Electronic Supplementary Information for The thermal isomerization of the GFP chromophore: a computational study

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Contents

1 Full citation of the Gaussian09 program

Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

2 Energy profile for the unassisted thermal isomerization in the gas phase

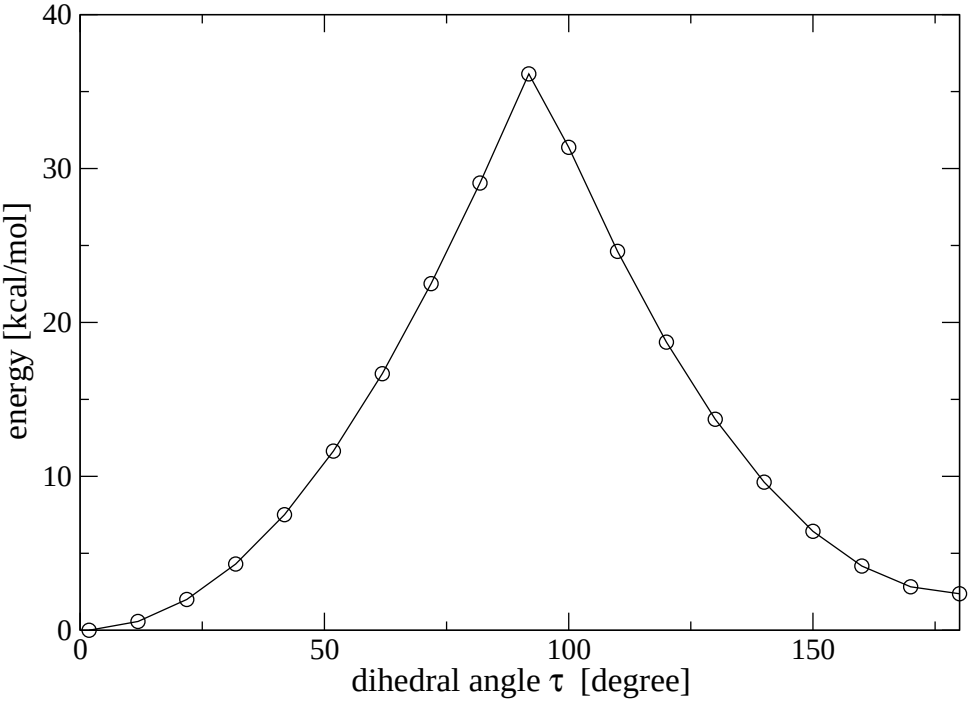

Figure S1: The potential energy profile of the unassisted thermal isomerization of HOBDI in the gas phase as a function of the dihedral-angle $N^1 - C^1 - C^2 - C^3$ (τ in degree). The energy maximum corresponds to a τ value of 92° and an energy of 36.2 kcal/mol.

3 TS1 of the reaction assisted by n-propylamine in the gas phase, in benzene and in MeCN

In our calculations, the isomerization assisted by n-propylamine in the gas phase, in benzene and in MeCN has barriers of 21.5, 3.6, 13.6 and 19.1, 3.7, 11.1 and 17.8, 3.0, 2.6 kcal/mol for the three reaction steps, see Fig. 13. This shows the solvent effect: with increase of the polarity of the environment, the barriers to the addition/elimination of n-propylamine decrease.

In view of the change of geometry of HOBDI during the isomerization, this is reasonable since there is less pyramidalization of C^2 in state TS1 (see Fig. S2) when the polarity of the environment becomes stronger. Accordingly, the hydrogen bond interaction between O^1 and the protons of n-propylamine becomes weaker due to the stabilization of the charged groups (O^1 and NH_2) in a polar environment. Actually, in our calculations we observe the proton transfer between O^1 and n-propylamine in the gas phase and in benzene, but not in MeCN.

