Supporting Information for

The Morita-Baylis-Hillman Reaction: ESI-MS(/MS) Investigation with Charge Tags and Ionic Liquid Effect Origin Revealed by DFT Calculations

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Summary

Figures S1-S12

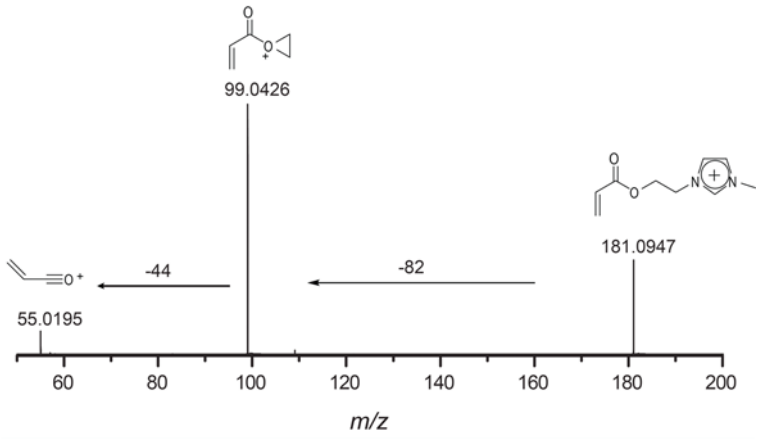


Figure S1. High-resolution ESI(+)-MS/MS of the charge-tagged acrylate derivative **11**.

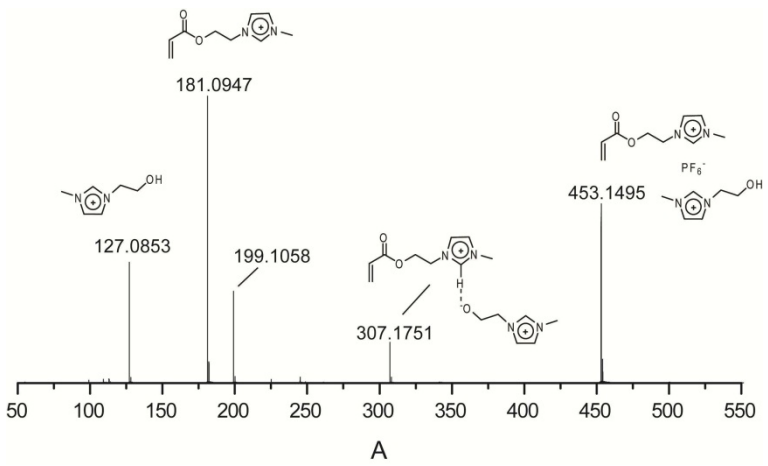


Figure S2. High-resolution ESI(+)-MS/MS of the ion of *m/z* 453.

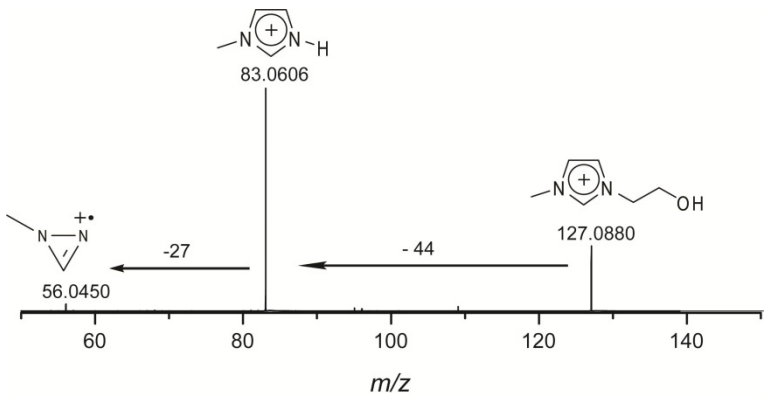


Figure S3. High-resolution ESI(+)-MS/MS of the charge-tagged alcohol.

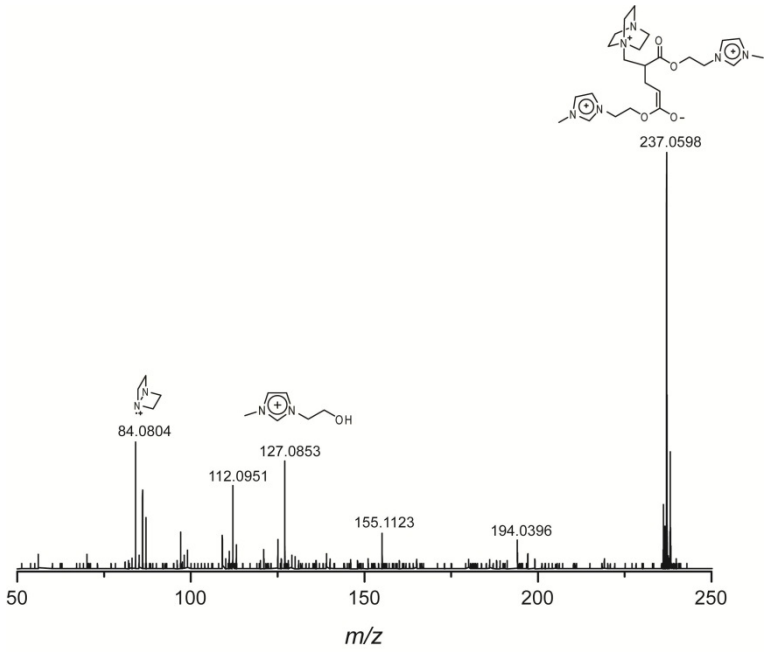


Figure S4. High-resolution ESI(+)-MS/MS of the ion of *m/z* 237. Note it is a dicharged specie.

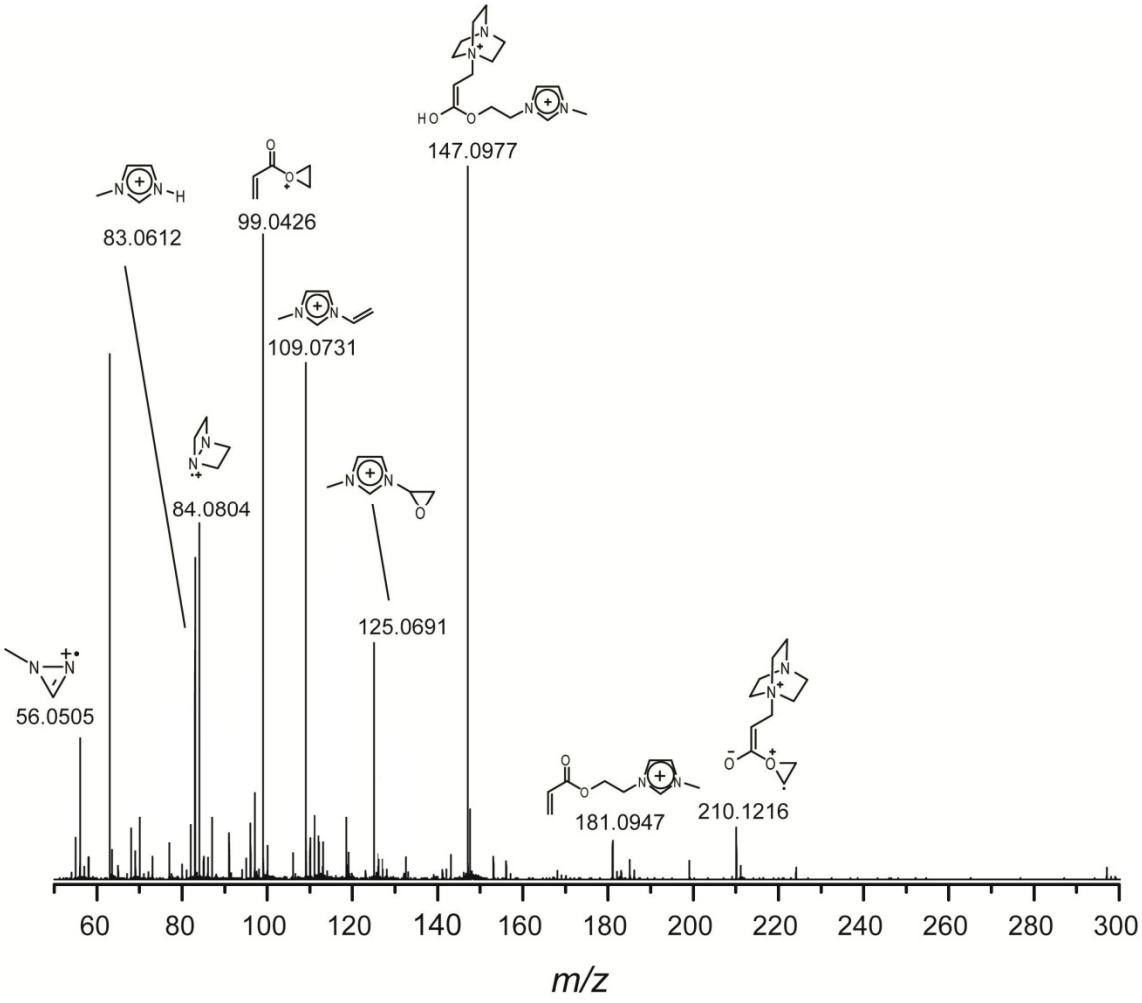


Figure S5. High-resolution ESI(+)-MS/MS of the ion of *m/z* 147. Note it is a dicharged specie.

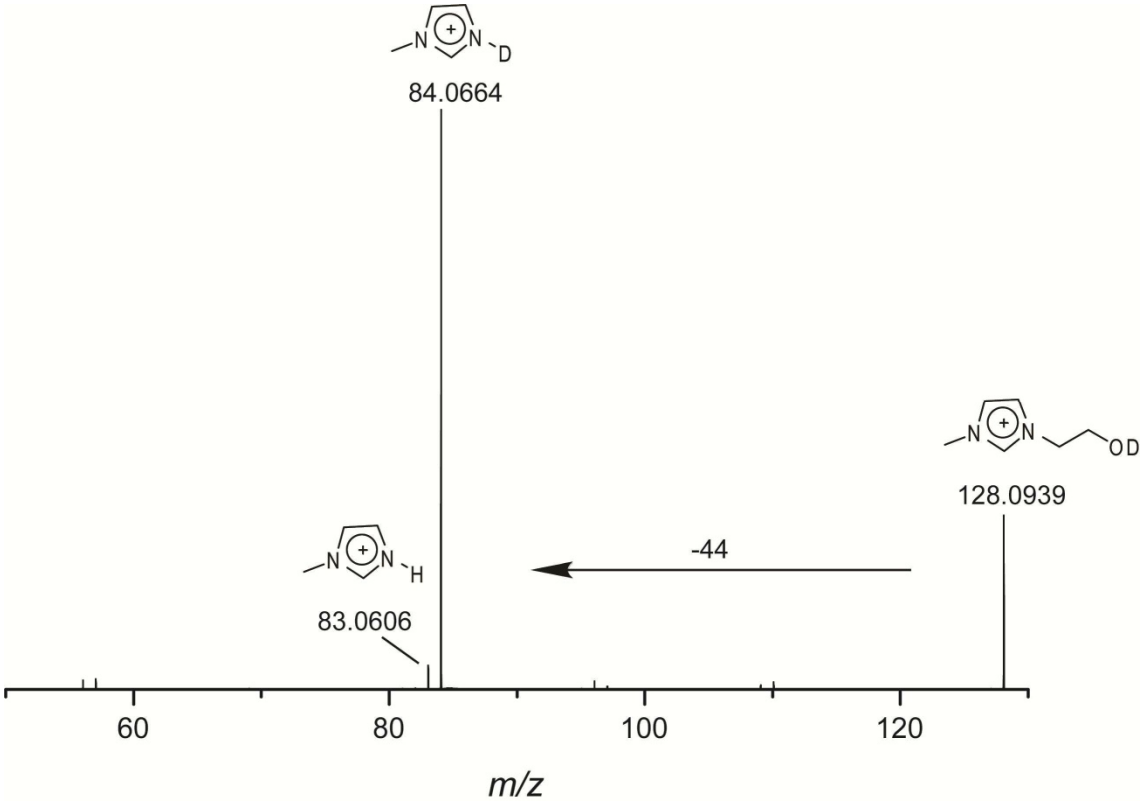
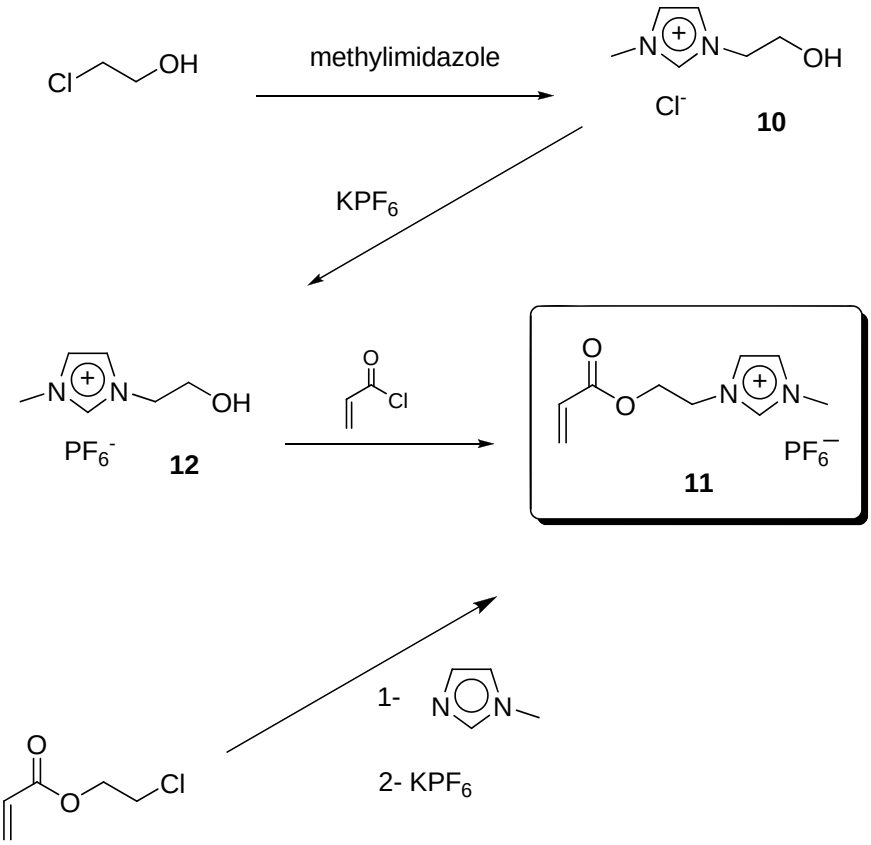
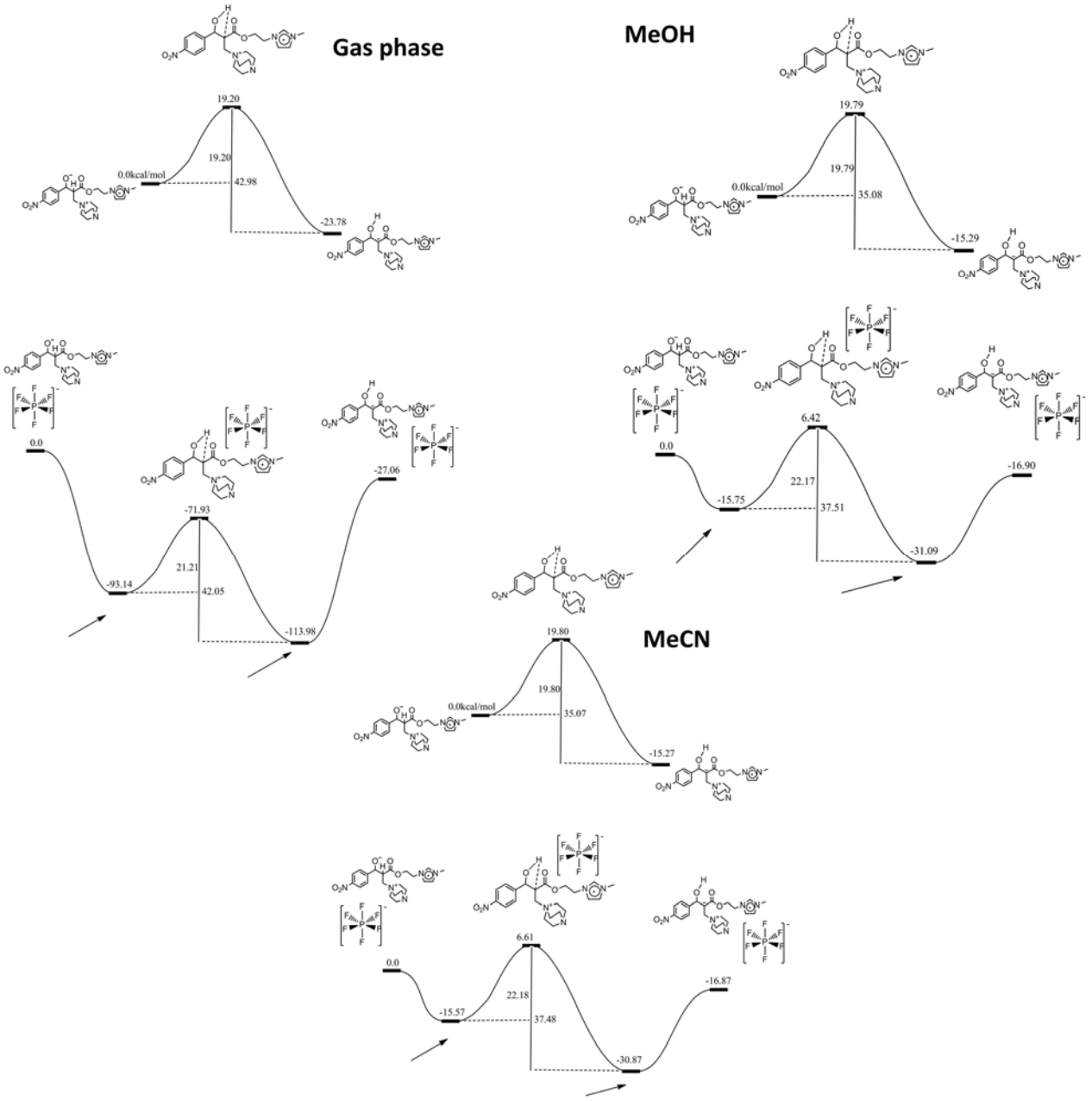


Figure S6. High-resolution ESI(+)-MS/MS of the charge-tagged deuterated alcohol.



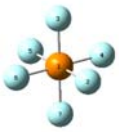
Scheme S1. Synthesis of **11** and **12**.



Scheme S2. Direct (intramolecular) H-transfer. The arrows indicate the electrostatic intermediate complex formation observed as the 'apparent negative activation energy' in the intrinsic reaction coordinate.

Cartesian coordinates (Angstroms and Degrees), energy (Hartree) and thermal corrections for all the calculated structures at M062X/6-311G(d,p) level. It was regarded for calculate the thermodynamics correction terms, a temperature at 295.15K.

$[PF_6]^-$ - Gas phase



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Zero-point correction=                           0.019664
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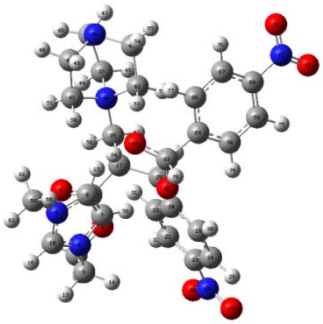
Thermal correction to Enthalpy=                  0.026589
Thermal correction to Gibbs Free Energy=        -0.007414
Sum of electronic and zero-point Energies=           -940.636435
Sum of electronic and thermal Energies=              -940.630453
Sum of electronic and thermal Enthalpies=            -940.629509
Sum of electronic and thermal Free Energies=         -940.663513
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.000000	0.000000	0.000000
2	9	0	0.000000	0.000000	1.630000
3	9	0	0.000000	1.630000	0.000000
4	9	0	1.630000	0.000000	0.000000
5	9	0	0.000000	0.000000	-1.630000
6	9	0	-1.630000	0.000000	0.000000
7	9	0	0.000000	-1.630000	0.000000

