220	-0.315825
56	6	0	5.886147	-1.743712	-0.791952
57	6	0	7.915134	-0.157454	0.215503
58	6	0	8.228173	-1.308907	-0.493771
59	6	0	7.209609	-2.101094	-0.996673
60	1	0	5.095707	-2.369138	-1.186257
61	1	0	6.359544	1.097811	0.975528
62	1	0	8.707263	0.462637	0.615681
63	1	0	9.262422	-1.586997	-0.650332
64	1	0	7.445102	-3.001702	-1.549274
65	6	0	0.551028	4.645654	-1.440911
66	6	0	1.199897	5.649466	-0.738317
67	6	0	2.233543	5.323710	0.126424
68	1	0	0.898147	6.681714	-0.861021
69	1	0	2.736510	6.102971	0.684906
70	1	0	3.423886	3.759169	0.970011
71	1	0	0.429971	2.539706	-1.818736
72	1	0	-0.258474	4.893341	-2.115672
73	7	0	1.647891	-2.370156	1.783567
74	6	0	2.591732	-1.704046	1.965388
75	6	0	3.766234	-0.903935	2.058763
76	6	0	3.681086	0.269249	2.868874
77	1	0	4.662199	-1.495410	2.243341
78	7	0	3.652690	1.283363	3.443649
79	8	0	-6.345193	1.484385	-1.708020

80	6	0	-7.720349	1.804426	-1.956160
81	1	0	-7.744864	2.314702	-2.920773
82	1	0	-8.349674	0.912087	-2.020646
83	1	0	-8.135433	2.474397	-1.197944

N-TS2-*Si*-1

Energy+zep = -1895.175434 au

Gibbs free energy = -1895.253762 au

Number of imaginary frequencies: 1 (-1638.8077 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.183346	-0.343780	1.899549
2	6	0	-0.867927	-1.053451	0.792952
3	6	0	0.569125	-1.353693	2.670745
4	6	0	-1.140572	0.318062	2.812429
5	6	0	-1.178839	-0.180005	-0.462200
6	6	0	-2.051194	-1.893993	1.348875
7	6	0	-0.352426	-2.535083	3.138086
8	6	0	-2.037234	-0.722086	3.549555
9	1	0	1.400330	-1.704204	2.054252
10	1	0	1.009051	-0.849283	3.537296
11	1	0	-0.561776	0.919894	3.520729
12	1	0	-1.747386	1.012321	2.230785
13	6	0	-2.324786	0.869162	-0.375886
14	6	0	-1.819652	-2.084664	2.865080
15	1	0	-3.011603	-1.386630	1.202100
16	1	0	-2.115421	-2.857490	0.830851
17	1	0	-0.254138	-2.643869	4.231180
18	1	0	-1.778019	-0.789256	4.613338
19	1	0	-3.094201	-0.434518	3.495155
20	6	0	-0.077846	-3.938186	2.555154
21	1	0	-1.454047	-0.908749	-1.239055
22	6	0	-2.036832	2.143359	-0.021789
23	6	0	-3.695593	0.567588	-0.733112
24	1	0	-2.516716	-2.829288	3.263645
25	6	0	-3.063524	3.135784	0.032091
26	6	0	-4.638283	1.609939	-0.650621
27	1	0	-1.021461	2.424281	0.219126
28	6	0	-4.145222	-0.706386	-1.180010
29	7	0	-4.327438	2.918358	-0.254096

30	1	0	-2.796378	4.146692	0.332003
31	6	0	-5.998516	1.349737	-0.994899
32	1	0	-0.116529	-1.758591	0.415104
33	6	0	-6.404770	0.126373	-1.410228
34	6	0	-5.451952	-0.932969	-1.511475
35	1	0	-3.452935	-1.528369	-1.271922
36	1	0	-7.439405	-0.041240	-1.665966
37	1	0	-6.701509	2.170052	-0.916221
38	6	0	0.953926	-4.340423	1.859141
39	1	0	-0.854277	-4.654786	2.804226
40	1	0	1.040180	-5.365519	1.527322
41	1	0	1.772406	-3.694462	1.578689
42	8	0	-5.742383	-2.236986	-1.933541
43	6	0	-7.107126	-2.467262	-2.303864
44	1	0	-7.166469	-3.511645	-2.615820
45	1	0	-7.797253	-2.316186	-1.468773
46	1	0	-7.424730	-1.837707	-3.140018
47	8	0	-0.002492	0.499463	-0.896362
48	1	0	1.084067	0.394316	-0.224183
49	6	0	2.594875	1.802749	-0.904842
50	6	0	2.469607	0.376790	-0.343411
51	6	0	2.469876	-0.729578	-1.256307
52	6	0	3.309816	-1.959991	-1.124565
53	8	0	1.568839	-0.752639	-2.196583
54	6	0	4.445753	-1.997964	-0.314756
55	6	0	2.953300	-3.095739	-1.854100
56	6	0	1.944997	2.922829	-0.054775
57	1	0	3.065072	0.217745	0.551339
58	6	0	1.906602	2.869046	1.334010
59	1	0	2.135038	1.830997	-1.897011
60	6	0	1.416523	4.038337	-0.698869
61	6	0	1.348749	3.909404	2.062166
62	6	0	0.825186	5.015658	1.412505
63	6	0	0.859305	5.077410	0.027518
64	1	0	1.436234	4.091816	-1.780019
65	1	0	2.306741	2.010380	1.855463
66	1	0	1.324539	3.853922	3.143088
67	1	0	0.390030	5.826501	1.982582
68	1	0	0.449421	5.936328	-0.488551
69	6	0	5.203545	-3.153624	-0.231651
70	6	0	4.836562	-4.279221	-0.957032
71	6	0	3.711329	-4.250283	-1.770097
72	1	0	5.432158	-5.182150	-0.890185
73	1	0	3.427630	-5.127614	-2.336759