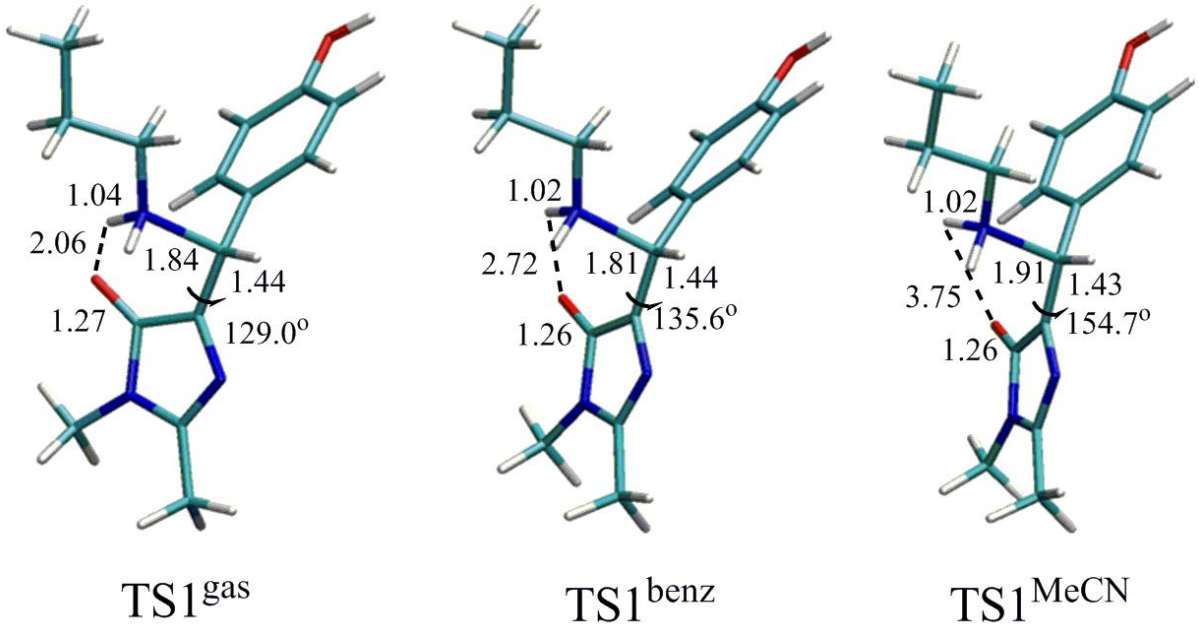

Figure S2: The optimized transition state for the adduct formation of E-HOBDI and n-propylamine in the gas phase ($TS1^{gas}$), in benzene ($TS1^{benz}$) and in acetonitrile ($TS1^{MeCN}$). The dihedral-angle values are given for $N^1 - C^1 - C^2 - C^3$. Some bond lengths or atom-atom distances are given in Å.

4 Coordinates (Å) and energies (kcal/mol) of fully optimized stationary points

E-HOBDI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.276153	-1.486321	-0.000030
2	6	0	3.321525	-0.719847	-0.000018
3	6	0	4.732189	-1.204089	-0.000029
4	1	0	4.727420	-2.294252	-0.000035
5	1	0	5.276798	-0.849986	0.883034
6	1	0	5.276787	-0.849978	-0.883096
7	7	0	3.015576	0.641962	0.000006
8	6	0	3.924007	1.770613	0.000031
9	1	0	4.559955	1.772132	0.891210
10	1	0	4.560051	1.772087	-0.891079
11	1	0	3.306922	2.670913	-0.000023
12	6	0	1.624047	0.778627	0.000011
13	8	0	1.040657	1.859531	0.000030
14	6	0	1.151245	-0.634598	-0.000014
15	6	0	-0.100005	-1.178827	-0.000021
16	1	0	-0.064702	-2.267455	-0.000040
17	6	0	-1.441222	-0.631711	-0.000009
18	6	0	-2.513470	-1.555913	-0.000022
19	1	0	-2.291117	-2.619541	-0.000039
20	6	0	-3.836297	-1.145918	-0.000012
21	1	0	-4.651953	-1.860798	-0.000022
22	6	0	-4.130677	0.223762	0.000010
23	8	0	-5.443520	0.584147	0.000018
24	1	0	-5.507821	1.548709	0.000034
25	6	0	-3.088442	1.160654	0.000022
26	1	0	-3.319056	2.224264	0.000039
27	6	0	-1.764317	0.743947	0.000013
28	1	0	-0.963978	1.474796	0.000022

Zero-point correction=	0.222194
Thermal correction to Energy=	0.236622
Thermal correction to Enthalpy=	0.237566
Thermal correction to Gibbs Free Energy=	0.180497
Sum of electronic and zero-point Energies=	-724.261626
Sum of electronic and thermal Energies=	-724.247198
Sum of electronic and thermal Enthalpies=	-724.246254
Sum of electronic and thermal Free Energies=	-724.303323

in DMSO:

DMSO:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.000011	1.507980	0.386264
2	16	0	-0.000001	0.241894	-0.439291
3	6	0	1.363508	-0.821441	0.180479
4	6	0	-1.363497	-0.821458	0.180478
5	1	0	-1.331797	-1.794722	-0.316648
6	1	0	-1.275488	-0.931494	1.264337
7	1	0	-2.298148	-0.312184	-0.061283
8	1	0	1.331824	-1.794700	-0.316658
9	1	0	2.298153	-0.312151	-0.061273
10	1	0	1.275497	-0.931491	1.264336

Zero-point correction=	0.079544
Thermal correction to Energy=	0.085206
Thermal correction to Enthalpy=	0.086151
Thermal correction to Gibbs Free Energy=	0.051207
Sum of electronic and zero-point Energies=	-553.115975
Sum of electronic and thermal Energies=	-553.110312
Sum of electronic and thermal Enthalpies=	-553.109368
Sum of electronic and thermal Free Energies=	-553.144311

TS:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.895213	-0.909382	0.745734
2	6	0	-1.648046	-0.079289	-0.353127
3	6	0	-2.740422	0.410048	-1.081104
4	6	0	-4.046923	0.085193	-0.734124
5	6	0	-4.277134	-0.744392	0.368931
6	6	0	-3.196845	-1.240845	1.108302
7	6	0	-0.245584	0.329789	-0.720115
8	8	0	-0.022819	1.584290	0.118006
9	16	0	1.297658	2.497729	-0.243148
10	6	0	1.709499	3.148764	1.396700
11	8	0	-5.575327	-1.039511	0.674374
12	6	0	0.838033	-0.650543	-0.438728
13	7	0	0.736905	-1.991998	-0.780897
14	6	0	1.879731	-2.536732	-0.432732
15	7	0	2.739047	-1.602357	0.124820
16	6	0	2.079288	-0.365676	0.124574
17	8	0	2.616587	0.723141	0.568180
18	6	0	4.075876	-1.796847	0.638092
19	6	0	2.237906	-3.976638	-0.595603