Structure 13 - Gas phase



```
Zero-point correction=                           0.646709
Thermal correction to Energy=                    0.683952
Thermal correction to Enthalpy=                  0.684896
Thermal correction to Gibbs Free Energy=         0.573261
Sum of electronic and zero-point Energies=          -2055.060192
Sum of electronic and thermal Energies=             -2055.022950
Sum of electronic and thermal Enthalpies=           -2055.022006
Sum of electronic and thermal Free Energies=        -2055.133641
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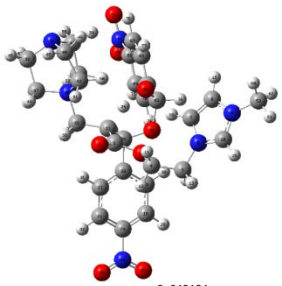
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.890388	-1.144625	1.251469
2	8	0	-2.153432	-1.821227	2.209273
3	8	0	-2.737060	-0.950879	0.225841
4	6	0	-3.944979	-1.708396	0.191561
5	6	0	-4.144223	-2.145893	-1.253669
6	7	0	-3.024977	-2.986360	-1.692931
7	6	0	-1.732478	-2.527254	-1.839643
8	6	0	-0.959800	-3.606081	-2.123102
9	7	0	-1.798265	-4.702010	-2.165261
10	6	0	-3.040034	-4.304590	-1.893594
11	1	0	-3.868801	-2.561287	0.867459
12	1	0	-4.775270	-1.072131	0.502454
13	1	0	-5.068669	-2.714212	-1.358108
14	1	0	-4.184313	-1.277620	-1.911807
15	1	0	0.109341	-3.645601	-2.256886
16	1	0	-3.908273	-4.941908	-1.847615
17	6	0	-0.541406	-0.508537	1.003457
18	6	0	-3.028083	3.409610	-0.761551
19	6	0	-2.043786	2.441180	-0.906362
20	6	0	-1.595657	1.709840	0.193680
21	6	0	-2.158407	1.958223	1.448099
22	6	0	-3.143215	2.922205	1.611243
23	6	0	-3.559177	3.632248	0.497585
24	7	0	-4.619583	4.651386	0.658191
25	6	0	-0.487460	0.685138	0.006131
26	8	0	-0.485749	0.258190	-1.326398
27	8	0	-4.965015	5.250616	-0.333377
28	8	0	-5.069587	4.810350	1.769982
29	1	0	-3.389141	3.987174	-1.601926
30	1	0	-1.628449	2.229912	-1.882379
31	1	0	-1.854172	1.391278	2.321879
32	1	0	-3.593634	3.125258	2.573328
33	1	0	0.463767	1.200313	0.217108
34	1	0	-0.004677	-1.279107	0.420011
35	6	0	0.170957	-0.248769	2.332859
36	7	0	1.502366	-0.940968	2.467615
37	6	0	2.118039	-0.574244	3.793779
38	6	0	3.384985	-1.444086	4.009940
39	7	0	3.778126	-2.076831	2.747738
40	6	0	2.769042	-3.062350	2.373129
41	6	0	1.350420	-2.440899	2.419723
42	6	0	2.449183	-0.520119	1.362802
43	6	0	3.859159	-1.057055	1.702393
44	1	0	1.364238	-0.735745	4.565248
45	1	0	2.348087	0.491125	3.741204
46	1	0	3.198843	-2.224633	4.740483
47	1	0	4.203635	-0.824863	4.368412
48	1	0	2.824331	-3.916243	3.049562
49	1	0	2.991103	-3.411597	1.363610
50	1	0	0.772036	-2.691685	1.532828
51	1	0	0.782765	-2.721678	3.308932
52	1	0	2.420125	0.569922	1.306462
53	1	0	2.050056	-0.948865	0.436589
54	1	0	4.306940	-1.489107	0.806626
55	1	0	4.516117	-0.258233	2.050435
56	1	0	-1.477378	-1.485435	-1.711477
57	1	0	0.383705	0.814232	2.469889
58	1	0	-0.435849	-0.600658	3.168807
59	6	0	-1.388596	-6.072867	-2.471190
60	1	0	-0.958674	-6.104379	-3.470735
61	1	0	-0.653515	-6.400558	-1.738215
62	1	0	-2.261154	-6.720968	-2.429059
63	6	0	0.743556	-0.477639	-1.815315
64	8	0	0.976661	-1.604438	-1.167784
65	6	0	1.921747	0.511370	-1.812213
66	6	0	3.209351	-0.018100	-1.711201
67	6	0	4.323432	0.809466	-1.699736
68	6	0	4.124158	2.178661	-1.793932
69	6	0	2.863240	2.738566	-1.925026
70	6	0	1.761583	1.891270	-1.941414
71	7	0	5.300900	3.073631	-1.752870
72	8	0	6.383985	2.557772	-1.590199
73	8	0	5.100955	4.260220	-1.875038
74	1	0	0.766635	2.309301	-2.042469
75	1	0	2.764284	3.812546	-2.009622
76	1	0	5.331010	0.422416	-1.624318
77	1	0	3.311816	-1.094794	-1.637001
78	1	0	0.430111	-0.606577	-2.870884

Structure 14 - Gas phase



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Thermal correction to Gibbs Free Energy=         0.567779
Sum of electronic and zero-point Energies=          -2055.059315
Sum of electronic and thermal Energies=             -2055.022241
Sum of electronic and thermal Enthalpies=           -2055.021296
Sum of electronic and thermal Free Energies=        -2055.133660
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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.386434	0.498599	1.809808
2	8	0	1.578577	0.758296	2.975122
3	8	0	2.251432	0.889656	0.841492
4	6	0	3.382150	1.640142	1.250837
5	6	0	4.008186	2.149995	-0.030108
6	7	0	3.200578	3.214121	-0.658223
7	6	0	1.828454	3.236351	-0.827146
8	6	0	1.541760	4.391304	-1.483931
9	7	0	2.731661	5.048130	-1.710819
10	6	0	3.717233	4.316109	-1.200809
11	1	0	3.085638	2.453335	1.917868
12	1	0	4.093137	0.999691	1.778277
13	1	0	4.994102	2.571410	0.166607
14	1	0	4.100158	1.327615	-0.741349
15	1	0	0.595156	4.792414	-1.804401
16	1	0	4.764016	4.573465	-1.224168
17	6	0	0.204748	-0.154067	1.230558
18	6	0	3.402885	-2.892477	-1.389702
19	6	0	2.311282	-2.036264	-1.338182
20	6	0	1.625594	-1.828458	-0.140595
21	6	0	2.050065	-2.494643	1.010554
22	6	0	3.135242	-3.358941	0.975546
23	6	0	3.795059	-3.538054	-0.228760
24	7	0	4.964363	-4.442283	-0.272348
25	6	0	0.413618	-0.910413	-0.105549
26	8	0	0.518025	-0.040205	-1.214823
27	8	0	5.540201	-4.552549	-1.330574
28	8	0	5.268106	-5.005290	0.754549
29	1	0	3.949644	-3.067530	-2.306435
30	1	0	1.989707	-1.510767	-2.226895
31	1	0	1.547048	-2.336926	1.958024
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36	7	0	-1.897309	-0.188070	2.670855
37	6	0	-2.496012	-0.890300	3.857601
38	6	0	-3.924133	-0.332660	4.083816
39	7	0	-4.095158	0.922646	3.358080
40	6	0	-2.969120	1.801844	3.669479
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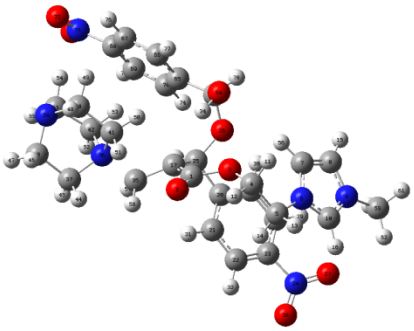
42	6	0	-2.884724	-0.232324	1.536385
43	6	0	-4.100601	0.643424	1.922247
44	1	0	-1.831407	-0.695470	4.701086
45	1	0	-2.489614	-1.960006	3.644618
46	1	0	-4.094781	-0.165760	5.147762
47	1	0	-4.676539	-1.040351	3.731838
48	1	0	-2.879315	1.872461	4.755008
49	1	0	-3.174626	2.801954	3.286591
50	1	0	-1.421931	1.773560	2.105620
51	1	0	-0.800442	1.292617	3.699846
52	1	0	-3.147133	-1.282417	1.388326
53	1	0	-2.375761	0.147770	0.654304
54	1	0	-4.065854	1.593540	1.385415
55	1	0	-5.028721	0.139286	1.651103
56	1	0	1.151035	2.464436	-0.474845
57	1	0	-0.907872	-1.875225	1.948083
58	1	0	-0.041215	-0.971059	3.212949
59	6	0	2.880750	6.333383	-2.395212
60	1	0	2.338789	7.100193	-1.844485
61	1	0	3.936784	6.590608	-2.435603
62	1	0	2.487202	6.247762	-3.406523
63	6	0	-0.557245	0.907903	-1.395432
64	8	0	-0.753721	1.681682	-0.291565
65	6	0	-1.830354	0.198089	-1.863103
66	6	0	-3.055440	0.838808	-1.668325
67	6	0	-4.240191	0.242791	-2.075429
68	6	0	-4.173308	-1.002919	-2.682089
69	6	0	-2.973015	-1.655236	-2.913244
70	6	0	-1.796081	-1.039778	-2.503653
71	7	0	-5.432782	-1.659730	-3.096464
72	8	0	-6.467248	-1.090092	-2.830449
73	8	0	-5.343359	-2.723636	-3.664137
74	1	0	-0.842405	-1.527112	-2.672627
75	1	0	-2.976903	-2.619775	-3.402851
76	1	0	-5.203382	0.715612	-1.936503
77	1	0	-3.058968	1.805007	-1.176874
78	1	0	-0.185792	1.499705	-2.249199

Structure 15 - Gas phase

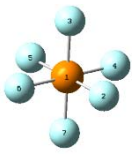


Zero-point correction= 0.646973
Thermal correction to Energy= 0.684038
Thermal correction to Enthalpy= 0.684982
Thermal correction to Gibbs Free Energy= 0.576708
Sum of electronic and zero-point Energies= -2055.080757
Sum of electronic and thermal Energies= -2055.043692
Sum of electronic and thermal Enthalpies= -2055.042748
Sum of electronic and thermal Free Energies= -2055.151023

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.342582	1.676278	-1.043221
2	8	0	0.163620	2.831131	-1.403001
3	8	0	1.353065	0.914712	-1.625937
4	6	0	2.274220	1.569181	-2.470482
5	6	0	3.636040	1.527572	-1.807232
6	7	0	4.092398	0.136838	-1.583474
7	6	0	3.400410	-1.032870	-1.825000
8	6	0	4.240375	-2.053509	-1.507543
9	7	0	5.420246	-1.495067	-1.067772
10	6	0	5.302847	-0.173798	-1.119374
11	1	0	2.290115	1.052515	-3.434078
12	1	0	1.978340	2.607642	-2.626014
13	1	0	4.380185	2.024502	-2.431858
14	1	0	3.583640	2.016620	-0.833230
15	1	0	4.094416	-3.119478	-1.541318
16	1	0	6.070243	0.529059	-0.835436
17	6	0	-0.383922	0.937528	-0.076352
18	6	0	3.797722	-1.003327	1.700598
19	6	0	2.481619	-1.181542	1.308678
20	6	0	1.630624	-0.085506	1.128280
21	6	0	2.092631	1.185566	1.472150
22	6	0	3.400960	1.383225	1.899121
23	6	0	4.242608	0.285318	1.957163
24	7	0	5.671354	0.500714	2.222030
25	6	0	0.221987	-0.294927	0.551069
26	8	0	0.394822	-1.479664	-0.262642
27	8	0	6.442467	-0.336048	1.776205
28	8	0	5.998666	1.496216	2.815535
29	1	0	4.480150	-1.837325	1.803346
30	1	0	2.118765	-2.174068	1.080579
31	1	0	1.442859	2.045364	1.359941
32	1	0	3.780288	2.366085	2.148882
33	1	0	-0.428359	-0.570025	1.393909
34	1	0	-0.618739	-0.224469	-2.139390
35	6	0	-1.213330	1.820950	0.775467
36	7	0	-2.725801	1.999940	0.411443
37	6	0	-3.222890	3.278652	1.018671
38	6	0	-4.697417	3.500948	0.584692
39	7	0	-5.203449	2.339025	-0.135315
40	6	0	-4.440765	2.165605	-1.367761
41	6	0	-2.921094	2.071491	-1.075497
42	6	0	-3.539406	0.864767	0.957062
43	6	0	-5.044152	1.150962	0.695924
44	1	0	-2.565892	4.075415	0.669999
45	1	0	-3.109757	3.178774	2.100164
46	1	0	-4.771665	4.371893	-0.068071
47	1	0	-5.327232	3.682751	1.456200
48	1	0	-4.646286	3.004088	-2.034255
49	1	0	-4.791730	1.255323	-1.857793
50	1	0	-2.468566	1.169318	-2.488222
51	1	0	-2.344171	2.929653	-1.422513
52	1	0	-3.313555	0.789287	2.021875
53	1	0	-3.179591	-0.031369	0.457047
54	1	0	-5.517739	0.303153	0.198733
55	1	0	-5.570734	1.315609	1.637446
56	1	0	2.365402	-1.038995	-2.132772
57	1	0	-1.245221	1.503401	1.821722
58	1	0	-0.843796	2.847269	0.722632
59	6	0	6.593963	-2.229259	-0.591639
60	1	0	6.320131	-2.808296	0.288747
61	1	0	6.950918	-2.883114	-1.385375
62	1	0	7.362835	-1.514338	-0.311491
63	6	0	-0.559421	-1.887430	-1.206937
64	8	0	-0.504325	-1.149926	-2.388692
65	6	0	-1.967455	-2.011099	-0.647103
66	6	0	-3.071721	-1.756246	-1.461684
67	6	0	-4.360041	-1.936588	-0.974571
68	6	0	-4.515338	-2.383755	0.328724
69	6	0	-3.438756	-2.691414	1.146925
70	6	0	-2.157817	-2.502391	0.645759
71	7	0	-5.882798	-2.524441	0.871760
72	8	0	-6.779181	-2.002483	0.243793
73	8	0	-6.010526	-3.129351	1.909202
74	1	0	-1.295997	-2.743897	1.257522
75	1	0	-3.617420	-3.071596	2.144078
76	1	0	-5.235603	-1.742521	-1.580919
77	1	0	-2.911469	-1.429363	-2.481633
78	1	0	-0.237667	-2.895494	-1.484068

$[PF_6]$ – Solvent: Methanol

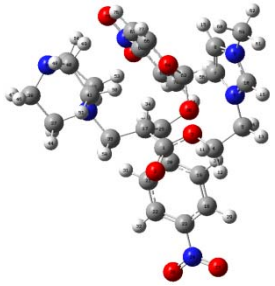


Zero-point correction= 0.019332
Thermal correction to Energy= 0.025373
Thermal correction to Enthalpy= 0.026317
Thermal correction to Gibbs Free Energy= -0.007778
Sum of electronic and zero-point Energies= -940.720957
Sum of electronic and thermal Energies= -940.714916
Sum of electronic and thermal Enthalpies= -940.713972
Sum of electronic and thermal Free Energies= -940.748067

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.000000	0.000000	0.000000
2	9	0	0.000000	0.000000	1.622353
3	9	0	0.000000	1.622353	0.000000
4	9	0	1.622353	0.000000	0.000000
5	9	0	0.000000	0.000000	-1.622353
6	9	0	-1.622353	0.000000	0.000000
7	9	0	0.000000	-1.622353	0.000000

Structure 13 - Solvent: Methanol

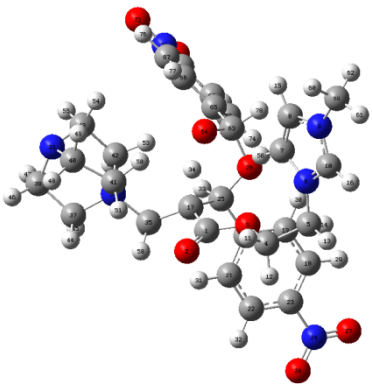


Zero-point correction= 0.646438
Thermal correction to Energy= 0.684226
Thermal correction to Enthalpy= 0.685170
Thermal correction to Gibbs Free Energy= 0.570334
Sum of electronic and zero-point Energies= -2055.156707
Sum of electronic and thermal Energies= -2055.118919
Sum of electronic and thermal Enthalpies= -2055.117974
Sum of electronic and thermal Free Energies= -2055.232811

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.033587	0.683085	1.126650
2	8	0	-2.535166	1.286975	2.038322
3	8	0	-2.688733	0.361912	0.007465
4	6	0	-4.056659	0.746608	-0.113275
5	6	0	-4.497758	0.200930	-1.454876
6	7	0	-4.450674	-1.266692	-1.482945
7	6	0	-3.321307	-2.064783	-1.408473
8	6	0	-3.757554	-3.348957	-1.485192
9	7	0	-5.129849	-3.315716	-1.607071
10	6	0	-5.523232	-2.048551	-1.602712
11	1	0	-4.637543	0.326066	0.709637
12	1	0	-4.146260	1.834778	-0.100924
13	1	0	-5.521242	0.503692	-1.669441
14	1	0	-3.845294	0.572708	-2.245002
15	1	0	-3.213511	-4.277427	-1.465589
16	1	0	-6.542139	-1.708138	-1.687965
17	6	0	-0.621405	0.158395	1.050522
18	6	0	-1.154896	4.355883	-0.621327
19	6	0	-0.986786	2.983102	-0.710029
20	6	0	0.072096	2.351924	-0.050003
21	6	0	0.983198	3.118313	0.677594
22	6	0	0.829664	4.494614	0.778738
23	6	0	-0.244248	5.084288	0.131467
24	7	0	-0.416617	6.543088	0.235163
25	6	0	0.195787	0.844116	-0.107046
26	8	0	-0.212502	0.409415	-1.367580
27	8	0	-1.361457	7.045022	-0.336213
28	8	0	0.394033	7.165060	0.888776
29	1	0	-1.968220	4.860983	-1.123472
30	1	0	-1.665487	2.385537	-1.305055
31	1	0	1.834427	2.646162	1.154864
32	1	0	1.526839	5.102888	1.337517
33	1	0	1.248378	0.581688	0.066937
34	1	0	-0.706566	-0.866884	0.678699
35	6	0	0.067448	0.224008	2.408754
36	7	0	0.738000	-1.070289	2.791978
37	6	0	1.503760	-0.863351	4.075606
38	6	0	2.007807	-2.239776	4.572330
39	7	0	1.890988	-3.244207	3.515741
40	6	0	0.474176	-3.490768	3.249866
41	6	0	-0.279762	-2.158569	3.027473
42	6	0	1.711895	-1.532145	1.730764
43	6	0	2.516280	-2.728164	2.297571
44	1	0	0.829761	-0.384009	4.784758
45	1	0	2.320660	-0.181165	3.840407
46	1	0	1.423548	-2.572658	5.430830
47	1	0	3.049710	-2.157533	4.881349
48	1	0	0.031177	-4.023219	4.091469
49	1	0	0.396830	-4.123743	2.365019
50	1	0	-0.935398	-2.204336	2.160766
51	1	0	-0.858346	-1.852915	3.899861
52	1	0	2.357145	-0.683944	1.499376
53	1	0	1.122767	-1.799388	0.847843
54	1	0	2.562122	-3.521664	1.550713
55	1	0	3.537206	-2.427578	2.536063
56	1	0	-2.308292	-1.691953	-1.280613
57	1	0	0.845704	0.988758	2.444749
58	1	0	-0.650958	0.444420	3.198665
59	6	0	-6.003056	-4.483686	-1.724810
60	1	0	-5.907118	-5.091753	-0.827931
61	1	0	-7.028575	-4.140845	-1.831346
62	1	0	-5.712284	-5.057257	-2.602262
63	6	0	0.186222	-0.986469	-1.726511
64	8	0	-0.249142	-1.915166	-0.902985
65	6	0	1.719401	-0.970156	-1.906005
66	6	0	2.445290	-2.113571	-1.575760
67	6	0	3.823473	-2.156341	-1.740868
68	6	0	4.458020	-1.031040	-2.247252
69	6	0	3.766390	0.123183	-2.593260
70	6	0	2.390148	0.141934	-2.421747
71	7	0	5.917265	-1.060815	-2.425323
72	8	0	6.508970	-2.075797	-2.119324
73	8	0	6.457821	-0.068960	-2.870148
74	1	0	1.825863	1.032581	-2.673068
75	1	0	4.382532	0.977515	-2.982677
76	1	0	4.400978	-3.034417	-1.485994
77	1	0	1.904394	-2.964614	-1.179899
78	1	0	-0.252025	-1.021941	-2.746733

Structure 14 - Solvent: Methanol

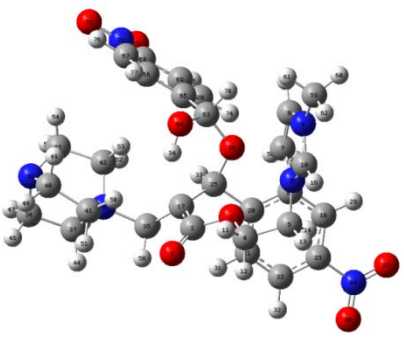


Zero-point correction= 0.642246
Thermal correction to Energy= 0.679361
Thermal correction to Enthalpy= 0.680305
Thermal correction to Gibbs Free Energy= 0.567949
Sum of electronic and zero-point Energies= -2055.152097
Sum of electronic and thermal Energies= -2055.114982
Sum of electronic and thermal Enthalpies= -2055.114038
Sum of electronic and thermal Free Energies= -2055.226393

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.469851	0.717861	1.697338
2	8	0	1.709340	1.133168	2.812696
3	8	0	2.346218	0.873888	0.680227
4	6	0	3.553619	1.579122	0.958539
5	6	0	4.172499	1.902033	-0.383771
6	7	0	3.425593	2.955492	-1.087786
7	6	0	2.063633	2.990684	-1.319176
8	6	0	1.817606	4.131564	-2.013454
9	7	0	3.025293	4.767709	-2.197970
10	6	0	3.978763	4.039369	-1.628886
11	1	0	3.341590	2.483055	1.531732
12	1	0	4.231181	0.943877	1.532258
13	1	0	5.191047	2.262442	-0.250370
14	1	0	4.188722	1.011979	-1.013464
15	1	0	0.895721	4.542619	-2.387539
16	1	0	5.027988	4.284757	-1.608935
17	6	0	0.226387	0.077232	1.252231
18	6	0	3.084828	-3.265645	-1.065429
19	6	0	2.073683	-2.316379	-1.095319
20	6	0	1.469291	-1.878668	0.085203
21	6	0	1.896561	-2.408716	1.305127
22	6	0	2.901746	-3.362639	1.354432
23	6	0	3.479411	-3.774031	0.162745
24	7	0	4.550924	-4.780415	0.204653
25	6	0	0.334789	-0.867987	0.032884
26	8	0	0.460201	-0.167136	-1.193019
27	8	0	5.063830	-5.108971	-0.844789
28	8	0	4.866493	-5.230233	1.286658
29	1	0	3.563058	-3.609226	-1.972119
30	1	0	1.754826	-1.897617	-2.039704
31	1	0	1.456744	-2.074668	2.237148
32	1	0	3.240903	-3.777090	2.293412
33	1	0	-0.604909	-1.444130	0.012807
34	1	0	-0.349095	1.013899	0.550382
35	6	0	-0.579624	-0.454871	2.413570
36	7	0	-1.835836	0.335099	2.739970
37	6	0	-2.423240	-0.183836	4.025197
38	6	0	-3.821033	0.448621	4.211565
39	7	0	-3.973859	1.613594	3.337315
40	6	0	-2.801465	2.477042	3.502196
41	6	0	-1.540893	1.804005	2.909681
42	6	0	-2.859866	0.183267	1.649595
43	6	0	-4.029463	1.150882	1.948224
44	1	0	-1.729076	0.094787	4.818730
45	1	0	-2.462156	-1.270642	3.953751
46	1	0	-3.950180	0.752863	5.250284
47	1	0	-4.604155	-0.270488	3.968059
48	1	0	-2.669452	2.675714	4.566769
49	1	0	-2.976765	3.428302	2.999518
50	1	0	-1.302226	2.189210	1.918733
51	1	0	-0.662988	1.887654	3.549481
52	1	0	-3.166299	-0.863990	1.648270
53	1	0	-2.365455	0.427043	0.712951
54	1	0	-3.978195	2.022899	1.293374
55	1	0	-4.980043	0.648140	1.768950
56	1	0	1.388821	2.228941	-0.960421
57	1	0	-0.935795	-1.473413	2.240249
58	1	0	0.002044	-0.440324	3.337382
59	6	0	3.218066	6.040185	-2.894910
60	1	0	2.682834	6.822931	-2.361707
61	1	0	4.280361	6.267687	-2.917666
62	1	0	2.838307	5.947890	-3.909888
63	6	0	-0.598259	0.764952	-1.490955
64	8	0	-0.790481	1.666995	-0.490589
65	6	0	-1.875633	0.010136	-1.877660
66	6	0	-3.104624	0.656683	-1.737585
67	6	0	-4.284838	0.024680	-2.100056
68	6	0	-4.208528	-1.265618	-2.606173
69	6	0	-3.003368	-1.933365	-2.769054
70	6	0	-1.833289	-1.280574	-2.406149
71	7	0	-5.453687	-1.951589	-2.986663
72	8	0	-6.499302	-1.352853	-2.843278
73	8	0	-5.370473	-3.080410	-3.424060
74	1	0	-0.879046	-1.780690	-2.522278
75	1	0	-2.991737	-2.938112	-3.167750
76	1	0	-5.245589	0.509182	-1.993683
77	1	0	-3.121636	1.658265	-1.325019
78	1	0	-0.224620	1.245497	-2.410808

Structure 15 - Solvent: Methanol

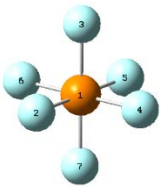


Zero-point correction= 0.646906
Thermal correction to Energy= 0.684486
Thermal correction to Enthalpy= 0.685430
Thermal correction to Gibbs Free Energy= 0.572410
Sum of electronic and zero-point Energies= -2055.162503
Sum of electronic and thermal Energies= -2055.124924
Sum of electronic and thermal Enthalpies= -2055.123980
Sum of electronic and thermal Free Energies= -2055.237000

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.031770	-0.662396	2.007001
2	8	0	-1.045818	-1.039822	3.176834
3	8	0	-2.106939	-0.940995	1.191254
4	6	0	-3.193126	-1.615694	1.804932
5	6	0	-4.306315	-1.661168	0.780404
6	7	0	-3.941548	-2.486221	-0.378179
7	6	0	-2.943381	-2.199943	-1.286537
8	6	0	-2.937415	-3.215456	-2.188765
9	7	0	-3.927391	-4.098965	-1.815599
10	6	0	-4.518378	-3.636368	-0.719852
11	1	0	-2.898795	-2.622816	2.110906
12	1	0	-3.538240	-1.071163	2.685981
13	1	0	-5.208740	-2.086993	1.215952
14	1	0	-4.525754	-0.656500	0.417330
15	1	0	-2.323055	-3.391346	-3.054739
16	1	0	-5.331899	-4.112201	-0.196900
17	6	0	0.000971	0.044317	1.337876
18	6	0	-3.243044	2.844379	-1.175425
19	6	0	-2.190417	1.940236	-1.163049
20	6	0	-1.481079	1.680202	0.013451
21	6	0	-1.841442	2.354514	1.182658
22	6	0	-2.885666	3.266727	1.188616
23	6	0	-3.572145	3.493247	0.004689
24	7	0	-4.683652	4.455234	0.001250
25	6	0	-0.286728	0.722747	0.014839
26	8	0	-0.531498	-0.138714	-1.119165
27	8	0	-5.276004	4.636708	-1.042484
28	8	0	-4.952275	5.018759	1.042089
29	1	0	-3.800809	3.048399	-2.078811
30	1	0	-1.922919	1.422658	-2.073664
31	1	0	-1.311497	2.157800	2.106418
32	1	0	-3.172427	3.791650	2.089076
33	1	0	0.591562	1.339086	-0.220186
34	1	0	0.525892	-1.654453	0.294402
35	6	0	0.964816	0.710526	2.249098
36	7	0	2.322198	0.804825	2.484646
37	6	0	3.183922	0.856288	3.370364
38	6	0	4.434341	0.034926	3.767912
39	7	0	4.582318	-1.131420	2.893159
40	6	0	3.483789	-2.063055	3.165438
41	6	0	2.125015	-1.324717	3.152532
42	6	0	3.041931	-0.215315	1.190233
43	6	0	4.482088	-0.685739	1.500981
44	1	0	2.584493	1.146993	4.232571
45	1	0	3.438055	1.749344	2.798137
46	1	0	4.349279	-0.317899	4.796600
47	1	0	5.324778	0.659494	3.695274
48	1	0	3.638382	-2.531263	4.137849
49	1	0	3.503482	-2.845672	2.405149
50	1	0	1.351546	-1.856198	2.601028
51	1	0	1.746904	-1.114895	4.153561
52	1	0	3.015444	0.718754	0.625409
53	1	0	2.473228	-0.968983	0.653601
54	1	0	4.751675	-1.507723	0.836006
55	1	0	5.196271	0.124352	1.345791
56	1	0	-2.318957	-1.324238	-1.183523
57	1	0	1.259125	1.703229	1.895984
58	1	0	0.559887	0.799247	3.260580
59	6	0	-4.269208	-5.337880	-2.514871
60	1	0	-4.555123	-5.101286	-3.537455
61	1	0	-3.405980	-5.999695	-2.508173
62	1	0	-5.100953	-5.809592	-1.998778
63	6	0	0.445937	-1.061284	-1.515413
64	8	0	0.626478	-2.086803	-0.576156
65	6	0	1.760333	-0.404039	-1.926509
66	6	0	2.948969	-1.131570	-1.855976
67	6	0	4.148336	-0.565298	-2.262148
68	6	0	4.129217	0.733601	-2.749256
69	6	0	2.960716	1.471500	-2.863369
70	6	0	1.770008	0.886728	-2.455000
71	7	0	5.398428	1.349019	-3.174494
72	8	0	6.407977	0.682759	-3.088512
73	8	0	5.365388	2.488881	-3.587247
74	1	0	0.842395	1.440979	-2.539465
75	1	0	2.991089	2.476254	-3.260663
76	1	0	5.080708	-1.109886	-2.205620
77	1	0	2.930913	-2.140993	-1.463570
78	1	0	0.027513	-1.528028	-2.413550

$[PF_6]^-$ – Solvent: Acetonitrile

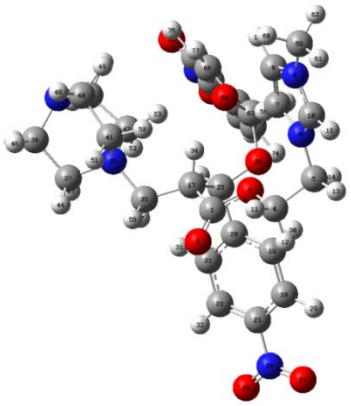


Zero-point correction= 0.019335
Thermal correction to Energy= 0.025374
Thermal correction to Enthalpy= 0.026318
Thermal correction to Gibbs Free Energy= -0.007774
Sum of electronic and zero-point Energies= -940.721187
Sum of electronic and thermal Energies= -940.715148
Sum of electronic and thermal Enthalpies= -940.714204
Sum of electronic and thermal Free Energies= -940.748295

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.000000	0.000000	0.000000
2	9	0	0.000000	0.000000	1.622348
3	9	0	0.000000	1.622348	0.000000
4	9	0	1.622348	0.000000	0.000000
5	9	0	0.000000	0.000000	-1.622348
6	9	0	-1.622348	0.000000	0.000000
7	9	0	0.000000	-1.622348	0.000000

Structure 13 - Solvent: Acetonitrile

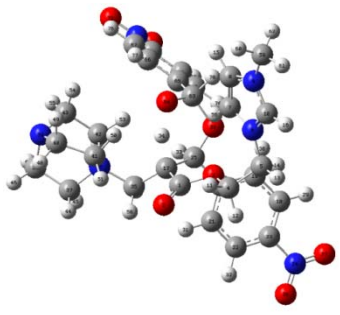


Zero-point correction= 0.646439 (Hartree/Particle)
Thermal correction to Energy= 0.684221
Thermal correction to Enthalpy= 0.685165
Thermal correction to Gibbs Free Energy= 0.570372
Sum of electronic and zero-point Energies= -2055.157076
Sum of electronic and thermal Energies= -2055.119294
Sum of electronic and thermal Enthalpies= -2055.118350
Sum of electronic and thermal Free Energies= -2055.233143

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.032726	0.685294	1.126367
2	8	0	-2.533308	1.291301	2.037209
3	8	0	-2.688299	0.363526	0.007683
4	6	0	-4.055604	0.750299	-0.113885
5	6	0	-4.496643	0.205103	-1.455686
6	7	0	-4.451998	-1.262573	-1.483365
7	6	0	-3.324123	-2.062743	-1.408410
8	6	0	-3.762820	-3.346131	-1.484599
9	7	0	-5.135065	-3.310327	-1.606535
10	6	0	-5.526022	-2.042438	-1.602812
11	1	0	-4.637573	0.330663	0.708718
12	1	0	-4.143559	1.838596	-0.101702
13	1	0	-5.519482	0.509448	-1.671044
14	1	0	-3.842991	0.575665	-2.245403
15	1	0	-3.220709	-4.275727	-1.464390
16	1	0	-6.544262	-1.700062	-1.688177
17	6	0	-0.621185	0.158818	1.050727
18	6	0	-1.150269	4.357058	-0.620648
19	6	0	-0.983629	2.984092	-0.709252
20	6	0	0.074745	2.351833	-0.049413
21	6	0	0.986783	3.117306	0.677973
22	6	0	0.834740	4.493788	0.778994
23	6	0	-0.238648	5.084570	0.131853
24	7	0	-0.409371	6.543537	0.235374
25	6	0	0.196877	0.843883	-0.106564
26	8	0	-0.211872	0.409934	-1.367278
27	8	0	-1.354089	7.046429	-0.335391
28	8	0	0.402468	7.164843	0.888179
29	1	0	-1.963233	4.862891	-1.122642
30	1	0	-1.663237	2.387255	-1.303980
31	1	0	1.837562	2.644320	1.155213
32	1	0	1.532688	5.101330	1.337591
33	1	0	1.249188	0.580310	0.067349
34	1	0	-0.707432	-0.866314	0.678935
35	6	0	0.067391	0.223626	2.409164
36	7	0	0.736877	-1.071289	2.792148
37	6	0	1.502650	-0.865244	4.075946
38	6	0	2.005418	-2.242213	4.572430
39	7	0	1.888125	-3.246294	3.515510
40	6	0	0.471160	-3.491681	3.249127
41	6	0	-0.281745	-2.158829	3.027381
42	6	0	1.710592	-1.533591	1.730993
43	6	0	2.514073	-2.730266	2.297643
44	1	0	0.828936	-0.385487	4.785081
45	1	0	2.320148	-0.183692	3.840992
46	1	0	1.420655	-2.574908	5.430658
47	1	0	3.047299	-2.160887	4.881758
48	1	0	0.027540	-4.024333	4.090270
49	1	0	0.393630	-4.124039	2.363854
50	1	0	-0.937659	-2.203770	2.160840
51	1	0	-0.859927	-1.853057	3.899989
52	1	0	2.356524	-0.685826	1.499938
53	1	0	1.121452	-1.800230	0.847909
54	1	0	2.559642	-3.523570	1.550557
55	1	0	3.535118	-2.430384	2.536512
56	1	0	-2.310367	-1.691646	-1.280943
57	1	0	0.846208	0.987772	2.445517
58	1	0	-0.651016	0.444361	3.198984
59	6	0	-6.010552	-4.476634	-1.723578
60	1	0	-5.919334	-5.082118	-0.824460
61	1	0	-7.034834	-4.131670	-1.835012
62	1	0	-5.717994	-5.053555	-2.598228
63	6	0	0.185271	-0.986123	-1.726786
64	8	0	-0.251152	-1.914838	-0.903837
65	6	0	1.718518	-0.971485	-1.906253
66	6	0	2.443160	-2.115647	-1.575900
67	6	0	3.821297	-2.159945	-1.741008
68	6	0	4.457070	-1.035394	-2.247530
69	6	0	3.766703	0.119576	-2.593597
70	6	0	2.390494	0.139842	-2.422073
71	7	0	5.916235	-1.066798	-2.425686
72	8	0	6.506927	-2.082326	-2.119494
73	8	0	6.457865	-0.075699	-2.870949
74	1	0	1.827203	1.031104	-2.673433
75	1	0	4.303767	0.973338	-2.982994
76	1	0	4.397833	-3.038609	-1.485985
77	1	0	1.901345	-2.966038	-1.179900
78	1	0	-0.252925	-1.020636	-2.747083

Structure 14 - Solvent: Acetonitrile

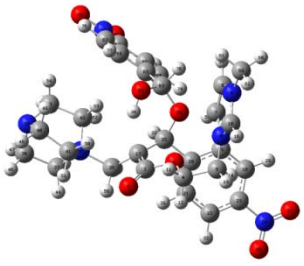


Zero-point correction= 0.642236
Thermal correction to Energy= 0.679353
Thermal correction to Enthalpy= 0.680298
Thermal correction to Gibbs Free Energy= 0.567935
Sum of electronic and zero-point Energies= -2055.152426
Sum of electronic and thermal Energies= -2055.115309
Sum of electronic and thermal Enthalpies= -2055.114364
Sum of electronic and thermal Free Energies= -2055.226727

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.470256	0.718787	1.696867
2	8	0	1.709751	1.134752	2.811999
3	8	0	2.346835	0.873836	0.679794
4	6	0	3.554397	1.579017	0.957785
5	6	0	4.173354	1.901354	-0.384627
6	7	0	3.426505	2.954534	-1.089068
7	6	0	2.064666	2.989117	-1.321212
8	6	0	1.818495	4.129856	-2.015661
9	7	0	3.026012	4.766515	-2.199527
10	6	0	3.979490	4.038642	-1.629876
11	1	0	3.342513	2.483199	1.530622
12	1	0	4.231859	0.943859	1.531715
13	1	0	5.191912	2.261754	-0.251311
14	1	0	4.189585	1.011067	-1.013990
15	1	0	0.896657	4.540517	-2.390290
16	1	0	5.028593	4.284490	-1.609377
17	6	0	0.226635	0.078204	1.252148
18	6	0	3.082902	-3.267590	-1.064456
19	6	0	2.072186	-2.317884	-1.094602
20	6	0	1.468798	-1.878685	0.085892
21	6	0	1.896681	-2.407675	1.306066
22	6	0	2.901487	-3.361981	1.355650
23	6	0	3.478121	-3.774886	0.163978
24	7	0	4.549150	-4.781725	0.296164
25	6	0	0.334668	-0.867608	0.033254
26	8	0	0.460179	-0.167353	-1.193021
27	8	0	5.060277	-5.112627	-0.843422
28	8	0	4.866202	-5.229657	1.288535
29	1	0	3.560287	-3.612309	-1.971155
30	1	0	1.752903	-1.899965	-2.039216
31	1	0	1.457643	-2.072503	2.238050
32	1	0	3.241097	-3.775571	2.294844
33	1	0	-0.605211	-1.443465	0.013486
34	1	0	-0.348862	1.014673	0.549823
35	6	0	-0.579331	-0.453358	2.413792
36	7	0	-1.835504	0.336754	2.739983
37	6	0	-2.422808	-0.181732	4.025447
38	6	0	-3.820532	0.450880	4.211778
39	7	0	-3.973486	1.615489	3.337036
40	6	0	-2.801070	2.479021	3.501391
41	6	0	-1.540518	1.805695	2.909162
42	6	0	-2.859630	0.184504	1.649764
43	6	0	-4.029237	1.152178	1.948138
44	1	0	-1.728556	0.097096	4.818821
45	1	0	-2.461813	-1.268554	3.954322
46	1	0	-3.949422	0.755624	5.250380
47	1	0	-4.603739	-0.268302	3.968765
48	1	0	-2.668957	2.678245	4.565845
49	1	0	-2.976414	3.430004	2.998206
50	1	0	-1.301747	2.190555	1.918106
51	1	0	-0.662679	1.889529	3.549021
52	1	0	-3.166063	-0.862744	1.648831
53	1	0	-2.365305	0.427950	0.712993
54	1	0	-3.978140	2.023922	1.292912
55	1	0	-4.979788	0.649261	1.769209
56	1	0	1.390157	2.227017	-0.962725
57	1	0	-0.935522	-1.471959	2.240903
58	1	0	0.002386	-0.438487	3.337562
59	6	0	3.218622	6.039144	-2.896227
60	1	0	2.684201	6.821944	-2.362294
61	1	0	4.280993	6.266179	-2.919931
62	1	0	2.837856	5.947265	-3.910858
63	6	0	-0.598241	0.764662	-1.491338
64	8	0	-0.790381	1.667138	-0.491353
65	6	0	-1.875672	0.009747	-1.877672
66	6	0	-3.104669	0.656250	-1.737460
67	6	0	-4.284917	0.024142	-2.099629
68	6	0	-4.208629	-1.266214	-2.605607
69	6	0	-3.003463	-1.933944	-2.768581
70	6	0	-1.833360	-1.281047	-2.405968
71	7	0	-5.453787	-1.952238	-2.985859
72	8	0	-6.499403	-1.353399	-2.842813
73	8	0	-5.370689	-3.081255	-3.422822
74	1	0	-0.879134	-1.781175	-2.522143
75	1	0	-2.991816	-2.938758	-3.167102
76	1	0	-5.245653	0.508627	-1.993074
77	1	0	-3.121693	1.657873	-1.325002
78	1	0	-0.224613	1.244780	-2.411420

Structure 15 - Solvent: Acetonitrile



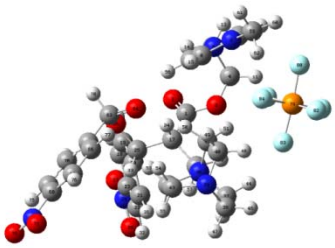
Zero-point correction= 0.646888
Thermal correction to Energy= 0.684470
Thermal correction to Enthalpy= 0.685415
Thermal correction to Gibbs Free Energy= 0.572272
Sum of electronic and zero-point Energies= -2055.162839
Sum of electronic and thermal Energies= -2055.125257
Sum of electronic and thermal Enthalpies= -2055.124312
Sum of electronic and thermal Free Energies= -2055.237455

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.030349	-0.659555	2.009179
2	8	0	-1.043786	-1.035600	3.179516
3	8	0	-2.105724	-0.939561	1.194225
4	6	0	-3.191065	-1.614728	1.808953
5	6	0	-4.305553	-1.669323	0.785854
6	7	0	-3.942349	-2.485223	-0.373325
7	6	0	-2.945065	-2.199188	-1.282750
8	6	0	-2.940931	-3.214225	-2.185518
9	7	0	-3.931104	-4.097208	-1.811624
10	6	0	-4.520437	-3.634761	-0.714938
11	1	0	-2.896068	-2.621841	2.114326
12	1	0	-3.535290	-1.070512	2.690529
13	1	0	-5.287247	-2.086390	1.222663
14	1	0	-4.525734	-0.655654	0.423221
15	1	0	-2.327829	-3.390060	-3.052387
16	1	0	-5.333761	-4.110230	-0.191338
17	6	0	0.001872	0.046718	1.338862
18	6	0	-3.244922	2.839458	-1.178526
19	6	0	-2.191647	1.936074	-1.164799
20	6	0	-1.481178	1.679401	0.011729
21	6	0	-1.841027	2.356348	1.179598
22	6	0	-2.885896	3.267808	1.184191
23	6	0	-3.573538	3.490950	0.000276
24	7	0	-4.685664	4.452145	-0.004565
25	6	0	-0.286254	0.722630	0.014650
26	8	0	-0.530783	-0.140985	-1.117723
27	8	0	-5.278137	4.631770	-1.048566
28	8	0	-4.954705	5.017045	1.035440
29	1	0	-3.803472	3.040857	-2.082012

30	1	0	-1.924510	1.416499	-2.074382
31	1	0	-1.310195	2.162225	2.103397
32	1	0	-3.172288	3.794734	2.083605
33	1	0	0.591645	1.339078	-0.221550
34	1	0	0.527772	-1.653693	0.298768
35	6	0	0.965913	0.714396	2.248813
36	7	0	2.323661	0.809521	2.484567
37	6	0	3.185193	0.861993	3.369495
38	6	0	4.435987	0.041423	3.767422
39	7	0	4.584412	-1.125422	2.893355
40	6	0	3.486326	-2.057406	3.166347
41	6	0	2.127265	-1.319637	3.153428
42	6	0	3.043220	-0.211212	1.190148
43	6	0	4.483700	-0.680596	1.500918