74	1	0	2.073410	-3.055199	-2.485074
75	1	0	4.745402	-1.121579	0.245515
76	1	0	6.084598	-3.176264	0.396475
77	7	0	5.198158	0.680771	-3.023997
78	6	0	4.737162	1.344392	-2.190986
79	6	0	4.116570	2.194573	-1.162274
80	6	0	4.918714	2.164698	0.072867
81	1	0	4.136066	3.226389	-1.538518
82	7	0	5.526113	2.143430	1.061372
83	1	0	0.710387	-0.124948	-1.792631

N-TS1-*Re*-2

Energy+zep = -1895.204240 au

Gibbs free energy = -1895.284167 au

Number of imaginary frequencies: 1 (-243.3655 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.103077	0.515682	1.573111
2	7	0	0.737023	1.116923	1.645411
3	6	0	1.507042	1.080340	0.334834
4	6	0	0.265070	2.529090	1.892795
5	6	0	1.546873	0.630599	2.818793
6	6	0	1.453589	-0.341011	-0.328558
7	6	0	2.869553	1.757537	0.596134
8	6	0	1.488760	3.487414	1.864470
9	6	0	2.682240	1.642843	3.087279
10	1	0	-0.481181	2.732808	1.127560
11	1	0	-0.238525	2.517394	2.859935
12	1	0	0.848378	0.520968	3.648903
13	1	0	1.921739	-0.357447	2.556349
14	8	0	0.164310	-0.875213	-0.141054
15	6	0	2.472064	-1.414586	0.137817
16	6	0	2.773021	2.604172	1.886128
17	1	0	3.665623	1.015665	0.715080
18	1	0	3.135727	2.380405	-0.262504
19	1	0	1.485125	4.055003	2.807385
20	1	0	2.492623	2.204252	4.008306
21	1	0	3.628958	1.110703	3.223210
22	1	0	1.637657	-0.143070	-1.396345
23	6	0	2.083268	-2.368511	1.014470

24	6	0	3.816112	-1.489206	-0.393396
25	1	0	3.656614	3.241839	1.981708
26	6	0	2.998247	-3.387097	1.431504
27	6	0	4.644025	-2.525756	0.075368
28	1	0	1.070617	-2.383028	1.395590
29	6	0	4.341181	-0.599749	-1.370588
30	7	0	4.239116	-3.487865	1.012278
31	1	0	2.657153	-4.133081	2.145973
32	6	0	5.975489	-2.634989	-0.426063
33	1	0	-0.529964	-0.229666	-0.478587
34	6	0	-3.351352	-1.253085	-0.329017
35	6	0	-3.686319	0.111230	-0.519090
36	6	0	-2.751108	1.145250	-0.714791
37	8	0	-1.475681	1.034010	-0.730085
38	1	0	-4.731386	0.387673	-0.593118
39	1	0	-2.300736	-1.508891	-0.439112
40	1	0	0.898773	1.708540	-0.319885
41	6	0	-3.283669	2.559155	-0.999739
42	6	0	-4.412671	3.076170	-0.369946
43	6	0	-2.593105	3.366414	-1.900321
44	6	0	-4.841458	4.366732	-0.638626
45	1	0	-4.955033	2.470122	0.343851
46	6	0	-3.025315	4.652678	-2.178142
47	1	0	-1.712228	2.969164	-2.388430
48	6	0	-4.152030	5.156541	-1.545931
49	1	0	-5.717888	4.758232	-0.137882
50	1	0	-2.483813	5.264654	-2.888289
51	1	0	-4.491020	6.162329	-1.758615
52	6	0	-4.282793	-2.363837	-0.753521
53	6	0	-5.671342	-2.237687	-0.684108
54	6	0	-3.746088	-3.551289	-1.249255
55	6	0	-6.494673	-3.267047	-1.103558
56	1	0	-6.109748	-1.329571	-0.293471
57	6	0	-4.571847	-4.580466	-1.673835
58	1	0	-2.671227	-3.667971	-1.303891
59	6	0	-5.948074	-4.441417	-1.602240
60	1	0	-7.569543	-3.154822	-1.041442
61	1	0	-4.137294	-5.494375	-2.058141
62	1	0	-6.594598	-5.245035	-1.930815
63	6	0	1.542974	4.534351	0.734059
64	1	0	2.442593	5.138043	0.780039
65	6	0	0.657114	4.766678	-0.199015
66	1	0	-0.266132	4.214976	-0.306818
67	1	0	0.812892	5.550983	-0.927246