20	6	0	0.315122	3.956419	-0.812912
21	1	0	-0.144367	3.679326	-1.763489
22	1	0	0.998463	4.795218	-0.974296
23	1	0	-0.458430	4.217156	-0.088393
24	1	0	2.282283	2.362861	1.882150
25	1	0	0.774144	3.363247	1.916362
26	1	0	2.292848	4.061945	1.256290
27	1	0	4.435657	-0.819181	0.965612
28	1	0	4.750958	-2.186391	-0.132449
29	1	0	4.088398	-2.485577	1.491148
30	1	0	3.118231	-4.121542	-1.236528
31	1	0	2.454922	-4.467902	0.362783
32	1	0	1.391519	-4.488115	-1.057631
33	1	0	-2.563806	1.050721	-1.942094
34	1	0	-4.894658	0.453843	-1.301767
35	1	0	-5.591139	-1.634273	1.435832
36	1	0	-3.377502	-1.892678	1.960838
37	1	0	-1.053575	-1.307306	1.301134
38	1	0	-0.257391	0.692899	-1.760405

Zero-point correction=	0.303681
Thermal correction to Energy=	0.323716
Thermal correction to Enthalpy=	0.324660
Thermal correction to Gibbs Free Energy=	0.255358
Sum of electronic and zero-point Energies=	-1277.320558
Sum of electronic and thermal Energies=	-1277.300523
Sum of electronic and thermal Enthalpies=	-1277.299579
Sum of electronic and thermal Free Energies=	-1277.368881

in methanol:

Methanol:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.749296	0.122042	-0.000017
2	6	0	0.661644	-0.019433	-0.000014
3	1	0	1.038088	-0.543214	-0.891726
4	1	0	1.082064	0.989509	-0.000147
5	1	0	1.038168	-0.542773	0.891935
6	1	0	-1.133819	-0.763254	0.000156

Zero-point correction=	0.051404
Thermal correction to Energy=	0.054707
Thermal correction to Enthalpy=	0.055651
Thermal correction to Gibbs Free Energy=	0.028675
Sum of electronic and zero-point Energies=	-115.672560
Sum of electronic and thermal Energies=	-115.669257

Sum of electronic and thermal Enthalpies= -115.668313
Sum of electronic and thermal Free Energies= -115.695288

TS1:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.041267	-0.255423	-1.555373
2	6	0	-3.039554	-0.746095	-0.863197
3	6	0	-4.275103	-1.353473	-1.438114
4	1	0	-4.222613	-1.272265	-2.524797
5	1	0	-5.186025	-0.846062	-1.095780
6	1	0	-4.376425	-2.414299	-1.175223
7	7	0	-2.819144	-0.662582	0.516268
8	6	0	-3.729317	-0.979322	1.598419
9	1	0	-4.688522	-0.467424	1.471166
10	1	0	-3.912319	-2.056966	1.667990
11	1	0	-3.263265	-0.635755	2.523901
12	6	0	-1.575121	-0.081434	0.689047
13	8	0	-1.091150	0.378918	1.793286
14	6	0	-1.084279	0.110300	-0.612118
15	6	0	0.153283	0.810247	-0.831443
16	1	0	0.171355	1.437640	-1.724428
17	6	0	1.477348	0.240732	-0.497746
18	6	0	2.646759	0.937306	-0.854538
19	1	0	2.560313	1.898567	-1.353756
20	6	0	3.905356	0.428367	-0.573863
21	1	0	4.808431	0.961805	-0.850037
22	6	0	4.019609	-0.806410	0.079779
23	8	0	5.277035	-1.268420	0.327748
24	1	0	5.219591	-2.118705	0.783761
25	6	0	2.868151	-1.517426	0.437621
26	1	0	2.957349	-2.481366	0.933890
27	6	0	1.611873	-0.996654	0.146913
28	1	0	0.721080	-1.557721	0.405269
29	8	0	0.104514	2.089800	0.499005
30	6	0	-0.875873	3.103725	0.275830
31	1	0	-1.179040	3.524088	1.239922
32	1	0	-0.435883	3.891035	-0.342282
33	1	0	-1.761108	2.692496	-0.225448
34	1	0	-0.332020	1.369409	1.239731

Zero-point correction= 0.272700
Thermal correction to Energy= 0.290098
Thermal correction to Enthalpy= 0.291042
Thermal correction to Gibbs Free Energy= 0.227158
Sum of electronic and zero-point Energies= -839.890579
Sum of electronic and thermal Energies= -839.873181

Sum of electronic and thermal Enthalpies= -839.872237
Sum of electronic and thermal Free Energies= -839.936121