44	1	0	2.585811	1.153062	4.231607
45	1	0	3.438900	1.754724	2.796589
46	1	0	4.351186	-0.310808	4.796335
47	1	0	5.326128	0.666353	3.694285
48	1	0	3.641316	-2.525103	4.138940
49	1	0	3.506156	-2.840373	2.406419
50	1	0	1.353823	-1.851790	2.602549
51	1	0	1.749459	-1.109277	4.154456
52	1	0	3.016086	0.722411	0.624626
53	1	0	2.474882	-0.965678	0.654254
54	1	0	4.753634	-1.502781	0.836330
55	1	0	5.197378	0.129823	1.345142
56	1	0	-2.319820	-1.324019	-1.180172
57	1	0	1.259665	1.706810	1.894431
58	1	0	0.561366	0.804092	3.260351
59	6	0	-4.274591	-5.335565	-2.511051
60	1	0	-4.562649	-5.098228	-3.532856
61	1	0	-3.411430	-5.997476	-2.506602
62	1	0	-5.105281	-5.807526	-1.993498
63	6	0	0.446630	-1.064266	-1.512295
64	8	0	0.627677	-2.087819	-0.570981
65	6	0	1.760789	-0.407754	-1.925349
66	6	0	2.949405	-1.135307	-1.854308
67	6	0	4.148549	-0.569897	-2.262296
68	6	0	4.129273	0.728196	-2.751580
69	6	0	2.960794	1.466054	-2.866117
70	6	0	1.770265	0.882095	-2.456044
71	7	0	5.398242	1.342705	-3.178712
72	8	0	6.407558	0.675932	-3.093802
73	8	0	5.365347	2.482401	-3.591980
74	1	0	0.842661	1.436283	-2.540921
75	1	0	2.991016	2.470161	-3.265056
76	1	0	5.080893	-1.114496	-2.205443
77	1	0	2.931507	-2.144010	-1.460021
78	1	0	0.027965	-1.533012	-2.409262

Structure 16 – Gas phase

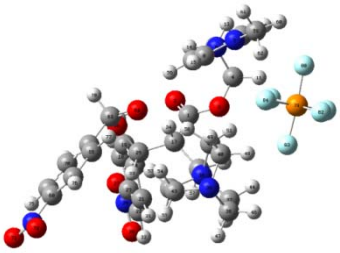


Zero-point correction= 0.669569
Thermal correction to Energy= 0.713924
Thermal correction to Enthalpy= 0.714869
Thermal correction to Gibbs Free Energy= 0.588633
Sum of electronic and zero-point Energies= -2995.849548
Sum of electronic and thermal Energies= -2995.805193
Sum of electronic and thermal Enthalpies= -2995.804248
Sum of electronic and thermal Free Energies= -2995.930484

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.029474	2.057405	-0.712018
2	8	0	0.475365	2.815493	-1.490178
3	8	0	-1.348183	2.105712	-0.397614
4	6	0	-2.144731	2.998069	-1.165646
5	6	0	-2.351121	2.427002	-2.563436
6	7	0	-2.935460	1.082901	-2.529481
7	6	0	-2.235687	-0.108255	-2.536986
8	6	0	-3.166506	-1.095306	-2.462383
9	7	0	-4.405996	-0.496412	-2.406903
10	6	0	-4.237670	0.817620	-2.427391
11	1	0	-3.082894	3.083972	-0.624212
12	1	0	-1.654319	3.969029	-1.253338
13	1	0	-3.011432	3.073956	-3.142662
14	1	0	-1.396625	2.350179	-3.083242
15	1	0	-3.049030	-2.164791	-2.443060
16	1	0	-5.025625	1.545713	-2.327549
17	6	0	0.593439	0.853817	-0.064703
18	6	0	4.138897	3.860848	-0.622325
19	6	0	3.333071	2.788966	-0.973425
20	6	0	2.986402	1.826437	-0.024434
21	6	0	3.485392	1.934046	1.274877
22	6	0	4.288149	3.004731	1.645935
23	6	0	4.592907	3.953498	0.685222
24	7	0	5.448545	5.096018	1.065168
25	6	0	2.096304	0.659210	-0.398832
26	8	0	2.228439	0.387966	-1.765246
27	8	0	5.697247	5.916357	0.210172
28	8	0	5.845220	5.141685	2.209146
29	1	0	4.419109	4.621922	-1.337377
30	1	0	2.953605	2.683983	-1.979521
31	1	0	3.277381	1.156401	2.002864
32	1	0	4.689550	3.106322	2.644583
33	1	0	2.442078	-0.199508	0.196446
34	1	0	0.164752	0.044399	-0.684783
35	6	0	0.156744	0.642083	1.379971
36	7	0	-0.379939	-0.744916	1.659301
37	6	0	-0.904429	-0.763776	3.073457
38	6	0	-1.226767	-2.225326	3.461482
39	7	0	-1.315699	-3.053869	2.263843
40	6	0	-2.200690	-2.379579	1.309451
41	6	0	-1.516177	-1.120746	0.725670
42	6	0	0.681627	-1.798516	1.497328
43	6	0	0.015748	-3.185098	1.680315
44	1	0	-1.797874	-0.137621	3.071399
45	1	0	-0.141401	-0.316778	3.712233
46	1	0	-2.176929	-2.256527	3.995693
47	1	0	-0.454361	-2.637716	4.113952
48	1	0	-3.123303	-2.109911	1.819242
49	1	0	-2.449939	-3.064592	0.497876
50	1	0	-1.051400	-1.329700	-0.239440
51	1	0	-2.184647	-0.264257	0.649879
52	1	0	1.456848	-1.592765	2.239601
53	1	0	1.079757	-1.697823	0.488725
54	1	0	-0.078862	-3.675522	0.709495
55	1	0	0.635873	-3.817486	2.317392
56	1	0	-1.148111	-0.200879	-2.567648
57	1	0	0.980552	0.789874	2.082259
58	1	0	-0.656650	1.316595	1.649679
59	6	0	-5.685451	-1.196138	-2.300397
60	1	0	-6.470520	-0.459981	-2.152907
61	1	0	-5.855621	-1.768091	-3.211520
62	1	0	-5.649595	-1.840199	-1.425110
63	6	0	1.747476	-0.950936	-2.203249
64	8	0	0.485361	-1.222292	-1.892770
65	6	0	2.743462	-1.983582	-1.640983
66	6	0	2.278253	-3.263723	-1.341711
67	6	0	3.130877	-4.229100	-0.822520
68	6	0	4.458705	-3.887107	-0.612707
69	6	0	4.959325	-2.628774	-0.914613
70	6	0	4.090800	-1.679150	-1.435268
71	7	0	5.370743	-4.898908	-0.044692
72	8	0	4.903510	-5.983162	0.230895
73	8	0	6.529206	-4.583566	0.116433
74	1	0	4.448074	-0.682839	-1.669934
75	1	0	6.004129	-2.414884	-0.735114
76	1	0	2.794725	-5.228581	-0.581312
77	1	0	1.229765	-3.470670	-1.521693
78	1	0	1.942495	-0.859940	-3.287206
79	15	0	-5.002943	0.398387	1.112531
80	9	0	-5.998522	0.716742	-0.141894
81	9	0	-5.465514	1.730938	1.860562
82	9	0	-6.130409	-0.472847	1.831707
83	9	0	-3.933561	0.061714	2.299811
84	9	0	-4.481010	-0.944347	0.313954
85	9	0	-3.823687	1.239128	0.336623

Structure 17 – Gas phase

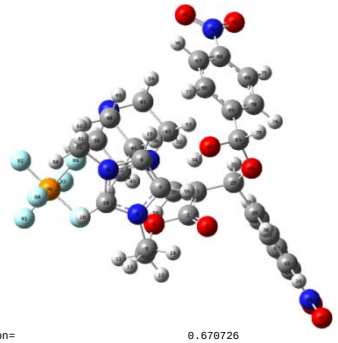


Zero-point correction= 0.671107
Thermal correction to Energy= 0.713815
Thermal correction to Enthalpy= 0.714759
Thermal correction to Gibbs Free Energy= 0.594754
Sum of electronic and zero-point Energies= -2978.708142
Sum of electronic and thermal Energies= -2978.665434
Sum of electronic and thermal Enthalpies= -2978.664490
Sum of electronic and thermal Free Energies= -2978.784495

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.088917	-1.929233	-0.745244
2	8	0	-0.528487	-2.601308	-1.646728
3	8	0	1.202299	-2.081126	-0.317768
4	6	0	1.976821	-3.066633	-0.979240
5	6	0	2.316676	-2.649029	-2.407615
6	7	0	2.892205	-1.303210	-2.468612
7	6	0	2.170571	-0.130763	-2.552627
8	6	0	3.076724	0.880688	-2.523760
9	7	0	4.327097	0.311893	-2.420091
10	6	0	4.185851	-1.005469	-2.367446
11	1	0	2.875312	-3.171474	-0.375971
12	1	0	1.431769	-4.012062	-1.027258
13	1	0	3.037176	-3.346513	-2.837066
14	1	0	1.417464	-2.642443	-3.020055
15	1	0	2.938863	1.946929	-2.568110
16	1	0	4.986748	-1.709975	-2.216723
17	6	0	-0.742726	-0.803174	-0.070635
18	6	0	-4.071438	-4.012504	-0.624756
19	6	0	-3.363031	-2.869750	-0.964049
20	6	0	-3.071141	-1.908655	0.004971
21	6	0	-3.522624	-2.093144	1.313063
22	6	0	-4.227909	-3.233742	1.670667
23	6	0	-4.483680	-4.176906	0.689286
24	7	0	-5.235905	-5.393436	1.055441
25	6	0	-2.263611	-0.677574	-0.344477
26	8	0	-2.503506	-0.363524	-1.699069
27	8	0	-5.439597	-6.209060	0.183894
28	8	0	-5.600934	-5.500872	2.206045
29	1	0	-4.305866	-4.774343	-1.355362
30	1	0	-3.017815	-2.708821	-1.974874
31	1	0	-3.348426	-1.326584	2.061037
32	1	0	-4.591426	-3.394979	2.675924
33	1	0	-2.629540	0.141708	0.295467
34	1	0	-0.451852	0.132903	-0.897423
35	6	0	-0.287326	-0.552731	1.345215
36	7	0	0.302406	0.827158	1.609480
37	6	0	0.842460	0.855180	3.014891
38	6	0	1.205048	2.316301	3.372969
39	7	0	1.290078	3.125983	2.160847
40	6	0	2.147205	2.419999	1.294246
41	6	0	1.439748	1.152360	0.665784
42	6	0	-0.739928	1.895822	1.457365
43	6	0	-0.046972	3.272753	1.593380
44	1	0	1.719716	0.207004	3.016176
45	1	0	0.075741	0.438894	3.669904
46	1	0	2.166257	2.335522	3.887615
47	1	0	0.455040	2.756532	4.033545
48	1	0	3.076755	2.153623	1.702353
49	1	0	2.387792	3.085581	0.373702
50	1	0	0.982277	1.326011	-0.307045
51	1	0	2.092881	0.281535	0.618884
52	1	0	-1.491445	1.721108	2.231161
53	1	0	-1.186425	1.773163	0.472779
54	1	0	0.044384	3.741564	0.611360
55	1	0	-0.645202	3.932673	2.223746
56	1	0	1.087663	-0.087066	-2.611340
57	1	0	-1.107984	-0.638031	2.064092
58	1	0	0.499885	-1.245487	1.639932
59	6	0	5.590773	1.045051	-2.359992
60	1	0	6.382996	0.347821	-2.102699
61	1	0	5.779328	1.511881	-3.326004
62	1	0	5.516293	1.786050	-1.568065
63	6	0	-1.929679	0.875562	-2.163798
64	8	0	-0.603471	1.002240	-1.879976
65	6	0	-2.749389	2.047413	-1.606142
66	6	0	-2.133482	3.291418	-1.461617
67	6	0	-2.833759	4.376433	-0.953687
68	6	0	-4.161307	4.191774	-0.596080
69	6	0	-4.808572	2.973971	-0.742114
70	6	0	-4.091763	1.900843	-1.255402
71	7	0	-4.911449	5.333955	-0.036250
72	8	0	-4.308665	6.372450	0.127642
73	8	0	-6.080209	5.160409	0.228781
74	1	0	-4.565207	0.932914	-1.374653
75	1	0	-5.846728	2.884786	-0.452565
76	1	0	-2.379671	5.350327	-0.828365
77	1	0	-1.090597	3.381321	-1.741830
78	1	0	-2.116045	0.821537	-3.246502
79	15	0	4.922088	-0.395688	1.119649
80	9	0	5.928480	-0.777375	-0.110067
81	9	0	5.333038	-1.722525	1.907516
82	9	0	6.065814	0.458426	1.833830
83	9	0	3.848255	0.002889	2.282653
84	9	0	4.452713	0.939919	0.279304
85	9	0	3.730628	-1.219772	0.345904

Structure 18 – Gas phase

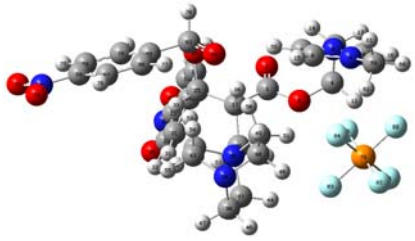


Zero-point correction= 0.670726
Thermal correction to Energy= 0.714980
Thermal correction to Enthalpy= 0.715925
Thermal correction to Gibbs Free Energy= 0.591498
Sum of electronic and zero-point Energies= -2995.858307
Sum of electronic and thermal Energies= -2995.814053
Sum of electronic and thermal Enthalpies= -2995.813109
Sum of electronic and thermal Free Energies= -2995.937536

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.799550	-1.744072	0.476202
2	8	0	1.271855	-2.401985	1.399194
3	8	0	-0.362363	-2.197523	-0.144085
4	6	0	-0.693331	-3.559570	0.022360
5	6	0	-1.169142	-3.915490	1.438065
6	7	0	-1.940633	-2.831127	2.049345
7	6	0	-1.388905	-1.828348	2.815522
8	6	0	-2.400915	-0.982815	3.138219
9	7	0	-3.549504	-1.487759	2.567573
10	6	0	-3.241908	-2.594379	1.900003
11	1	0	-1.489724	-3.737257	-0.696244
12	1	0	0.165698	-4.197697	-0.203852
13	1	0	-1.799897	-4.805083	1.408204
14	1	0	-0.318593	-4.090632	2.090363
15	1	0	-2.398637	-0.078938	2.721885
16	1	0	-3.929801	-3.168200	1.300185
17	6	0	1.233040	-0.496771	-0.035406
18	6	0	5.162464	-2.744798	0.388475
19	6	0	4.134523	-1.917347	0.812721
20	6	0	3.738290	-0.829926	0.028671
21	6	0	4.403550	-0.571206	-1.171046
22	6	0	5.431722	-1.392830	-1.611231
23	6	0	5.789505	-2.471299	-0.819127
24	7	0	6.884595	-3.349587	-1.271058
25	6	0	2.572273	0.048838	0.438573
26	8	0	2.725277	0.239303	1.852966
27	8	0	7.189896	-4.279226	-0.556785
28	8	0	7.412402	-3.088525	-2.330846
29	1	0	5.486094	-3.594102	0.974293
30	1	0	3.616813	-2.106753	1.741705
31	1	0	4.128606	0.294581	-1.765138
32	1	0	5.960965	-1.207566	-2.535505
33	1	0	2.714472	1.016218	-0.061644
34	1	0	0.311165	0.051832	1.840339
35	6	0	0.806995	-0.158416	-1.410677
36	7	0	-0.253213	0.977439	-1.612111
37	6	0	-0.882107	0.794478	-2.964376
38	6	0	-1.918628	1.923355	-3.203236
39	7	0	-1.979839	2.818223	-2.052090
40	6	0	-2.363162	2.046385	-0.871145
41	6	0	-1.340937	0.914968	-0.579510
42	6	0	0.398767	2.324328	-1.555908
43	6	0	-0.669834	3.416153	-1.837475
44	1	0	-1.359058	0.185066	-3.751571
45	1	0	-0.067928	0.798626	-3.692308
46	1	0	-2.902943	1.482790	-3.355298
47	1	0	-1.655362	2.508349	-4.086131
48	1	0	-3.348561	1.614581	-1.033780
49	1	0	-2.419519	2.729924	-0.020756
50	1	0	-0.853009	1.034138	0.386022
51	1	0	-1.774354	-0.082174	-0.636147
52	1	0	1.194041	2.324037	-2.303753
53	1	0	0.846283	2.416793	-0.566143
54	1	0	-0.734178	4.116053	-1.003583
55	1	0	-0.397947	3.989755	-2.725628
56	1	0	-0.333350	-1.802335	3.035917
57	1	0	1.634077	0.175630	-2.046087
58	1	0	0.331886	-1.013467	-1.885264
59	6	0	-4.877175	-0.880317	2.642911
60	1	0	-5.542079	-1.428690	1.981033
61	1	0	-5.230428	-0.916995	3.672677
62	1	0	-4.809911	0.144839	2.286658
63	6	0	1.791443	1.008843	2.552045
64	8	0	0.554309	0.373446	2.724835
65	6	0	1.622388	2.405452	1.961582
66	6	0	0.384670	3.046586	2.010265
67	6	0	0.226084	4.316582	1.471522
68	6	0	1.326591	4.926093	0.889666
69	6	0	2.582095	4.336483	0.868453
70	6	0	2.723273	3.069074	1.416363
71	7	0	1.150511	6.248336	0.256810
72	8	0	0.013296	6.631877	0.082944
73	8	0	2.147973	6.854940	-0.058897
74	1	0	3.688198	2.574374	1.408912
75	1	0	3.413958	4.867466	0.425507
76	1	0	-0.724877	4.832852	1.486159
77	1	0	-0.453332	2.537366	2.469236
78	1	0	2.218074	1.112414	3.552812
79	15	0	-4.485397	-1.348629	-1.195407
80	9	0	-5.360937	-2.209021	-0.113728
81	9	0	-4.953080	-2.303745	-2.383911
82	9	0	-5.711643	-0.349431	-1.434625
83	9	0	-3.547262	-0.482218	-2.209916
84	9	0	-3.970217	-0.393591	0.045937
85	9	0	-3.209922	-2.329280	-0.890084

Structure 16 – Solvent: Methanol

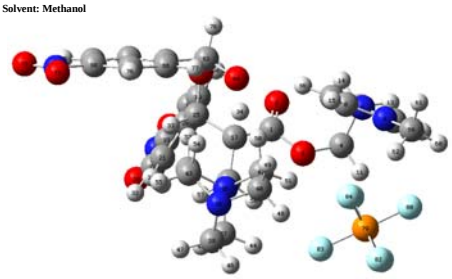


Zero-point correction= 0.668467
Thermal correction to Energy= 0.713101
Thermal correction to Enthalpy= 0.714045
Thermal correction to Gibbs Free Energy= 0.586378
Sum of electronic and zero-point Energies= -2995.900359
Sum of electronic and thermal Energies= -2995.855725
Sum of electronic and thermal Enthalpies= -2995.854780
Sum of electronic and thermal Free Energies= -2995.982448

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.088984	2.022896	-0.746150
2	8	0	0.432622	2.804815	-1.493310
3	8	0	-1.410170	2.036968	-0.476676
4	6	0	-2.214450	2.928653	-1.250973
5	6	0	-2.425545	2.349596	-2.642166
6	7	0	-3.033296	1.018153	-2.577505
7	6	0	-2.355993	-0.177970	-2.445214
8	6	0	-3.302531	-1.148709	-2.360944
9	7	0	-4.531316	-0.532259	-2.441145
10	6	0	-4.342639	0.774616	-2.557993
11	1	0	-3.153768	3.009487	-0.711372
12	1	0	-1.732515	3.902581	-1.333799
13	1	0	-3.078693	2.998149	-3.225100
14	1	0	-1.475908	2.249842	-3.166401
15	1	0	-3.211520	-2.216510	-2.258927
16	1	0	-5.120539	1.517320	-2.625220
17	6	0	0.550870	0.827908	-0.088293
18	6	0	4.101914	3.874508	-0.598800
19	6	0	3.298199	2.805260	-0.960147
20	6	0	2.932890	1.841153	-0.018163
21	6	0	3.410410	1.946898	1.289975
22	6	0	4.210121	3.015530	1.673143
23	6	0	4.535679	3.963773	0.717190
24	7	0	5.388878	5.097283	1.107302
25	6	0	2.059447	0.665702	-0.410515
26	8	0	2.213384	0.404411	-1.780579
27	8	0	5.653505	5.926574	0.261960
28	8	0	5.782419	5.145584	2.254324
29	1	0	4.392914	4.630180	-1.315905
30	1	0	2.937411	2.707563	-1.973294
31	1	0	3.185148	1.175429	2.017927
32	1	0	4.588381	3.108069	2.681350
33	1	0	2.414986	-0.190842	0.179260
34	1	0	0.134078	0.004505	-0.686920
35	6	0	0.125831	0.635975	1.366159
36	7	0	-0.386804	-0.752585	1.673834
37	6	0	-0.882663	-0.755815	3.100231
38	6	0	-1.170520	-2.213999	3.518017
39	7	0	-1.283278	-3.064957	2.333388
40	6	0	-2.192749	-2.413693	1.384818
41	6	0	-1.532829	-1.156818	0.771086
42	6	0	0.686436	-1.796699	1.514079
43	6	0	0.039771	-3.188574	1.722376
44	1	0	-1.783804	-0.141806	3.105394
45	1	0	-0.116122	-0.287967	3.716891
46	1	0	-2.100558	-2.250962	4.085691
47	1	0	-0.368861	-2.601053	4.148624
48	1	0	-3.106406	-2.142875	1.910839
49	1	0	-2.451289	-3.110223	0.586348
50	1	0	-1.088899	-1.376650	-0.200569
51	1	0	-2.212880	-0.309920	0.697732
52	1	0	1.464130	-1.572342	2.246128
53	1	0	1.071327	-1.705072	0.499207
54	1	0	-0.071110	-3.694775	0.761440
55	1	0	0.680317	-3.800943	2.357558
56	1	0	-1.273038	-0.268618	-2.436970
57	1	0	0.948516	0.810207	2.060793
58	1	0	-0.691111	1.306255	1.629704
59	6	0	-5.823475	-1.215766	-2.406071
60	1	0	-6.610875	-0.470769	-2.475108
61	1	0	-5.881034	-1.903821	-3.247026
62	1	0	-5.905813	-1.746990	-1.461284
63	6	0	1.822808	-0.968762	-2.208694
64	8	0	0.581747	-1.315860	-1.916663
65	6	0	2.886100	-1.927452	-1.631761
66	6	0	2.501981	-3.221788	-1.282961
67	6	0	3.424629	-4.128737	-0.778654
68	6	0	4.740339	-3.712738	-0.634043
69	6	0	5.160216	-2.433261	-0.976132
70	6	0	4.221526	-1.545026	-1.479812
71	7	0	5.727678	-4.659533	-0.095370
72	8	0	5.344590	-5.769014	0.215070
73	8	0	6.877356	-4.284553	0.012938
74	1	0	4.517982	-0.536528	-1.744029
75	1	0	6.195583	-2.152027	-0.842839
76	1	0	3.142391	-5.134594	-0.499396
77	1	0	1.461403	-3.494764	-1.407501
78	1	0	2.036236	-0.874867	-3.292626
79	15	0	-5.095705	0.312170	1.108189
80	9	0	-6.114945	0.594916	-0.124082
81	9	0	-5.544999	1.694296	1.812923
82	9	0	-6.251142	-0.488508	1.900014
83	9	0	-4.048899	0.024659	2.324405
84	9	0	-4.624804	-1.074772	0.393905
85	9	0	-3.919419	1.101566	0.304621

Structure 17 – Solvent: Methanol



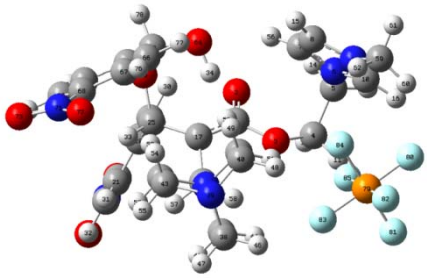
Zero-point correction= 0.664372
Thermal correction to Energy= 0.708532
Thermal correction to Enthalpy= 0.709477
Thermal correction to Gibbs Free Energy= 0.583497
Sum of electronic and zero-point Energies= -2995.897238
Sum of electronic and thermal Energies= -2995.853077
Sum of electronic and thermal Enthalpies= -2995.852133
Sum of electronic and thermal Free Energies= -2995.978113

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.097903	1.900138	-0.813494
2	8	0	0.559332	2.583052	-1.702002
3	8	0	-1.210589	2.016176	-0.445315
4	6	0	-1.995618	2.962989	-1.161497
5	6	0	-2.324223	2.467380	-2.563166
6	7	0	-2.980941	1.159276	-2.532906
7	6	0	-2.334663	-0.056877	-2.463515
8	6	0	-3.302680	-1.006834	-2.390164
9	7	0	-4.515515	-0.355513	-2.414550
10	6	0	-4.294746	0.950198	-2.487961
11	1	0	-2.901869	3.084477	-0.573122
12	1	0	-1.466769	3.913420	-1.245047
13	1	0	-2.991262	3.172358	-3.058631
14	1	0	-1.416852	2.362859	-3.154615
15	1	0	-3.238631	-2.079560	-2.330011
16	1	0	-5.053453	1.715227	-2.503237
17	6	0	0.762694	0.804677	-0.105316
18	6	0	4.080267	4.052519	-0.631151
19	6	0	3.387727	2.901035	-0.971649
20	6	0	3.073620	1.948732	0.000566
21	6	0	3.487950	2.152775	1.319011
22	6	0	4.176189	3.302593	1.679583
23	6	0	4.455164	4.235536	0.692905
24	7	0	5.188344	5.456029	1.060527
25	6	0	2.288357	0.703701	-0.353068

26	8	0	2.559922	0.383670	-1.706068
27	8	0	5.404494	6.273945	0.190330
28	8	0	5.539011	5.584126	2.215579
29	1	0	4.328110	4.801109	-1.370739
30	1	0	3.073900	2.729850	-1.990467
31	1	0	3.296688	1.398955	2.074357
32	1	0	4.504794	3.471153	2.695397
33	1	0	2.659178	-0.104594	0.294915
34	1	0	0.504257	-0.160741	-0.942600
35	6	0	0.295250	0.570128	1.310791
36	7	0	-0.272694	-0.813269	1.598347
37	6	0	-0.798279	-0.827602	3.010497
38	6	0	-1.134574	-2.286786	3.392882
39	7	0	-1.232551	-3.116071	2.190726
40	6	0	-2.104095	-2.427875	1.232054
41	6	0	-1.408420	-1.166218	0.668380
42	6	0	0.782217	-1.873349	1.460992
43	6	0	0.102991	-3.255601	1.608824
44	1	0	-1.681693	-0.189120	3.011722
45	1	0	-0.032266	-0.393936	3.652588
46	1	0	-2.082852	-2.311997	3.930472
47	1	0	-0.363127	-2.705135	4.041067
48	1	0	-3.026486	-2.154643	1.741162
49	1	0	-2.352242	-3.103080	0.412033
50	1	0	-0.955972	-1.356482	-0.303616
51	1	0	-2.070776	-0.303168	0.602146
52	1	0	1.528990	-1.684112	2.234216
53	1	0	1.229058	-1.757069	0.476289
54	1	0	0.004329	-3.734397	0.632348
55	1	0	0.714009	-3.900188	2.241553
56	1	0	-1.255614	-0.153421	-2.483759
57	1	0	1.101814	0.685611	2.038696
58	1	0	-0.505492	1.255578	1.583834
59	6	0	-5.824583	-1.005792	-2.379352
60	1	0	-6.587857	-0.238873	-2.286789
61	1	0	-5.964805	-1.574571	-3.296434
62	1	0	-5.859144	-1.655592	-1.508586
63	6	0	2.016628	-0.870318	-2.164480
64	8	0	0.686279	-1.010672	-1.904512
65	6	0	2.846762	-2.024903	-1.587164
66	6	0	2.246631	-3.274604	-1.426210
67	6	0	2.965490	-4.347414	-0.919126
68	6	0	4.296122	-4.144008	-0.581641
69	6	0	4.926673	-2.917353	-0.737642
70	6	0	4.190067	-1.857511	-1.247948
71	7	0	5.068288	-5.271016	-0.035048
72	8	0	4.494282	-6.327489	0.129436
73	8	0	6.239446	-5.086071	0.223560
74	1	0	4.652617	-0.885389	-1.371422
75	1	0	5.965152	-2.804519	-0.459192
76	1	0	2.514540	-5.320571	-0.781144
77	1	0	1.201510	-3.386684	-1.687639
78	1	0	2.221006	-0.829166	-3.245283
79	15	0	-4.970237	0.376776	1.156842
80	9	0	-6.020131	0.743017	-0.027725
81	9	0	-5.322577	1.760514	1.912168
82	9	0	-6.136037	-0.385186	1.972710
83	9	0	-3.896957	0.004417	2.325855
84	9	0	-4.597654	-1.012610	0.393479
85	9	0	-3.786877	1.127477	0.328795

Structure 18 – Solvent: Methanol

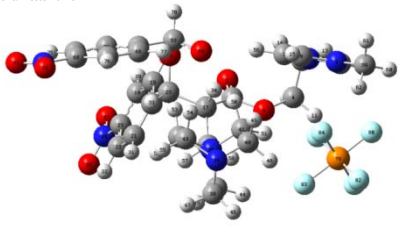


Zero-point correction= 0.668910
Thermal correction to Energy= 0.713689
Thermal correction to Enthalpy= 0.714634
Thermal correction to Gibbs Free Energy= 0.587633
Sum of electronic and zero-point Energies= -2995.903781
Sum of electronic and thermal Energies= -2995.859002
Sum of electronic and thermal Enthalpies= -2995.858058
Sum of electronic and thermal Free Energies= -2995.985058

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.738009	-1.754143	0.736579
2	8	0	1.224520	-2.362369	1.689792
3	8	0	-0.469904	-2.193205	0.208350
4	6	0	-0.908270	-3.488871	0.570805
5	6	0	-1.427604	-3.574599	2.006138
6	7	0	-2.229904	-2.400483	2.353338
7	6	0	-1.719531	-1.261052	2.932261
8	6	0	-2.749159	-0.381458	3.044133
9	7	0	-3.865408	-1.002715	2.529511
10	6	0	-3.524208	-2.214825	2.106071
11	1	0	-1.710813	-3.714081	-0.128575
12	1	0	-0.104462	-4.220482	0.459856
13	1	0	-2.045650	-4.463647	2.129397
14	1	0	-0.602785	-3.604202	2.711641
15	1	0	-2.789825	0.614971	3.448893
16	1	0	-4.187570	-2.918415	1.629929
17	6	0	1.212056	-0.580097	0.102478
18	6	0	5.047380	-3.001852	0.410592
19	6	0	4.095183	-2.096371	0.850281
20	6	0	3.692580	-1.037672	0.028604
21	6	0	4.277805	-0.887508	-1.231549
22	6	0	5.227884	-1.788649	-1.689764
23	6	0	5.593005	-2.835433	-0.856667
24	7	0	6.602992	-3.793248	-1.324544
25	6	0	2.605460	-0.074052	0.462096
26	8	0	2.863830	0.186649	1.850870
27	8	0	6.929256	-4.690852	-0.574660
28	8	0	7.061123	-3.641512	-2.438980
29	1	0	5.370326	-3.826761	1.030481
30	1	0	3.642233	-2.200721	1.825181
31	1	0	4.002599	-0.046983	-1.859084
32	1	0	5.688755	-1.680694	-2.661668
33	1	0	2.764176	0.853364	-0.101983
34	1	0	0.437202	0.215766	1.927993
35	6	0	0.749707	-0.334272	-1.286549
36	7	0	-0.212018	0.859938	-1.548772
37	6	0	-0.803720	0.688632	-2.918967
38	6	0	-1.741553	1.884394	-3.220143
39	7	0	-1.786380	2.808605	-2.087609
40	6	0	-2.261819	2.088749	-0.904034
41	6	0	-1.331896	0.896968	-0.554005
42	6	0	0.536376	2.157994	-1.505160
43	6	0	-0.440848	3.316437	-1.836073
44	1	0	-1.349347	-0.253701	-2.907324
45	1	0	0.030648	0.618461	-3.617731
46	1	0	-2.749159	1.515884	-3.409196
47	1	0	-1.395471	2.427263	-4.100322
48	1	0	-3.268096	1.721841	-1.097530
49	1	0	-2.301872	2.788640	-0.067192
50	1	0	-0.874055	1.004642	0.427760
51	1	0	-1.833889	-0.069449	-0.601805
52	1	0	1.346355	2.081559	-2.231496
53	1	0	0.960507	2.242175	-0.505565
54	1	0	-0.484671	4.026852	-1.010040
55	1	0	-0.096997	3.852933	-2.721470
56	1	0	-0.680322	-1.188814	3.211722
57	1	0	1.569528	-0.135406	-1.983731
58	1	0	0.186570	-1.187448	-1.658123
59	6	0	-5.211686	-0.432464	2.485739
60	1	0	-5.819966	-1.045894	1.827007
61	1	0	-5.626481	-0.415806	3.491785
62	1	0	-5.147102	0.573317	2.079143
63	6	0	2.017844	1.058059	2.552328
64	8	0	0.752828	0.513047	2.800042
65	6	0	1.915706	2.432212	1.900475
66	6	0	0.723370	3.153769	1.967778
67	6	0	0.623496	4.402873	1.370146
68	6	0	1.735878	4.907892	0.714895
69	6	0	2.948529	4.234639	0.666364
70	6	0	3.031177	2.989540	1.272255
71	7	0	1.620605	6.208151	0.034933
72	8	0	0.505156	6.652398	-0.144343
73	8	0	2.641938	6.758532	-0.315073
74	1	0	3.960354	2.432477	1.240775
75	1	0	3.793423	4.677616	0.157433
76	1	0	-0.294428	4.974471	1.400232
77	1	0	-0.129306	2.729073	2.481487
78	1	0	2.494973	1.177153	3.527825
79	15	0	-4.551463	-1.290820	-1.307910
80	9	0	-5.429460	-2.142562	-0.231538
81	9	0	-4.876312	-2.380654	-2.453189
82	9	0	-5.861618	-0.443502	-1.719065
83	9	0	-3.653428	-0.433276	-2.360689
84	9	0	-4.214469	-0.197410	-0.148260
85	9	0	-3.228594	-2.130367	-0.874768

Structure 16 – Solvent: Acetonitrile

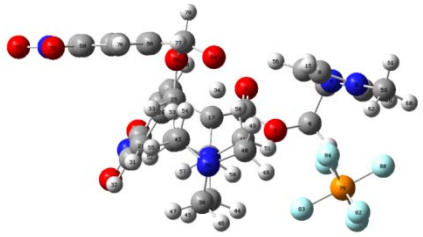


Zero-point correction= 0.668460
Thermal correction to Energy= 0.713095
Thermal correction to Enthalpy= 0.714039
Thermal correction to Gibbs Free Energy= 0.586372
Sum of electronic and zero-point Energies= -2995.900608
Sum of electronic and thermal Energies= -2995.855973
Sum of electronic and thermal Enthalpies= -2995.855029
Sum of electronic and thermal Free Energies= -2995.982696

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.088813	2.022732	-0.746549
2	8	0	0.432861	2.804631	-1.493719
3	8	0	-1.409979	2.036797	-0.477182
4	6	0	-2.214256	2.928487	-1.251559
5	6	0	-2.425467	2.349284	-2.642664
6	7	0	-3.033353	1.017924	-2.577732
7	6	0	-2.356191	-0.178260	-2.445254
8	6	0	-3.302844	-1.148874	-2.360781
9	7	0	-4.531556	-0.532284	-2.441101
10	6	0	-4.342724	0.774550	-2.558198
11	1	0	-3.153553	3.009407	-0.711941
12	1	0	-1.732274	3.902376	-1.334453
13	1	0	-3.078578	2.997828	-3.225639
14	1	0	-1.475887	2.249366	-3.166965
15	1	0	-3.211984	-2.216671	-2.258560
16	1	0	-5.120507	1.517346	-2.625777
17	6	0	0.551087	0.827767	-0.088671
18	6	0	4.101985	3.874755	-0.598627
19	6	0	3.298415	2.805442	-0.960096
20	6	0	2.933008	1.841275	-0.018196
21	6	0	3.410313	1.947028	1.290024
22	6	0	4.209878	3.015736	1.673325
23	6	0	4.535514	3.964021	0.717443
24	7	0	5.388547	5.097593	1.107702
25	6	0	2.059719	0.665763	-0.410765
26	8	0	2.213904	0.404677	-1.780879
27	8	0	5.653959	5.927065	0.262487
28	8	0	5.782232	5.145668	2.254685
29	1	0	4.393041	4.630439	-1.314795
30	1	0	2.937843	2.707750	-1.973316
31	1	0	3.185021	1.175608	2.017989
32	1	0	4.587927	3.108256	2.681612
33	1	0	2.415271	-0.190817	0.178921
34	1	0	0.134343	0.004372	-0.687318
35	6	0	0.126083	0.635812	1.365806
36	7	0	-0.386420	-0.752796	1.673495
37	6	0	-0.881983	-0.756124	3.100004
38	6	0	-1.169600	-2.214330	3.517790
39	7	0	-1.282694	-3.065247	2.333128
40	6	0	-2.192387	-2.413912	1.384814
41	6	0	-1.532614	-1.157013	0.770995
42	6	0	0.686812	-1.796889	1.513444
43	6	0	0.040226	-3.188797	1.721771
44	1	0	-1.783167	-0.142181	3.105356
45	1	0	-0.115396	-0.288218	3.716540
46	1	0	-2.099432	-2.251384	4.085797
47	1	0	-0.367681	-2.601334	4.148085
48	1	0	-3.105884	-2.143088	1.911124
49	1	0	-2.451176	-3.110373	0.586366
50	1	0	-1.088941	-1.376772	-0.200790
51	1	0	-2.212734	-0.310160	0.689787
52	1	0	1.464671	-1.572602	2.245314
53	1	0	1.071500	-1.705178	0.498509
54	1	0	-0.070878	-3.694963	0.760840
55	1	0	0.680944	-3.801161	2.356776
56	1	0	-1.273236	-0.268997	-2.437931
57	1	0	0.948737	0.810141	2.060431
58	1	0	-0.690912	1.306018	1.629358
59	6	0	-5.823782	-1.215651	-2.405820
60	1	0	-6.611104	-0.470576	-2.474949
61	1	0	-5.881474	-1.903862	-3.246626
62	1	0	-5.906072	-1.746730	-1.460943
63	6	0	1.823409	-0.968387	-2.209403
64	8	0	0.582094	-1.315329	-1.918265
65	6	0	2.886227	-1.927323	-1.632012
66	6	0	2.501684	-3.221601	-1.283469
67	6	0	3.423916	-4.128773	-0.778793
68	6	0	4.739643	-3.713041	-0.633599
69	6	0	5.159943	-2.433620	-0.975395
70	6	0	4.221661	-1.545171	-1.479433
71	7	0	5.726555	-4.660062	-0.094567
72	8	0	5.343148	-5.769509	0.215615
73	8	0	6.876276	-4.285338	0.014282
74	1	0	4.518464	-0.536718	-1.743426
75	1	0	6.195297	-2.152598	-0.841571
76	1	0	3.141311	-5.134562	-0.499667
77	1	0	1.461108	-3.494380	-1.408409
78	1	0	2.037548	-0.874355	-3.293202
79	15	0	-5.095601	0.312474	1.108458
80	9	0	-6.115134	0.595066	-0.123521
81	9	0	-5.544970	1.694662	1.813266
82	9	0	-6.250952	-0.488171	1.900656
83	9	0	-4.048719	0.025174	2.324593
84	9	0	-4.624825	-1.074523	0.394313
85	9	0	-3.919579	1.101920	0.304718

Structure 17 – Solvent: Acetonitrile

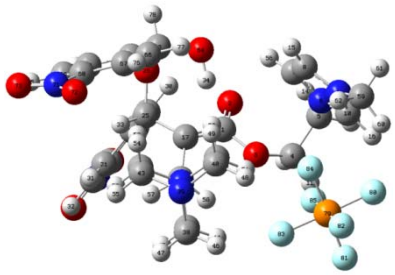


Zero-point correction= 0.664361
Thermal correction to Energy= 0.708524
Thermal correction to Enthalpy= 0.709468
Thermal correction to Gibbs Free Energy= 0.583479
Sum of electronic and zero-point Energies= -2995.897477
Sum of electronic and thermal Energies= -2995.853314
Sum of electronic and thermal Enthalpies= -2995.852370
Sum of electronic and thermal Free Energies= -2995.978359

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.698100	1.900063	-0.814050
2	8	0	0.559350	2.582766	-1.792857
3	8	0	-1.210246	2.016329	-0.445549
4	6	0	-1.995397	2.963157	-1.161633
5	6	0	-2.324524	2.467505	-2.563145
6	7	0	-2.981423	1.159511	-2.532586
7	6	0	-2.335350	-0.056762	-2.463315
8	6	0	-3.303520	-1.006571	-2.389999
9	7	0	-4.516236	-0.355023	-2.414318
10	6	0	-4.295257	0.950652	-2.487644
11	1	0	-2.901467	3.084785	-0.573013
12	1	0	-1.466497	3.913537	-1.245395
13	1	0	-2.991649	3.172562	-3.058369
14	1	0	-1.417403	2.362847	-3.154948
15	1	0	-3.239669	-2.079315	-2.329945
16	1	0	-5.053847	1.715795	-2.502910
17	6	0	0.763016	0.804686	-0.105908
18	6	0	4.080315	4.052718	-0.630875
19	6	0	3.387534	2.901467	-0.971656
20	6	0	3.074067	1.948511	0.000150
21	6	0	3.489273	2.151691	1.318459
22	6	0	4.177794	3.301257	1.679308
23	6	0	4.456134	4.234841	0.693050
24	7	0	5.189633	5.455035	1.060936
25	6	0	2.288664	0.703647	-0.353732
26	8	0	2.560286	0.383740	-1.706776
27	8	0	5.404957	6.273672	0.191197
28	8	0	5.541430	5.582252	2.215747
29	1	0	4.327680	4.801760	-1.370167
30	1	0	3.073066	2.731003	-1.990392
31	1	0	3.298429	1.397410	2.073450
32	1	0	4.507080	3.469099	2.695020
33	1	0	2.659370	-0.104771	0.294134
34	1	0	0.504472	-0.160669	-0.943294
35	6	0	0.295897	0.570210	1.310331
36	7	0	-0.272178	-0.813091	1.598019
37	6	0	-0.797357	-0.827381	3.010330
38	6	0	-1.133494	-2.286551	3.392828
39	7	0	-1.232168	-3.115787	2.190664
40	6	0	-2.103948	-2.427385	1.232340
41	6	0	-1.408231	-1.165860	0.668413
42	6	0	0.782536	-1.873347	1.460325
43	6	0	0.103136	-3.255498	1.608205
44	1	0	-1.680797	-0.188932	3.011750
45	1	0	-0.031208	-0.393672	3.652216
46	1	0	-2.081440	-2.311739	3.931007
47	1	0	-0.361649	-2.704933	4.040514
48	1	0	-3.026051	-2.153952	1.741862
49	1	0	-2.352581	-3.102491	0.412388
50	1	0	-0.956132	-1.356232	-0.303730
51	1	0	-2.070484	-0.302706	0.602331
52	1	0	1.529537	-1.684298	2.233358
53	1	0	1.229159	-1.757065	0.475528
54	1	0	0.003986	-3.734157	0.631713
55	1	0	0.714302	-3.900248	2.240621
56	1	0	-1.256322	-0.153430	-2.483669
57	1	0	1.102692	0.685576	2.037992
58	1	0	-0.504636	1.255802	1.583612
59	6	0	-5.825437	-1.005027	-2.379012
60	1	0	-6.588564	-0.237895	-2.286933
61	1	0	-5.965640	-1.574177	-3.295859
62	1	0	-5.860221	-1.654465	-1.507981
63	6	0	2.016818	-0.870163	-2.165269
64	8	0	0.686369	-1.010159	-1.905624
65	6	0	2.846524	-2.024951	-1.587737
66	6	0	2.246072	-3.274544	-1.427119
67	6	0	2.964495	-4.347514	-0.919758
68	6	0	4.295909	-4.144372	-0.581643
69	6	0	4.925870	-2.917829	-0.737284
70	6	0	4.189705	-1.857833	-1.247897
71	7	0	5.066704	-5.271537	-0.034772
72	8	0	4.492459	-6.327932	0.129426
73	8	0	6.237810	-5.086875	0.224333
74	1	0	4.652513	-0.885796	-1.371055
75	1	0	5.964219	-2.805159	-0.458291
76	1	0	2.513244	-5.320562	-0.781995
77	1	0	1.201029	-3.386434	-1.688941
78	1	0	2.221462	-0.829104	-3.246033
79	15	0	-4.970323	0.377120	1.157404
80	9	0	-6.020046	0.743620	-0.027192
81	9	0	-5.323157	1.760561	1.913189
82	9	0	-6.136303	-0.385267	1.972798
83	9	0	-3.897421	0.004583	2.326684
84	9	0	-4.597447	-1.011977	0.393774
85	9	0	-3.786897	1.128282	0.329994

Structure 18 – Solvent: Acetonitrile



Zero-point correction= 0.668909
Thermal correction to Energy= 0.713688
Thermal correction to Enthalpy= 0.714632
Thermal correction to Gibbs Free Energy= 0.587636
Sum of electronic and zero-point Energies= -2995.904017
Sum of electronic and thermal Energies= -2995.859238
Sum of electronic and thermal Enthalpies= -2995.858294