68	7	0	-1.691511	0.056819	2.768250
69	6	0	-2.429970	-0.758358	2.369808
70	6	0	-3.307774	-1.717665	1.809108
71	6	0	5.617630	-0.726676	-1.845071
72	6	0	6.457850	-1.771890	-1.352043
73	1	0	3.731837	0.195697	-1.769806
74	1	0	7.467610	-1.879678	-1.716703
75	1	0	6.591407	-3.439878	-0.043316
76	6	0	-2.916142	-3.082477	1.959944
77	7	0	-2.599703	-4.205314	2.012672
78	1	0	-4.360299	-1.521624	1.997424
79	8	0	5.996838	0.227019	-2.796237
80	6	0	7.294882	0.031529	-3.372122
81	1	0	7.417334	0.816451	-4.120720
82	1	0	8.096277	0.129384	-2.634107
83	1	0	7.389032	-0.938863	-3.867650

N-TS2-*Re*-2

Energy+zep = -1895.163166 au

Gibbs free energy = -1895.242194 au

Number of imaginary frequencies: 1 (-1010.9969 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.894466	-2.843127	-0.136940
2	6	0	1.740995	-1.560519	0.579944
3	6	0	1.757456	-3.915150	0.872593
4	6	0	3.226671	-2.973123	-0.769182
5	6	0	1.215564	-0.378764	-0.271592
6	6	0	3.013870	-1.247578	1.414956
7	6	0	2.738329	-3.699412	2.079116
8	6	0	4.364042	-3.015716	0.294955
9	1	0	0.714369	-3.955671	1.192667
10	1	0	1.970162	-4.865588	0.373576
11	1	0	3.212910	-3.880828	-1.380297
12	1	0	3.367949	-2.137602	-1.455863
13	8	0	-0.127205	-0.756460	-0.744211
14	6	0	1.994182	0.096601	-1.513640
15	6	0	3.747268	-2.591192	1.640796
16	1	0	3.689379	-0.560707	0.890653
17	1	0	2.741272	-0.772061	2.363911

18	1	0	3.329544	-4.619443	2.217022
19	1	0	4.793813	-4.021208	0.378853
20	1	0	5.182294	-2.339429	0.019085
21	1	0	1.075975	0.454979	0.426835
22	6	0	1.778421	-0.497783	-2.710030
23	6	0	2.925525	1.201370	-1.452996
24	1	0	4.525104	-2.472909	2.402068
25	6	0	2.479321	-0.047493	-3.873578
26	6	0	3.569134	1.568022	-2.649919
27	1	0	1.074272	-1.314205	-2.808726
28	6	0	3.220741	1.943108	-0.276707
29	7	0	3.350881	0.935535	-3.882003
30	1	0	2.287628	-0.546691	-4.820580
31	6	0	4.497695	2.651300	-2.638431
32	1	0	-0.713849	-1.154084	0.042719
33	1	0	0.928367	-1.731843	1.296447
34	6	0	2.128174	-3.387296	3.462224
35	1	0	2.884944	-3.195922	4.216398
36	6	0	0.867037	-3.354020	3.807536
37	1	0	0.053554	-3.538704	3.121457
38	1	0	0.572109	-3.138237	4.824984
39	6	0	4.110686	2.982108	-0.288492
40	6	0	4.769146	3.340966	-1.504738
41	1	0	2.741305	1.704639	0.659507
42	1	0	5.474685	4.156995	-1.524687
43	1	0	4.980287	2.907903	-3.573828
44	8	0	4.299519	3.616095	0.943863
45	6	0	5.207553	4.725069	0.927688
46	1	0	5.231839	5.113177	1.947597
47	1	0	6.221790	4.428276	0.645576
48	1	0	4.875787	5.525084	0.259757
49	6	0	-3.313149	0.190716	-1.415551
50	6	0	-2.282590	0.783661	-0.426436
51	6	0	-2.051426	0.260488	0.872081
52	8	0	-1.778361	-0.991227	1.050023
53	1	0	-2.329261	1.869908	-0.471692
54	1	0	-3.168976	0.691007	-2.378031
55	6	0	-1.903581	1.155120	2.098826
56	6	0	-1.227559	0.652801	3.209394
57	6	0	-2.447657	2.435524	2.167586
58	6	0	-1.082852	1.413282	4.356579
59	1	0	-0.822477	-0.350212	3.157901
60	6	0	-2.306292	3.198649	3.316078
61	1	0	-2.996004	2.836782	1.325579

62	6	0	-1.621238	2.691256	4.409855
63	1	0	-0.552822	1.012033	5.210829
64	1	0	-2.735440	4.191453	3.359238
65	1	0	-1.511199	3.289504	5.305925
66	6	0	-4.749826	0.551230	-0.935121
67	6	0	-5.293764	-0.017682	0.215473
68	6	0	-5.499067	1.490873	-1.631476
69	6	0	-6.556508	0.341710	0.651039
70	1	0	-4.725250	-0.747827	0.776635
71	6	0	-6.764442	1.856137	-1.193436
72	1	0	-5.092439	1.943357	-2.526799
73	6	0	-7.297189	1.282038	-0.052468
74	1	0	-6.966656	-0.112030	1.544497
75	1	0	-7.334313	2.590147	-1.749149
76	1	0	-8.284607	1.563339	0.289880
77	7	0	-1.377949	-1.820321	-3.573305
78	6	0	-2.160128	-1.631069	-2.737683
79	6	0	-3.183703	-1.359997	-1.710451
80	6	0	-4.453787	-1.950934	-2.173477
81	7	0	-5.447933	-2.432028	-2.530358
82	1	0	-2.897845	-1.871139	-0.782500
83	1	0	-0.828416	0.114269	-0.824475