IM1:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.632137	-0.792079	-1.251819
2	6	0	-2.677164	-1.230325	-0.581420
3	6	0	-3.592302	-2.327935	-1.010508
4	1	0	-3.242515	-2.704843	-1.972674
5	1	0	-4.627927	-1.985432	-1.131639
6	1	0	-3.605958	-3.162363	-0.297884
7	7	0	-2.843462	-0.533183	0.604845
8	6	0	-3.884567	-0.697443	1.603801
9	1	0	-4.875410	-0.559864	1.160238
10	1	0	-3.836685	-1.690478	2.061715
11	1	0	-3.736923	0.054885	2.378862
12	6	0	-1.818757	0.383493	0.656371
13	8	0	-1.708208	1.238226	1.699339
14	6	0	-1.079701	0.221498	-0.489128
15	6	0	0.162803	0.994232	-0.836223
16	1	0	0.195102	1.142672	-1.927373
17	6	0	1.466589	0.329913	-0.400446
18	6	0	2.553213	1.085017	0.058165
19	1	0	2.448867	2.159983	0.149566
20	6	0	3.755107	0.476115	0.410553
21	1	0	4.594737	1.058553	0.775613
22	6	0	3.892667	-0.909770	0.294709
23	8	0	5.094459	-1.460525	0.650556
24	1	0	5.050599	-2.416584	0.518712
25	6	0	2.818817	-1.675035	-0.170687
26	1	0	2.919967	-2.754848	-0.262957
27	6	0	1.616733	-1.056857	-0.510244
28	1	0	0.785608	-1.656158	-0.868626
29	8	0	0.090482	2.292770	-0.198769
30	6	0	-0.696354	3.230255	-0.924687
31	1	0	-0.707516	4.154964	-0.343117
32	1	0	-0.254770	3.431554	-1.909862
33	1	0	-1.725427	2.875354	-1.064252
34	1	0	-0.968923	1.826734	1.451960

Zero-point correction= 0.277947
Thermal correction to Energy= 0.295785
Thermal correction to Enthalpy= 0.296729
Thermal correction to Gibbs Free Energy= 0.230853
Sum of electronic and zero-point Energies= -839.922793
Sum of electronic and thermal Energies= -839.904955

Sum of electronic and thermal Enthalpies= -839.904011
Sum of electronic and thermal Free Energies= -839.969886

TS2:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.472477	-1.006189	-1.034122
2	6	0	-2.589040	-1.381740	-0.447227
3	6	0	-3.364656	-2.618386	-0.755856
4	1	0	-2.846175	-3.155051	-1.551705
5	1	0	-4.384275	-2.398217	-1.096957
6	1	0	-3.447686	-3.285584	0.111507
7	7	0	-2.980559	-0.468957	0.516900
8	6	0	-4.152453	-0.515495	1.372545
9	1	0	-5.070713	-0.539551	0.777449
10	1	0	-4.129348	-1.395834	2.022663
11	1	0	-4.157902	0.380362	1.993665
12	6	0	-2.027296	0.525899	0.515248
13	8	0	-2.141031	1.580570	1.354493
14	6	0	-1.103592	0.187614	-0.441283
15	6	0	0.138003	0.956845	-0.809154
16	1	0	0.168033	1.060035	-1.903901
17	6	0	1.444816	0.300231	-0.361081
18	6	0	2.370147	0.969783	0.445340
19	1	0	2.146912	1.975311	0.783299
20	6	0	3.565017	0.362038	0.827780
21	1	0	4.282479	0.879127	1.456599
22	6	0	3.851536	-0.936395	0.401332
23	8	0	5.038688	-1.490310	0.801074
24	1	0	5.099926	-2.386151	0.444721
25	6	0	2.933185	-1.618375	-0.404582
26	1	0	3.149011	-2.632337	-0.736434
27	6	0	1.741476	-1.002681	-0.780036
28	1	0	1.021220	-1.543346	-1.386345
29	8	0	0.017323	2.274604	-0.225433
30	6	0	0.060443	3.336906	-1.167388
31	1	0	-0.028024	4.268977	-0.603762
32	1	0	1.011086	3.343464	-1.715997
33	1	0	-0.767352	3.274100	-1.886746
34	1	0	-1.401309	2.164346	1.097608

Zero-point correction= 0.277721
Thermal correction to Energy= 0.294818
Thermal correction to Enthalpy= 0.295763
Thermal correction to Gibbs Free Energy= 0.231776
Sum of electronic and zero-point Energies= -839.921177
Sum of electronic and thermal Energies= -839.904080

Sum of electronic and thermal Enthalpies= -839.903136
Sum of electronic and thermal Free Energies= -839.967122