Sum of electronic and thermal Free Energies= -2995.985290

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.738683	-1.753343	0.737772
2	8	0	1.225515	-2.361166	1.691149
3	8	0	-0.469153	-2.192916	0.209889
4	6	0	-0.907531	-3.488319	0.573388
5	6	0	-1.426886	-3.572905	2.008741
6	7	0	-2.229640	-2.398758	2.354733
7	6	0	-1.719808	-1.258728	2.932961
8	6	0	-2.749722	-0.379353	3.043890
9	7	0	-3.865616	-1.001381	2.529451
10	6	0	-3.523940	-2.213713	2.107013
11	1	0	-1.710127	-3.714071	-0.125765
12	1	0	-0.103751	-4.220032	0.462962
13	1	0	-2.044625	-4.462060	2.132717
14	1	0	-0.602155	-3.601579	2.714384
15	1	0	-2.790799	0.617398	3.447821
16	1	0	-4.186951	-2.917839	1.631167
17	6	0	1.213396	-0.579546	0.103098
18	6	0	5.048025	-3.001007	0.411085
19	6	0	4.096083	-2.095233	0.850720
20	6	0	3.692893	-1.037124	0.028564
21	6	0	4.277237	-0.887877	-1.232128
22	6	0	5.227049	-1.789312	-1.690284
23	6	0	5.592800	-2.835485	-0.856658
24	7	0	6.602512	-3.793558	-1.324465
25	6	0	2.605994	-0.073255	0.462069
26	8	0	2.864945	0.188049	1.850642
27	8	0	6.929122	-4.690806	-0.574275
28	8	0	7.060093	-3.642541	-2.439232
29	1	0	5.371417	-3.825427	1.031391
30	1	0	3.643808	-2.198922	1.825996
31	1	0	4.001559	-0.047859	-1.860119
32	1	0	5.687249	-1.681991	-2.662577
33	1	0	2.764493	0.853905	-0.102451
34	1	0	0.437995	0.216989	1.928970
35	6	0	0.749885	-0.334291	-1.285971
36	7	0	-0.212090	0.859573	-1.548543
37	6	0	-0.803519	0.687748	-2.918769
38	6	0	-1.741548	1.883215	-3.220421
39	7	0	-1.786934	2.807651	-2.088063
40	6	0	-2.262371	2.087857	-0.904419
41	6	0	-1.332047	0.896548	-0.553904
42	6	0	0.535992	2.157835	-1.505279
43	6	0	-0.441569	3.315930	-1.836328
44	1	0	-1.348869	-0.254736	-2.906979
45	1	0	0.030953	0.617647	-3.617393
46	1	0	-2.749018	1.514438	-3.409753
47	1	0	-1.395281	2.425982	-4.100585
48	1	0	-3.268428	1.720488	-1.098185
49	1	0	-2.302947	2.787838	-0.067689
50	1	0	-0.874389	1.004737	0.427885
51	1	0	-1.833743	-0.070040	-0.601430
52	1	0	1.345907	2.081407	-2.231668
53	1	0	0.960164	2.242372	-0.505744
54	1	0	-0.485805	4.026265	-1.010258
55	1	0	-0.097705	3.852547	-2.721640
56	1	0	-0.680733	-1.186042	3.212747
57	1	0	1.569564	-0.135483	-1.983320
58	1	0	0.186876	-1.187719	-1.657164
59	6	0	-5.212112	-0.431720	2.484994
60	1	0	-5.819969	-1.045829	1.826502
61	1	0	-5.627180	-0.414712	3.490917
62	1	0	-5.147832	0.573904	2.077971
63	6	0	2.019037	1.059479	2.552214
64	8	0	0.754386	0.514043	2.800809
65	6	0	1.915992	2.433358	1.899974
66	6	0	0.723302	3.154314	1.967558
67	6	0	0.622578	4.403170	1.369569
68	6	0	1.734451	4.908527	0.713707
69	6	0	2.947409	4.235848	0.664816
70	6	0	3.030926	2.990999	1.271081
71	7	0	1.618252	6.208486	0.033397
72	8	0	0.502507	6.651961	-0.145986
73	8	0	2.639182	6.759566	-0.316734
74	1	0	3.960349	2.434374	1.239262
75	1	0	3.791843	4.678975	0.155256
76	1	0	-0.295665	4.974243	1.399837
77	1	0	-0.129021	2.729358	2.481644
78	1	0	2.496630	1.179070	3.527427
79	15	0	-4.550651	-1.292844	-1.308871
80	9	0	-5.428459	-2.144774	-0.231748
81	9	0	-4.874578	-2.383303	-2.453167
82	9	0	-5.861366	-0.446563	-1.720912
83	9	0	-3.652990	-0.435113	-2.361021
84	9	0	-4.214740	-0.198809	-0.148874
85	9	0	-3.227453	-2.131465	-0.874394

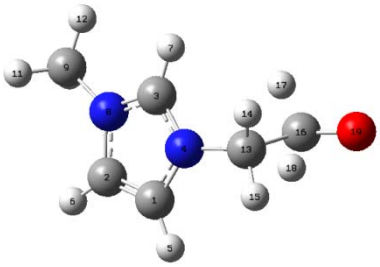
Structure 19 – Gas phase

Zero-point correction= 0.175832
Thermal correction to Energy= 0.185081
Thermal correction to Enthalpy= 0.186025
Thermal correction to Gibbs Free Energy= 0.141060
Sum of electronic and zero-point Energies= -419.504811
Sum of electronic and thermal Energies= -419.495562
Sum of electronic and thermal Enthalpies= -419.494618
Sum of electronic and thermal Free Energies= -419.539582

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.434337	1.372236	-0.113680
2	6	0	-1.751224	1.178405	0.157228
3	6	0	-0.847749	-0.781906	-0.261859
4	7	0	0.110461	0.134649	-0.376321
5	1	0	0.154272	2.273675	-0.151701
6	1	0	-2.533441	1.877324	0.401399
7	1	0	-0.720679	-1.842415	-0.412809
8	7	0	-1.987266	-0.174841	0.059104
9	6	0	-3.284259	-0.829296	0.263744
10	1	0	-3.629751	-0.627880	1.276078
11	1	0	-3.997295	-0.445920	-0.463822
12	1	0	-3.160429	-1.900881	0.125659
13	6	0	1.523959	-0.132772	-0.672611
14	1	0	1.598757	-1.122702	-1.121882
15	1	0	1.867164	0.602495	-1.400080
16	6	0	2.382266	-0.067819	0.585652
17	1	0	2.022411	-0.807640	1.312250
18	1	0	2.302603	0.929463	1.037440
19	8	0	3.675423	-0.346758	0.126363
20	1	0	4.298704	-0.313204	0.856236

Structure 19 (Anion) – Gas phase

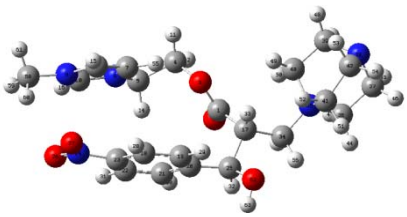


Zero-point correction= 0.158844
Thermal correction to Energy= 0.167114
Thermal correction to Enthalpy= 0.168058
Thermal correction to Gibbs Free Energy= 0.125174
Sum of electronic and zero-point Energies= -419.037500
Sum of electronic and thermal Energies= -419.029230
Sum of electronic and thermal Enthalpies= -419.028286
Sum of electronic and thermal Free Energies= -419.071170

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.464861	1.493513	-0.108289
2	6	0	1.720952	1.078939	-0.423260
3	6	0	0.647037	-0.596013	0.520916
4	7	0	-0.181408	0.443630	0.505374
5	1	0	-0.029141	2.436097	-0.266221
6	1	0	2.538150	1.591655	-0.900257
7	1	0	0.410429	-1.569686	0.914570
8	7	0	1.821938	-0.231707	-0.018552
9	6	0	2.992532	-1.084589	-0.163257
10	1	0	3.284405	-1.130737	-1.211875
11	1	0	3.815322	-0.695027	0.435731
12	1	0	2.738777	-2.085296	0.179602
13	6	0	-1.618418	0.327417	0.714129
14	1	0	-1.813479	-0.252697	1.614528
15	1	0	-2.043696	1.324874	0.804463
16	6	0	-2.284253	-0.436940	-0.535489
17	1	0	-1.636007	-1.384745	-0.564091
18	1	0	-1.909400	0.169892	-1.420247
19	8	0	-3.546917	-0.572720	-0.377807

Structure 20 – Gas phase

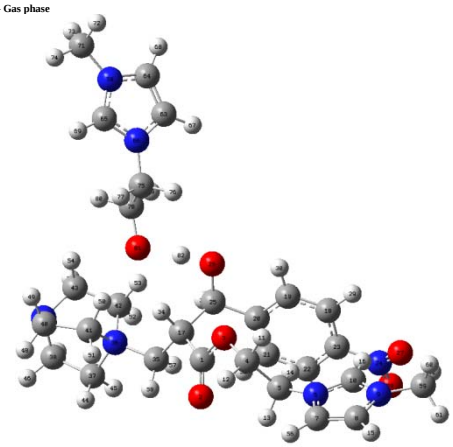


Zero-point correction= 0.542440
Thermal correction to Energy= 0.570742
Thermal correction to Enthalpy= 0.571686
Thermal correction to Gibbs Free Energy= 0.482822
Sum of electronic and zero-point Energies= -1505.514908
Sum of electronic and thermal Energies= -1505.486606
Sum of electronic and thermal Enthalpies= -1505.485662
Sum of electronic and thermal Free Energies= -1505.574526

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.995213	-0.340287	-0.955180
2	8	0	-1.054446	-0.499946	-2.141228
3	8	0	-0.320697	-1.159086	-0.124695
4	6	0	0.303508	-2.299815	-0.743952
5	6	0	1.659906	-1.959534	-1.332513
6	7	0	2.705613	-1.810901	-0.304095
7	6	0	2.531988	-1.546629	1.039522
8	6	0	3.771266	-1.489345	1.595035
9	7	0	4.679792	-1.711970	0.585287
10	6	0	4.015674	-1.898288	-0.548766
11	1	0	0.380557	-3.053770	0.038632
12	1	0	-0.336063	-2.667455	-1.545835
13	1	0	1.967170	-2.770729	-1.994249
14	1	0	1.598264	-1.036452	-1.910862
15	1	0	4.085680	-1.298648	2.607828
16	1	0	4.465854	-2.083771	-1.511845
17	6	0	-1.665562	0.810149	-0.226402
18	6	0	2.528954	1.877702	1.116858
19	6	0	1.166889	2.077160	0.943251
20	6	0	0.598216	1.966479	-0.326493
21	6	0	1.402333	1.698984	-1.434977
22	6	0	2.766694	1.491272	-1.277321
23	6	0	3.293730	1.563575	0.002867
24	7	0	4.720596	1.235804	0.195979
25	6	0	-0.896108	2.130041	-0.507882
26	8	0	5.350171	0.876592	-0.776080
27	8	0	5.157727	1.284217	1.324361
28	1	0	2.999258	1.959464	2.088158
29	1	0	0.542321	2.337405	1.789780
30	1	0	0.965413	1.663249	-2.427828
31	1	0	3.417504	1.293705	-2.119752
32	1	0	-1.092370	2.421177	-1.548892
33	1	0	-1.608765	0.646341	0.851391
34	6	0	-3.096067	1.029034	-0.730876
35	7	0	-4.166651	0.196193	-0.085543
36	6	0	-5.447762	0.361571	-0.881933
37	6	0	-6.602807	-0.305388	-0.091278
38	7	0	-6.060556	-1.165506	0.954309
39	6	0	-5.073291	-2.066836	0.378724
40	6	0	-3.815745	-1.271418	-0.070614
41	6	0	-4.441534	0.657950	1.329115
42	6	0	-5.431308	-0.343064	1.980183
43	1	0	-5.269797	-0.112609	-1.848597
44	1	0	-5.597816	1.430851	-1.035137
45	1	0	-7.222776	-0.894858	-0.766830
46	1	0	-7.240087	0.447856	0.373530
47	1	0	-5.525585	-2.581569	-0.469961
48	1	0	-4.791515	-2.819723	1.115094
49	1	0	-2.983801	-1.389259	0.626503
50	1	0	-3.485340	-1.534052	-1.077855
51	1	0	-4.856766	1.663277	1.242028
52	1	0	-3.492015	0.721006	1.858714
53	1	0	-4.915198	-0.998620	2.683168
54	1	0	-6.196113	0.201536	2.533911
55	1	0	1.558023	-1.403796	1.475395
56	1	0	-3.377116	2.067745	-0.553840
57	1	0	-3.129603	0.818854	-1.802636
58	6	0	6.144780	-1.711630	0.735082
59	1	0	6.590889	-1.838302	-0.248263
60	1	0	6.448336	-0.751751	1.150467
61	1	0	6.432995	-2.532952	1.388524
62	8	0	-1.465292	3.044369	0.398063
63	1	0	-1.133507	3.931235	0.219628

Structure 21 – Gas phase

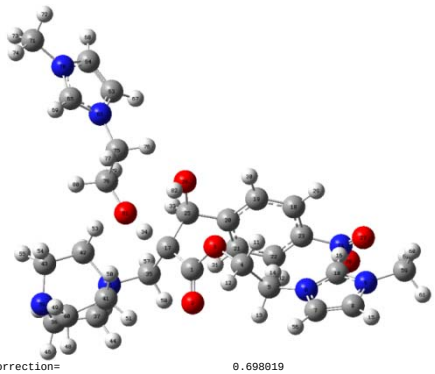


Zero-point correction= 0.704896
Thermal correction to Energy= 0.742801
Thermal correction to Enthalpy= 0.743745
Thermal correction to Gibbs Free Energy= 0.630277
Sum of electronic and zero-point Energies= -1924.658065
Sum of electronic and thermal Energies= -1924.620159
Sum of electronic and thermal Enthalpies= -1924.619215
Sum of electronic and thermal Free Energies= -1924.732684

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.965829	1.286111	-1.152455
2	8	0	1.653407	2.207327	-1.508233
3	8	0	1.243980	0.012388	-1.460559
4	6	0	2.446048	-0.211199	-2.198377
5	6	0	3.674942	0.250318	-1.402705
6	7	0	4.871317	-0.528828	-1.744014
7	6	0	5.574049	-0.474740	-2.929777
8	6	0	6.646591	-1.297698	-2.791999
9	7	0	6.581600	-1.834572	-1.525256
10	6	0	5.500996	-1.360487	-0.914635
11	1	0	2.477896	-1.288608	-2.353501
12	1	0	2.384971	0.300034	-3.161497
13	1	0	3.892294	1.302312	-1.573581
14	1	0	3.487419	0.100541	-0.338953
15	1	0	7.445847	-1.535863	-3.473578
16	1	0	5.213087	-1.595243	0.101807
17	6	0	-0.277120	1.391644	-0.293939
18	6	0	3.000573	-1.409959	1.850014
19	6	0	1.701533	-1.127671	1.453478
20	6	0	1.234190	0.187591	1.440447
21	6	0	2.076035	1.219638	1.862371
22	6	0	3.373560	0.956154	2.284542
23	6	0	3.815076	-0.357734	2.249924
24	7	0	5.210901	-0.643644	2.621459
25	6	0	-0.194409	0.461673	0.991187
26	8	0	-0.851158	-0.725962	0.769570
27	8	0	5.711811	-1.650337	2.134827
28	8	0	5.778113	0.128888	3.344101
29	1	0	3.379019	-2.424165	1.876174
30	1	0	1.022096	-1.912853	1.151341
31	1	0	1.723644	2.245236	1.880808
32	1	0	4.034725	1.739100	2.633025
33	1	0	-0.660191	1.043794	1.805184
34	1	0	-1.088542	0.947618	-0.876057
35	6	0	-0.555897	2.871970	-0.016651
36	7	0	-2.002946	3.286121	-0.053967
37	6	0	-2.054668	4.793611	0.034629
38	6	0	-3.528401	5.223638	0.233964
39	7	0	-4.420721	4.126825	-0.124811
40	6	0	-4.029618	3.614951	-1.436260
41	6	0	-2.683922	2.856405	-1.337293
42	6	0	-2.791694	2.720809	1.105502
43	6	0	-4.281637	3.059841	0.864589
44	1	0	-1.632091	5.172412	-0.897621
45	1	0	-1.412183	5.097280	0.861935
46	1	0	-3.747361	6.093888	-0.385488
47	1	0	-3.716022	5.499197	1.272854
48	1	0	-3.966969	4.455425	-2.129656
49	1	0	-4.797686	2.934197	-1.804459
50	1	0	-2.851204	1.779931	-1.249362
51	1	0	-2.002142	3.085675	-2.158571
52	1	0	-2.385372	3.182148	2.008255
53	1	0	-2.653163	1.640007	1.099434
54	1	0	-4.792492	2.170159	0.491205
55	1	0	-4.754774	3.364127	1.798891
56	1	0	5.267109	0.149773	-3.751861
57	1	0	-0.189490	3.167218	0.969068
58	1	0	-0.048573	3.490136	-0.758050
59	6	0	7.548071	-2.759573	-0.918738
60	1	0	7.447950	-3.742641	-1.375525
61	1	0	8.551758	-2.369468	-1.075135
62	1	0	7.341808	-2.814252	0.148804
63	6	0	-4.889986	-3.929178	0.858320
64	6	0	-6.052733	-4.629456	0.926523
65	6	0	-6.128727	-3.345412	-0.856308
66	7	0	-4.955210	-3.139235	-0.266776
67	1	0	-4.026423	-3.927009	1.501820
68	1	0	-6.400799	-5.358330	1.639027
69	1	0	-6.467838	-2.865019	-1.760003
70	7	0	-6.813653	-4.248628	-0.155528
71	6	0	-8.146988	-4.763397	-0.481511
72	1	0	-8.087952	-5.838287	-0.642912
73	1	0	-8.827603	-4.541213	0.338385
74	1	0	-8.497668	-4.277124	-1.388860
75	6	0	-3.944519	-2.141400	-0.661152
76	1	0	-2.962148	-2.603823	-0.557107
77	1	0	-4.106060	-1.893550	-1.710134
78	6	0	-4.023360	-0.871346	0.209334
79	1	0	-3.956244	-1.199103	1.265745
80	1	0	-5.037855	-0.449387	0.082561
81	8	0	-3.030102	-0.004809	-0.152969
82	1	0	-1.797387	-0.481148	0.379510

Structure 22 – Gas phase

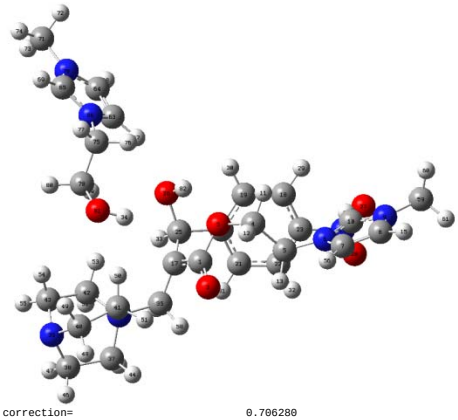


Zero-point correction=	0.698019
Thermal correction to Energy=	0.736784
Thermal correction to Enthalpy=	0.737728
Thermal correction to Gibbs Free Energy=	0.617308
Sum of electronic and zero-point Energies=	1.251561
Sum of electronic and thermal Energies=	1.290327
Sum of electronic and thermal Enthalpies=	1.291271
Sum of electronic and thermal Free Energies=	1.170851

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.486660	1.087105	-0.706331
2	8	0	0.941202	2.111215	-1.165195
3	8	0	0.924603	-0.124766	-1.121263
4	6	0	2.041643	-0.126148	-2.001438
5	6	0	3.272875	0.469429	-1.302236
6	7	0	4.522918	-0.093327	-1.826696
7	6	0	5.064568	0.138501	-3.073599
8	6	0	6.238340	-0.544288	-3.128778
9	7	0	6.392865	-1.176700	-1.915824
10	6	0	5.344526	-0.894101	-1.148634
11	1	0	2.214398	-1.175884	-2.237106
12	1	0	1.800928	0.424364	-2.912958
13	1	0	3.308804	1.551516	-1.411080
14	1	0	3.230593	0.225312	-0.238851
15	1	0	6.971548	-0.626894	-3.913532
16	1	0	5.209762	-1.245674	-0.133661
17	6	0	-0.570856	0.970436	0.322520
18	6	0	3.110880	-1.773148	1.702395
19	6	0	1.761625	-1.623857	1.415119
20	6	0	1.107364	-0.421641	1.685938
21	6	0	1.809710	0.614351	2.307030
22	6	0	3.153765	0.476349	2.628954
23	6	0	3.784536	-0.711749	2.292150
24	7	0	5.229724	-0.839714	2.538620
25	6	0	-0.352290	-0.224941	1.287142
26	8	0	-0.873246	-1.428381	0.755412
27	8	0	5.839959	-1.622886	1.820540
28	8	0	5.724517	-0.159522	3.394770
29	1	0	3.636951	-2.696600	1.494980
30	1	0	1.200075	-2.429413	0.962438
31	1	0	1.309362	1.546937	2.545949
32	1	0	3.711285	1.263461	3.120265
33	1	0	-0.911370	-0.003897	2.205629
34	1	0	-1.589922	0.542896	-0.346093
35	6	0	-0.818660	2.314735	0.978695
36	7	0	-2.011237	3.085626	0.431897
37	6	0	-1.984444	4.492309	0.973895
38	6	0	-3.333870	5.173083	0.626332
39	7	0	-4.017410	4.425804	-0.424339
40	6	0	-3.076549	4.183240	-1.516363
41	6	0	-1.993554	3.166079	-1.081870
42	6	0	-3.302195	2.449068	0.870218
43	6	0	-4.459381	3.141494	0.112059
44	1	0	-1.133580	4.987329	0.503307
45	1	0	-1.807728	4.430640	2.048729
46	1	0	-3.157759	6.195798	0.292594
47	1	0	-3.983600	5.216898	1.502099
48	1	0	-2.630483	5.137234	-1.802665
49	1	0	-3.615915	3.796349	-2.381388
50	1	0	-2.206563	2.159399	-1.445511
51	1	0	-0.984815	3.454712	-1.373824
52	1	0	-3.365719	2.598128	1.950384
53	1	0	-3.234500	1.387182	0.659207
54	1	0	-4.792351	2.519345	-0.721020
55	1	0	-5.305838	3.294868	0.782582
56	1	0	4.584255	0.774109	-3.798353
57	1	0	-1.027100	2.211087	2.046304
58	1	0	0.030299	2.990227	0.846602
59	6	0	7.528073	-2.013757	-1.505558
60	1	0	7.514785	-2.944655	-2.069662
61	1	0	8.452109	-1.470835	-1.694062
62	1	0	7.434445	-2.216329	-0.440008
63	6	0	-4.528490	-3.564880	0.691285
64	6	0	-5.698471	-4.208019	0.945929
65	6	0	-5.863736	-3.243809	-1.023601
66	7	0	-4.652166	-2.975246	-0.546438
67	1	0	-3.620086	-3.478374	1.265284
68	1	0	-6.613216	-4.797630	1.790542
69	1	0	-6.248423	-2.915832	-1.976241
70	7	0	-6.519684	-3.992818	-0.138356
71	6	0	-7.876478	-4.526052	-0.299346
72	1	0	-7.833134	-5.612708	-0.349277
73	1	0	-8.486970	-4.210581	0.544650
74	1	0	-8.298819	-4.133768	-1.221602
75	6	0	-3.626461	-2.130233	-1.579015
76	1	0	-2.673424	-2.651636	-1.082828
77	1	0	-3.864445	-2.034658	-2.237982
78	6	0	-3.532652	-0.742122	-0.527129
79	1	0	-3.396090	-0.901633	0.561279
80	1	0	-4.512751	-0.245130	-0.655548
81	8	0	-2.495565	-0.059685	-1.112383
82	1	0	-1.140695	-1.243359	-0.157509

Structure 23 – Gas phase

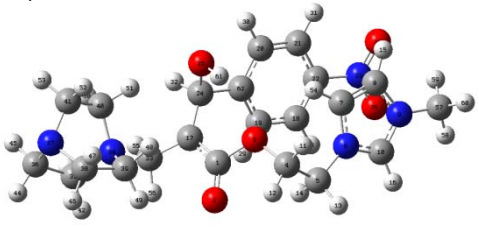


Zero-point correction=	0.706280
Thermal correction to Energy=	0.745196
Thermal correction to Enthalpy=	0.746140
Thermal correction to Gibbs Free Energy=	0.631226
Sum of electronic and zero-point Energies=	-1924.662653
Sum of electronic and thermal Energies=	-1924.623738
Sum of electronic and thermal Enthalpies=	-1924.622794
Sum of electronic and thermal Free Energies=	-1924.737707

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.326923	-1.494069	-0.726818
2	8	0	-0.720049	-2.555871	-1.187230
3	8	0	-0.816150	-0.293828	-1.285881
4	6	0	-2.018977	-0.419799	-2.021881
5	6	0	-3.136236	-0.912105	-1.091194
6	7	0	-4.471401	-0.547412	-1.578604
7	6	0	-5.146257	-1.123770	-2.633222
8	6	0	-6.356360	-0.509658	-2.712293
9	7	0	-6.398304	0.427977	-1.704318
10	6	0	-5.248483	0.390037	-1.038139
11	1	0	-2.251941	0.580803	-2.389723
12	1	0	-1.884815	-1.103345	-2.862561
13	1	0	-3.093109	-1.993559	-0.973720
14	1	0	-3.011920	-0.446286	-0.111603
15	1	0	-7.183468	-0.664495	-3.384472
16	1	0	-5.008534	1.011569	-0.185360
17	6	0	0.575991	-1.249525	0.326303
18	6	0	-2.748043	1.990612	1.309374
19	6	0	-1.430919	1.710560	0.968742
20	6	0	-0.796910	0.560310	1.440408
21	6	0	-1.479751	-0.262402	2.341691
22	6	0	-2.779217	0.022298	2.735925
23	6	0	-3.402306	1.129334	2.176214
24	7	0	-4.819947	1.374628	2.483249
25	6	0	0.591286	0.131739	0.943065
26	8	0	1.117603	1.135546	0.050814
27	8	0	-5.466040	1.978341	1.634885
28	8	0	-5.261029	0.949788	3.515337
29	1	0	-3.261079	2.864014	0.926744
30	1	0	-0.901061	2.384745	0.309807
31	1	0	-1.000332	-1.155551	2.725734
32	1	0	-3.317702	-0.602063	3.436506
33	1	0	1.267306	0.133202	1.803973
34	1	0	2.382708	-0.294102	-1.056553
35	6	0	0.944568	-2.450340	1.109508
36	7	0	2.248623	-3.177269	0.694807
37	6	0	2.362928	-4.487238	1.421642
38	6	0	3.786162	-5.054334	1.170706
39	7	0	4.403205	-4.380790	0.031014
40	6	0	3.459297	-4.392681	-1.086443
41	6	0	2.258263	-3.464692	-0.786378
42	6	0	3.445597	-2.349541	1.049837
43	6	0	4.687442	-2.993085	0.391170
44	1	0	1.579232	-5.134061	1.024233
45	1	0	2.163603	-4.301883	2.478350
46	1	0	3.731367	-6.125282	0.974741
47	1	0	4.421486	-4.908296	2.046074
48	1	0	3.131396	-5.421160	-1.247054
49	1	0	3.966795	-4.060146	-1.992394
50	1	0	2.349707	-2.502184	-1.285187
51	1	0	1.288756	-3.894737	-1.037706
52	1	0	3.505786	-2.344891	2.140659
53	1	0	3.255345	-1.341228	0.690393
54	1	0	4.951362	-2.448828	-0.517811
55	1	0	5.537425	-2.958677	1.074028
56	1	0	-4.719176	-1.922274	-3.216531
57	1	0	1.106209	-2.234759	2.170096
58	1	0	0.185692	-3.232702	1.012244
59	6	0	-7.522878	1.315981	-1.384379
60	1	0	-7.621370	2.073708	-2.159782
61	1	0	-8.432446	0.721966	-1.320515
62	1	0	-7.324178	1.784030	-0.421580
63	6	0	3.254644	3.731828	0.186811
64	6	0	3.895547	4.846015	0.627641
65	6	0	4.970670	4.104649	-1.142917
66	7	0	3.942312	3.289058	-0.922567
67	1	0	2.379111	3.204701	0.537024
68	1	0	3.687082	5.502784	1.455466
69	1	0	5.687593	4.010958	-1.943443
70	7	0	4.963895	5.059874	-0.216313
71	6	0	5.924774	6.164415	-0.110766
72	1	0	5.400686	7.110193	-0.235764
73	1	0	6.407833	6.124434	0.863833
74	1	0	6.672130	6.053487	-0.892965
75	6	0	3.594044	2.075998	-1.673640
76	1	0	2.519426	2.102317	-1.847642
77	1	0	4.105886	2.104879	-2.635118
78	6	0	3.952364	0.816811	-0.874620
79	1	0	3.684647	0.980390	0.175791
80	1	0	5.026560	0.627953	-0.935360
81	8	0	3.287127	-0.294353	-1.411509
82	1	0	0.543705	1.070920	-0.727745

Structure 24 – Gas phase



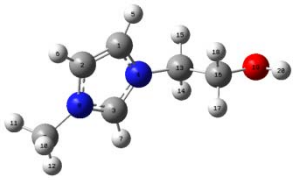
Zero-point correction=	0.528439
Thermal correction to Energy=	0.556527
Thermal correction to Enthalpy=	0.557471
Thermal correction to Gibbs Free Energy=	0.469126
Sum of electronic and zero-point Energies=	-1505.194996
Sum of electronic and thermal Energies=	-1505.166909
Sum of electronic and thermal Enthalpies=	-1505.165965

Sum of electronic and thermal Free Energies= -1505.254310

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.176644	1.201997	0.319362
2	8	0	-1.582292	2.188584	0.922878
3	8	0	-0.122088	1.376480	-0.626847
4	6	0	0.494374	2.646896	-0.578901
5	6	0	1.661378	2.635611	0.394159
6	7	0	2.824098	1.892645	-0.141428
7	6	0	2.841207	1.068885	-1.243335
8	6	0	4.121024	0.631551	-1.391852
9	7	0	4.859710	1.182760	-0.370838
10	6	0	4.052300	1.935658	0.372604
11	1	0	0.823529	2.899851	-1.588840
12	1	0	-0.220926	3.394091	-0.235925
13	1	0	1.997499	3.652928	0.599706
14	1	0	1.344569	2.161655	1.325181
15	1	0	4.560543	-0.046832	-2.103985
16	1	0	4.349434	2.499826	1.242043
17	6	0	-1.613959	-0.122320	0.390929
18	6	0	2.457765	-1.077859	1.410337
19	6	0	1.101777	-0.938662	1.152321
20	6	0	1.356228	-2.122591	-0.931020
21	6	0	2.711216	-2.282131	-0.687562
22	6	0	3.243654	-1.720744	0.465607
23	7	0	4.701576	-1.680375	0.625279
24	6	0	-0.939200	-1.228014	-0.356789
25	8	0	-1.108232	-1.161287	-1.780400
26	8	0	5.153451	-1.162277	1.626147
27	8	0	5.382905	-2.096160	-0.292289
28	1	0	2.911233	-0.687095	2.311958
29	1	0	0.462979	-0.430569	1.864907
30	1	0	0.914535	-2.517480	-1.837192
31	1	0	3.358705	-2.799854	-1.382838
32	1	0	-1.423475	-2.171586	-0.075664
33	6	0	-2.768914	-0.379681	1.253308
34	7	0	-4.164654	-0.264764	0.544624
35	6	0	-5.261867	-0.465654	1.542984
36	6	0	-6.610219	-0.551677	0.781257
37	7	0	-6.449497	-0.070330	-0.587586
38	6	0	-5.791111	1.235632	-0.552897
39	6	0	-4.325585	1.095251	-0.075408
40	6	0	-4.297226	-1.296505	-0.535564
41	6	0	-5.601391	-1.007076	-1.322600
42	1	0	-5.221802	0.384391	2.226405
43	1	0	-5.036452	-1.374243	2.103393
44	1	0	-7.367761	0.045814	1.289570
45	1	0	-6.968519	-1.581880	0.743949
46	1	0	-6.357924	1.885694	0.116146
47	1	0	-5.821500	1.679493	-1.548667
48	1	0	-3.607460	1.138597	-0.894232
49	1	0	-4.027243	1.833829	0.668657
50	1	0	-4.320683	-2.268088	-0.036112
51	1	0	-3.404358	-1.236214	-1.160103
52	1	0	-5.372681	-0.569173	-2.295616
53	1	0	-6.150324	-1.933365	-1.495892
54	1	0	1.941459	0.823547	-1.781460
55	1	0	-2.788024	-1.392868	1.665224
56	1	0	-2.844260	0.350952	2.062111
57	6	0	6.302579	1.003770	-0.160856
58	1	0	6.536997	1.260004	0.869440
59	1	0	6.549889	-0.043561	-0.328454
60	1	0	6.848549	1.645847	-0.850335
61	1	0	-0.873299	-0.257787	-2.021182
62	6	0	0.545648	-1.417036	-0.035829

Structure 19 – Solvent: Methanol

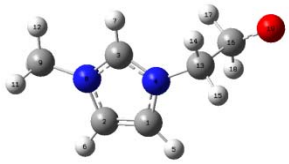


Zero-point correction= 0.175778
Thermal correction to Energy= 0.185155
Thermal correction to Enthalpy= 0.186099
Thermal correction to Gibbs Free Energy= 0.140943
Sum of electronic and zero-point Energies= -419.582204
Sum of electronic and thermal Energies= -419.572828
Sum of electronic and thermal Enthalpies= -419.571884
Sum of electronic and thermal Free Energies= -419.617040

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.434164	1.377410	-0.108572
2	6	0	-1.747099	1.176600	0.170483
3	6	0	-0.844554	-0.778730	-0.275874
4	7	0	0.109801	0.142226	-0.388760
5	1	0	0.153133	2.278962	-0.139733
6	1	0	-2.530220	1.867630	0.429786
7	1	0	-0.714949	-1.836738	-0.435619
8	7	0	-1.979758	-0.176369	0.059198
9	6	0	-3.270255	-0.835291	0.270327
10	1	0	-3.603031	-0.642055	1.287689
11	1	0	-3.990036	-0.442530	-0.444419
12	1	0	-3.142411	-1.903585	0.118885
13	6	0	1.517320	-0.123220	-0.691778
14	1	0	1.582887	-1.103902	-1.160564
15	1	0	1.860883	0.629053	-1.400806
16	6	0	2.361061	-0.085136	0.574257
17	1	0	2.000499	-0.846132	1.275179
18	1	0	2.271071	0.898833	1.048091
19	8	0	3.681012	-0.342316	0.147676
20	1	0	4.259921	-0.311814	0.913988

Structure 19 (Anion) – Solvent: Methanol

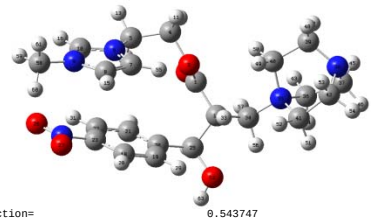


Zero-point correction= 0.160868
Thermal correction to Energy= 0.169788
Thermal correction to Enthalpy= 0.170732
Thermal correction to Gibbs Free Energy= 0.126083
Sum of electronic and zero-point Energies= -419.084190
Sum of electronic and thermal Energies= -419.075270
Sum of electronic and thermal Enthalpies= -419.074326
Sum of electronic and thermal Free Energies= -419.118975

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.420475	1.429091	0.018376
2	6	0	1.715277	1.143370	-0.280222
3	6	0	0.735330	-0.711781	0.379217
4	7	0	-0.168829	0.259743	0.440622
5	1	0	-0.128758	2.353683	-0.023109
6	1	0	2.519163	1.768704	-0.627625
7	1	0	0.562435	-1.743050	0.639594
8	7	0	1.890565	-0.201467	-0.047826
9	6	0	3.140503	-0.939594	-0.222565
10	1	0	3.481274	-0.824963	-1.249297
11	1	0	3.886802	-0.551071	0.467325
12	1	0	2.955339	-1.989676	-0.012402
13	6	0	-1.600225	0.070452	0.708392
14	1	0	-1.706380	-0.745028	1.423297
15	1	0	-1.979157	0.990118	1.153105
16	6	0	-2.412955	-0.262364	-0.578666
17	1	0	-1.873777	-1.151610	-1.015699
18	1	0	-2.164242	0.576048	-1.289065
19	8	0	-3.699411	-0.433266	-0.295360

Structure 20 – Solvent: Methanol

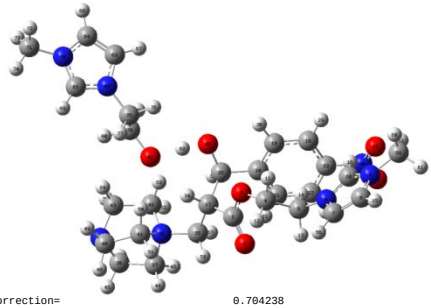


Zero-point correction= 0.543747
Thermal correction to Energy= 0.571761
Thermal correction to Enthalpy= 0.572705
Thermal correction to Gibbs Free Energy= 0.485019
Sum of electronic and zero-point Energies= -1505.725787
Sum of electronic and thermal Energies= -1505.697773
Sum of electronic and thermal Enthalpies= -1505.696829
Sum of electronic and thermal Free Energies= -1505.784515

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.010326	-0.322524	-1.012011
2	8	0	-1.045805	-0.451964	-2.206052
3	8	0	-0.417393	-1.189236	-0.182575
4	6	0	0.159989	-2.358099	-0.793166
5	6	0	1.525816	-2.062337	-1.373563
6	7	0	2.544305	-1.858813	-0.327554
7	6	0	2.338629	-1.573007	1.006355
8	6	0	3.564423	-1.490428	1.586770
9	7	0	4.495262	-1.719303	0.598095
10	6	0	3.856653	-1.934208	-0.547115
11	1	0	0.207553	-3.105259	-0.003304
12	1	0	-0.493013	-2.707801	-1.591002
13	1	0	1.842229	-2.912812	-1.976722
14	1	0	1.489567	-1.174173	-2.005099
15	1	0	3.852957	-1.282976	2.603109
16	1	0	4.325761	-2.147038	-1.494781
17	6	0	-1.624726	0.853139	-0.276501
18	6	0	2.554146	1.855734	1.117366
19	6	0	1.202029	2.064301	0.896385
20	6	0	0.667911	1.918999	-0.384892
21	6	0	1.496222	1.574031	-1.453560
22	6	0	2.852745	1.356015	-1.249303
23	6	0	3.350110	1.498613	0.037354
24	7	0	4.779535	1.240730	0.273488
25	6	0	-0.816331	2.131099	-0.610107
26	8	0	5.469533	0.932066	-0.675881
27	8	0	5.188881	1.320081	1.413962
28	1	0	2.990327	1.960128	2.101275
29	1	0	0.556204	2.356511	1.714841
30	1	0	1.084002	1.485533	-2.452806
31	1	0	3.513409	1.092892	-2.064517
32	1	0	-0.982532	2.377540	-1.665910
33	1	0	-1.539532	0.695999	0.800324
34	6	0	-3.064032	1.093958	-0.735021
35	7	0	-4.109022	0.251948	-0.060873
36	6	0	-5.401930	0.391641	-0.835082
37	6	0	-6.533845	-0.262694	-0.010576
38	7	0	-5.971535	-1.128651	1.025933
39	6	0	-4.981596	-2.015238	0.417179
40	6	0	-3.737228	-1.209810	-0.032304
41	6	0	-4.361988	0.719974	1.352860
42	6	0	-5.311660	-0.296243	2.031413
43	1	0	-5.239941	-0.103854	-1.792356
44	1	0	-5.564726	1.454873	-1.006787
45	1	0	-7.172617	-0.849135	-0.670474
46	1	0	-7.147728	0.498965	0.470915
47	1	0	-5.442082	-2.513064	-0.436632
48	1	0	-4.679035	-2.777072	1.135041
49	1	0	-2.910551	-1.314057	0.671073
50	1	0	-3.404058	-1.483258	-1.034445
51	1	0	-4.802616	1.713489	1.269265
52	1	0	-3.405223	0.800195	1.864906
53	1	0	-4.756514	-0.946720	2.708109
54	1	0	-6.061251	0.240723	2.612186
55	1	0	1.355067	-1.432287	1.422128
56	1	0	-3.336007	2.139931	-0.539961
57	1	0	-3.138374	0.895860	-1.806025
58	6	0	5.949620	-1.764446	0.781821
59	1	0	6.415073	-1.836519	-0.197241
60	1	0	6.266953	-0.848274	1.275824
61	1	0	6.203402	-2.633444	1.384955
62	8	0	-1.349375	3.122652	0.236918
63	1	0	-1.011935	3.982556	-0.036220

Structure 21 – Solvent: Methanol



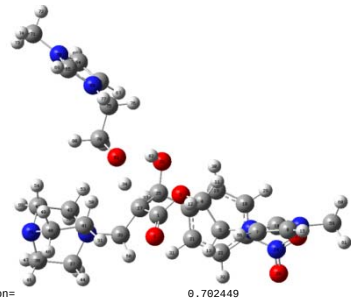
Zero-point correction= 0.704238
Thermal correction to Energy= 0.743152
Thermal correction to Enthalpy= 0.744097
Thermal correction to Gibbs Free Energy= 0.626718
Sum of electronic and zero-point Energies= -1924.849613
Sum of electronic and thermal Energies= -1924.810698
Sum of electronic and thermal Enthalpies= -1924.809754
Sum of electronic and thermal Free Energies= -1924.927133

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.930536	1.140124	-1.217753
2	8	0	1.602437	1.978427	-1.762066
3	8	0	1.169896	-0.170732	-1.326941

4	6	0	2.306857	-0.555424	-2.106924
5	6	0	3.607555	-0.026334	-1.490341
6	7	0	4.726224	-0.926707	-1.778175
7	6	0	5.249502	-1.200354	-3.024107
8	6	0	6.275287	-2.070183	-2.838129
9	7	0	6.361231	-2.307764	-1.484559
10	6	0	5.415515	-1.609941	-0.866736
11	1	0	2.297307	-1.643344	-2.088228
12	1	0	2.181260	-0.199908	-3.130635
13	1	0	3.858259	0.964894	-1.859801
14	1	0	3.500898	0.018905	-0.406611
15	1	0	6.948018	-2.530435	-3.540801
16	1	0	5.251537	-1.590529	0.200723
17	6	0	-0.257134	1.396727	-0.317159
18	6	0	3.206842	-0.919860	2.102254
19	6	0	1.877140	-0.732171	1.752491
20	6	0	1.382304	0.547207	1.497539
21	6	0	2.233974	1.649658	1.616803
22	6	0	3.563415	1.485805	1.979519
23	6	0	4.025643	0.196825	2.204107
24	7	0	5.440493	0.004507	2.543518
25	6	0	-0.079187	0.725185	1.109744
26	8	0	-0.741028	-0.482661	1.182992
27	8	0	5.925982	-1.092905	2.326543
28	8	0	6.050596	0.939842	3.006680
29	1	0	3.604798	-1.906521	2.301454
30	1	0	1.202111	-1.572032	1.668569
31	1	0	1.865578	2.652606	1.433240
32	1	0	4.234323	2.328278	2.077580
33	1	0	-0.487737	1.456949	1.826444
34	1	0	-1.086324	0.846608	-0.767793
35	6	0	-0.563420	2.896065	-0.287928
36	7	0	-2.026447	3.241793	-0.315701
37	6	0	-2.152400	4.743951	-0.410130
38	6	0	-3.633597	5.123919	-0.190731
39	7	0	-4.490870	3.954332	-0.386861
40	6	0	-4.110758	3.309832	-1.646258
41	6	0	-2.730356	2.629081	-1.508621
42	6	0	-2.743764	2.786318	0.932665
43	6	0	-4.255889	3.014610	0.712793
44	1	0	-1.791786	5.021968	-1.400885
45	1	0	-1.494434	5.177484	0.341993
46	1	0	-3.915464	5.908624	-0.892896
47	1	0	-3.788371	5.501149	0.820796
48	1	0	-4.101545	4.067389	-2.431600
49	1	0	-4.854576	2.556904	-1.909050
50	1	0	-2.841876	1.567058	-1.284708
51	1	0	-2.093142	2.782408	-2.380135
52	1	0	-2.336909	3.374660	1.756576
53	1	0	-2.545468	1.723215	1.057216
54	1	0	-4.731822	2.063997	0.463721
55	1	0	-4.707199	3.400857	1.626929
56	1	0	4.856787	-0.752971	-3.920853
57	1	0	-0.164112	3.369804	0.610787
58	1	0	-0.121587	3.389927	-1.153084
59	6	0	7.328814	-3.188704	-0.826502
60	1	0	7.119612	-4.220127	-1.101788
61	1	0	8.330868	-2.907712	-1.141620
62	1	0	7.230989	-3.061462	0.248879
63	6	0	-4.918641	-4.014194	1.100489
64	6	0	-6.134950	-4.615522	1.165243
65	6	0	-6.134549	-3.262546	-0.568132
66	7	0	-4.937965	-3.179409	0.005598
67	1	0	-4.947676	-4.110137	1.725579
68	1	0	-6.533167	-5.339502	1.854918
69	1	0	-6.446921	-2.719926	-1.445478
70	7	0	-6.878085	-4.130165	0.112972
71	6	0	-8.253168	-4.514852	-0.207493
72	1	0	-8.285873	-5.581651	-0.417653
73	1	0	-8.894624	-4.276262	0.637917
74	1	0	-8.571949	-3.955824	-1.083004
75	6	0	-3.864142	-2.258257	-0.389781
76	1	0	-2.915248	-2.780756	-0.267287
77	1	0	-4.001268	-2.020675	-1.444229
78	6	0	-3.877085	-0.968259	0.447087
79	1	0	-3.785015	-1.262857	1.509901
80	1	0	-4.879048	-0.516409	0.336443
81	8	0	-2.869473	-0.133809	0.029005
82	1	0	-1.694621	-0.378279	0.697870

Structure 22 – Solvent: Methanol

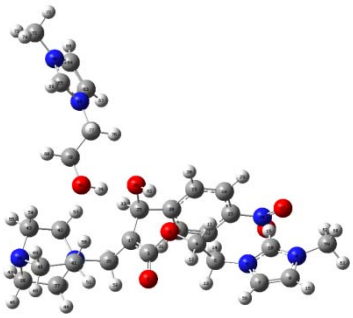