N-TS1-*Si*-2

Energy+zep = -1895.197392 au

Gibbs free energy = -1895.275954 au

Number of imaginary frequencies: 1 (-275.6115 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.140833	0.059204	1.123792
2	7	0	0.915480	0.639068	1.483680
3	6	0	1.875207	0.928272	0.336344
4	6	0	0.352576	1.952982	1.973384
5	6	0	1.565468	-0.098588	2.628408
6	6	0	1.947914	-0.273767	-0.664034
7	6	0	3.161069	1.505266	0.959818
8	6	0	1.527591	2.906553	2.328245
9	6	0	2.587727	0.844367	3.300653
10	1	0	-0.290517	2.321479	1.177268
11	1	0	-0.271298	1.716810	2.835553

12	1	0	0.755282	-0.414813	3.285632
13	1	0	2.032936	-0.986743	2.205475
14	8	0	0.642555	-0.770843	-0.835946
15	6	0	2.867854	-1.470166	-0.303794
16	6	0	2.829890	2.048235	2.369046
17	1	0	3.943315	0.743046	1.040961
18	1	0	3.547746	2.299399	0.315073
19	1	0	1.358732	3.264191	3.354595
20	1	0	2.219203	1.185512	4.273884
21	1	0	3.523432	0.305929	3.480952
22	6	0	1.704201	4.167185	1.458338
23	1	0	2.316471	0.174695	-1.599633
24	1	0	0.025877	-0.020003	-1.126020
25	6	0	4.280868	-1.481961	-0.595126
26	6	0	2.323062	-2.580055	0.252615
27	1	0	3.659661	2.654187	2.744060
28	6	0	5.006805	-2.630105	-0.235842
29	6	0	3.141673	-3.701361	0.576794
30	6	0	4.970606	-0.406685	-1.242925
31	1	0	1.258917	-2.628776	0.440835
32	7	0	4.440510	-3.756199	0.368408
33	6	0	6.416092	-2.682682	-0.503061
34	1	0	2.679764	-4.574664	1.031540
35	1	0	1.355689	1.709547	-0.221773
36	6	0	6.305030	-0.487078	-1.498105
37	6	0	7.044544	-1.655315	-1.106901
38	1	0	4.411939	0.462965	-1.539357
39	1	0	8.104866	-1.678638	-1.321430
40	1	0	6.950297	-3.577559	-0.208010
41	6	0	1.038509	4.516476	0.388182
42	1	0	1.261723	5.442588	-0.124004
43	1	0	0.242416	3.929541	-0.049013
44	1	0	2.488986	4.813913	1.834732
45	6	0	-4.004402	-0.602273	-0.433071
46	6	0	-2.664790	-0.296345	-0.823812
47	6	0	-2.183439	0.982677	-1.120750
48	8	0	-0.932557	1.260847	-1.246692
49	1	0	-1.918306	-1.081606	-0.759353
50	1	0	-4.746294	0.157836	-0.669726
51	6	0	-4.546088	-2.009693	-0.589224
52	6	0	-3.762935	-3.136104	-0.334510
53	6	0	-5.860425	-2.195529	-1.012610
54	6	0	-4.279853	-4.407966	-0.506538
55	1	0	-2.743602	-3.015388	0.006091

56	6	0	-6.376783	-3.469612	-1.190007
57	1	0	-6.484087	-1.332722	-1.208933
58	6	0	-5.587766	-4.579554	-0.937757
59	1	0	-3.660299	-5.272044	-0.303057
60	1	0	-7.399123	-3.594293	-1.523383
61	1	0	-5.989455	-5.575568	-1.072980
62	6	0	-3.147851	2.164294	-1.352100
63	6	0	-3.072535	3.308322	-0.563504
64	6	0	-4.070633	2.135825	-2.395238
65	6	0	-3.904196	4.391554	-0.800081
66	1	0	-2.360908	3.351373	0.250155
67	6	0	-4.898007	3.220405	-2.639173
68	1	0	-4.136323	1.256813	-3.023818
69	6	0	-4.819210	4.350881	-1.840070
70	1	0	-3.837628	5.270882	-0.171885
71	1	0	-5.608145	3.183774	-3.455758
72	1	0	-5.467716	5.196714	-2.027908
73	7	0	-1.737522	-0.474115	2.376728
74	6	0	-2.872824	-0.394713	2.112956
75	6	0	-4.196083	-0.248384	1.607252
76	8	0	7.094888	0.479406	-2.121804
77	6	0	6.383051	1.630296	-2.592807
78	1	0	7.120684	2.268574	-3.082462
79	1	0	5.608652	1.369828	-3.320054
80	1	0	5.923053	2.194577	-1.776328
81	6	0	-5.212463	-1.061328	2.208083
82	7	0	-6.073850	-1.729036	2.624298
83	1	0	-4.484913	0.800182	1.533571