IM2:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.315156	-1.099654	-0.867347
2	6	0	-2.505189	-1.461091	-0.443128
3	6	0	-3.147395	-2.788520	-0.671969
4	1	0	-2.458467	-3.402509	-1.253744
5	1	0	-4.089886	-2.706283	-1.228349
6	1	0	-3.367512	-3.313211	0.266550
7	7	0	-3.119722	-0.441249	0.265437
8	6	0	-4.423251	-0.451619	0.903725
9	1	0	-5.211032	-0.673002	0.177063
10	1	0	-4.464337	-1.195927	1.705779
11	1	0	-4.604086	0.535353	1.329909
12	6	0	-2.233552	0.613318	0.267150
13	8	0	-2.562018	1.770801	0.885025
14	6	0	-1.124402	0.198363	-0.429667
15	6	0	0.111348	0.995130	-0.741529
16	1	0	0.157254	1.205878	-1.823666
17	6	0	1.406961	0.307243	-0.344589
18	6	0	2.373584	-0.022708	-1.299122
19	1	0	2.190092	0.206668	-2.345925
20	6	0	3.564239	-0.650430	-0.939168
21	1	0	4.312158	-0.913028	-1.679781
22	6	0	3.806361	-0.948231	0.404084
23	8	0	4.989922	-1.559119	0.714158
24	1	0	5.020323	-1.719653	1.666382
25	6	0	2.851590	-0.617842	1.374590
26	1	0	3.038973	-0.850386	2.421220
27	6	0	1.663474	-0.000399	0.996599
28	1	0	0.920961	0.246437	1.749564
29	8	0	-0.054081	2.254848	-0.045081
30	6	0	0.848991	3.268825	-0.455953
31	1	0	0.628254	4.155872	0.141972
32	1	0	1.890398	2.970469	-0.286562
33	1	0	0.718975	3.511722	-1.520639
34	1	0	-1.785062	2.343449	0.734639

Zero-point correction= 0.277545
Thermal correction to Energy= 0.295545
Thermal correction to Enthalpy= 0.296489
Thermal correction to Gibbs Free Energy= 0.229460
Sum of electronic and zero-point Energies= -839.923861
Sum of electronic and thermal Energies= -839.905861

Sum of electronic and thermal Enthalpies= -839.904917
Sum of electronic and thermal Free Energies= -839.971946

TS3:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.279019	-1.390967	0.294123
2	6	0	2.567694	-1.561804	0.133885
3	6	0	3.266726	-2.877901	0.067064
4	1	0	2.517286	-3.667568	0.137285
5	1	0	3.983887	-3.007868	0.887552
6	1	0	3.819938	-3.007480	-0.871849
7	7	0	3.255071	-0.344666	0.052248
8	6	0	4.661826	-0.116881	-0.213930
9	1	0	5.286464	-0.448545	0.622122
10	1	0	4.978711	-0.639959	-1.121322
11	1	0	4.797162	0.956679	-0.356282
12	6	0	2.312255	0.649131	0.182565
13	8	0	2.500949	1.917600	-0.013347
14	6	0	1.092647	-0.013339	0.370781
15	6	0	-0.112497	0.749886	0.527138
16	1	0	-0.090287	1.506465	1.313263
17	6	0	-1.445603	0.184824	0.308080
18	6	0	-2.558663	0.743943	0.964091
19	1	0	-2.409550	1.576972	1.645903
20	6	0	-3.839804	0.246534	0.771765
21	1	0	-4.697472	0.671147	1.281934
22	6	0	-4.032942	-0.832408	-0.099913
23	8	0	-5.306192	-1.286663	-0.260849
24	1	0	-5.303489	-2.031335	-0.877161
25	6	0	-2.938563	-1.401836	-0.765831
26	1	0	-3.092972	-2.241498	-1.440195
27	6	0	-1.661064	-0.896658	-0.565098
28	1	0	-0.812992	-1.347835	-1.065048
29	8	0	0.200191	2.093610	-0.744052
30	6	0	-0.503174	3.291480	-0.475266
31	1	0	-0.145037	4.078735	-1.149435
32	1	0	-1.573970	3.141631	-0.651914
33	1	0	-0.362677	3.639812	0.560419
34	1	0	1.353759	2.183861	-0.425881

Zero-point correction= 0.272030
Thermal correction to Energy= 0.289643
Thermal correction to Enthalpy= 0.290587
Thermal correction to Gibbs Free Energy= 0.226337
Sum of electronic and zero-point Energies= -839.896512
Sum of electronic and thermal Energies= -839.878898

Sum of electronic and thermal Enthalpies=	-839.877954
Sum of electronic and thermal Free Energies=	-839.942204

in Benzene:

n-propylamine

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.897771	-0.178747	-0.093893
2	1	0	2.647180	0.509125	-0.075723
3	1	0	2.048077	-0.776315	0.716979
4	6	0	0.599425	0.493660	0.029201
5	1	0	0.512059	1.204509	-0.802759
6	6	0	-0.544607	-0.518187	-0.055854
7	1	0	0.485341	1.086373	0.956192
8	6	0	-1.927988	0.132802	0.021582
9	1	0	-0.437680	-1.082780	-0.989171
10	1	0	-0.437245	-1.248236	0.759283
11	1	0	-2.723944	-0.616303	-0.034421
12	1	0	-2.058630	0.685379	0.959103
13	1	0	-2.080533	0.839829	-0.801802

Zero-point correction=	0.121608
Thermal correction to Energy=	0.127246
Thermal correction to Enthalpy=	0.128190
Thermal correction to Gibbs Free Energy=	0.093767
Sum of electronic and zero-point Energies=	-174.378287
Sum of electronic and thermal Energies=	-174.372648
Sum of electronic and thermal Enthalpies=	-174.371704
Sum of electronic and thermal Free Energies=	-174.406127