```
Zero-point correction=                           0.702449
Thermal correction to Energy=                    0.739849
Thermal correction to Enthalpy=                  0.740793
Thermal correction to Gibbs Free Energy=         0.630684
Sum of electronic and zero-point Energies=          -1924.837296
Sum of electronic and thermal Energies=             -1924.799897
Sum of electronic and thermal Enthalpies=           -1924.798952
Sum of electronic and thermal Free Energies=        -1924.909061
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.541365	1.005794	-0.759350
2	8	0	0.936939	2.030351	-1.276467
3	8	0	1.032763	-0.199958	-1.122224
4	6	0	2.154695	-0.197852	-1.999944
5	6	0	3.364873	0.447953	-1.312531
6	7	0	4.620895	-0.092041	-1.835770
7	6	0	5.135023	0.124517	-3.096257
8	6	0	6.303854	-0.563069	-3.168711
9	7	0	6.481744	-1.183117	-1.952107
10	6	0	5.452805	-0.887550	-1.166433
11	1	0	2.357449	-1.248306	-2.203026
12	1	0	1.905184	0.318761	-2.927646
13	1	0	3.373767	1.527446	-1.442808
14	1	0	3.333497	0.222289	-0.245674
15	1	0	7.020068	-0.668341	-3.966038
16	1	0	5.329178	-1.226269	-0.148018
17	6	0	-0.503173	0.884010	0.276258
18	6	0	3.260579	-1.689861	1.764822
19	6	0	1.912073	-1.590778	1.454421
20	6	0	1.211039	-0.407273	1.689507
21	6	0	1.871587	0.670776	2.286874
22	6	0	3.214888	0.586736	2.624398
23	6	0	3.889213	-0.592038	2.337692
24	7	0	5.323404	-0.675379	2.631289
25	6	0	-0.251825	-0.273761	1.278975
26	8	0	-0.721159	-1.518099	0.798400
27	8	0	5.976029	-1.502677	2.016265
28	8	0	5.785794	0.082081	3.452437
29	1	0	3.817540	-2.598175	1.574362
30	1	0	1.391344	-2.423772	1.003936
31	1	0	1.341166	1.594568	2.489245
32	1	0	3.738114	1.414288	3.083863
33	1	0	-0.817513	-0.027415	2.186852
34	1	0	-1.493003	0.369210	-0.421057
35	6	0	-0.795656	2.231299	0.904599
36	7	0	-2.035987	2.939640	0.378745
37	6	0	-2.044095	4.356698	0.891175
38	6	0	-3.421807	4.982624	0.567266
39	7	0	-4.119778	4.186087	-0.443050
40	6	0	-3.202654	3.940386	-1.558294
41	6	0	-2.065681	2.983805	-1.130037
42	6	0	-3.284619	2.263465	0.869270
43	6	0	-4.495267	2.900221	0.148066
44	1	0	-1.224060	4.871873	0.390465
45	1	0	-1.841884	4.321810	1.961334
46	1	0	-3.284011	5.999039	0.198530
47	1	0	-4.044038	5.027045	1.462094
48	1	0	-2.799695	4.898971	-1.888062
49	1	0	-3.752902	3.500429	-2.390377
50	1	0	-2.238179	1.961034	-1.467656
51	1	0	-1.081698	3.311231	-1.460867
52	1	0	-3.315971	2.418292	1.948490
53	1	0	-3.185645	1.200859	0.665600
54	1	0	-4.854296	2.248624	-0.650255
55	1	0	-5.308135	3.046648	0.859322
56	1	0	4.637446	0.749727	-3.817586
57	1	0	-0.968042	2.148766	1.979306
58	1	0	0.015994	2.940958	0.731130
59	6	0	7.618406	-2.026124	-1.575042
60	1	0	7.605757	-2.933777	-2.174313
61	1	0	8.538776	-1.472520	-1.745978
62	1	0	7.526265	-2.273136	-0.520242
63	6	0	-4.858638	-3.444141	0.784532
64	6	0	-6.134417	-3.839158	1.029201
65	6	0	-6.066750	-2.971939	-0.991136
66	7	0	-4.838292	-2.910792	-0.485537
67	1	0	-3.969931	-3.498848	1.390104
68	1	0	-6.579001	-4.307990	1.889694
69	1	0	-6.359758	-2.628999	-1.969865
70	7	0	-6.870961	-3.534023	-0.093666
71	6	0	-8.298829	-3.802041	-0.271984
72	1	0	-8.468574	-4.875487	-0.225865
73	1	0	-8.854580	-3.297618	0.515226
74	1	0	-8.604011	-3.420216	-1.242404
75	6	0	-3.669701	-2.294563	-1.124576
76	1	0	-2.811103	-2.937742	-0.929512
77	1	0	-3.848168	-2.262689	-2.198502
78	6	0	-3.409361	-0.886214	-0.580276
79	1	0	-3.327169	-0.968667	0.519845
80	1	0	-4.302091	-0.273219	-0.792549
81	8	0	-2.257931	-0.389248	-1.165196
82	1	0	-1.112290	-1.360442	-0.080513