N-TS2-*Si*-2

Energy+zep = -1895.178656 au

Gibbs free energy = -1895.254358 au

Number of imaginary frequencies: 1 (-1599.8004 cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.565768	0.184180	1.632824
2	6	0	1.388109	0.864487	0.593287
3	6	0	-0.104518	1.246607	2.422315
4	6	0	1.395375	-0.626053	2.559857
5	6	0	1.706104	0.042212	-0.693615

6	6	0	2.620847	1.538090	1.259211
7	6	0	0.919786	2.282451	2.999558
8	6	0	2.362535	0.268610	3.388343
9	1	0	-0.847820	1.726525	1.780968
10	1	0	-0.650931	0.760189	3.236959
11	1	0	0.715787	-1.184162	3.212478
12	1	0	1.945743	-1.360432	1.972194
13	8	0	0.515717	-0.403811	-1.332795
14	6	0	2.660239	-1.183242	-0.576750
15	6	0	2.336529	1.678865	2.770244
16	1	0	3.525157	0.933063	1.129299
17	1	0	2.816208	2.512474	0.797760
18	1	0	0.774863	2.342591	4.090628
19	1	0	2.058680	0.312473	4.441082
20	1	0	3.380513	-0.137726	3.365460
21	6	0	0.837144	3.736559	2.487347
22	1	0	2.180861	0.777388	-1.359395
23	1	0	-0.114166	0.412929	-2.135414
24	6	0	4.086496	-1.099794	-0.788637
25	6	0	2.132978	-2.410007	-0.334706
26	1	0	3.092225	2.316324	3.240762
27	6	0	4.832010	-2.287052	-0.684326
28	6	0	2.970206	-3.559013	-0.251067
29	6	0	4.776168	0.112736	-1.118804
30	1	0	1.066727	-2.532374	-0.207652
31	7	0	4.278221	-3.538701	-0.403066
32	6	0	6.252996	-2.246128	-0.884084
33	1	0	2.514771	-4.524977	-0.044699
34	1	0	0.737695	1.662981	0.215256
35	6	0	6.122277	0.122599	-1.313040
36	6	0	6.878449	-1.091456	-1.183885
37	1	0	4.207830	1.019443	-1.221090
38	1	0	7.947750	-1.042599	-1.341155
39	1	0	6.799478	-3.176378	-0.789380
40	6	0	-0.110829	4.295690	1.780626
41	1	0	-0.062223	5.339924	1.505732
42	1	0	-0.988370	3.768779	1.436909
43	1	0	1.681479	4.340815	2.804004
44	8	0	6.910267	1.229224	-1.640465
45	6	0	6.188172	2.455318	-1.804194
46	1	0	6.927118	3.214961	-2.065524
47	1	0	5.449014	2.397264	-2.608484
48	1	0	5.682020	2.764325	-0.884966
49	6	0	-2.947114	-0.747333	0.100861

50	6	0	-1.996458	-0.419575	-1.047819
51	6	0	-1.978713	0.839289	-1.736049
52	8	0	-0.948053	1.095799	-2.487805
53	1	0	-3.182556	0.180099	0.634713
54	6	0	-4.287737	-1.447525	-0.249982
55	6	0	-4.373492	-2.420178	-1.241213
56	6	0	-5.437076	-1.121522	0.465606
57	6	0	-5.579250	-3.048189	-1.511863
58	1	0	-3.496087	-2.697059	-1.809534
59	6	0	-6.642985	-1.748311	0.196507
60	1	0	-5.389237	-0.368214	1.241622
61	6	0	-6.717474	-2.714555	-0.794651
62	1	0	-5.628069	-3.803026	-2.286530
63	1	0	-7.526088	-1.481328	0.763083
64	1	0	-7.658482	-3.205696	-1.007056
65	6	0	-2.936086	1.989611	-1.605290
66	6	0	-2.432199	3.286327	-1.721171
67	6	0	-4.305718	1.802692	-1.431855
68	6	0	-3.279236	4.377230	-1.638479
69	1	0	-1.368913	3.426155	-1.873953
70	6	0	-5.154351	2.895717	-1.361641
71	1	0	-4.712728	0.802618	-1.371877
72	6	0	-4.642166	4.181566	-1.457563
73	1	0	-2.880193	5.380049	-1.719573
74	1	0	-6.218268	2.743204	-1.233784
75	1	0	-5.307600	5.034636	-1.397036
76	7	0	-1.487812	-3.984539	0.276695
77	6	0	-1.792252	-2.941334	0.685009
78	6	0	-2.138059	-1.596433	1.170134
79	6	0	-2.845474	-1.675150	2.456826
80	7	0	-3.391194	-1.672306	3.481792
81	1	0	-1.182448	-1.060244	1.343734
82	1	0	-0.656924	-0.433910	-0.787738
83	1	0	-1.802541	-1.254037	-1.727290