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.939144	-0.093184	0.736645
2	6	0	1.476549	-0.289134	-0.591530
3	6	0	0.137110	-0.023496	-1.033724
4	7	0	-0.131968	1.687783	-0.414495
5	7	0	3.318590	-0.318118	0.634047
6	6	0	4.227079	-0.208069	1.753314
7	1	0	4.990806	0.558842	1.581080
8	1	0	3.624696	0.077827	2.618654
9	1	0	4.728991	-1.159307	1.963611

10	6	0	3.610853	-0.565697	-0.707445
11	6	0	4.993630	-0.862419	-1.185097
12	1	0	5.697412	-0.051795	-0.954758
13	1	0	4.962061	-0.995617	-2.267775
14	1	0	5.399845	-1.778492	-0.736511
15	7	0	2.544382	-0.519346	-1.462624
16	1	0	0.095215	0.110786	-2.116355
17	6	0	-1.067612	-0.752360	-0.534679
18	6	0	-1.226818	-1.146786	0.809446
19	1	0	-0.456074	-0.882786	1.528652
20	6	0	-2.355049	-1.847315	1.214544
21	1	0	-2.481584	-2.153172	2.247902
22	6	0	-2.079493	-1.085716	-1.446269
23	1	0	-1.975821	-0.801421	-2.490594
24	6	0	-3.210850	-1.797531	-1.049402
25	1	0	-3.977067	-2.056926	-1.777006
26	6	0	-3.351681	-2.180324	0.286981
27	8	0	-4.433409	-2.874643	0.747946
28	1	0	-5.030781	-3.056961	0.010593
29	1	0	0.604673	2.224986	-0.869769
30	1	0	0.175952	1.509695	0.559023
31	6	0	-1.446221	2.354624	-0.485238
32	1	0	-1.698890	2.486887	-1.543372
33	1	0	-2.176942	1.660747	-0.060678
34	6	0	-1.485901	3.697620	0.252293
35	1	0	-0.733494	4.372442	-0.176729
36	1	0	-1.201306	3.538742	1.299999
37	6	0	-2.869198	4.352828	0.182229
38	1	0	-3.633842	3.713091	0.635479
39	1	0	-3.167000	4.546277	-0.854156
40	1	0	-2.876543	5.308504	0.714018
41	8	0	1.341336	0.319290	1.774277

Zero-point correction=	0.346490
Thermal correction to Energy=	0.366789
Thermal correction to Enthalpy=	0.367733
Thermal correction to Gibbs Free Energy=	0.296544
Sum of electronic and zero-point Energies=	-898.605650
Sum of electronic and thermal Energies=	-898.585351
Sum of electronic and thermal Enthalpies=	-898.584407
Sum of electronic and thermal Free Energies=	-898.655596

IM1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.222634	-0.614231	-1.371213
2	6	0	1.359883	0.133975	-0.592519

3	6	0	-0.077441	0.430324	-0.927253
4	6	0	-1.041748	-0.648325	-0.442211
5	6	0	2.004256	0.528577	0.555191
6	8	0	1.591104	1.265390	1.613017
7	7	0	-0.387406	1.750464	-0.298281
8	1	0	0.721197	1.623789	1.305338
9	1	0	0.256248	2.419867	-0.721402
10	6	0	-1.756167	2.244557	-0.503756
11	1	0	-2.447043	1.541660	-0.028287
12	1	0	-2.021602	2.270248	-1.575863
13	6	0	-1.933086	3.637080	0.103040
14	1	0	-1.213516	4.329392	-0.356719
15	1	0	-1.680060	3.592138	1.169348
16	6	0	-3.352143	4.183604	-0.078080
17	1	0	-3.451577	5.180049	0.362925
18	1	0	-3.617221	4.261379	-1.138351
19	1	0	-4.091449	3.532465	0.401101
20	6	0	-1.850086	-1.337781	-1.347731
21	1	0	-1.793704	-1.097090	-2.406161
22	6	0	-2.725949	-2.339759	-0.924067
23	1	0	-3.342305	-2.868898	-1.648205
24	6	0	-2.807833	-2.660019	0.432155
25	8	0	-3.646127	-3.626163	0.918022
26	1	0	-4.126242	-4.023970	0.180007
27	6	0	-2.005951	-1.977747	1.356028
28	1	0	-2.076618	-2.241666	2.406132
29	6	0	-1.132297	-0.990586	0.916967
30	1	0	-0.503993	-0.479584	1.640033
31	1	0	-0.178161	0.485584	-2.023261
32	6	0	3.358539	-0.670668	-0.710035
33	6	0	4.595670	-1.374970	-1.157483
34	1	0	5.446203	-0.691975	-1.280436
35	1	0	4.390025	-1.841593	-2.121927
36	1	0	4.906132	-2.158946	-0.455077
37	7	0	3.282480	0.024071	0.488914
38	6	0	4.315749	0.202368	1.492419
39	1	0	5.220774	0.626422	1.047058
40	1	0	3.939690	0.889281	2.251203
41	1	0	4.571086	-0.748275	1.972305