Structure 23 – Solvent: Methanol



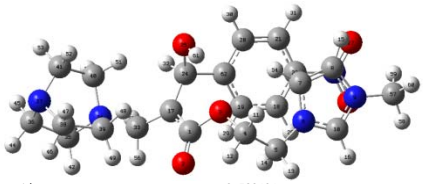
```
Zero-point correction=                           0.707358
Thermal correction to Energy=                    0.746256
Thermal correction to Enthalpy=                  0.747200
Thermal correction to Gibbs Free Energy=         0.631746
Sum of electronic and zero-point Energies=          -1924.855642
Sum of electronic and thermal Energies=             -1924.816743
Sum of electronic and thermal Enthalpies=           -1924.815799
Sum of electronic and thermal Free Energies=        -1924.931254
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.784572	1.692795	-0.748591
2	8	0	1.210648	2.737129	-1.245922
3	8	0	1.171934	0.465912	-1.325016
4	6	0	2.411037	0.460455	-2.005823
5	6	0	3.538838	0.750001	-1.009384
6	7	0	4.833016	0.285192	-1.511069
7	6	0	5.567772	0.851315	-2.529886
8	6	0	6.684329	0.092440	-2.680295
9	7	0	6.609738	-0.920750	-1.750897
10	6	0	5.482423	-0.786421	-1.061768
11	1	0	2.526247	-0.543848	-2.414618
12	1	0	2.412959	1.190708	-2.817280
13	1	0	3.610106	1.816004	-0.798524
14	1	0	3.343330	0.217297	-0.078029
15	1	0	7.518611	0.186413	-3.353499
16	1	0	5.159877	-1.437639	-0.262426
17	6	0	-0.065511	1.492431	0.340981
18	6	0	2.788772	-2.201571	1.203322
19	6	0	1.533445	-1.732048	0.836898
20	6	0	1.042800	-0.531638	1.352090
21	6	0	1.798406	0.155562	2.308462
22	6	0	3.034251	-0.314657	2.720844
23	6	0	3.519969	-1.476496	2.132390
24	7	0	4.863306	-1.940361	2.489594
25	6	0	-0.267167	0.097045	0.873921
26	8	0	-0.922321	-0.780997	-0.060825
27	8	0	5.448304	-2.644856	1.682971
28	8	0	5.326471	-1.592188	3.551064
29	1	0	3.193594	-3.114044	0.784894
30	1	0	0.946502	-2.297883	0.126166
31	1	0	1.425430	1.088636	2.714937
32	1	0	3.628385	0.212969	3.453737
33	1	0	-0.936370	0.138437	1.738637
34	1	0	-2.315386	0.052315	-0.920694
35	6	0	-0.492049	2.688258	1.083602
36	7	0	-1.880088	3.274788	0.700473
37	6	0	-2.063154	4.607616	1.359316
38	6	0	-3.530756	5.056163	1.146790
39	7	0	-4.161260	4.259744	0.091013
40	6	0	-3.279458	4.255947	-1.080165
41	6	0	-1.989309	3.455531	-0.787352
42	6	0	-2.979189	2.367297	1.159725
43	6	0	-4.309815	2.880466	0.564191
44	1	0	-1.348228	5.287892	0.895173
45	1	0	-1.809273	4.493188	2.413424
46	1	0	-3.558211	6.110677	0.871607
47	1	0	-4.107312	4.929155	2.064302
48	1	0	-3.046139	5.290645	-1.336357
49	1	0	-3.804324	3.806781	-1.923989
50	1	0	-2.020690	2.454809	-1.214076
51	1	0	-1.079417	3.954214	-1.120717
52	1	0	-2.969276	2.389069	2.250525
53	1	0	-2.736062	1.365781	0.812069
54	1	0	-4.600086	2.257501	-0.283676
55	1	0	-5.096807	2.834928	1.317598
56	1	0	5.241779	1.738879	-3.044208
57	1	0	-0.582822	2.526480	2.161246
58	1	0	0.190081	3.521316	0.900536
59	6	0	7.604849	-1.974299	-1.542122
60	1	0	7.619878	-2.631149	-2.409059
61	1	0	8.579673	-1.513914	-1.399300
62	1	0	7.326993	-2.533638	-0.651869
63	6	0	-4.637759	-3.647788	0.521608
64	6	0	-5.747631	-4.413091	0.680090
65	6	0	-5.910065	-3.378137	-1.254100
66	7	0	-4.757148	-3.014524	-0.696267
67	1	0	-3.779320	-3.503417	1.154868
68	1	0	-6.048281	-5.069673	1.477802
69	1	0	-6.277729	-3.040422	-2.209616
70	7	0	-6.526829	-4.228029	-0.440232
71	6	0	-7.813212	-4.879433	-0.694801
72	1	0	-7.661254	-5.954833	-0.754125
73	1	0	-8.497090	-4.638305	0.115700
74	1	0	-8.209013	-4.508241	-1.636047
75	6	0	-3.813234	-2.041024	-1.251663
76	1	0	-2.808562	-2.351743	-0.964292

77	1	0	-3.896027	-2.066276	-2.337229
78	6	0	-4.102242	-0.634613	-0.726448
79	1	0	-4.054259	-0.639025	0.370367
80	1	0	-5.107428	-0.328223	-1.022906
81	8	0	-3.189221	0.279752	-1.286187
82	1	0	-0.351214	-0.774874	-0.844222

Structure 24 – Solvent: Methanol



Zero-point correction= 0.528494
Thermal correction to Energy= 0.556516
Thermal correction to Enthalpy= 0.557461
Thermal correction to Gibbs Free Energy= 0.469637
Sum of electronic and zero-point Energies= -1505.268409
Sum of electronic and thermal Energies= -1505.240387
Sum of electronic and thermal Enthalpies= -1505.239442
Sum of electronic and thermal Free Energies= -1505.327266

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.195719	1.253119	-0.357322
2	8	0	1.612549	2.216629	-1.005409
3	8	0	0.155723	1.467094	0.579540
4	6	0	-0.501890	2.718093	0.485063
5	6	0	-1.684211	2.637570	-0.462894
6	7	0	-2.819191	1.897373	0.124712
7	6	0	-2.807055	1.121238	1.261934
8	6	0	-4.075161	0.666722	1.444757
9	7	0	-4.835123	1.161466	0.408990
10	6	0	-4.053183	1.899086	-0.375333
11	1	0	-0.819099	3.000524	1.489808
12	1	0	0.186760	3.470153	0.104551
13	1	0	-2.044007	3.637558	-0.703913
14	1	0	-1.383638	2.131266	-1.382127
15	1	0	-4.495575	0.029021	2.203864
16	1	0	-4.370997	2.428006	-1.259398
17	6	0	1.617128	-0.075080	-0.378237
18	6	0	-2.473191	-1.023965	-1.382284
19	6	0	-1.122303	-0.856832	-1.110470
20	6	0	-1.367392	-2.071786	0.954497
21	6	0	-2.714099	-2.264240	0.696983
22	6	0	-3.248968	-1.708349	-0.458676
23	7	0	-4.699036	-1.762336	-0.661409
24	6	0	0.916358	-1.134702	0.413769
25	8	0	1.043819	-0.983812	1.838984
26	8	0	-5.159216	-1.262805	-1.668920
27	8	0	-5.379890	-2.263120	0.213846
28	1	0	-2.924816	-0.615718	-2.276680
29	1	0	-0.494648	-0.319620	-1.810805
30	1	0	-0.931996	-2.460110	1.866058
31	1	0	-3.352556	-2.800161	1.385829
32	1	0	1.405676	-2.092793	0.202101
33	6	0	2.764836	-0.405456	-1.230606
34	7	0	4.159641	-0.303989	-0.532078
35	6	0	5.244326	-0.605517	-1.520523
36	6	0	6.588957	-0.704277	-0.758564
37	7	0	6.458170	-0.137793	0.585335
38	6	0	5.847321	1.189796	0.475219
39	6	0	4.376929	1.079217	0.009820
40	6	0	4.255248	-1.277127	0.604043
41	6	0	5.571080	-0.998423	1.371835
42	1	0	5.237788	0.206140	-2.248943
43	1	0	4.982415	-1.535167	-2.025655
44	1	0	7.364600	-0.166672	-1.304449
45	1	0	6.900430	-1.745593	-0.663557
46	1	0	6.432258	1.776234	-0.235223
47	1	0	5.893146	1.689065	1.443639
48	1	0	3.665043	1.200759	0.825634
49	1	0	4.117644	1.784224	-0.778506
50	1	0	4.233781	-2.275584	0.163141
51	1	0	3.371533	-1.137320	1.227218
52	1	0	5.361962	-0.498312	2.318742
53	1	0	6.079304	-1.938128	1.589554
54	1	0	-1.903397	0.932192	1.815076
55	1	0	2.748292	-1.434816	-1.597821
56	1	0	2.861050	0.281445	-2.073890
57	6	0	-6.278679	0.968310	0.240516
58	1	0	-6.564194	1.333217	-0.742222
59	1	0	-6.504123	-0.093917	0.316898
60	1	0	-6.803551	1.523183	1.015413
61	1	0	0.780067	-0.072938	2.018072
62	6	0	-0.562481	-1.342574	0.072207

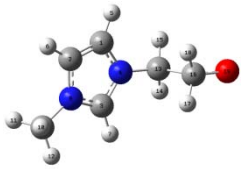
Structure 19 – Solvent: Acetonitrile

Zero-point correction= 0.175773
Thermal correction to Energy= 0.185153
Thermal correction to Enthalpy= 0.186097
Thermal correction to Gibbs Free Energy= 0.140932
Sum of electronic and zero-point Energies= -419.582434
Sum of electronic and thermal Energies= -419.573055
Sum of electronic and thermal Enthalpies= -419.572110
Sum of electronic and thermal Free Energies= -419.617275

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.434199	1.377446	-0.108522
2	6	0	-1.747130	1.176608	0.170516
3	6	0	-0.844541	-0.778714	-0.275813
4	7	0	0.109792	0.142266	-0.388703
5	1	0	0.153085	2.279003	-0.139703
6	1	0	-2.530279	1.867604	0.429817
7	1	0	-0.714924	-1.836721	-0.435535
8	7	0	-1.979750	-0.176371	0.059230
9	6	0	-3.270213	-0.835365	0.270250
10	1	0	-3.603047	-0.642266	1.287617
11	1	0	-3.989977	-0.442556	-0.444483
12	1	0	-3.142280	-1.903626	0.118669
13	6	0	1.517279	-0.123150	-0.691808
14	1	0	1.582790	-1.103800	-1.160672
15	1	0	1.860781	0.629204	-1.400783
16	6	0	2.361057	-0.085152	0.574200
17	1	0	2.000518	-0.846163	1.275095
18	1	0	2.271130	0.898791	1.048078
19	8	0	3.681067	-0.342347	0.147650
20	1	0	4.259851	-0.311990	0.914066

Structure 19 (Anion) – Solvent: Acetonitrile

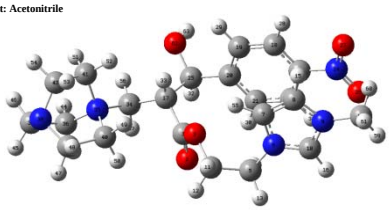


Zero-point correction= 0.160870
Thermal correction to Energy= 0.169789
Thermal correction to Enthalpy= 0.170734
Thermal correction to Gibbs Free Energy= 0.126087
Sum of electronic and zero-point Energies= -419.084399
Sum of electronic and thermal Energies= -419.075480
Sum of electronic and thermal Enthalpies= -419.074536
Sum of electronic and thermal Free Energies= -419.119182

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.420138	1.428763	0.018971
2	6	0	1.715052	1.143615	-0.279663
3	6	0	0.735705	-0.712218	0.378747
4	7	0	-0.168811	0.258972	0.440530
5	1	0	-0.129365	2.353217	-0.022013
6	1	0	2.518774	1.769386	-0.626666
7	1	0	0.563184	-1.743677	0.638626
8	7	0	1.890758	-0.201287	-0.047949
9	6	0	3.140988	-0.938894	-0.222931
10	1	0	3.481842	-0.823522	-1.249547
11	1	0	3.887032	-0.550461	0.467277
12	1	0	2.956140	-1.989145	-0.013370
13	6	0	-1.600104	0.069288	0.708456
14	1	0	-1.705912	-0.747418	1.422117
15	1	0	-1.978906	0.988129	1.154834
16	6	0	-2.413239	-0.261459	-0.578774
17	1	0	-1.874409	-1.149984	-1.017511
18	1	0	-2.164888	0.578086	-1.287889
19	8	0	-3.699795	-0.432811	-0.295346

Structure 20 – Solvent: Acetonitrile

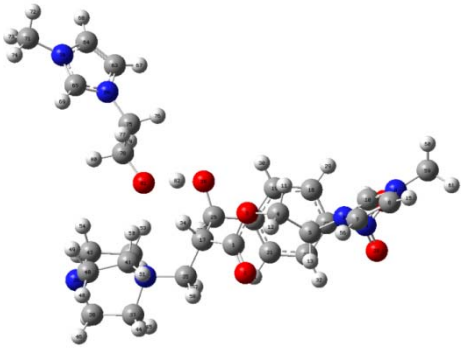


Zero-point correction= 0.543718
Thermal correction to Energy= 0.571745
Thermal correction to Enthalpy= 0.572689
Thermal correction to Gibbs Free Energy= 0.484930
Sum of electronic and zero-point Energies= -1505.726440
Sum of electronic and thermal Energies= -1505.698414
Sum of electronic and thermal Enthalpies= -1505.697469
Sum of electronic and thermal Free Energies= -1505.785228

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.010438	-0.322996	-1.013324
2	8	0	-1.045949	-0.452079	-2.207417
3	8	0	-0.417674	-1.189979	-0.184138
4	6	0	0.159955	-2.358559	-0.794875
5	6	0	1.526049	-2.062574	-1.374472
6	7	0	2.543749	-1.858812	-0.327762
7	6	0	2.336999	-1.572000	1.005768
8	6	0	3.562311	-1.489562	1.587218
9	7	0	4.493935	-1.719327	0.599478
10	6	0	3.856243	-1.934811	-0.546141
11	1	0	0.207225	-3.106001	-0.005264
12	1	0	-0.492692	-2.708142	-1.593085
13	1	0	1.843089	-2.912919	-1.977454
14	1	0	1.489986	-1.174399	-2.005990
15	1	0	3.850010	-1.281570	2.603681
16	1	0	4.326091	-2.148531	-1.493229
17	6	0	-1.624445	0.852653	-0.277455
18	6	0	2.554358	1.856536	1.116907
19	6	0	1.202264	2.064814	0.895531
20	6	0	0.668343	1.918362	-0.385702
21	6	0	1.496864	1.572474	-1.453922
22	6	0	2.853366	1.354700	-1.249278
23	6	0	3.350521	1.498533	0.037331
24	7	0	4.779892	1.240884	0.273940
25	6	0	-0.815870	2.139433	-0.611322
26	8	0	5.470134	0.931495	-0.675023
27	8	0	5.189072	1.321254	1.414419
28	1	0	2.990308	1.961689	2.100835
29	1	0	0.556289	2.357589	1.713656
30	1	0	1.084784	1.483017	-2.453140
31	1	0	3.514110	1.090766	-2.064161
32	1	0	-0.981848	2.376436	-1.667252
33	1	0	-1.538907	0.695338	0.799312
34	6	0	-3.063882	1.093760	-0.735409
35	7	0	-4.108765	0.252125	-0.060610
36	6	0	-5.402116	0.392409	-0.833951
37	6	0	-6.533718	-0.261769	-0.008907
38	7	0	-5.971122	-1.127818	1.027386
39	6	0	-4.981766	-0.914779	0.418216
40	6	0	-3.737546	-1.209783	-0.032457
41	6	0	-4.360574	0.720173	1.353309
42	6	0	-5.310416	-0.295508	2.032405
43	1	0	-5.240914	-0.102883	-1.791459
44	1	0	-5.564707	1.455730	-1.005269
45	1	0	-7.172856	-0.848112	-0.668539
46	1	0	-7.147258	0.499993	0.472862
47	1	0	-5.442938	-2.512865	-0.435070
48	1	0	-4.678804	-2.776383	1.136148
49	1	0	-2.910203	-1.314399	0.670060
50	1	0	-3.405529	-1.483297	-1.034954
51	1	0	-4.800607	1.713977	1.270045
52	1	0	-3.403461	0.799677	1.864798
53	1	0	-4.755228	-0.946095	2.708965
54	1	0	-6.059514	0.241902	2.613407
55	1	0	1.354024	-1.430623	1.420582
56	1	0	-3.335533	2.130821	-0.540395
57	1	0	-3.138776	0.895515	-1.806341
58	6	0	5.948109	-1.764787	0.784395
59	1	0	6.414308	-1.837039	-0.194304
60	1	0	6.265239	-0.848640	1.278575
61	1	0	6.201236	-2.633778	1.387799
62	8	0	-1.348881	3.122468	0.235155
63	1	0	-1.012018	3.982275	-0.039005

Structure 21 – Solvent: Acetonitrile

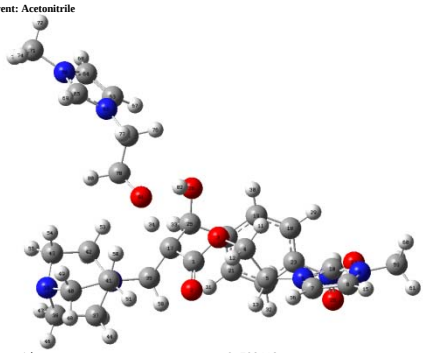


Zero-point correction= 0.704200
Thermal correction to Energy= 0.743130
Thermal correction to Enthalpy= 0.744074
Thermal correction to Gibbs Free Energy= 0.626525
Sum of electronic and zero-point Energies= -1924.850238
Sum of electronic and thermal Energies= -1924.811308
Sum of electronic and thermal Enthalpies= -1924.810364
Sum of electronic and thermal Free Energies= -1924.927912

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.930070	1.139777	-1.218280
2	8	0	1.602019	1.977762	-1.763039
3	8	0	1.169218	-0.171140	-1.326930
4	6	0	2.305921	-0.556400	-2.107066
5	6	0	3.607002	-0.026068	-1.492282
6	7	0	4.725289	-0.927392	-1.778588
7	6	0	5.248542	-1.202762	-3.024156
8	6	0	6.273686	-2.073097	-2.837099
9	7	0	6.359256	-2.309277	-1.483254
10	6	0	5.413909	-1.610166	-0.866329
11	1	0	2.296806	-1.644290	-2.086855
12	1	0	2.179441	-0.202439	-3.131207
13	1	0	3.857875	0.964181	-1.864215
14	1	0	3.500961	0.021877	-0.408590
15	1	0	6.946247	-2.534533	-3.539148
16	1	0	5.249845	-1.589503	0.201067
17	6	0	-0.257337	1.397006	-0.317525
18	6	0	3.207330	-0.918549	2.101585
19	6	0	1.877582	-0.730979	1.751948
20	6	0	1.382549	0.548342	1.497128
21	6	0	2.234118	1.650895	1.616242
22	6	0	3.563635	1.487158	1.978715
23	6	0	4.026025	0.198229	2.203326
24	7	0	5.440890	0.006070	2.542787
25	6	0	-0.079043	0.726097	1.109608
26	8	0	-0.740880	-0.481747	1.183539
27	8	0	5.926218	-1.091637	2.327042
28	8	0	6.051197	0.941808	3.004933
29	1	0	3.605338	-1.905192	2.300764
30	1	0	1.202683	-1.570938	1.668031
31	1	0	1.865607	2.653807	1.432737
32	1	0	4.234484	2.329698	2.076548
33	1	0	-0.487437	1.458128	1.826116
34	1	0	-1.086781	0.846853	-0.767649
35	6	0	-0.563407	2.896390	-0.288872
36	7	0	-2.026438	3.242222	-0.316198
37	6	0	-2.152306	4.744401	-0.410623
38	6	0	-3.633385	5.124482	-0.190733
39	7	0	-4.490856	3.954978	-0.386753
40	6	0	-4.111124	3.310444	-1.646156
41	6	0	-2.730761	2.629556	-1.508905
42	6	0	-2.743446	2.786783	0.932342
43	6	0	-4.255628	3.015243	0.712937
44	1	0	-1.792025	5.022361	-1.401511
45	1	0	-1.494085	5.177916	0.341282
46	1	0	-3.915383	5.909255	-0.892771
47	1	0	-3.787789	5.501657	0.820870
48	1	0	-4.101990	4.068003	-2.431496
49	1	0	-4.855082	2.557600	-1.908786
50	1	0	-2.842293	1.567548	-1.284978
51	1	0	-2.093830	2.782790	-2.380640
52	1	0	-2.336298	3.374988	1.756194
53	1	0	-2.545271	1.723647	1.056784
54	1	0	-4.731775	2.064677	0.464073
55	1	0	-4.706554	3.401573	1.627231
56	1	0	4.856247	-0.755886	-3.921334
57	1	0	-0.163687	3.370556	0.609419
58	1	0	-0.121904	3.389798	-1.154443
59	6	0	7.325852	-3.190518	-0.824157
60	1	0	7.115294	-4.222051	-1.097981
61	1	0	8.328197	-2.911217	-1.139855
62	1	0	7.228377	-3.061641	0.251061
63	6	0	-4.916643	-4.015125	1.100481
64	6	0	-6.132724	-4.616852	1.165760
65	6	0	-6.133775	-3.263331	-0.567197
66	7	0	-4.936879	-3.180001	0.005849
67	1	0	-4.045267	-4.110974	1.725011
68	1	0	-6.530331	-5.341202	1.855399
69	1	0	-6.446816	-2.720620	-1.444246
70	7	0	-6.876598	-4.131448	0.114026
71	6	0	-8.251772	-4.516323	-0.205780
72	1	0	-8.284481	-5.583193	-0.415556
73	1	0	-8.892938	-4.277472	0.639776
74	1	0	-8.570866	-3.957602	-1.081371
75	6	0	-3.863662	-2.258299	-0.389817
76	1	0	-2.914502	-2.780569	-0.268386
77	1	0	-4.001733	-2.020117	-1.444008
78	6	0	-3.876446	-0.968850	0.447899
79	1	0	-3.783567	-1.264149	1.510455
80	1	0	-4.878593	-0.517224	0.338218
81	8	0	-2.869363	-0.133732	0.029789
82	1	0	-1.694622	-0.377606	0.698264

Structure 22 – Solvent: Acetonitrile

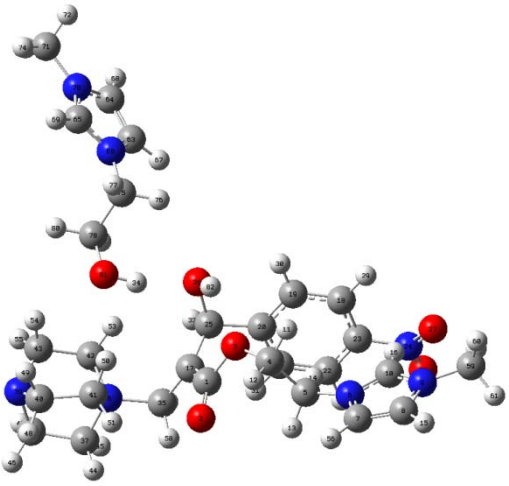


Zero-point correction= 0.702413
Thermal correction to Energy= 0.739819
Thermal correction to Enthalpy= 0.740763
Thermal correction to Gibbs Free Energy= 0.630610
Sum of electronic and zero-point Energies= -1924.837921
Sum of electronic and thermal Energies= -1924.800515
Sum of electronic and thermal Enthalpies= -1924.799571
Sum of electronic and thermal Free Energies= -1924.909725

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.542027	1.002559	-0.760544
2	8	0	0.936275	2.026093	-1.280757
3	8	0	1.033863	-0.203740	-1.121066
4	6	0	2.155122	-0.202886	-1.999682
5	6	0	3.365422	0.445090	-1.314554
6	7	0	4.621376	-0.095440	-1.837324
7	6	0	5.135216	0.119358	-3.098223
8	6	0	6.304152	-0.568128	-3.169886
9	7	0	6.482367	-1.186368	-1.952406
10	6	0	5.453540	-0.889805	-1.166978
11	1	0	2.358315	-1.253649	-2.200676
12	1	0	1.904656	0.311604	-2.928308
13	1	0	3.373728	1.524281	-1.447302
14	1	0	3.334891	0.221836	-0.247173
15	1	0	7.020246	-0.666466	-3.967185
16	1	0	5.330165	-1.226949	-0.148021
17	6	0	-0.501222	0.882740	0.276497
18	6	0	3.264766	-1.686449	1.767603
19	6	0	1.915951	-1.588444	1.458144
20	6	0	1.214701	-0.404676	1.691255
21	6	0	1.875438	0.674887	2.285687
22	6	0	3.219071	0.592018	2.622077
23	6	0	3.893541	-0.587182	2.337515
24	7	0	5.327970	-0.669436	2.630168
25	6	0	-0.248589	-0.272564	1.281746
26	8	0	-0.717902	-1.518265	0.804724
27	8	0	5.980342	-1.498178	2.016856
28	8	0	5.790849	0.090229	3.449054
29	1	0	3.821801	-2.595011	1.578561
30	1	0	1.395167	-2.422594	1.009885
31	1	0	1.344964	1.598977	2.486541
32	1	0	3.742425	1.420801	3.079254
33	1	0	-0.813454	-0.024092	2.189570
34	1	0	-1.491681	0.365463	-0.418815
35	6	0	-0.793701	2.231356	0.901952
36	7	0	-2.035035	2.937839	0.375934
37	6	0	-2.043252	4.356087	0.885078
38	6	0	-3.421802	4.980398	0.561658
39	7	0	-4.120529	4.181268	-0.446144
40	6	0	-3.204484	3.933647	-1.561873
41	6	0	-2.066619	2.978497	-1.132863
42	6	0	-3.282701	2.262187	0.869603
43	6	0	-4.494533	2.896436	0.148217
44	1	0	-1.224267	4.870613	0.381983
45	1	0	-1.839477	4.323830	1.955016
46	1	0	-3.285141	5.996125	0.190607
47	1	0	-4.042934	5.026243	1.457185
48	1	0	-2.802277	4.891723	-1.894015
49	1	0	-3.755406	3.491684	-2.392445
50	1	0	-2.239086	1.954883	-1.467943
51	1	0	-1.083203	3.305569	-1.465719
52	1	0	-3.312892	2.419734	1.948446
53	1	0	-3.183355	1.199098	0.668633
54	1	0	-4.853944	2.242846	-0.648309
55	1	0	-5.306769	3.043834	0.859992
56	1	0	4.637327	0.743367	-3.820363
57	1	0	-0.964778	2.151294	1.977043
58	1	0	0.017372	2.941013	0.725841
59	6	0	7.619222	-2.028613	-1.574302
60	1	0	7.606700	-2.937064	-2.172358
61	1	0	8.539462	-1.475059	-1.746074
62	1	0	7.527178	-2.274216	-0.519167
63	6	0	-4.868856	-3.442512	0.788570
64	6	0	-6.146507	-3.832751	1.031133
65	6	0	-6.072289	-2.965632	-0.989015
66	7	0	-4.844427	-2.909159	-0.481436
67	1	0	-3.981415	-3.500507	1.395664
68	1	0	-6.594248	-4.300036	1.890844
69	1	0	-6.362417	-2.621422	-1.968155
70	7	0	-6.880078	-3.524677	-0.092890
71	6	0	-8.308620	-3.787218	-0.273839
72	1	0	-8.482233	-4.860183	-0.231290
73	1	0	-8.863590	-3.283236	0.514200
74	1	0	-8.611148	-3.401215	-1.243441
75	6	0	-3.672784	-2.297074	-1.118838
76	1	0	-2.816574	-2.943037	-0.922519
77	1	0	-3.849697	-2.264801	-2.193005
78	6	0	-3.408619	-0.889400	-0.574795
79	1	0	-3.326360	-0.971627	0.525315
80	1	0	-4.299700	-0.274074	-0.787166
81	8	0	-2.255892	-0.395714	-1.160193
82	1	0	-1.111682	-1.362698	-0.073443

Structure 23 – Solvent: Acetonitrile



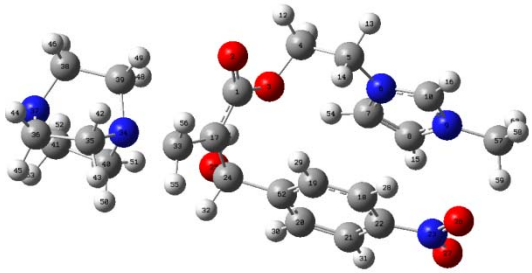
Zero-point correction= 0.707344
Thermal correction to Energy= 0.746248
Thermal correction to Enthalpy= 0.747192
Thermal correction to Gibbs Free Energy= 0.631713
Sum of electronic and zero-point Energies= -1924.856246
Sum of electronic and thermal Energies= -1924.817342
Sum of electronic and thermal Enthalpies= -1924.816397
Sum of electronic and thermal Free Energies= -1924.931877

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.784656	1.693498	-0.747608
2	8	0	1.210571	2.738064	-1.244745
3	8	0	1.172342	0.466857	-1.324199
4	6	0	2.411304	0.461664	-2.005265
5	6	0	3.539271	0.750422	-1.008805
6	7	0	4.833325	0.285734	-1.510895
7	6	0	5.567961	0.852303	-2.529549
8	6	0	6.684300	0.093255	-2.680698
9	7	0	6.609697	-0.920481	-1.751902

10	6	0	5.482599	-0.786303	-1.062401
11	1	0	2.526290	-0.542388	-2.414716
12	1	0	2.413134	1.192441	-2.816251
13	1	0	3.610728	1.816279	-0.797267
14	1	0	3.343756	0.217151	-0.077783
15	1	0	7.518442	0.187460	-3.354036
16	1	0	5.160130	-1.437860	-0.263306
17	6	0	-0.065528	1.492737	0.341756
18	6	0	2.789226	-2.201085	1.203982
19	6	0	1.533814	-1.731754	0.837600
20	6	0	1.043112	-0.531260	1.352566
21	6	0	1.798744	0.156211	2.308720
22	6	0	3.034679	-0.313806	2.720251
23	6	0	3.520463	-1.475739	2.132802
24	7	0	4.863868	-1.939352	2.489929
25	6	0	-0.266951	0.097156	0.874312
26	8	0	-0.921706	-0.780831	-0.060760
27	8	0	5.448699	-2.644341	1.683650
28	8	0	5.327278	-1.590615	3.551162
29	1	0	3.194048	-3.113599	0.785646
30	1	0	0.946867	-2.297810	0.127053
31	1	0	1.425727	1.089340	2.715028
32	1	0	3.628883	0.214121	3.453666
33	1	0	-0.936327	0.138164	1.738904
34	1	0	-2.314175	0.051741	-0.922135
35	6	0	-0.493177	2.688177	1.084378
36	7	0	-1.881476	3.273755	0.700729
37	6	0	-2.066086	4.606070	1.360196
38	6	0	-3.533919	5.053489	1.146960
39	7	0	-4.163108	4.257146	0.090314
40	6	0	-3.280466	4.254748	-1.080260
41	6	0	-1.989888	3.455200	-0.787043
42	6	0	-2.980124	2.365087	1.158753
43	6	0	-4.310788	2.877444	0.562647
44	1	0	-1.351437	5.287210	0.896896
45	1	0	-1.812835	4.491260	2.414407
46	1	0	-3.562069	6.108131	0.872338
47	1	0	-4.110957	4.925490	2.064027
48	1	0	-3.047751	5.289792	-1.335599
49	1	0	-3.804377	3.805710	-1.924747
50	1	0	-2.020222	2.454678	-1.214307
51	1	0	-1.080220	3.954833	-1.119575
52	1	0	-2.970943	2.386245	2.249550
53	1	0	-2.735918	1.363973	0.810716
54	1	0	-4.600052	2.254745	-0.285759
55	1	0	-5.098199	2.830808	1.315545
56	1	0	5.242078	1.740265	-3.043244
57	1	0	-0.584249	2.526116	2.161956
58	1	0	0.188398	3.521783	0.901742
59	6	0	7.604620	-1.974379	-1.544125
60	1	0	7.619623	-2.630339	-2.411730
61	1	0	8.579503	-1.514290	-1.400742
62	1	0	7.326601	-2.534621	-0.654497
63	6	0	-4.637255	-3.647313	0.522055
64	6	0	-5.747432	-4.412161	0.680572
65	6	0	-5.908968	-3.378038	-1.254131
66	7	0	-4.756094	-3.014546	-0.696131
67	1	0	-3.778981	-3.502952	1.155539
68	1	0	-6.048518	-5.068234	1.478535
69	1	0	-6.276225	-3.040625	-2.209903
70	7	0	-6.526248	-4.227360	-0.440067
71	6	0	-7.812655	-4.878601	-0.694888
72	1	0	-7.660731	-5.953969	-0.754942
73	1	0	-8.496405	-4.638003	0.115876
74	1	0	-8.208589	-4.506773	-1.635828
75	6	0	-3.811787	-2.041609	-1.251836
76	1	0	-2.807335	-2.351950	-0.963302
77	1	0	-3.893697	-2.068115	-2.337444
78	6	0	-4.101275	-0.634614	-0.728496
79	1	0	-4.054279	-0.637684	0.368367
80	1	0	-5.106170	-0.328524	-1.026230
81	8	0	-3.187673	0.279099	-1.288505
82	1	0	-0.350084	-0.774951	-0.843797

Structure 24 – Solvent: Acetonitrile

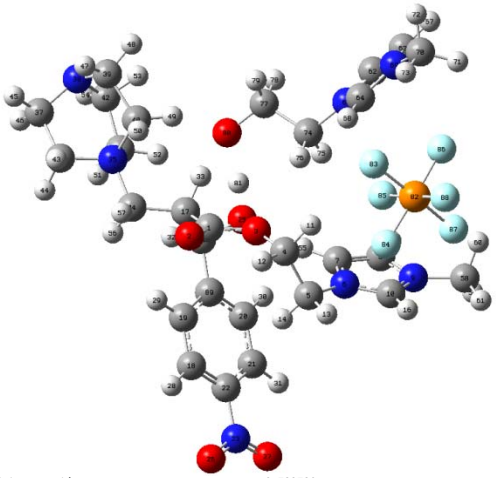


Zero-point correction= 0.528477
Thermal correction to Energy= 0.556508
Thermal correction to Enthalpy= 0.557453
Thermal correction to Gibbs Free Energy= 0.469584
Sum of electronic and zero-point Energies= -1505.268679
Sum of electronic and thermal Energies= -1505.240648
Sum of electronic and thermal Enthalpies= -1505.239704
Sum of electronic and thermal Free Energies= -1505.327573

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.195564	1.253245	-0.356818
2	8	0	1.612352	2.216908	-1.004817
3	8	0	0.155917	1.467089	0.580308
4	6	0	-0.501500	2.718271	0.486521
5	6	0	-1.683596	2.638612	-0.461737
6	7	0	-2.818742	1.897896	0.124869
7	6	0	-2.807314	1.121470	1.261915
8	6	0	-4.075510	0.666856	1.443796
9	7	0	-4.834808	1.161784	0.407618
10	6	0	-4.052393	1.899671	-0.375982
11	1	0	-0.818818	3.000008	1.491416
12	1	0	0.187321	3.470514	0.106685
13	1	0	-2.043305	3.638840	-0.701864
14	1	0	-1.382820	2.133205	-1.381393
15	1	0	-4.496382	0.028949	2.202473
16	1	0	-4.369638	2.428819	-1.260109
17	6	0	1.616952	-0.074939	-0.378083
18	6	0	-2.473510	-1.023928	-1.381645
19	6	0	-1.122636	-0.856549	-1.109884
20	6	0	-1.367348	-2.071817	0.954945
21	6	0	-2.714050	-2.264415	0.697552
22	6	0	-3.249073	-1.708616	-0.458089
23	7	0	-4.699085	-1.763069	-0.660884
24	6	0	0.916305	-1.134650	0.413939
25	8	0	1.044025	-0.983953	1.839166
26	8	0	-5.159235	-1.265248	-1.669248
27	8	0	-5.379993	-2.262572	0.215082
28	1	0	-2.925274	-0.615444	-2.275861
29	1	0	-0.495199	-0.318987	-1.810141
30	1	0	-0.931852	-2.460129	1.866460
31	1	0	-3.352362	-2.800396	1.386481
32	1	0	1.405577	-2.092715	0.202072
33	6	0	2.764486	-0.405338	-1.230693
34	7	0	4.159418	-0.304032	-0.532408
35	6	0	5.243885	-0.606054	-1.520950
36	6	0	6.588626	-0.704845	-0.759189
37	7	0	6.458162	-0.138132	0.584672
38	6	0	5.847535	1.189561	0.474465
39	6	0	4.377099	1.079233	0.009137
40	6	0	4.254957	-1.276946	0.603907
41	6	0	5.571005	-0.998493	1.371415
42	1	0	5.237387	0.205379	-2.249616
43	1	0	4.981751	-1.535831	-2.025715
44	1	0	7.364224	-0.167405	-1.305294
45	1	0	6.899956	-1.746191	-0.664067
46	1	0	6.432530	1.775837	-0.236059
47	1	0	5.893481	1.688883	1.442852
48	1	0	3.665254	1.201190	0.824922
49	1	0	4.118070	1.784103	-0.779393
50	1	0	4.233094	-2.275484	0.163233
51	1	0	3.371410	-1.136700	1.227214
52	1	0	5.362192	-0.498260	2.318326
53	1	0	6.079040	-1.938319	1.589054
54	1	0	-1.904067	0.932329	1.815684
55	1	0	2.747749	-1.434680	-1.597926
56	1	0	2.860631	0.281559	-2.073988
57	6	0	-6.278297	0.968922	0.238265
58	1	0	-6.563024	1.333558	-0.744801
59	1	0	-6.504082	-0.093209	0.314921
60	1	0	-6.803544	1.524191	1.012621
61	1	0	0.779993	-0.073195	2.018443
62	6	0	-0.562594	-1.342472	0.072610

Structure 25 – Gas Phase



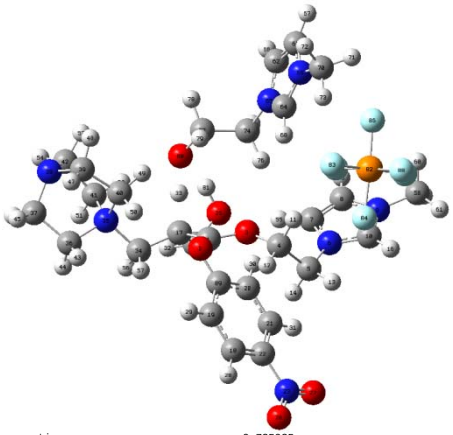
Zero-point correction= 0.728726
Thermal correction to Energy= 0.773901
Thermal correction to Enthalpy= 0.774846
Thermal correction to Gibbs Free Energy= 0.648026
Sum of electronic and zero-point Energies= -2865.516558
Sum of electronic and thermal Energies= -2865.471383
Sum of electronic and thermal Enthalpies= -2865.470438
Sum of electronic and thermal Free Energies= -2865.597258

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.678729	0.354822	-1.408405
2	8	0	-1.949045	0.511373	-2.567535
3	8	0	-0.444743	0.485113	-0.894643
4	6	0	0.589940	1.025333	-1.730874
5	6	0	1.087310	2.311861	-1.098819
6	7	0	1.810575	2.077859	0.155611
7	6	0	1.312743	1.473811	1.292601
8	6	0	2.336896	1.429584	2.182921
9	7	0	3.436296	1.996579	1.576086
10	6	0	3.094145	2.367899	0.350448
11	1	0	1.385846	0.287789	-1.797274
12	1	0	0.188261	1.233786	-2.722020
13	1	0	1.780645	2.801660	-1.782147
14	1	0	0.248895	2.982130	-0.889474
15	1	0	2.382183	1.044046	3.186571
16	1	0	3.762355	2.780949	-0.386525
17	6	0	-2.644195	-0.049213	-0.321676
18	6	0	-2.495235	4.285953	-0.662992
19	6	0	-2.753611	2.939187	-0.440319
20	6	0	-1.562121	3.036881	1.650572
21	6	0	-1.287436	4.380973	1.440647
22	6	0	-1.753394	4.978241	0.279691
23	7	0	-1.450200	6.406768	0.039707
24	6	0	-2.542375	0.822961	0.972654
25	8	0	-1.574987	0.318634	1.840214
26	8	0	-1.916933	6.911928	-0.954743
27	8	0	-0.750345	6.966763	0.852332
28	1	0	-2.848315	4.798674	-1.547542
29	1	0	-3.316215	2.395758	-1.191209
30	1	0	-1.217481	2.540253	2.548053
31	1	0	-0.728082	4.969583	2.155219
32	1	0	-3.536925	0.764915	1.447882
33	1	0	-2.267899	-1.019644	0.035812
34	6	0	-4.057867	-0.216123	-0.862360
35	7	0	-4.665898	-1.558176	-0.535342
36	6	0	-6.019641	-1.640068	-1.190699
37	6	0	-6.737175	-2.914363	-0.668315
38	7	0	-5.773189	-3.815769	-0.047050
39	6	0	-4.648332	-3.998630	-0.961988
40	6	0	-3.809930	-2.699744	-1.046723
41	6	0	-4.843298	-1.746772	0.954979
42	6	0	-5.284839	-3.210345	1.192052
43	1	0	-5.840050	-1.677811	-2.266756
44	1	0	-6.560382	-0.729485	-0.952535
45	1	0	-7.238540	-3.422847	-1.492477
46	1	0	-7.494313	-2.652819	0.072670
47	1	0	-5.041274	-4.285188	-1.939406
48	1	0	-4.017271	-4.812229	-0.603185
49	1	0	-2.946975	-2.748131	-0.379837
50	1	0	-3.501709	-2.445989	-2.062720
51	1	0	-5.591368	-1.015568	1.269057
52	1	0	-3.882247	-1.566040	1.436873
53	1	0	-4.430353	-3.786677	1.550990
54	1	0	-6.067925	-3.249501	1.949945
55	1	0	0.295440	1.109805	1.362876
56	1	0	-4.743526	0.526285	-0.446101
57	1	0	-4.068843	-0.128469	-1.950613
58	6	0	4.784986	2.057679	2.135706
59	1	0	4.740714	2.519473	3.120500
60	1	0	5.189765	1.049181	2.188923
61	1	0	5.410179	2.651609	1.473988
62	6	0	2.240801	-3.817432	2.214433
63	6	0	3.282565	-4.493302	1.663178
64	6	0	2.417792	-3.194485	0.115592
65	7	0	1.719077	-3.007179	1.229836
66	1	0	1.831057	-3.838369	3.209413
67	1	0	3.963527	-5.212287	2.085184
68	1	0	2.272039	-2.674135	-0.817594
69	7	0	3.369923	-4.991935	0.349093
70	6	0	4.387598	-4.508183	-0.617670
71	1	0	5.366544	-4.205020	-0.253207
72	1	0	4.333239	-5.587091	-0.752971
73	1	0	4.194564	-3.993254	-1.555631
74	6	0	0.540120	-2.141750	1.358985
75	1	0	0.677412	-1.509857	2.238891
76	1	0	0.509814	-1.493143	0.480860
77	6	0	-0.756402	-2.968879	1.475289
78	1	0	-0.675637	-3.588878	2.388016
79	1	0	-0.747182	-3.682566	0.625947
80	8	0	-1.857610	-2.157089	1.475111
81	1	0	-1.652661	-0.714077	1.833522
82	15	0	4.277097	-0.459142	-1.205441
83	9	0	3.352758	-1.446951	-2.124747
84	9	0	3.594792	0.837781	-1.922112
85	9	0	3.043742	-0.440536	-0.104856
86	9	0	4.887922	-1.750717	-0.440592
87	9	0	5.122674	0.530598	-0.238110

88	9	0	5.442801	-0.488399	-2.283177
89	6	0	-2.276976	2.297361	0.706174

Structure 26 – Gas Phase

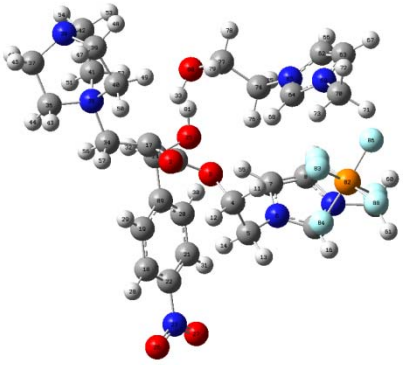


Zero-point correction= 0.725035
Thermal correction to Energy= 0.769984
Thermal correction to Enthalpy= 0.770928
Thermal correction to Gibbs Free Energy= 0.645479
Sum of electronic and zero-point Energies= -2865.513455
Sum of electronic and thermal Energies= -2865.468507
Sum of electronic and thermal Enthalpies= -2865.467563
Sum of electronic and thermal Free Energies= -2865.593012

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.657755	0.181343	-0.988416
2	8	0	-1.865580	-0.066321	-2.153778
3	8	0	-0.421314	0.493775	-0.522517
4	6	0	0.584375	0.851792	-1.476626
5	6	0	1.229010	2.141339	-1.001249
6	7	0	1.994975	1.961759	0.238552
7	6	0	1.512303	1.497714	1.446087
8	6	0	2.579170	1.419493	2.282480
9	7	0	3.687190	1.834968	1.576697
10	6	0	3.306965	2.148568	0.345943
11	1	0	1.318495	0.051606	-1.547593
12	1	0	0.125621	1.010546	-2.452696