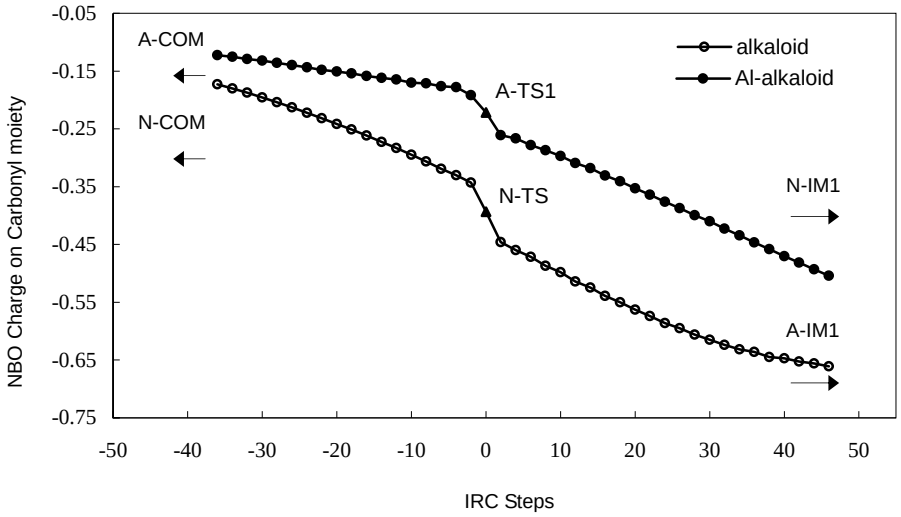

Figure S1. Evolution of charge populations on carbonyl groups in the formation of the C-C bond for the Michael addition reaction catalyzed by cinchona alkaloid and Al(III)-cinchona alkaloid complex, respectively.

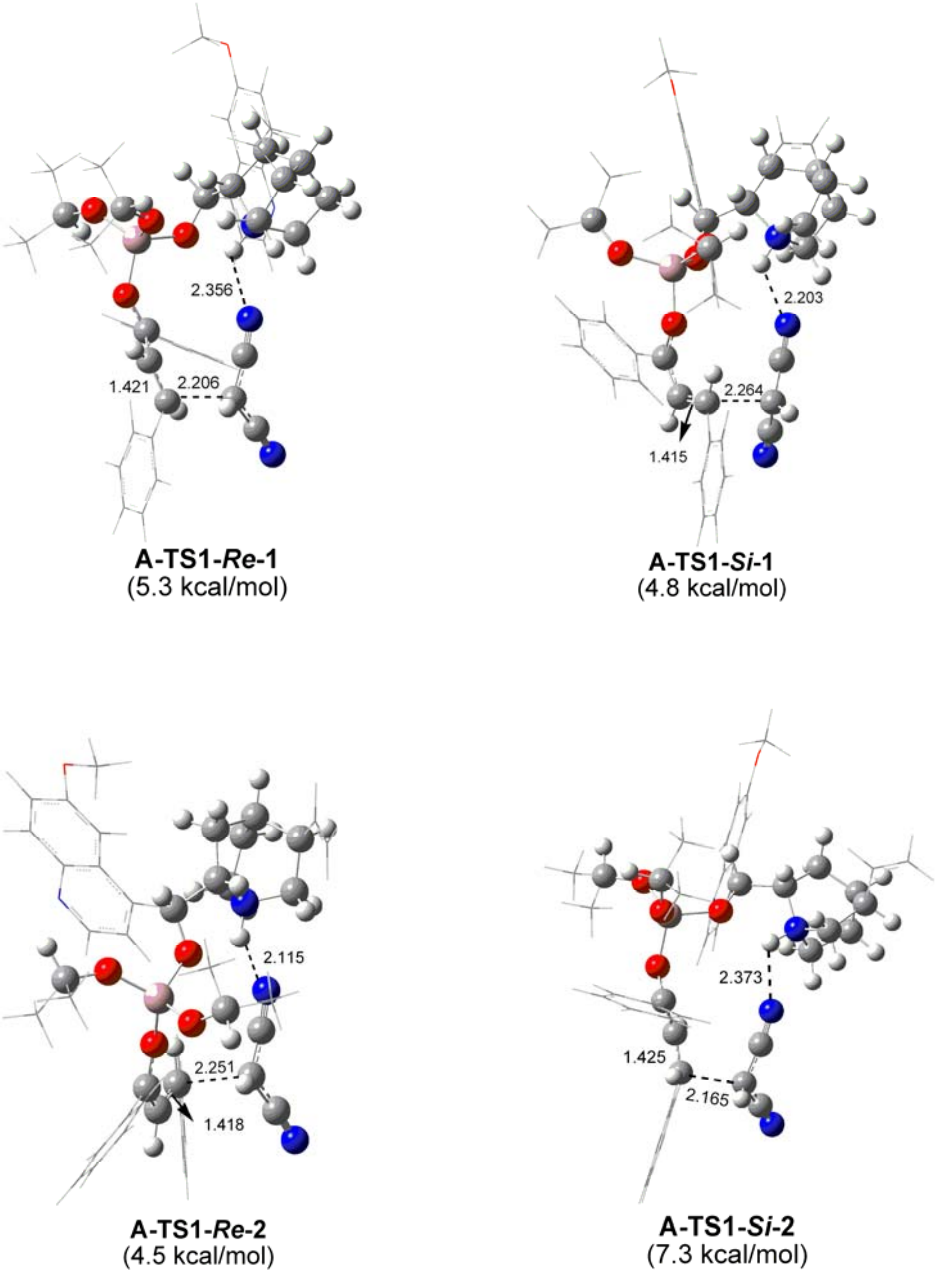

Figure S2. Optimized geometries and relative Gibbs free energies of transition states for C-C formation step in Michael addition reaction catalyzed by Al^{III}-complex.