Zero-point correction=	0.348069
Thermal correction to Energy=	0.368533
Thermal correction to Enthalpy=	0.369477
Thermal correction to Gibbs Free Energy=	0.297661
Sum of electronic and zero-point Energies=	-898.630017
Sum of electronic and thermal Energies=	-898.609553
Sum of electronic and thermal Enthalpies=	-898.608609
Sum of electronic and thermal Free Energies=	-898.680425

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.898967	-1.433011	0.738660
2	6	0	-1.353509	-0.169773	0.575301
3	6	0	0.004813	0.227212	1.089665
4	6	0	1.142453	-0.627589	0.542863
5	6	0	-2.262459	0.638747	-0.066359
6	8	0	-2.217348	1.936473	-0.424694
7	7	0	0.175475	1.721057	0.848792
8	1	0	-1.334693	2.205363	-0.041228
9	1	0	0.157761	2.177957	1.757141
10	6	0	1.377309	2.187077	0.135768
11	1	0	1.379930	1.740083	-0.863126
12	1	0	2.308894	1.860484	0.622679
13	6	0	1.367919	3.712704	0.017252
14	1	0	1.315556	4.155702	1.022327
15	1	0	0.456976	4.029322	-0.505945
16	6	0	2.602393	4.251496	-0.711845
17	1	0	2.573933	5.342961	-0.783081
18	1	0	3.525449	3.975430	-0.190326
19	1	0	2.666056	3.853177	-1.730343
20	6	0	2.238483	-0.943161	1.351958
21	1	0	2.259493	-0.599696	2.383729
22	6	0	3.306121	-1.700195	0.869366
23	1	0	4.145206	-1.940226	1.519434
24	6	0	3.287833	-2.160170	-0.450307
25	8	0	4.298397	-2.908445	-0.988118
26	1	0	4.972735	-3.058133	-0.312614
27	6	0	2.196155	-1.861817	-1.273442
28	1	0	2.190065	-2.236757	-2.291596
29	6	0	1.139441	-1.108546	-0.774207
30	1	0	0.283945	-0.899806	-1.409000
31	1	0	0.018748	0.083270	2.179347
32	6	0	-3.098869	-1.389217	0.204905
33	6	0	-4.064879	-2.524594	0.133619
34	1	0	-5.007326	-2.305950	0.652133
35	1	0	-3.604726	-3.391430	0.610157
36	1	0	-4.317587	-2.794361	-0.900004
37	7	0	-3.379394	-0.131281	-0.307910
38	6	0	-4.587744	0.322611	-0.969556
39	1	0	-5.460519	0.197934	-0.320658
40	1	0	-4.470271	1.381438	-1.202359
41	1	0	-4.760579	-0.227045	-1.900844

Zero-point correction= 0.347388

Thermal correction to Energy= 0.367133
Thermal correction to Enthalpy= 0.368078
Thermal correction to Gibbs Free Energy= 0.298285
Sum of electronic and zero-point Energies= -898.624275
Sum of electronic and thermal Energies= -898.604530
Sum of electronic and thermal Enthalpies= -898.603586
Sum of electronic and thermal Free Energies= -898.673378

IM2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.733121	-1.439925	0.532341
2	6	0	-1.316140	-0.133027	0.345364
3	6	0	0.069486	0.385330	0.630587
4	6	0	1.187276	-0.602985	0.328941
5	6	0	-2.390289	0.635628	-0.042379
6	8	0	-2.502888	1.947816	-0.330440
7	7	0	0.217949	1.681120	-0.115867
8	1	0	-1.558756	2.253484	-0.264592
9	1	0	0.394154	1.441486	-1.092567
10	6	0	1.317524	2.535017	0.356092
11	1	0	1.097989	2.814097	1.394632
12	1	0	2.278644	1.996487	0.368692
13	6	0	1.447249	3.796675	-0.498742
14	1	0	1.635963	3.507292	-1.541966
15	1	0	0.489677	4.331792	-0.494885
16	6	0	2.567932	4.722228	-0.016451
17	1	0	2.391017	5.057271	1.011609
18	1	0	2.642894	5.613122	-0.647161
19	1	0	3.539564	4.216568	-0.038073
20	1	0	0.149523	0.656980	1.693865
21	7	0	-3.478647	-0.203700	-0.106815
22	6	0	-4.821358	0.183526	-0.497541
23	1	0	-5.141840	-0.356604	-1.394348
24	1	0	-4.818813	1.252683	-0.711553
25	1	0	-5.536525	-0.014677	0.307125
26	6	0	-3.018026	-1.461204	0.256930
27	6	0	-3.902892	-2.661667	0.311700
28	1	0	-4.349762	-2.898308	-0.662654
29	1	0	-4.726837	-2.541369	1.026868
30	1	0	-3.298327	-3.513576	0.626336
31	6	0	1.215071	-1.321581	-0.876496
32	1	0	0.383736	-1.228189	-1.569260
33	6	0	2.268215	-2.172559	-1.188760
34	1	0	2.284831	-2.733314	-2.117496
35	6	0	3.325961	-2.330578	-0.284973
36	8	0	4.336162	-3.182360	-0.639199

37	1	0	4.984087	-3.214927	0.076722
38	6	0	3.313376	-1.632859	0.924737
39	1	0	4.127810	-1.758381	1.635537
40	6	0	2.249291	-0.778651	1.219968
41	1	0	2.245472	-0.247801	2.168812