13	1	0	1.928326	2.494402	-1.758692
14	1	0	0.465383	2.902260	-0.823342
15	1	0	2.647537	1.109021	3.310535
16	1	0	3.963832	2.448173	-0.452838
17	6	0	-2.652860	0.144062	0.099967
18	6	0	-2.031012	4.334234	-0.861598
19	6	0	-2.412405	3.063188	-0.452089
20	6	0	-1.251572	3.363119	1.634203
21	6	0	-0.850895	4.632050	1.237391
22	6	0	-1.242493	5.091172	-0.010273
23	7	0	-0.801495	6.433201	-0.449244
24	6	0	-2.426123	1.160506	1.241361
25	8	0	-1.470764	0.718153	2.188833
26	8	0	-1.184129	6.815299	-1.531055
27	8	0	-0.081437	7.051470	0.301010
28	1	0	-2.322647	4.737864	-1.821745
29	1	0	-3.006639	2.462468	-1.131300
30	1	0	-0.961020	2.981969	2.604430
31	1	0	-0.248568	5.266621	1.873682
32	1	0	-3.395122	1.266895	1.754149
33	1	0	-2.342001	-0.962422	0.745569
34	6	0	-4.058495	0.151430	-0.453629
35	7	0	-4.800902	-1.176085	-0.383952
36	6	0	-6.105591	-1.042476	-1.119436
37	6	0	-6.948743	-2.315434	-0.856006
38	7	0	-6.101979	-3.377731	-0.322212
39	6	0	-4.925281	-3.513299	-1.189775
40	6	0	-4.002480	-2.280582	-1.031957
41	6	0	-5.097785	-1.567803	1.040479
42	6	0	-5.667724	-3.007094	1.024512
43	1	0	-5.854910	-0.917919	-2.174242
44	1	0	-6.591738	-0.132903	-0.764658
45	1	0	-7.415116	-2.651434	-1.782687
46	1	0	-7.743633	-2.113112	-0.136301
47	1	0	-5.264674	-3.628918	-2.211664
48	1	0	-4.380253	-4.417126	-0.906624
49	1	0	-3.169543	-2.475645	-0.359252
50	1	0	-3.619750	-1.894020	-1.977229
51	1	0	-5.815157	-0.835026	1.416061
52	1	0	-4.165715	-1.513665	1.601814
53	1	0	-4.902059	-3.714498	1.348358
54	1	0	-6.510071	-3.085342	1.712749
55	1	0	0.469986	1.253650	1.599527
56	1	0	-4.702595	0.852048	0.084569
57	1	0	-4.066942	0.408130	-1.515868
58	6	0	5.066398	1.820935	2.060005
59	1	0	5.122861	2.375588	2.994904
60	1	0	5.382951	0.788321	2.191956
61	1	0	5.701509	2.286725	1.310027
62	6	0	1.941193	-4.079078	2.081892
63	6	0	2.834956	-4.809960	1.366584
64	6	0	1.975414	-3.292645	0.030493
65	7	0	1.421802	-3.130186	1.228405
66	1	0	1.637778	-4.142824	3.112679
67	1	0	3.468939	-5.630872	1.653874
68	1	0	1.795148	-2.678340	-0.836060
69	7	0	2.834564	-4.303680	0.086295
70	6	0	3.694712	-4.743669	-1.015256
71	1	0	4.731400	-4.685101	-0.691781
72	1	0	3.427158	-5.761124	-1.296005
73	1	0	3.553277	-4.059702	-1.848523
74	6	0	0.370866	-2.154908	1.540616
75	1	0	0.441548	-1.919019	2.603461
76	1	0	0.571357	-1.248272	0.965593
77	6	0	-1.018653	-2.728535	1.219034
78	1	0	-1.105820	-3.704917	1.720359
79	1	0	-1.035422	-2.933155	0.129696
80	8	0	-2.026182	-1.872998	1.614176
81	1	0	-1.617726	-0.239326	2.317509
82	15	0	4.202002	-0.817372	-1.137116
83	9	0	3.179547	-1.710173	-2.055543
84	9	0	3.623167	0.534000	-1.844014
85	9	0	2.992211	-0.692028	-0.015584
86	9	0	4.697113	-2.165899	-0.390346
87	9	0	5.144810	0.087636	-0.180441
88	9	0	5.345418	-0.946246	-2.231370
89	6	0	-2.017203	2.556639	0.788592

Structure 27 – Gas Phase

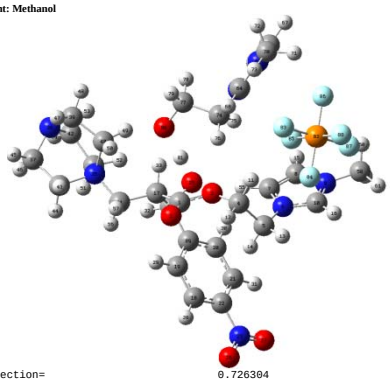


Zero-point correction= 0.728525
Thermal correction to Energy= 0.774462
Thermal correction to Enthalpy= 0.775406
Thermal correction to Gibbs Free Energy= 0.646341
Sum of electronic and zero-point Energies= -2865.519002
Sum of electronic and thermal Energies= -2865.473065
Sum of electronic and thermal Enthalpies= -2865.472121
Sum of electronic and thermal Free Energies= -2865.601186

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.624604	0.928135	-0.874928
2	8	0	-1.677390	-0.556145	-1.947249
3	8	0	-0.415449	0.498228	-0.398778
4	6	0	0.608337	0.759390	-1.356206
5	6	0	1.297344	2.042437	-0.926173
6	7	0	2.005374	1.889601	0.353199
7	6	0	1.456780	1.495810	1.558105
8	6	0	2.485392	1.414902	2.441400
9	7	0	3.636090	1.759738	1.766311
10	6	0	3.317177	2.035661	0.508958
11	1	0	1.319816	-0.065331	-1.394887
12	1	0	0.169388	0.895720	-2.345689
13	1	0	2.041028	2.327222	-1.669425
14	1	0	0.563262	2.842087	-0.812031
15	1	0	2.499680	1.153459	3.485346
16	1	0	4.017047	2.277400	-0.272653
17	6	0	-2.695754	0.284538	0.033720
18	6	0	-1.797357	4.355249	-1.121666
19	6	0	-2.257969	3.125650	-0.670859
20	6	0	-1.241084	3.506850	1.475945
21	6	0	-0.756305	4.732470	1.037203
22	6	0	-1.039814	5.131945	-0.258882
23	7	0	-0.512470	6.427268	-0.739046
24	6	0	-2.504008	1.332680	1.115767
25	8	0	-1.635257	0.939003	2.183609
26	8	0	-0.821980	6.771902	-1.856525
27	8	0	0.198893	7.050118	0.016315
28	1	0	-2.002307	4.713080	-2.121621
29	1	0	-2.823404	2.498225	-1.350131
30	1	0	-1.037848	3.176931	2.486121
31	1	0	-0.171644	5.379018	1.677832
32	1	0	-3.496411	1.535299	1.547368
33	1	0	-2.173416	-1.256103	1.082565
34	6	0	-4.035717	0.213971	-0.598784
35	7	0	-4.868657	-1.075229	-0.378142
36	6	0	-6.159391	-0.967088	-1.136542
37	6	0	-7.065357	-2.158456	-0.731155
38	7	0	-6.273631	-3.189269	-0.063573
39	6	0	-5.101508	-3.481954	-0.887515
40	6	0	-4.125361	-2.280652	-0.886136
41	6	0	-5.193415	-1.275044	1.072103
42	6	0	-5.825542	-2.679135	1.231666
43	1	0	-5.900623	-0.978815	-2.196672
44	1	0	-6.604480	-0.000409	-0.897551
45	1	0	-7.543642	-2.582716	-1.614422
46	1	0	-7.852597	-1.831535	-0.049739
47	1	0	-5.441852	-3.708371	-1.899601
48	1	0	-4.601703	-4.370286	-0.499199
49	1	0	-3.295135	-2.428344	-0.199763
50	1	0	-3.719805	-2.027246	-1.865683
51	1	0	-5.878940	-0.471228	1.349551
52	1	0	-4.267916	-1.173628	1.635854
53	1	0	-5.093840	-3.377173	1.642558
54	1	0	-6.671372	-2.635581	1.918615
55	1	0	0.398887	1.307056	1.676419
56	1	0	-4.701061	1.003036	-0.234532
57	1	0	-3.973389	0.271799	-1.690272
58	6	0	4.994444	1.706792	2.302287
59	1	0	5.037738	2.282943	3.224821
60	1	0	5.266072	0.666715	2.471963
61	1	0	5.674961	2.128365	1.567033
62	6	0	2.200183	-3.921390	1.753919
63	6	0	2.990734	-4.630204	0.908645
64	6	0	1.701082	-3.332063	-0.304001
65	7	0	1.401161	-3.115635	0.973657
66	1	0	2.143063	-3.911360	2.828383
67	1	0	3.770512	-5.346412	1.101057
68	1	0	1.271237	-2.807446	-1.141961
69	7	0	2.654142	-4.252582	-0.370680
70	6	0	3.354028	-4.671057	-1.587032
71	1	0	4.375451	-4.298439	-1.534635
72	1	0	3.328940	-5.756944	-1.656576
73	1	0	2.858290	-4.220964	-2.442452
74	6	0	0.380299	-2.173751	1.436264
75	1	0	0.612973	-1.906245	2.467144
76	1	0	0.442177	-1.270419	0.824944
77	6	0	-1.004003	-2.820092	1.343566
78	1	0	-1.035511	-3.710780	1.975465
79	1	0	-1.172834	-3.137957	0.304636
80	8	0	-2.012022	-1.944163	1.779539
81	1	0	-1.902923	0.068181	2.496603
82	15	0	4.200137	-0.946881	-0.937925
83	9	0	3.209451	-1.795797	-1.923513
84	9	0	3.695981	0.426293	-1.658101
85	9	0	2.943125	-0.801445	0.126684
86	9	0	4.623054	-2.319077	-0.187065
87	9	0	5.117542	-0.078217	0.076751
88	9	0	5.399475	-1.094856	-1.971615
89	6	0	-1.977936	2.681003	0.623408

Structure 25 – Solvent: Methanol

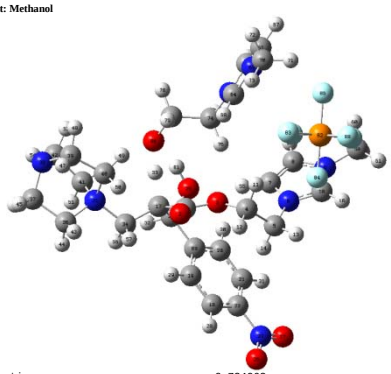


Zero-point correction=	0.726304
Thermal correction to Energy=	0.771480
Thermal correction to Enthalpy=	0.772424
Thermal correction to Gibbs Free Energy=	0.644734
Sum of electronic and zero-point Energies=	-2865.608771
Sum of electronic and thermal Energies=	-2865.563595
Sum of electronic and thermal Enthalpies=	-2865.562651
Sum of electronic and thermal Free Energies=	-2865.690340

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.567738	0.349601	-1.404916
2	8	0	-1.785708	0.514853	-2.575121
3	8	0	-0.353606	0.454135	-0.844410
4	6	0	0.742193	0.933337	-1.638915
5	6	0	1.269800	2.207085	-1.007994
6	7	0	1.927910	1.953787	0.277012
7	6	0	1.362892	1.359766	1.388615
8	6	0	2.345216	1.275771	2.322188
9	7	0	3.485543	1.813337	1.766693
10	6	0	3.209012	2.208527	0.531851
11	1	0	1.504308	0.156645	-1.647728
12	1	0	0.400773	1.138889	-2.651919
13	1	0	2.011092	2.655951	-1.667545
14	1	0	0.455860	2.918387	-0.848805
15	1	0	2.335691	0.882441	3.323947
16	1	0	3.912039	2.639095	-0.160819
17	6	0	-2.589088	-0.008349	-0.348744
18	6	0	-2.319636	4.315180	-0.879058
19	6	0	-2.637657	2.993942	-0.598296
20	6	0	-1.428910	3.125214	1.481324
21	6	0	-1.098255	4.446600	1.217277
22	6	0	-1.546616	5.015749	0.034391
23	7	0	-1.196090	6.414952	-0.259139
24	6	0	-2.527974	0.933375	0.907811
25	8	0	-1.645990	0.441458	1.861986
26	8	0	-1.609484	6.898501	-1.291830
27	8	0	-0.513064	7.009550	0.547821
28	1	0	-2.656628	4.795544	-1.786813
29	1	0	-3.235462	2.448629	-1.319120
30	1	0	-1.094555	2.653351	2.395051
31	1	0	-0.505376	5.029934	1.908077
32	1	0	-3.556445	0.953676	1.305287
33	1	0	-2.257169	-0.965938	0.063197
34	6	0	-3.981058	-0.170587	-0.955912
35	7	0	-4.689937	-1.427256	-0.522545
36	6	0	-5.999515	-1.510487	-1.269790
37	6	0	-6.841000	-2.652507	-0.658556
38	7	0	-5.988020	-3.542546	0.129241
39	6	0	-4.816289	-3.893166	-0.676053
40	6	0	-3.881583	-2.670852	-0.825442
41	6	0	-4.981495	-1.429399	0.958890
42	6	0	-5.543308	-2.823411	1.325592
43	1	0	-5.745742	-1.690149	-2.314950
44	1	0	-6.488895	-0.541189	-1.182781
45	1	0	-7.325044	-3.215906	-1.456327
46	1	0	-7.617097	-2.251416	-0.005615
47	1	0	-5.159330	-4.247907	-1.648882
48	1	0	-4.269659	-4.702922	-0.192274
49	1	0	-3.084801	-2.702808	-0.082024
50	1	0	-3.468283	-2.565189	-1.828631
51	1	0	-5.690679	-0.620219	1.138276
52	1	0	-4.041550	-1.256967	1.481253
53	1	0	-4.764884	-3.410992	1.815260
54	1	0	-6.378828	-2.713713	2.016934
55	1	0	0.328633	1.041166	1.417778
56	1	0	-4.643002	0.651391	-0.676234
57	1	0	-3.925367	-0.210698	-2.044098
58	6	0	4.801170	1.858183	2.401332
59	1	0	4.702955	2.311944	3.385018
60	1	0	5.188761	0.844962	2.481140
61	1	0	5.465311	2.454789	1.781891
62	6	0	2.285800	-3.523259	1.965544
63	6	0	3.163504	-4.248925	1.224882
64	6	0	1.827047	-3.183974	-0.155430
65	7	0	1.461677	-2.864735	1.081533
66	1	0	2.177252	-3.413620	3.030825
67	1	0	3.976528	-4.890898	1.515631
68	1	0	1.383110	-2.799538	-1.058634
69	7	0	2.852944	-4.025529	-0.097220
70	6	0	3.573074	-4.576770	-1.243615
71	1	0	4.602399	-4.227832	-1.205432
72	1	0	3.528566	-5.663063	-1.202971
73	1	0	3.100920	-4.214495	-2.152422
74	6	0	0.334999	-1.993904	1.424983
75	1	0	0.613509	-1.423208	2.318131
76	1	0	0.199397	-1.292563	0.600478
77	6	0	-0.950438	-2.803108	1.673416
78	1	0	-0.757139	-3.475180	2.529019
79	1	0	-1.078946	-3.464103	0.792589
80	8	0	-2.033764	-1.976985	1.873369
81	1	0	-1.785627	-0.626539	1.941585
82	15	0	4.386929	-0.719616	-1.014811
83	9	0	3.469491	-1.638920	-1.995736
84	9	0	3.807978	0.619489	-1.744413
85	9	0	3.152735	-0.656936	0.047197
86	9	0	4.945833	-2.050169	-0.278218
87	9	0	5.277960	0.210902	-0.028237
88	9	0	5.599180	-0.779974	-2.077474
89	6	0	-2.184877	2.379509	0.573680

Structure 26 – Solvent: Methanol

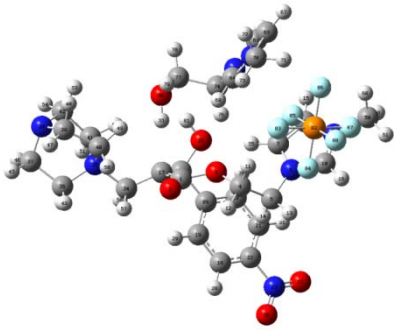


Zero-point correction=	0.724962
Thermal correction to Energy=	0.770080
Thermal correction to Enthalpy=	0.771024
Thermal correction to Gibbs Free Energy=	0.645043
Sum of electronic and zero-point Energies=	-2865.600678
Sum of electronic and thermal Energies=	-2865.555559
Sum of electronic and thermal Enthalpies=	-2865.554615
Sum of electronic and thermal Free Energies=	-2865.680596

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.635580	0.112943	-0.972680
2	8	0	-1.759934	-0.250553	-2.122440
3	8	0	-0.452761	0.561246	-0.487148
4	6	0	0.603845	0.841285	-1.408884
5	6	0	1.284059	2.108668	-0.928688
6	7	0	2.010794	1.897658	0.328130
7	6	0	1.486959	1.422990	1.515670
8	6	0	2.529419	1.305863	2.378190
9	7	0	3.662183	1.714077	1.708721
10	6	0	3.322314	2.061625	0.475322
11	1	0	1.381378	0.003109	-1.431164
12	1	0	0.192382	1.001525	-2.405149
13	1	0	2.010592	2.440885	-1.668354
14	1	0	0.541525	2.893999	-0.773208
15	1	0	2.565030	0.974823	3.401701
16	1	0	4.002102	2.386946	-0.293322
17	6	0	-2.674444	0.097834	0.071344
18	6	0	-2.125549	4.286824	-0.979272
19	6	0	-2.503785	3.025887	-0.542736
20	6	0	-1.322455	3.364436	1.527706
21	6	0	-0.929051	4.627325	1.107182
22	6	0	-1.334717	5.064086	-0.145197
23	7	0	-0.914351	6.396385	-0.604430
24	6	0	-2.511329	1.158397	1.184710
25	8	0	-1.595091	0.763382	2.193258
26	8	0	-1.280633	6.760586	-1.702353
27	8	0	-0.222698	7.061031	0.138350
28	1	0	-2.426448	4.661988	-1.947317
29	1	0	-3.108435	2.413804	-1.201997
30	1	0	-1.013179	3.001318	2.498318
31	1	0	-0.317845	5.264550	1.731418
32	1	0	-3.505227	1.270948	1.643565
33	1	0	-2.373277	-0.977066	0.784449
34	6	0	-4.060915	0.051344	-0.535375
35	7	0	-4.807299	-1.263364	-0.389080
36	6	0	-6.090364	-1.175735	-1.171609
37	6	0	-6.951783	-2.416317	-0.836740
38	7	0	-6.130534	-3.449176	-0.203066
39	6	0	-4.928020	-3.649906	-1.016673
40	6	0	-4.000760	-2.416493	-0.928416
41	6	0	-5.152044	-1.545005	1.049463
42	6	0	-5.728968	-2.978485	1.125394
43	1	0	-5.809573	-1.135336	-2.224530
44	1	0	-6.579450	-0.241390	-0.898097
45	1	0	-7.394044	-2.812278	-1.750930
46	1	0	-7.760646	-2.150571	-0.154966
47	1	0	-5.237676	-3.839179	-2.047206
48	1	0	-4.393705	-4.532559	-0.664294
49	1	0	-3.188315	-2.571224	-0.221784
50	1	0	-3.594202	-2.108571	-1.891334
51	1	0	-5.875217	-0.784453	1.347358
52	1	0	-4.239086	-1.450857	1.634379
53	1	0	-4.979307	-3.666039	1.521061
54	1	0	-6.590554	-2.993463	1.793063
55	1	0	0.433706	1.213471	1.641749
56	1	0	-4.725194	0.792241	-0.084588
57	1	0	-4.029255	0.224625	-1.613002
58	6	0	5.023285	1.688355	2.239698
59	1	0	5.054732	2.257087	3.166432
60	1	0	5.313917	0.654113	2.412452
61	1	0	5.688850	2.132592	1.504977
62	6	0	2.388384	-3.377198	2.027473
63	6	0	3.223274	-4.131576	1.267144
64	6	0	1.696787	-3.266557	-0.054491
65	7	0	1.441457	-2.847416	1.181348
66	1	0	2.384845	-3.169904	3.083251
67	1	0	4.093148	-4.708585	1.528222
68	1	0	1.143411	-2.993013	-0.937766
69	7	0	2.767013	-4.051936	-0.028253
70	6	0	3.385387	-4.692751	-1.187550
71	1	0	4.398033	-4.311308	-1.291429
72	1	0	3.388325	-5.770291	-1.038045
73	1	0	2.807364	-4.437236	-2.071248
74	6	0	0.334061	-1.960655	1.550544
75	1	0	0.492151	-1.657270	2.585928
76	1	0	0.381314	-1.073415	0.917618
77	6	0	-1.020132	-2.667179	1.398774
78	1	0	-1.014015	-3.561389	2.037243
79	1	0	-1.094014	-3.027283	0.356118
80	8	0	-2.065001	-1.818147	1.731774
81	1	0	-1.704226	-0.205115	2.311850
82	15	0	4.301943	-0.869459	-1.115087
83	9	0	3.305264	-1.816404	-1.983268
84	9	0	3.636044	0.449470	-1.805026
85	9	0	3.179574	-0.799603	0.065893
86	9	0	4.953940	-2.177612	-0.417991
87	9	0	5.274938	0.089484	-0.236533
88	9	0	5.403840	-0.931356	-2.292399
89	6	0	-2.099106	2.543808	0.705310

Structure 27 – Solvent: Methanol

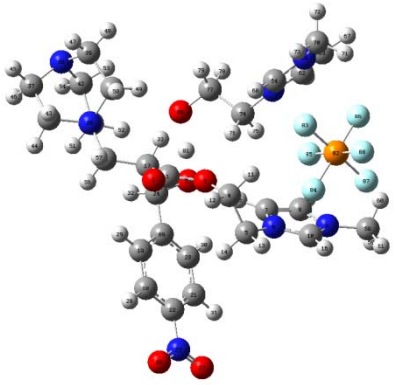


Zero-point correction= 0.728145
Thermal correction to Energy= 0.774181
Thermal correction to Enthalpy= 0.775126
Thermal correction to Gibbs Free Energy= 0.646420
Sum of electronic and zero-point Energies= -2865.608340
Sum of electronic and thermal Energies= -2865.562304
Sum of electronic and thermal Enthalpies= -2865.561360
Sum of electronic and thermal Free Energies= -2865.690065

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.741688	0.089164	-0.983676
2	8	0	-1.815594	-0.378918	-2.115551
3	8	0	-0.519460	0.509970	-0.490217
4	6	0	0.533610	0.756251	-1.413764
5	6	0	1.245239	2.014670	-0.951869
6	7	0	1.966576	1.798190	0.309183
7	6	0	1.440500	1.309101	1.489868
8	6	0	2.478213	1.198229	2.359210
9	7	0	3.610756	1.624357	1.700804
10	6	0	3.274573	1.976089	0.467027
11	1	0	1.225272	-0.089101	-1.433849
12	1	0	0.128725	0.911728	-2.413999
13	1	0	1.982695	2.321583	-1.691735
14	1	0	0.521787	2.818791	-0.803045
15	1	0	2.510480	0.860862	3.380850
16	1	0	3.956275	2.312955	-0.294997
17	6	0	-2.781288	0.263489	-0.030255
18	6	0	-1.914552	4.385120	-0.963631
19	6	0	-2.380398	3.143555	-0.558961
20	6	0	-1.212876	3.361011	1.534104
21	6	0	-0.726253	4.601563	1.143406
22	6	0	-1.083567	5.090336	-0.104199
23	7	0	-0.566772	6.399099	-0.529822
24	6	0	-2.561473	1.241572	1.112063
25	8	0	-1.686506	0.789225	2.152430
26	8	0	-0.888642	6.807990	-1.626279
27	8	0	0.154751	7.002910	0.236747
28	1	0	-2.176116	4.799724	-1.927103
29	1	0	-3.011015	2.576640	-1.233033
30	1	0	-0.944599	2.962966	2.502998
31	1	0	-0.081754	5.184192	1.787240
32	1	0	-3.547474	1.432312	1.560759
33	1	0	-2.252756	-1.389315	1.004295
34	6	0	-4.149274	0.198184	-0.609465
35	7	0	-4.942424	-1.115251	-0.431147
36	6	0	-6.246660	-1.000954	-1.168280
37	6	0	-7.124276	-2.221332	-0.797670
38	7	0	-6.305472	-3.271146	-0.186948
39	6	0	-5.137177	-3.501784	-1.041573
40	6	0	-4.186446	-2.282897	-1.001572
41	6	0	-5.249769	-1.379688	1.012873
42	6	0	-5.842195	-2.803622	1.122706
43	1	0	-6.004294	-0.969834	-2.230886
44	1	0	-6.705943	-0.055222	-0.882045
45	1	0	-7.607143	-2.612477	-1.693245
46	1	0	-7.902428	-1.933763	-0.089183
47	1	0	-5.487507	-3.685582	-2.058450
48	1	0	-4.607781	-4.391762	-0.700211
49	1	0	-3.336480	-2.452804	-0.345116
50	1	0	-3.815669	-1.983360	-1.980693
51	1	0	-5.955441	-0.608385	1.325295
52	1	0	-4.327004	-1.275718	1.579120
53	1	0	-5.086833	-3.501451	1.488757
54	1	0	-6.675024	-2.803252	1.826182
55	1	0	0.388293	1.091141	1.605310
56	1	0	-4.813612	0.951179	-0.176683
57	1	0	-4.133091	0.323601	-1.695981
58	6	0	4.968505	1.607200	2.239881
59	1	0	4.987256	2.161323	3.175787
60	1	0	5.271949	0.574240	2.398300
61	1	0	5.633000	2.071932	1.516998
62	6	0	2.385809	-3.309235	2.051702
63	6	0	3.262278	-4.064086	1.341072
64	6	0	1.725220	-3.328941	-0.045603
65	7	0	1.432158	-2.861451	1.165398
66	1	0	2.357302	-3.049341	3.095684
67	1	0	4.150756	-4.591240	1.641588
68	1	0	1.177406	-3.119505	-0.949780
69	7	0	2.824307	-4.066704	0.036394
70	6	0	3.476178	-4.753948	-1.077814
71	1	0	4.500870	-4.398708	-1.147290
72	1	0	3.447071	-5.826815	-0.899471
73	1	0	2.942593	-4.508375	-1.991558
74	6	0	0.281352	-2.013860	1.479420
75	1	0	0.457504	-1.566351	2.457421
76	1	0	0.225334	-1.212793	0.739394
77	6	0	-1.005722	-2.839390	1.480772
78	1	0	-0.957185	-3.596833	2.270101
79	1	0	-1.117813	-3.351501	0.523320
80	8	0	-2.119672	-2.015708	1.754538
81	1	0	-1.952282	-0.102326	2.408850
82	15	0	4.315330	-0.925192	-1.134203
83	9	0	3.340514	-1.907251	-1.987708
84	9	0	3.611651	0.368942	-1.830339
85	9	0	3.199777	-0.876095	0.053403
86	9	0	5.007808	-2.209322	-0.429031
87	9	0	5.269319	0.066063	-0.269812
88	9	0	5.412334	-0.969153	-2.317446
89	6	0	-2.027998	2.608615	0.683422

Structure 25 – Solvent: Acetonitrile

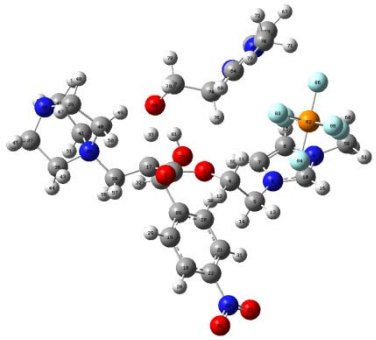


Zero-point correction= 0.726310
Thermal correction to Energy= 0.771476
Thermal correction to Enthalpy= 0.772420
Thermal correction to Gibbs Free Energy= 0.644800
Sum of electronic and zero-point Energies= -2865.609124
Sum of electronic and thermal Energies= -2865.563958
Sum of electronic and thermal Enthalpies= -2865.563014
Sum of electronic and thermal Free Energies= -2865.690634

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.567647	0.349387	-1.404650
2	8	0	-1.785815	0.515091	-2.574768
3	8	0	-0.353536	0.454304	-0.844206
4	6	0	0.742079	0.933751	-1.638746
5	6	0	1.269522	2.207558	-1.007793
6	7	0	1.927658	1.954234	0.277216
7	6	0	1.362737	1.360034	1.388766
8	6	0	2.345039	1.276269	2.322400
9	7	0	3.485249	1.814167	1.766996
10	6	0	3.208675	2.209354	0.532153
11	1	0	1.584325	0.157174	-1.647613
12	1	0	0.400575	1.139307	-2.651719
13	1	0	2.010786	2.656508	-1.667318
14	1	0	0.455541	2.918800	-0.848564
15	1	0	2.335539	0.883054	3.324206
16	1	0	3.911585	2.640140	-0.160497
17	6	0	-2.588791	-0.009200	-0.348517
18	6	0	-2.321612	4.314596	-0.878995
19	6	0	-2.638981	2.993233	-0.598062
20	6	0	-1.429124	3.124942	1.480880
21	6	0	-1.099152	4.446465	1.216683
22	6	0	-1.548431	5.015492	0.034064
23	7	0	-1.198828	6.414828	-0.259496
24	6	0	-2.527997	0.932752	0.907121
25	8	0	-1.645840	0.441341	1.862241
26	8	0	-1.612943	6.898289	-1.291973
27	8	0	-0.516489	7.010090	0.547591
28	1	0	-2.659370	4.794731	-1.786582
29	1	0	-3.237072	2.447738	-1.318501
30	1	0	-1.094033	2.653256	2.394416
31	1	0	-0.506057	5.029940	1.907178
32	1	0	-3.556475	0.952692	1.305390
33	1	0	-2.256562	-0.966600	0.063642
34	6	0	-3.980705	-0.171831	-0.955782
35	7	0	-4.689429	-1.428604	-0.522527
36	6	0	-5.998971	-1.511927	-1.269863
37	6	0	-6.840459	-2.653903	-0.658607
38	7	0	-5.987471	-3.544002	0.129205
39	6	0	-4.815667	-3.894490	-0.676123
40	6	0	-3.881035	-2.672120	-0.825494
41	6	0	-4.981003	-1.430807	0.958866
42	6	0	-5.542756	-2.824833	1.325553
43	1	0	-5.745092	-1.691681	-2.314967
44	1	0	-6.488345	-0.542620	-1.183031
45	1	0	-7.324469	-3.217310	-1.456398
46	1	0	-7.616521	-2.252778	-0.005644
47	1	0	-5.158667	-4.249125	-1.649009
48	1	0	-4.268990	-4.704255	-0.192412
49	1	0	-3.084081	-2.704010	-0.082294
50	1	0	-3.467844	-2.566494	-1.828713
51	1	0	-5.690286	-0.621743	1.138334
52	1	0	-4.041043	-1.258321	1.481208
53	1	0	-4.764386	-3.412488	1.815230
54	1	0	-6.378304	-2.715100	2.016864
55	1	0	0.328519	1.041267	1.417864
56	1	0	-4.642923	0.649942	-0.676186
57	1	0	-3.924863	-0.211875	-2.043966
58	6	0	4.800748	1.859626	2.401868
59	1	0	4.702118	2.313234	3.385574
60	1	0	5.188846	0.846603	2.481747
61	1	0	5.464670	2.456690	1.782630
62	6	0	2.286771	-3.522428	1.965410
63	6	0	3.164778	-4.247964	1.224997
64	6	0	1.827866	-3.183994	-0.155687
65	7	0	1.462390	-2.864472	1.081182
66	1	0	2.178270	-3.412406	3.030653
67	1	0	3.977902	-4.889741	1.515885
68	1	0	1.383719	-2.800203	-1.059074
69	7	0	2.854103	-4.025121	-0.097183
70	6	0	3.574085	-4.576752	-1.243466
71	1	0	4.603412	-4.227727	-1.205616
72	1	0	3.529869	-5.663047	-1.202290
73	1	0	3.101440	-4.215193	-2.152292
74	6	0	0.335468	-1.993938	1.424543
75	1	0	0.613968	-1.422885	2.311181
76	1	0	0.199455	-1.292873	0.599861
77	6	0	-0.949649	-2.803352	1.673571
78	1	0	-0.755876	-3.475438	2.529045
79	1	0	-1.078784	-3.464234	0.792822
80	8	0	-2.032892	-1.977154	1.874307
81	1	0	-1.784766	-0.626819	1.941988
82	15	0	4.387319	-0.718636	-1.014951
83	9	0	3.470151	-1.637751	-1.996272
84	9	0	3.808356	0.629603	-1.744273
85	9	0	3.153235	-0.656384	0.046944
86	9	0	4.946441	-2.049439	-0.278870
87	9	0	5.278339	0.211639	-0.028134
88	9	0	5.599746	-0.778533	-2.077691
89	6	0	-2.185373	2.378965	0.573680

Structure 26 – Solvent: Acetonitrile

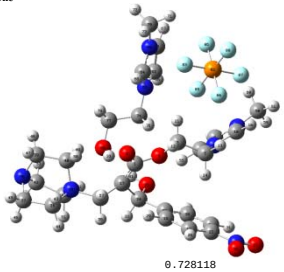


Zero-point correction=	0.724959
Thermal correction to Energy=	0.770078
Thermal correction to Enthalpy=	0.771022
Thermal correction to Gibbs Free Energy=	0.645039
Sum of electronic and zero-point Energies=	-2865.601010
Sum of electronic and thermal Energies=	-2865.555892
Sum of electronic and thermal Enthalpies=	-2865.554947
Sum of electronic and thermal Free Energies=	-2865.680930

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.635451	0.113144	-0.972258
2	8	0	-1.759488	-0.250699	-2.121960
3	8	0	-0.452836	0.561933	-0.486704
4	6	0	0.603853	0.841790	-1.408373
5	6	0	1.284496	2.108807	-0.927837
6	7	0	2.011180	1.897131	0.328889
7	6	0	1.487192	1.422277	1.516293
8	6	0	2.529628	1.304473	2.378753
9	7	0	3.662520	1.712516	1.709393
10	6	0	3.322752	2.060621	0.476120
11	1	0	1.301064	0.003345	-1.430887
12	1	0	0.192440	1.002467	-2.404590
13	1	0	2.011112	2.441054	-1.667401
14	1	0	0.542212	2.894322	-0.772111
15	1	0	2.565146	0.973054	3.402146
16	1	0	4.002616	2.386032	-0.292416
17	6	0	-2.674501	0.098145	0.071564
18	6	0	-2.125453	4.287135	-0.979286
19	6	0	-2.503931	3.026326	-0.542618
20	6	0	-1.322072	3.364649	1.527570
21	6	0	-0.928456	4.627432	1.106932
22	6	0	-1.334266	5.064248	-0.145388
23	7	0	-0.913692	6.396399	-0.604731
24	6	0	-2.511565	1.158874	1.184821
25	8	0	-1.595573	0.763930	2.193647
26	8	0	-1.279795	6.760571	-1.702743
27	8	0	-0.222052	7.061117	0.138020
28	1	0	-2.426468	4.662286	-1.947299
29	1	0	-3.108918	2.414386	-1.201698
30	1	0	-1.012626	3.001495	2.498112
31	1	0	-0.316927	5.264482	1.731029
32	1	0	-3.505557	1.271582	1.643415
33	1	0	-2.373622	-0.976719	0.785094
34	6	0	-4.060862	0.051564	-0.535447
35	7	0	-4.807209	-1.263197	-0.389423
36	6	0	-6.089885	-1.175713	-1.172610
37	6	0	-6.951433	-2.416236	-0.837926
38	7	0	-6.130428	-3.449085	-0.203851
39	6	0	-4.927531	-3.649772	-1.016934
40	6	0	-4.000366	-2.416331	-0.928267
41	6	0	-5.152692	-1.544719	1.048961
42	6	0	-5.729407	-2.978276	1.124756
43	1	0	-5.808560	-1.135521	-2.225390
44	1	0	-6.579128	-0.241328	-0.899530
45	1	0	-7.393365	-2.812253	-1.752253
46	1	0	-7.760504	-2.150388	-0.156445
47	1	0	-5.236726	-3.830032	-2.047604
48	1	0	-4.393325	-4.532398	-0.664321
49	1	0	-3.188264	-2.571004	-0.221239
50	1	0	-3.593361	-2.108483	-1.891414
51	1	0	-5.876181	-0.784282	1.346372
52	1	0	-4.240073	-1.450316	1.634361
53	1	0	-4.979779	-3.665717	1.520700
54	1	0	-6.591227	-2.993321	1.792124
55	1	0	0.433852	1.213173	1.642335
56	1	0	-4.725286	0.792365	-0.084738
57	1	0	-4.029015	0.224932	-1.613056
58	6	0	5.023614	1.686129	2.240351
59	1	0	5.055006	2.253676	3.167805
60	1	0	5.314249	0.651673	2.411861
61	1	0	5.689178	2.131383	1.506243
62	6	0	2.387786	-3.376009	2.027789
63	6	0	3.222521	-4.130554	1.267456
64	6	0	1.695543	-3.266103	-0.054021
65	7	0	1.440554	-2.846601	1.181770
66	1	0	2.384537	-3.168328	3.083496
67	1	0	4.092466	-4.707481	1.528482
68	1	0	1.141860	-2.992913	-0.937216
69	7	0	2.765858	-4.051369	-0.027838
70	6	0	3.383691	-4.692858	-1.187042
71	1	0	4.396532	-4.312014	-1.291182
72	1	0	3.386086	-5.778352	-1.037209
73	1	0	2.805637	-4.437318	-2.070709
74	6	0	0.333153	-1.959899	1.551076
75	1	0	0.491763	-1.655905	2.586202
76	1	0	0.379878	-1.073008	0.917634
77	6	0	-1.020972	-2.666760	1.400375
78	1	0	-1.014633	-3.560283	2.039789
79	1	0	-1.095151	-3.027955	0.358146
80	8	0	-2.065872	-1.817452	1.732787
81	1	0	-1.704836	-0.204558	2.312332
82	15	0	4.302169	-0.869878	-1.115817
83	9	0	3.305251	-1.816725	-1.983762
84	9	0	3.636020	0.449133	-1.805307
85	9	0	3.180448	-0.800269	0.065645
86	9	0	4.954701	-2.178114	-0.419355
87	9	0	5.275627	0.088951	-0.237619
88	9	0	5.403628	-0.931511	-2.293711
89	6	0	-2.099098	2.544184	0.705358

Structure 27 – Solvent: Acetonitrile

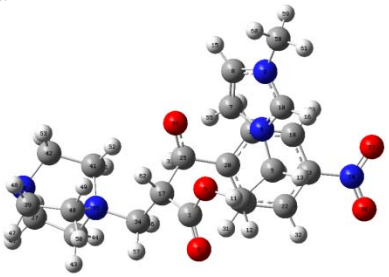


Zero-point correction=	0.728118
Thermal correction to Energy=	0.774165
Thermal correction to Enthalpy=	0.775109
Thermal correction to Gibbs Free Energy=	0.646331
Sum of electronic and zero-point Energies=	-2865.608707
Sum of electronic and thermal Energies=	-2865.562660
Sum of electronic and thermal Enthalpies=	-2865.561716
Sum of electronic and thermal Free Energies=	-2865.690494

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.742140	0.089629	-0.984031
2	8	0	-1.816003	-0.378090	-2.116096
3	8	0	-0.520035	0.510534	-0.490461
4	6	0	0.533376	0.756365	-1.413662
5	6	0	1.245343	2.014475	-0.951385
6	7	0	1.966560	1.797502	0.309653
7	6	0	1.440362	1.307909	1.490085
8	6	0	2.478003	1.196596	2.359458
9	7	0	3.610617	1.622993	1.701357
10	6	0	3.274556	1.975328	0.467710
11	1	0	1.224617	-0.089344	-1.433656
12	1	0	0.128863	0.912204	-2.413994
13	1	0	1.982858	2.321597	-1.691092
14	1	0	0.521982	2.818655	-0.802364
15	1	0	2.510131	0.858831	3.380974
16	1	0	3.956319	2.312843	-0.293979
17	6	0	-2.781669	0.263493	-0.030502
18	6	0	-1.915067	4.385344	-0.963002
19	6	0	-2.381071	3.143807	-0.558456
20	6	0	-1.212700	3.360444	1.534267
21	6	0	-0.725945	4.600987	1.143640
22	6	0	-1.083574	5.090170	-0.103723
23	7	0	-0.566647	6.398826	-0.529198
24	6	0	-2.561880	1.241360	1.112035
25	8	0	-1.686972	0.788835	2.152389
26	8	0	-0.888505	6.807914	-1.625625
27	8	0	0.154955	7.002523	0.237426
28	1	0	-2.176912	4.800189	-1.926291
29	1	0	-3.012114	2.577236	-1.232417
30	1	0	-0.944114	2.962117	2.502898
31	1	0	-0.081054	5.183255	1.787404
32	1	0	-3.547898	1.432043	1.560707
33	1	0	-2.252960	-1.389712	1.004125
34	6	0	-4.149724	0.198134	-0.609596
35	7	0	-4.942662	-1.115391	-0.431460
36	6	0	-6.246918	-1.001196	-1.168615
37	6	0	-7.124420	-2.221661	-0.798073
38	7	0	-6.305520	-3.271492	-0.187457
39	6	0	-5.137151	-3.501901	-1.042088
40	6	0	-4.186592	-2.282857	-1.002054
41	6	0	-5.250021	-1.380002	1.012526
42	6	0	-5.842232	-2.804016	1.122248
43	1	0	-6.004525	-0.970027	-2.231210
44	1	0	-6.706317	-0.055533	-0.882354
45	1	0	-7.607290	-2.612766	-1.693663
46	1	0	-7.902540	-1.934217	-0.089505
47	1	0	-5.487422	-3.685722	-2.058978
48	1	0	-4.607631	-4.391789	-0.700690
49	1	0	-3.336499	-2.452716	-0.345770
50	1	0	-3.816077	-1.983199	-1.981241
51	1	0	-5.955827	-0.608832	1.324964
52	1	0	-4.327309	-1.275937	1.578834
53	1	0	-5.086749	-3.501790	1.488151
54	1	0	-6.675026	-2.803824	1.825768
55	1	0	0.388092	1.090130	1.605445
56	1	0	-4.814109	0.950996	-0.176660
57	1	0	-4.133596	0.323786	-1.696082
58	6	0	4.968306	1.605577	2.240620
59	1	0	4.986493	2.157942	3.177575
60	1	0	5.272346	0.572530	2.397338
61	1	0	5.632647	2.072217	1.518831
62	6	0	2.386270	-3.306355	2.052665
63	6	0	3.263333	-4.061230	1.342813
64	6	0	1.725551	-3.328913	-0.044579
65	7	0	1.432162	-2.860377	1.165937
66	1	0	2.357635	-3.045198	3.096333
67	1	0	4.152212	-4.587412	1.643846
68	1	0	1.177571	-3.120941	-0.948998
69	7	0	2.825302	-4.065628	0.038162
70	6	0	3.477477	-4.753822	-1.075275
71	1	0	4.502475	-4.399348	-1.144113
72	1	0	3.447507	-5.826608	-0.896541
73	1	0	2.944745	-4.508262	-1.989509
74	6	0	0.280714	-2.013436	1.479348
75	1	0	0.456487	-1.565333	2.457135
76	1	0	0.224191	-1.212802	0.738893
77	6	0	-1.005962	-2.839562	1.487204
78	1	0	-0.957200	-3.596448	2.271044
79	1	0	-1.118031	-3.352265	0.524087
80	8	0	-2.120041	-2.015849	1.754565
81	1	0	-1.952717	-0.102809	2.408553
82	15	0	4.315523	-0.924964	-1.135386
83	9	0	3.340691	-1.907562	-1.988217
84	9	0	3.611094	0.368761	-1.831448
85	9	0	3.200814	-0.876075	0.052742
86	9	0	5.009037	-2.208714	-0.430527
87	9	0	5.269773	0.066810	-0.271880
88	9	0	5.411987	-0.968759	-2.319402
89	6	0	-2.028316	2.608444	0.683653

Structure 28 – Gas phase



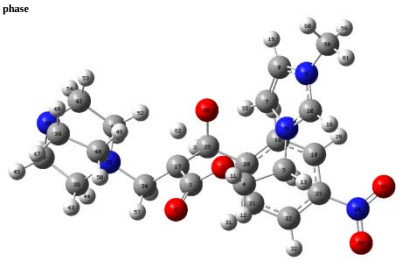
Zero-point correction=	0.528012
Thermal correction to Energy=	0.556047
Thermal correction to Enthalpy=	0.556991
Thermal correction to Gibbs Free Energy=	0.467527
Sum of electronic and zero-point Energies=	-1505.151873
Sum of electronic and thermal Energies=	-1505.123838
Sum of electronic and thermal Enthalpies=	-1505.122894
Sum of electronic and thermal Free Energies=	-1505.212358