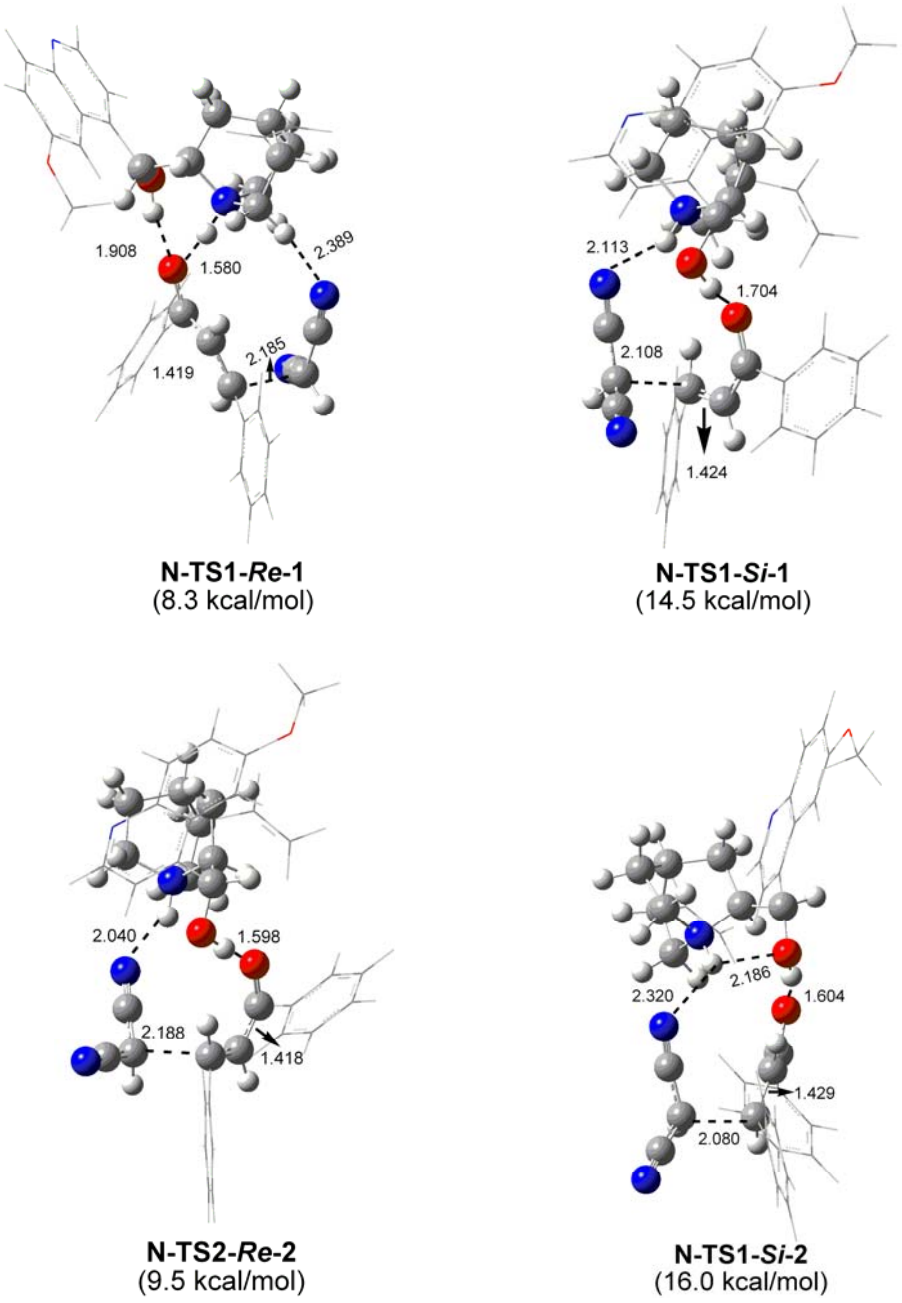

Figure S3. Optimized geometries and relative Gibbs free energies of transition states for C-C coupling step in Michael addition reaction catalyzed by quinine.

Table S1. Calculated total energies (include zero-point correction, in au), relative energies (kcal/mol) for the stationary points in gas phase and toluene solvent at the B3LYP/6-31++G** level.