Zero-point correction=	0.347763
Thermal correction to Energy=	0.368293
Thermal correction to Enthalpy=	0.369237
Thermal correction to Gibbs Free Energy=	0.296980
Sum of electronic and zero-point Energies=	-898.631191
Sum of electronic and thermal Energies=	-898.610661
Sum of electronic and thermal Enthalpies=	-898.609717
Sum of electronic and thermal Free Energies=	-898.681973

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.440969	0.479989	0.493642
2	6	0	-1.316242	-0.374871	0.385605
3	6	0	0.001390	0.129783	0.680307
4	7	0	0.073343	1.647813	-0.286585
5	1	0	0.064645	0.671220	1.629342
6	8	0	-2.503304	1.721960	0.743107
7	7	0	-3.512503	-0.337678	0.116207
8	6	0	-4.883249	0.117793	0.057561
9	1	0	-4.873077	1.178233	0.320023
10	1	0	-5.304212	0.001979	-0.947499
11	1	0	-5.521806	-0.420300	0.767502
12	6	0	-2.990558	-1.584762	-0.225252
13	6	0	-3.851469	-2.722569	-0.663363
14	1	0	-4.433144	-2.483952	-1.563596
15	1	0	-4.568090	-3.023326	0.112189
16	1	0	-3.207827	-3.575671	-0.884647
17	7	0	-1.688220	-1.629088	-0.097102
18	6	0	1.230195	-0.665857	0.417019
19	6	0	1.307856	-1.602477	-0.631189
20	1	0	0.421916	-1.799638	-1.222975
21	6	0	2.368661	-0.469356	1.212615
22	1	0	2.329005	0.237615	2.037470
23	6	0	3.547869	-1.173771	0.980617
24	1	0	4.416735	-1.012429	1.615179
25	6	0	3.605824	-2.096282	-0.069048
26	8	0	4.727637	-2.818252	-0.355436
27	1	0	5.418147	-2.600157	0.284477
28	1	0	2.538896	-3.038679	-1.673518
29	1	0	0.048666	1.354492	-1.262134

30	1	0	-0.875664	2.002107	-0.007971
31	6	0	1.147047	2.617883	-0.013246
32	1	0	2.107027	2.129443	-0.212174
33	1	0	1.108682	2.840936	1.058959
34	6	0	1.014180	3.910626	-0.825106
35	1	0	0.036820	4.364545	-0.620843
36	1	0	1.028663	3.667138	-1.895679
37	6	0	2.131499	4.909858	-0.507749
38	1	0	2.020424	5.822044	-1.100842
39	1	0	3.118107	4.487387	-0.727353
40	1	0	2.118733	5.197112	0.549192
41	6	0	2.478690	-2.308835	-0.873098

Zero-point correction=	0.346459
Thermal correction to Energy=	0.366700
Thermal correction to Enthalpy=	0.367645
Thermal correction to Gibbs Free Energy=	0.296499
Sum of electronic and zero-point Energies=	-898.609425
Sum of electronic and thermal Energies=	-898.589184
Sum of electronic and thermal Enthalpies=	-898.588240
Sum of electronic and thermal Free Energies=	-898.659385

Z-HOBDI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.290434	0.978390	-0.000008
2	6	0	-2.584120	1.129926	-0.000007
3	6	0	-3.275444	2.451234	-0.000018
4	1	0	-2.524364	3.241299	-0.000039
5	1	0	-3.915005	2.566078	0.882791
6	1	0	-3.915029	2.566051	-0.882814
7	7	0	-3.296459	-0.064100	0.000004
8	6	0	-4.730991	-0.265066	0.000016
9	1	0	-5.197741	0.166547	0.891374
10	1	0	-5.197755	0.166558	-0.891329
11	1	0	-4.893601	-1.344776	0.000011
12	6	0	-2.367612	-1.120527	0.000015
13	8	0	-2.645743	-2.310057	0.000028
14	6	0	-1.063062	-0.406086	0.000006
15	6	0	0.121993	-1.069812	0.000010
16	1	0	0.020846	-2.153930	0.000021
17	6	0	1.476300	-0.555475	0.000002
18	6	0	2.549451	-1.473701	0.000010
19	1	0	2.331984	-2.538396	0.000021
20	6	0	3.870444	-1.052942	0.000003
21	1	0	4.691613	-1.761499	0.000009
22	6	0	4.155929	0.318084	-0.000011

23	8	0	5.467365	0.687089	-0.000017
24	1	0	5.525810	1.651917	-0.000027
25	6	0	3.108381	1.250441	-0.000019
26	1	0	3.333794	2.315165	-0.000030
27	6	0	1.788368	0.822000	-0.000012
28	1	0	0.976892	1.540236	-0.000018

Zero-point correction=	0.222186
Thermal correction to Energy=	0.236697
Thermal correction to Enthalpy=	0.237641
Thermal correction to Gibbs Free Energy=	0.180264
Sum of electronic and zero-point Energies=	-724.265436
Sum of electronic and thermal Energies=	-724.250925
Sum of electronic and thermal Enthalpies=	-724.249981
Sum of electronic and thermal Free Energies=	-724.307358