Species	E_g	ΔE_g	G_g	ΔG_g	G_s	ΔG_s
Background Reaction						
R1	-224.945627		-224.973370		-224.977886	
R2	-270.463699		-270.494902		-270.497568	
R1+R2	-495.409326	0.0	-495.468272	0.0	-495.475454	0.0
B-TS	-495.313559	60.1	-495.354752	71.2	-495.362197	71.1
P	-495.420901	-7.3	-495.460237	5.0	-495.465888	6.0
Molononitrile Isomerization and Deprotonation						
1-TS1	-224.823148	76.9	-224.851094	76.7	-224.855674	76.7
2-TS1	-449.813754	53.2	-449.850136	56.5	-449.855976	56.4
3-TS1	-674.756667	61.7	-674.803814	67.0	-674.812964	65.9
CI	-690.675867		-690.716848		-690.720716	
R1	-224.945627		-224.973370		-224.977886	
CI+R1	-915.621494	0.0	-915.690218	0.0	-915.698601	0.0
CI-COM	-915.63076	-5.8	-915.68256	4.8	-915.687742	6.8
CI-TS	-915.621102	0.2	-915.669907	12.7	-915.677130	13.5
CI-IM1	-915.625468	-2.5	-915.675517	9.2	-915.684097	9.1
Al(III)-Alkaloid Complex Catalyzed Reaction						
A-COM	-1658.314115	0.0	-1658.387774	0.0	-1658.396101	0.0
A-TS1	-1658.30653	4.8	-1658.377998	6.1	-1658.385980	6.4
A-IM1	-1658.326503	-7.8	-1658.397962	-6.4	-1658.405752	-6.1
A-IM2	-1658.303597	6.6	-1658.375969	7.4	-1658.387450	5.4
A-TS2	-1658.297715	10.3	-1658.367767	12.6	-1658.376329	12.4
A-IM3	-1658.309281	3.0	-1658.381595	3.9	-1658.388630	4.7
Alkaloid Complex Catalyzed Reaction						
N-COM	-1186.091948	0.0	-1186.155803	0.0	-1186.164891	0.0
N-TS1	-1186.067434	15.4	-1186.126485	18.4	-1186.134895	18.8
N-IM1	-1186.100915	-5.6	-1186.162454	-4.2	-1186.168477	-2.3

N-IM2	-1186.093894	-1.2	-1186.156237	-0.3	-1186.161990	1.8
N-TS2	-1186.053041	24.4	-1186.110924	17.2	-1186.116501	30.4
N-IM3	-1186.112729	-13.0	-1186.175028	-12.1	-1186.180552	-9.8
CI+IM2	-1186.085421	4.1	-1186.165523	-6.1	-1186.174891	-6.3
CI+TS2	-1186.004924	54.6	-1186.085066	44.4	-1186.093437	44.8
CI+P	-1186.096768	-3.0	-1186.177085	-13.4	-1186.186604	-13.6

Table S2. Calculated total energies (include zero-point correction, in au) for molecular complexes and selected transition states and in gas phase at the ONIOM(B3LYP/6-31++G**:HF/STO-3G) level.(Experimental results are shown in parentheses)

Species	*E*	*ΔE*	*G*	*ΔG*	Configuration of main product
Al(III)-Alkaloid Complex Catalyzed Reaction (*S*-product, 93 % *ee***)**					
A-COM-*Re*-1	-2521.641752	0.0	-2521.738970	0.0	
A-TS1-*Re*-1	-2521.635245	4.1	-2521.730602	5.3	*S*
A-TS2-*Re*-1	-2521.628434	8.4	-2521.723352	9.8	
A-COM-*Si*-1	-2521.641686	0.0	-2521.737287	0.0	
A-TS1-*Si*-1	-2521.634862	4.3	-2521.729564	4.8	*R*
A-TS2-*Si*-1	-2521.615267	16.6	-2521.708576	18.0	
A-COM-*Re*-2	-2521.638355	0.0	-2521.736444	0.0	
A-TS1-*Re*-2	-2521.633843	2.8	-2521.729200	4.5	*S*
A-TS2-*Re*-2	-2521.623160	9.6	-2521.715878	12.9	
A-COM-*Si*-2	-2521.636370	0.0	-2521.735804	0.0	
A-TS1-*Si*-2	-2521.626616	6.1	-2521.724098	7.3	*R*
A-TS2-*Si*-2	-2521.599225	23.3	-2521.692404	27.2	
Alkaloid Complex Catalyzed Reaction (*S*-product, 69 % *ee***)**					
N-COM-*Re*-1	-1895.218940	0.0	-1895.301520	0.0	
N-TS1-*Re*-1	-1895.209492	5.9	-1895.288321	8.3	*S*
N-TS2-*Re*-1	-1895.180937	23.8	-1895.257019	27.9	
N-COM-*Si*-1	-1895.222705	0.0	-1895.304180	0.0	
N-TS1-*Si*-1	-1895.202543	12.7	-1895.281152	14.5	*R*
N-TS2-*Si*-1	-1895.175434	29.7	-1895.253762	31.6	
N-COM-*Re*-2	-1895.216190	0.0	-1895.299357	0.0	
N-TS1-*Re*-2	-1895.204240	7.5	-1895.284167	9.5	*S*
N-TS2-*Re*-2	-1895.163166	33.3	-1895.242194	35.9	
N-COM-*Si*-2	-1895.219120	0.0	-1895.300726	0.0	
N-TS1-*Si*-2	-1895.197407	13.6	-1895.275248	16.0	*R*
N-TS2-*Si*-2	-1895.178656	25.4	-1895.254358	29.1	