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.558668	-0.088443	1.741395
2	8	0	-0.597858	-0.867894	2.653212
3	8	0	0.369623	0.887424	1.623599
4	6	0	1.541043	0.817805	2.426704
5	6	0	2.729233	0.690580	1.489140
6	7	0	2.841128	1.842964	0.579960
7	6	0	1.942601	2.221605	-0.405922
8	6	0	2.480595	3.324190	-0.993778
9	7	0	3.680487	3.597565	-0.369816
10	6	0	3.873978	2.686201	0.576953
11	1	0	1.597510	1.732461	3.019485
12	1	0	1.497659	-0.046944	3.090359
13	1	0	3.656088	0.636668	2.062114
14	1	0	2.638494	-0.210317	0.881716
15	1	0	2.113588	3.929319	-1.805044
16	1	0	4.731864	2.632546	1.227479
17	6	0	-1.460351	-0.048475	0.550189
18	6	0	2.874250	-1.508328	-1.494775
19	6	0	1.682416	-0.799318	-1.547797
20	6	0	0.616449	-1.115434	-0.700986
21	6	0	0.744555	-2.205607	0.165572

22	6	0	1.932905	-2.923024	0.241342
23	6	0	2.983978	-2.547679	-0.581352
24	7	0	4.263326	-3.280460	-0.484221
25	6	0	-0.662472	-0.266498	-0.856094
26	8	0	-0.468627	0.902694	-1.442411
27	8	0	5.192496	-2.862767	-1.139435
28	8	0	4.301724	-4.239568	0.252004
29	1	0	3.711541	-1.276723	-2.139609
30	1	0	1.538567	0.019184	-2.242240
31	1	0	-0.074777	-2.501432	0.811029
32	1	0	2.056503	-3.756963	0.918926
33	1	0	-1.349045	-0.956612	-1.410627
34	6	0	-2.669104	-0.951018	0.724747
35	7	0	-3.925968	-0.353781	0.133118
36	6	0	-5.031473	-1.379089	0.200018
37	6	0	-6.252892	-0.842320	-0.585862
38	7	0	-6.118149	0.593141	-0.808004
39	6	0	-5.803384	1.237416	0.462287
40	6	0	-4.372142	0.858643	0.917388
41	6	0	-3.751221	0.055543	-1.318578
42	6	0	-5.021356	0.830989	-1.745487
43	1	0	-5.245858	-1.534601	1.258950
44	1	0	-4.640161	-2.306440	-0.217593
45	1	0	-7.170003	-1.042907	-0.031090
46	1	0	-6.334848	-1.335500	-1.555599
47	1	0	-6.541869	0.923577	1.202114
48	1	0	-5.880789	2.319449	0.352015
49	1	0	-3.658167	1.653099	0.708363
50	1	0	-4.316487	0.600460	1.975627
51	1	0	-3.626382	-0.873658	-1.877043
52	1	0	-2.836368	0.648664	-1.419533
53	1	0	-4.822697	1.903533	-1.776321
54	1	0	-5.323938	0.521694	-2.746231
55	1	0	1.001792	1.693384	-0.648303
56	1	0	-2.516068	-1.902449	0.209431
57	1	0	-2.888415	-1.162198	1.773747
58	6	0	4.586800	4.695051	-0.703531
59	1	0	4.903640	4.597045	-1.740492
60	1	0	4.074319	5.644255	-0.556633
61	1	0	5.456537	4.646165	-0.052157
62	1	0	-1.751300	0.993386	0.424716

Structure 29 – Gas phase

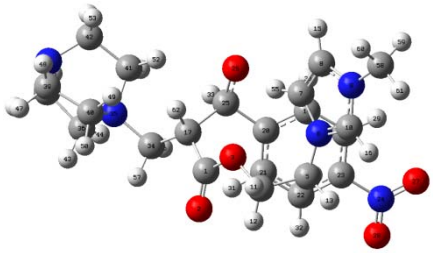


Zero-point correction= 0.526994
Thermal correction to Energy= 0.554391
Thermal correction to Enthalpy= 0.555335
Thermal correction to Gibbs Free Energy= 0.468862
Sum of electronic and zero-point Energies= -1496.451425
Sum of electronic and thermal Energies= -1496.424029
Sum of electronic and thermal Enthalpies= -1496.423084
Sum of electronic and thermal Free Energies= -1496.509557

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.801361	-0.105286	1.530047
2	8	0	-1.204067	-0.260391	2.657023
3	8	0	0.376822	0.512076	1.263591
4	6	0	1.308672	0.720939	2.304277
5	6	0	2.652078	0.771008	1.599913
6	7	0	2.732222	1.897014	0.649461
7	6	0	1.899328	2.149126	-0.430120
8	6	0	2.389615	3.266492	-1.030168
9	7	0	3.500945	3.673485	-0.321994
10	6	0	3.685278	2.827484	0.685763
11	1	0	1.089572	1.650682	2.836468
12	1	0	1.289051	-0.107469	3.016108
13	1	0	3.464420	0.894062	2.316572
14	1	0	2.803187	-0.152628	1.037046
15	1	0	2.043581	3.801008	-1.898388
16	1	0	4.482419	2.881754	1.409551
17	6	0	-1.478968	-0.449123	0.273803
18	6	0	3.083360	-1.436400	-1.470368
19	6	0	1.811954	-0.896402	-1.614967
20	6	0	0.762214	-1.311887	-0.794437
21	6	0	0.994159	-2.309655	0.155925
22	6	0	2.257405	-2.862830	0.316427
23	6	0	3.284996	-2.402748	-0.495153
24	7	0	4.642556	-2.954416	-0.308200
25	6	0	-0.604518	-0.678429	-0.986464
26	8	0	-0.561509	0.628188	-1.493387
27	8	0	5.535868	-2.463511	-0.962690
28	8	0	4.774271	-3.848434	0.496013
29	1	0	3.913109	-1.129789	-2.093193
30	1	0	1.608927	-0.135524	-2.358820
31	1	0	0.183329	-2.647452	0.794374
32	1	0	2.460725	-3.630403	1.051210
33	1	0	-1.164995	-1.367456	-1.649287
34	6	0	-2.726689	-1.254910	0.463939
35	7	0	-3.989656	-0.512864	0.051351
36	6	0	-5.192268	-1.372794	0.326674
37	6	0	-6.433185	-0.691613	-0.303122
38	7	0	-6.137025	0.703098	-0.616930
39	6	0	-5.551711	1.336886	0.562343
40	6	0	-4.137864	0.766414	0.835983
41	6	0	-3.969225	-0.182750	-1.420840
42	6	0	-5.170317	0.750066	-1.713100
43	1	0	-5.267278	-1.463582	1.411686
44	1	0	-4.993952	-2.359014	-0.094379
45	1	0	-7.276452	-0.739743	0.386441
46	1	0	-6.725866	-1.198221	-1.224134
47	1	0	-6.214518	1.160752	1.411348
48	1	0	-5.493370	2.413978	0.403434
49	1	0	-3.346033	1.430264	0.492944
50	1	0	-3.956268	0.525951	1.884877
51	1	0	-4.046048	-1.137886	-1.945008
52	1	0	-3.006381	0.274964	-1.658513
53	1	0	-4.834421	1.781567	-1.830652
54	1	0	-5.658097	0.451451	-2.641503
55	1	0	1.031479	1.539002	-0.695340
56	1	0	-2.725159	-2.164387	-0.141850
57	1	0	-2.878459	-1.522448	1.512612
58	6	0	4.338825	4.830127	-0.637105
59	1	0	4.792575	4.690696	-1.616949
60	1	0	3.726113	5.729899	-0.631980
61	1	0	5.118349	4.917139	0.116503
62	1	0	-1.444578	0.642888	-0.416889

Structure 28 – Solvent: Methanol

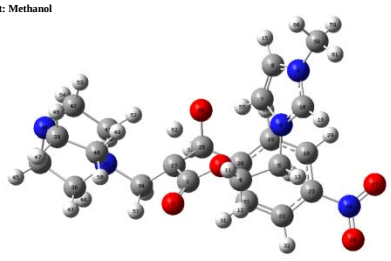


Zero-point correction= 0.528618
Thermal correction to Energy= 0.556823
Thermal correction to Enthalpy= 0.557767
Thermal correction to Gibbs Free Energy= 0.467403
Sum of electronic and zero-point Energies= -1505.241469
Sum of electronic and thermal Energies= -1505.213265
Sum of electronic and thermal Enthalpies= -1505.212320
Sum of electronic and thermal Free Energies= -1505.302684

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.547901	0.040249	1.639472
2	8	0	-0.592449	-0.717763	2.574234
3	8	0	0.382184	1.000707	1.499880
4	6	0	1.513702	0.997671	2.373774
5	6	0	2.751132	0.757780	1.531314
6	7	0	2.975166	1.849437	0.574939
7	6	0	2.146514	2.222630	-0.470853
8	6	0	2.753890	3.278060	-1.074512
9	7	0	3.927791	3.529485	-0.396623
10	6	0	4.037700	2.653878	0.593829
11	1	0	1.553283	1.970148	2.864411
12	1	0	1.412602	0.210356	3.119112
13	1	0	3.630873	0.696772	2.170958
14	1	0	2.655848	-0.174472	0.972603
15	1	0	2.458039	3.868791	-1.924275
16	1	0	4.854352	2.599426	1.294812
17	6	0	-1.459855	0.042782	0.448528
18	6	0	2.851941	-1.618176	-1.408159
19	6	0	1.699316	-0.853414	-1.508564
20	6	0	0.573500	-1.130879	-0.728926
21	6	0	0.607323	-2.235106	0.131333
22	6	0	1.752286	-3.009480	0.255623
23	6	0	2.861206	-2.679309	-0.512710
24	7	0	4.081668	-3.485787	-0.377467
25	6	0	-0.667269	-0.235595	-0.936811
26	8	0	-0.409105	0.901454	-1.577547
27	8	0	5.046834	-3.174729	-1.045028
28	8	0	4.064699	-4.421744	0.395612
29	1	0	3.730183	-1.402668	-2.001285
30	1	0	1.640978	-0.012173	-2.186589
31	1	0	-0.256854	-2.495853	0.731416
32	1	0	1.795018	-3.853020	0.930597
33	1	0	-1.369989	-0.915434	-1.478970
34	6	0	-2.668702	-0.854781	0.680090
35	7	0	-3.950476	-0.275003	0.137045
36	6	0	-5.051790	-1.295545	0.307717
37	6	0	-6.312639	-0.789048	-0.430711
38	7	0	-6.188093	0.635768	-0.736376
39	6	0	-5.798188	1.343789	0.482675
40	6	0	-4.353555	0.970533	0.891369
41	6	0	-3.848472	0.063395	-1.333132
42	6	0	-5.139223	0.813293	-1.742103
43	1	0	-5.209322	-1.403579	1.381059
44	1	0	-4.686345	-2.239386	-0.094055
45	1	0	-7.191436	-0.953380	0.192727
46	1	0	-6.453098	-1.331711	-1.366235
47	1	0	-6.501034	1.082157	1.274431
48	1	0	-5.860291	2.418873	0.314559
49	1	0	-3.647391	1.753700	0.624496
50	1	0	-4.260221	0.750923	1.954629
51	1	0	-3.737513	-0.887424	-1.856198
52	1	0	-2.949224	0.661927	-1.491384
53	1	0	-4.942260	1.880930	-1.847948
54	1	0	-5.489352	0.436740	-2.703176
55	1	0	1.206461	1.718909	-0.711973
56	1	0	-2.541506	-1.817763	0.181487
57	1	0	-2.843186	-1.040724	1.740493
58	6	0	4.888180	4.584382	-0.720265
59	1	0	5.263457	4.426815	-1.729083
60	1	0	4.392496	5.550162	-0.649436
61	1	0	5.709192	4.538150	-0.009768
62	1	0	-1.758039	1.079464	0.300886

Structure 29 – Solvent: Methanol



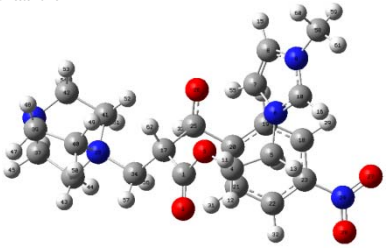
Zero-point correction= 0.523832
Thermal correction to Energy= 0.551955
Thermal correction to Enthalpy= 0.552899
Thermal correction to Gibbs Free Energy= 0.461702
Sum of electronic and zero-point Energies= -1505.209935
Sum of electronic and thermal Energies= -1505.181813
Sum of electronic and thermal Enthalpies= -1505.180869
Sum of electronic and thermal Free Energies= -1505.272066

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.784350	-0.025533	1.455439
2	8	0	-1.230125	-0.029565	2.584078
3	8	0	0.436382	0.476928	1.174276
4	6	0	1.306134	0.832293	2.237905
5	6	0	2.678349	0.912772	1.602055
6	7	0	2.762460	2.007907	0.623673
7	6	0	1.971367	2.192509	-0.498547
8	6	0	2.429035	3.318025	-1.106771
9	7	0	3.482809	3.796344	-0.357373
10	6	0	3.662591	2.988278	0.679588
11	1	0	1.004923	1.785939	2.677677
12	1	0	1.300696	0.061372	3.010611
13	1	0	3.442385	1.091851	2.356568
14	1	0	2.895696	-0.023700	1.083778
15	1	0	2.100331	3.818490	-2.001139
16	1	0	4.416803	3.104777	1.440518
17	6	0	-1.460482	-0.460328	0.231484
18	6	0	3.107506	-1.527805	-1.406132
19	6	0	1.842783	-0.981999	-1.579597
20	6	0	0.769615	-1.398858	-0.791162
21	6	0	0.973124	-2.398888	0.164945
22	6	0	2.228115	-2.953267	0.359024
23	6	0	3.278567	-2.501258	-0.431244
24	7	0	4.615179	-3.074317	-0.227547
25	6	0	-0.598842	-0.782724	-1.013465

26	8	0	-0.564276	0.484419	-1.625782
27	8	0	5.521206	-2.672369	-0.928944
28	8	0	4.748059	-3.920633	0.632866
29	1	0	3.949837	-1.210266	-2.005348
30	1	0	1.670536	-0.210421	-2.318847
31	1	0	0.144234	-2.732241	0.781072
32	1	0	2.402445	-3.714903	1.106312
33	1	0	-1.164484	-1.520566	-1.613316
34	6	0	-2.717878	-1.242009	0.475423
35	7	0	-3.986314	-0.508260	0.073358
36	6	0	-5.182617	-1.345914	0.436923
37	6	0	-6.440013	-0.692281	-0.183214
38	7	0	-6.154377	0.687627	-0.579963
39	6	0	-5.517155	1.375075	0.545264
40	6	0	-4.099132	0.809128	0.794976
41	6	0	-4.021209	-0.258178	-1.411281
42	6	0	-5.222455	0.669569	-1.710298
43	1	0	-5.220508	-1.376197	1.526057
44	1	0	-5.005861	-2.352025	0.058225
45	1	0	-7.254570	-0.702212	0.541003
46	1	0	-6.762740	-1.245267	-1.066253
47	1	0	-6.144721	1.243723	1.427837
48	1	0	-5.452955	2.441655	0.329902
49	1	0	-3.318523	1.451905	0.392396
50	1	0	-3.890791	0.619881	1.848043
51	1	0	-4.124153	-1.237191	-1.882120
52	1	0	-3.067487	0.180810	-1.705825
53	1	0	-4.882099	1.690544	-1.890218
54	1	0	-5.740243	0.322019	-2.604376
55	1	0	1.152494	1.531689	-0.765284
56	1	0	-2.736539	-2.171295	-0.097289
57	1	0	-2.849315	-1.475586	1.533736
58	6	0	4.269910	4.991917	-0.658053
59	1	0	4.748980	4.867008	-1.626821
60	1	0	3.611742	5.857791	-0.672339
61	1	0	5.024094	5.114118	0.114873
62	1	0	-1.410652	0.589821	-0.555996

Structure 28 – Solvent: Acetonitrile

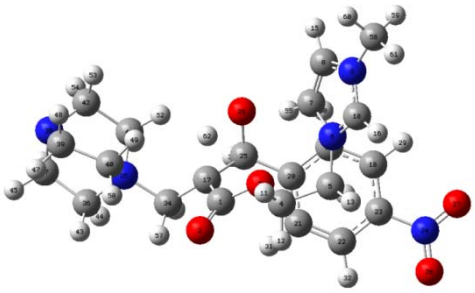


Zero-point correction= 0.528622
Thermal correction to Energy= 0.556828
Thermal correction to Enthalpy= 0.557772
Thermal correction to Gibbs Free Energy= 0.467378
Sum of electronic and zero-point Energies= -1505.241789
Sum of electronic and thermal Energies= -1505.213583
Sum of electronic and thermal Enthalpies= -1505.212639
Sum of electronic and thermal Free Energies= -1505.303033

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.547986	0.041695	1.638930
2	8	0	-0.592242	-0.716462	2.573592
3	8	0	0.381716	1.002568	1.499512
4	6	0	1.513034	0.999931	2.373732
5	6	0	2.750649	0.758095	1.532105
6	7	0	2.976143	1.848794	0.574996
7	6	0	2.148245	2.222159	-0.471335
8	6	0	2.756809	3.276689	-1.075366
9	7	0	3.930662	3.527417	-0.397154
10	6	0	4.039330	2.652347	0.593896
11	1	0	1.553084	1.973081	2.862973
12	1	0	1.411134	0.213746	3.120128
13	1	0	3.630013	0.696775	2.172237
14	1	0	2.654805	-0.174540	0.974122
15	1	0	2.461844	3.867259	-1.925551
16	1	0	4.855578	2.597670	1.295321
17	6	0	-1.459996	0.043940	0.447982
18	6	0	2.851552	-1.618581	-1.407405
19	6	0	1.699264	-0.853365	-1.508096
20	6	0	0.573044	-1.130492	-0.728922
21	6	0	0.606141	-2.234825	0.131231
22	6	0	1.750758	-3.009678	0.255828
23	6	0	2.860039	-2.679859	-0.512115
24	7	0	4.080058	-3.486954	-0.376713
25	6	0	-0.667406	-0.234799	-0.937110
26	8	0	-0.408734	0.902112	-1.578073
27	8	0	5.044580	-3.178150	-1.046261
28	8	0	4.063388	-4.421290	0.398376
29	1	0	3.730097	-1.403262	-2.000140
30	1	0	1.641579	-0.011974	-2.185979
31	1	0	-0.258341	-2.495300	0.730983
32	1	0	1.792891	-3.853286	0.930748
33	1	0	-1.370233	-0.914439	-1.479332
34	6	0	-2.668709	-0.853760	0.679853
35	7	0	-3.950673	-0.274306	0.136972
36	6	0	-5.051751	-1.295006	0.308211
37	6	0	-6.312930	-0.788930	-0.429952
38	7	0	-6.188687	0.635805	-0.736209
39	6	0	-5.798548	1.344329	0.482508
40	6	0	-4.353777	0.971411	0.891003
41	6	0	-3.849055	0.063689	-1.333291
42	6	0	-5.140105	0.813089	-1.742285
43	1	0	-5.208924	-1.402832	1.381614
44	1	0	-4.686255	-2.238850	-0.093491
45	1	0	-7.191457	-0.953103	0.193907
46	1	0	-6.453643	-1.331979	-1.365209
47	1	0	-6.501141	1.082880	1.274543
48	1	0	-5.860799	2.419344	0.314005
49	1	0	-3.647791	1.754596	0.623740
50	1	0	-4.260210	0.752153	1.954303
51	1	0	-3.737871	-0.887218	-1.856136
52	1	0	-2.950060	0.662511	-1.491790
53	1	0	-4.943416	1.880718	-1.848702
54	1	0	-5.490382	0.435949	-2.703077
55	1	0	1.207893	1.719055	-0.712423
56	1	0	-2.541479	-1.816804	0.181388
57	1	0	-2.842951	-1.039581	1.740311
58	6	0	4.892133	4.581304	-0.720885
59	1	0	5.266245	4.423948	-1.730160
60	1	0	4.397808	5.547694	-0.648890
61	1	0	5.713735	4.533399	-0.011190
62	1	0	-1.758357	1.080560	0.300230

Structure 29 – Solvent: Acetonitrile

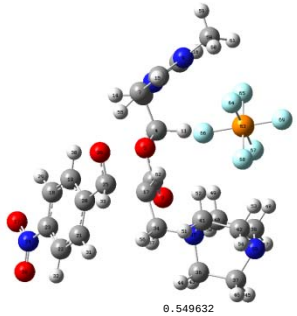


Zero-point correction= 0.523817
Thermal correction to Energy= 0.551948
Thermal correction to Enthalpy= 0.552893
Thermal correction to Gibbs Free Energy= 0.461614
Sum of electronic and zero-point Energies= -1505.210247
Sum of electronic and thermal Energies= -1505.182116
Sum of electronic and thermal Enthalpies= -1505.181172
Sum of electronic and thermal Free Energies= -1505.272450

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.783744	-0.025088	1.455077
2	8	0	-1.230063	-0.027275	2.583546
3	8	0	0.437487	0.476025	1.173878
4	6	0	1.306218	0.833787	2.237585
5	6	0	2.678619	0.915606	1.602356
6	7	0	2.761826	2.010353	0.623494
7	6	0	1.970919	2.193531	-0.499079
8	6	0	2.427464	3.319315	-1.107648
9	7	0	3.479600	3.799193	-0.358082
10	6	0	3.660766	2.991808	0.679300
11	1	0	1.003400	1.787458	2.676181
12	1	0	1.381521	0.063669	3.011094
13	1	0	3.442084	1.095986	2.357136
14	1	0	2.897378	-0.020849	1.084653
15	1	0	2.098473	3.819061	-2.002312
16	1	0	4.414545	3.109524	1.440465
17	6	0	-1.459831	-0.460845	0.231469
18	6	0	3.108173	-1.528760	-1.405188
19	6	0	1.843521	-0.982847	-1.578808
20	6	0	0.770082	-1.400076	-0.790946
21	6	0	0.973235	-2.400547	0.164776
22	6	0	2.228143	-2.955028	0.359013
23	6	0	3.278868	-2.502713	-0.430735
24	7	0	4.615320	-3.076028	-0.227006
25	6	0	-0.598352	-0.783972	-1.013386
26	8	0	-0.563830	0.482870	-1.626413
27	8	0	5.521543	-2.674146	-0.928213
28	8	0	4.747997	-3.922616	0.633197
29	1	0	3.950698	-1.210910	-2.003963
30	1	0	1.671558	-0.210931	-2.317760
31	1	0	0.144136	-2.734142	0.780486
32	1	0	2.402192	-3.716970	1.106050
33	1	0	-1.164117	-1.522082	-1.612776
34	6	0	-2.717289	-1.242270	0.476002
35	7	0	-3.985747	-0.508721	0.073663
36	6	0	-5.182008	-1.346167	0.437886
37	6	0	-6.439485	-0.692878	-0.182424
38	7	0	-6.153908	0.686811	-0.580047
39	6	0	-5.516477	1.374915	0.544683
40	6	0	-4.098445	0.809085	0.794529
41	6	0	-4.020854	-0.259515	-1.411104
42	6	0	-5.222138	0.668046	-1.710515
43	1	0	-5.219739	-1.375851	1.527038
44	1	0	-5.005331	-2.352482	0.059716
45	1	0	-7.253900	-0.702361	0.541957
46	1	0	-6.762355	-1.246373	-1.065089
47	1	0	-6.143902	1.244112	1.427433
48	1	0	-5.452251	2.441361	0.328670
49	1	0	-3.317886	1.451629	0.391478
50	1	0	-3.889982	0.620425	1.847671
51	1	0	-4.123839	-1.238789	-1.881379
52	1	0	-3.067192	0.179352	-1.706003
53	1	0	-4.881807	1.688910	-1.891106
54	1	0	-5.740046	0.319910	-2.604297
55	1	0	1.152933	1.531613	-0.765716
56	1	0	-2.736069	-2.171925	-0.096099
57	1	0	-2.848645	-1.475147	1.534471
58	6	0	4.266120	4.995634	-0.658916
59	1	0	4.745273	4.871154	-1.627692
60	1	0	3.606956	5.860747	-0.673260
61	1	0	5.020194	5.118739	0.113965
62	1	0	-1.410013	0.588912	-0.556687

Structure 30 – Gas phase



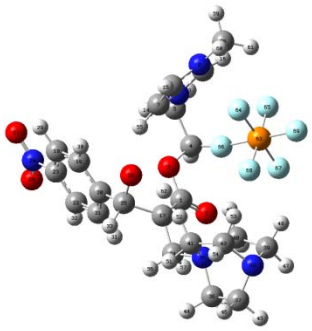
Zero-point correction= 0.549632
Thermal correction to Energy= 0.585037
Thermal correction to Enthalpy= 0.585981
Thermal correction to Gibbs Free Energy= 0.481628
Sum of electronic and zero-point Energies= -2445.936731
Sum of electronic and thermal Energies= -2445.901325
Sum of electronic and thermal Enthalpies= -2445.900381
Sum of electronic and thermal Free Energies= -2446.004735

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.928553	-0.070707	-0.536188
2	8	0	1.255947	0.450507	-1.575189
3	8	0	0.624656	-1.367056	-0.445480
4	6	0	0.350285	-2.087923	-1.626594
5	6	0	0.050955	-3.486135	-1.112841
6	7	0	-0.987997	-3.435221	-0.082101
7	6	0	-0.815679	-2.995656	1.220083
8	6	0	-2.053287	-3.015006	1.780121
9	7	0	-2.947870	-3.440382	0.820138
10	6	0	-2.279034	-3.673392	-0.299466
11	1	0	-0.517201	-1.646649	-2.127133
12	1	0	1.207759	-2.092947	-2.303261
13	1	0	-0.289143	-4.142966	-1.913650
14	1	0	0.942768	-3.913538	-0.654148
15	1	0	-2.380341	-2.717842	2.760377
16	1	0	-2.716972	-3.973560	-1.236346
17	6	0	0.840228	0.565935	0.809742

18	6	0	4.857527	-1.588465	-0.036959
19	6	0	3.645526	-1.489107	0.629019
20	6	0	3.237290	-0.282772	1.196890
21	6	0	4.087555	0.822134	1.125884
22	6	0	5.307369	0.745905	0.468815
23	6	0	5.665187	-0.461590	-0.112612
24	7	0	6.956174	-0.553896	-0.814968
25	6	0	1.860117	-0.240072	1.883289
26	8	0	1.383810	-1.395641	2.235793
27	8	0	7.252773	-1.619031	-1.312834
28	8	0	7.646982	0.442380	-0.858022
29	1	0	5.196629	-2.512356	-0.485850
30	1	0	2.983189	-2.336494	0.762123
31	1	0	3.808798	1.750331	1.615840
32	1	0	5.984330	1.586754	0.407465
33	1	0	1.931993	0.530434	2.694170
34	6	0	1.108749	2.047547	0.730013
35	7	0	-0.072326	2.942117	0.383515
36	6	0	0.441156	4.346995	0.239838
37	6	0	-0.745493	5.294927	-0.076184
38	7	0	-1.992270	4.550980	-0.166929
39	6	0	-1.870888	3.540699	-1.218723
40	6	0	-0.734313	2.539843	-0.914037
41	6	0	-1.107672	2.914535	1.477679
42	6	0	-2.254826	3.892595	1.108267
43	1	0	1.182814	4.323625	-0.559207
44	1	0	0.943502	4.597914	1.175368
45	1	0	-0.573005	5.808655	-1.023033
46	1	0	-0.844206	6.052061	0.703553
47	1	0	-1.693302	4.049618	-2.166053
48	1	0	-2.818499	2.998270	-1.296495
49	1	0	-1.111897	1.529782	-0.778334
50	1	0	0.048578	2.519561	-1.670311
51	1	0	-0.592476	3.189110	2.399951
52	1	0	-1.470679	1.892040	1.549780
53	1	0	-3.188714	3.340077	1.028047
54	1	0	-2.364936	4.657615	1.879021
55	1	0	0.132847	-2.587948	1.596845
56	1	0	1.463830	2.423332	1.693750
57	1	0	1.863138	2.246043	-0.034107
58	6	0	-4.391877	-3.587308	0.977908
59	1	0	-4.638254	-4.624752	1.203062
60	1	0	-4.711160	-2.932736	1.783422
61	1	0	-4.871820	-3.254723	0.059583
62	1	0	-0.119763	0.310839	1.259264
63	15	0	-3.518211	-0.172619	-0.587477
64	9	0	-4.029308	-0.856120	0.792065
65	9	0	-3.749485	-1.579542	-1.373502
66	9	0	-1.990590	-0.647764	-0.231321
67	9	0	-2.953419	0.517133	-1.939615
68	9	0	-3.241555	1.221140	0.226767
69	9	0	-5.006677	0.299243	-0.932943

Structure 31 – Gas phase

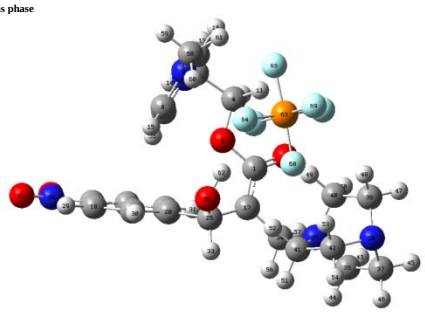


Zero-point correction= 0.546700
Thermal correction to Energy= 0.582813
Thermal correction to Enthalpy= 0.583757
Thermal correction to Gibbs Free Energy= 0.473136
Sum of electronic and zero-point Energies= -0.041758
Sum of electronic and thermal Energies= -0.005645
Sum of electronic and thermal Enthalpies= -0.004701
Sum of electronic and thermal Free Energies= -0.115322

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.391725	-1.111913	-0.962426
2	8	0	0.145746	-1.315502	-2.054060
3	8	0	-1.278871	-0.073795	-0.784852
4	6	0	-1.260131	0.975207	-1.794975
5	6	0	-2.111661	2.052350	-1.128707
6	7	0	-1.354391	2.624567	0.003752
7	6	0	-0.932673	1.934297	1.148251
8	6	0	-0.128447	2.802142	1.822877
9	7	0	-0.060005	3.986371	1.086708
10	6	0	-0.795627	3.844511	-0.019569
11	1	0	-0.237298	1.317057	-1.951536
12	1	0	-1.706862	0.629707	-2.729937
13	1	0	-2.352077	2.864946	-1.818003
14	1	0	-3.025025	1.594073	-0.742892
15	1	0	0.445042	2.659693	2.717491
16	1	0	-0.889422	4.565748	-0.809871
17	6	0	-0.146075	-1.812136	0.288067
18	6	0	-4.744832	-0.382138	1.142692
19	6	0	-3.444415	-0.646059	1.552621
20	6	0	-2.669665	-1.595334	0.879385
21	6	0	-3.214875	-2.306705	-0.193900
22	6	0	-4.513346	-2.047899	-0.617199
23	6	0	-5.255719	-1.083107	0.055379
24	7	0	-6.611246	-0.798511	-0.394478
25	6	0	-1.254496	-1.809026	1.376460
26	8	0	-0.774471	-0.685167	2.171988
27	8	0	-7.259222	0.103949	0.233217
28	8	0	-7.053667	-1.465178	-1.388069
29	1	0	-5.378310	0.343819	1.631877
30	1	0	-2.971241	-0.129635	2.378583
31	1	0	-2.609571	-3.039498	-0.717125
32	1	0	-4.970029	-2.559311	-1.452430
33	1	0	-1.229431	-2.770829	1.921843
34	6	0	0.730776	-3.009949	0.128771
35	7	0	2.252657	-2.692566	0.197110
36	6	0	2.972209	-4.021677	0.381833
37	6	0	4.513821	-3.780462	0.400451
38	7	0	4.800791	-2.335247	0.327108
39	6	0	4.290730	-1.801583	-0.961519
40	6	0	2.744807	-2.011142	-1.083486
41	6	0	2.583471	-1.746269	1.348897
42	6	0	4.140030	-1.645550	1.463943
43	1	0	2.656515	-4.662012	-0.446261
44	1	0	2.608137	-4.437890	1.324812
45	1	0	4.990200	-4.271019	-0.451602
46	1	0	4.944209	-4.177172	1.323394
47	1	0	4.815634	-2.311705	-1.772451
48	1	0	4.492393	-0.734119	-0.993835
49	1	0	2.228455	-1.059735	-1.170666
50	1	0	2.451485	-2.649781	-1.918200
51	1	0	2.086180	-2.124360	2.245992
52	1	0	2.167804	-0.783330	1.059842
53	1	0	4.413276	-0.592400	1.430415
54	1	0	4.498765	-2.100925	2.390757
55	1	0	-1.114732	0.873444	1.387136
56	1	0	0.563660	-3.722414	0.942680
57	1	0	0.614850	-3.508030	-0.842210
58	6	0	0.884124	5.082505	1.360049
59	1	0	0.723660	5.459739	2.370846
60	1	0	1.884415	4.665643	1.247647
61	1	0	0.720231	5.883325	0.637497
62	1	0	0.184787	-0.906368	1.170047
63	15	0	2.388224	1.793712	-0.617535
64	9	0	2.350879	2.648532	0.792756
65	9	0	1.200966	2.762864	-1.235750
66	9	0	1.208836	0.774186	-0.024857
67	9	0	2.372456	0.890265	-1.989388
68	9	0	3.511090	0.770743	0.043089
69	9	0	3.551605	2.763471	-1.207558

Structure 32 – Gas phase

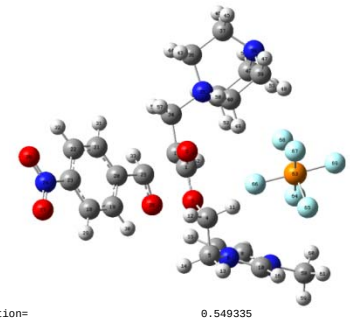


Zero-point correction= 0.550186
Thermal correction to Energy= 0.585870
Thermal correction to Enthalpy= 0.586814
Thermal correction to Gibbs Free Energy= 0.481340
Sum of electronic and zero-point Energies= -2445.969944
Sum of electronic and thermal Energies= -2445.934260
Sum of electronic and thermal Enthalpies= -2445.933316
Sum of electronic and thermal Free Energies= -2446.038790

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.156893	-1.207211	1.622875
2	8	0	-0.465644	-1.400085	2.662283
3	8	0	1.011353	-0.100137	1.558388
4	6	0	0.804045	0.828712	2.599518
5	6	0	1.763517	1.973786	2.345435
6	7	0	1.497580	2.600784	1.047107
7	6	0	1.886062	2.087313	-0.168385
8	6	0	1.325945	2.872795	-1.122914
9	7	0	0.602278	3.846519	-0.472884
10	6	0	0.705455	3.647224	0.835381
11	1	0	-0.231356	1.181515	2.589383
12	1	0	1.011166	0.384404	3.576038
13	1	0	1.668748	2.740629	3.115000
14	1	0	2.793551	1.616046	2.324559
15	1	0	1.343436	2.799449	-2.195789
16	1	0	0.192684	4.213560	1.594310
17	6	0	0.125379	-1.954652	0.433693
18	6	0	4.512808	-0.681343	-1.573485
19	6	0	3.132381	-0.798055	-1.646120
20	6	0	2.406967	-1.452453	-0.643943
21	6	0	3.099152	-2.015102	0.428295
22	6	0	4.480056	-1.906921	0.521506
23	6	0	5.163423	-1.234355	-0.479961
24	7	0	6.628443	-1.102208	-0.381008
25	6	0	0.887229	-1.580549	-0.796881
26	8	0	0.399478	-0.412262	-1.479017
27	8	0	7.197281	-0.487571	-1.257674
28	8	0	7.175743	-1.612152	0.572486
29	1	0	5.087988	-0.176843	-2.337882
30	1	0	2.590506	-0.364442	-2.477973
31	1	0	2.540630	-2.527599	1.201699
32	1	0	5.031019	-2.326814	1.352042
33	1	0	0.750019	-2.396735	-1.520306
34	6	0	-0.770560	-3.106098	0.443701
35	7	0	-2.269496	-2.820544	0.020915
36	6	0	-3.070227	-4.068331	0.181080
37	6	0	-4.522618	-3.799226	-0.298637
38	7	0	-4.702000	-2.397974	-0.653548
39	6	0	-4.350002	-1.561148	0.496960
40	6	0	-2.864711	-1.749480	0.891262
41	6	0	-2.334825	-2.373608	-1.407314
42	6	0	-3.813830	-2.069497	-1.767545
43	1	0	-3.024359	-4.337374	1.237642
44	1	0	-2.574748	-4.850272	-0.397889
45	1	0	-5.232494	-4.057624	0.488959
46	1	0	-4.755897	-4.410607	-1.172713
47	1	0	-5.004928	-1.831295	1.327662
48	1	0	-4.530991	-0.516787	0.246458
49	1	0	-2.276657	-0.851846	0.723243
50	1	0	-2.714502	-2.058971	1.924850
51	1	0	-1.918328	-3.187825	-2.006176
52	1	0	-1.693554	-1.496364	-1.501069
53	1	0	-3.927657	-1.011741	-1.997475
54	1	0	-4.119532	-2.649942	-2.640351
55	1	0	2.478356	1.190739	-0.237885
56	1	0	-0.479832	-3.897635	-0.253949
57	1	0	-0.888214	-3.515723	1.449700
58	6	0	-0.156688	4.922673	-1.107567
59	1	0	0.488147	5.788409	-1.255762
60	1	0	-0.538737	4.551189	-2.053852
61	1	0	-1.004942	5.163443	-0.471035
62	1	0	0.020255	0.167482	-0.804869
63	15	0	-2.450416	2.023759	-0.175653
64	9	0	-1.716491	2.652192	-1.483340
65	9	0	-2.072046	3.369100	0.668518
66	9	0	-0.997158	1.379911	0.278173
67	9	0	-3.118576	1.373359	1.140160
68	9	0	-2.755311	0.664406	-1.012382
69	9	0	-3.847304	2.658584	-0.623273

Structure 30 – Solvent: Methanol



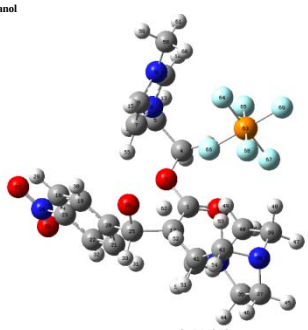
Zero-point correction= 0.549335
Thermal correction to Energy= 0.585185
Thermal correction to Enthalpy= 0.586129
Thermal correction to Gibbs Free Energy= 0.479422
Sum of electronic and zero-point Energies= -2445.987522
Sum of electronic and thermal Energies= -2445.951672
Sum of electronic and thermal Enthalpies= -2445.950727
Sum of electronic and thermal Free Energies= -2446.057435

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.948281	0.916844	-0.500881
2	8	0	1.272514	0.516580	-1.553647
3	8	0	0.692592	-1.279938	-0.367326

4	6	0	0.552741	-2.076788	-1.532226
5	6	0	0.315266	-3.474639	-0.993750
6	7	0	-0.802869	-3.472260	-0.048009
7	6	0	-0.770658	-2.969603	1.241442
8	6	0	-2.028754	-3.116307	1.731129
9	7	0	-2.799759	-3.685571	0.739516
10	6	0	-2.037052	-3.884745	-0.325733
11	1	0	-0.300833	-1.718176	-2.113465
12	1	0	1.456303	-2.047932	-2.143684
13	1	0	0.085537	-4.171432	-1.798078
14	1	0	1.197005	-3.827590	-0.459422
15	1	0	-2.452824	-2.838875	2.680163
16	1	0	-2.362903	-4.313847	-1.258818
17	6	0	0.831367	0.705976	0.825814
18	6	0	4.817871	-1.542063	0.062785
19	6	0	3.616033	-1.378909	0.734807
20	6	0	3.216064	-0.124070	1.197017
21	6	0	4.061425	0.972189	1.004945
22	6	0	5.271169	0.833280	0.340135
23	6	0	5.624230	-0.426507	-0.126104
24	7	0	6.902039	-0.585504	-0.830401
25	6	0	1.851680	-0.007493	1.903152
26	8	0	1.381229	-1.144046	2.377629
27	8	0	7.204904	-1.694378	-1.223399
28	8	0	7.595095	0.399728	-0.988349
29	1	0	5.140373	-2.506202	-0.306141
30	1	0	2.954330	-2.212402	0.936443
31	1	0	3.785036	1.946759	1.394172
32	1	0	5.937088	1.671096	0.187409
33	1	0	1.971417	0.806128	2.659345
34	6	0	1.049102	2.200774	0.699145
35	7	0	-0.166733	3.038793	0.361391
36	6	0	0.295075	4.465357	0.201196
37	6	0	-0.925114	5.362616	-0.124150
38	7	0	-2.150225	4.571920	-0.188787
39	6	0	-2.009659	3.551124	-1.225844
40	6	0	-0.823068	2.600375	-0.923685
41	6	0	-1.190130	2.985160	1.466301
42	6	0	-2.370459	3.922533	1.100956
43	1	0	1.034788	4.463413	-0.598718
44	1	0	0.782473	4.745430	1.134672
45	1	0	-0.776856	5.859394	-1.083161
46	1	0	-1.041774	6.128584	0.642825
47	1	0	-1.854220	4.048317	-2.183817
48	1	0	-2.929575	2.970942	-1.279077
49	1	0	-1.157485	1.575699	-0.777184
50	1	0	-0.050873	2.617443	-1.690766
51	1	0	-0.680388	3.283969	2.382203
52	1	0	-1.521327	1.952898	1.549451
53	1	0	-3.289243	3.341069	1.046044
54	1	0	-2.487582	4.692128	1.864415
55	1	0	0.106897	-2.461376	1.648779
56	1	0	1.414649	2.612025	1.642355
57	1	0	1.777412	2.411105	-0.085583
58	6	0	-4.223124	-3.997992	0.834838
59	1	0	-4.361786	-4.907694	1.416350
60	1	0	-4.722881	-3.157243	1.308480
61	1	0	-4.615336	-4.128898	-0.170617
62	1	0	-0.133383	0.447285	1.262605
63	15	0	-3.503988	-0.272247	-0.576169
64	9	0	-3.956679	-0.988427	0.806047
65	9	0	-3.666629	-1.676780	-1.369054
66	9	0	-1.949239	-0.631036	-0.257294
67	9	0	-3.936420	0.463735	-1.946660
68	9	0	-3.328184	1.137633	0.228786
69	9	0	5.043491	0.099742	-0.896004

Structure 31 – Solvent: Methanol

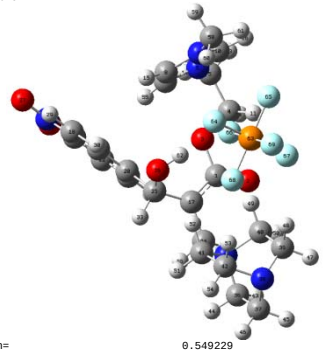


Zero-point correction= 0.544978
Thermal correction to Energy= 0.580646
Thermal correction to Enthalpy= 0.581590
Thermal correction to Gibbs Free Energy= 0.475074
Sum of electronic and zero-point Energies= -2445.952200
Sum of electronic and thermal Energies= -2445.916532
Sum of electronic and thermal Enthalpies= -2445.915588
Sum of electronic and thermal Free Energies= -2446.022105

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.460937	-0.870150	-1.143373
2	8	0	0.098478	-0.992554	-2.215456
3	8	0	-1.226606	0.208951	-0.870012
4	6	0	-1.156177	1.287738	-1.794680
5	6	0	-1.787775	2.470184	-1.093858
6	7	0	-0.993403	2.895360	0.063612
7	6	0	-0.844350	2.207647	1.250808
8	6	0	-0.044201	2.970945	2.038382
9	7	0	0.281369	4.101313	1.322358
10	6	0	-0.292297	4.025826	0.129765
11	1	0	-0.115763	1.492307	-2.048870
12	1	0	-1.717456	1.052447	-2.701550
13	1	0	-1.862339	3.318414	-1.772641
14	1	0	-2.785861	2.213062	-0.737100
15	1	0	0.339292	2.802834	3.029567
16	1	0	-0.214825	4.763781	-0.651276
17	6	0	-0.335684	-1.770521	0.002363
18	6	0	-4.850823	-0.149036	1.093148
19	6	0	-3.541046	-0.455048	1.434913
20	6	0	-2.822012	-1.412511	0.721234
21	6	0	-3.442547	-2.086789	-0.334986
22	6	0	-4.747971	-1.796379	-0.694343
23	6	0	-5.430415	-0.823615	0.027946
24	7	0	-6.811746	-0.503028	-0.348047
25	6	0	-1.398468	-1.741833	1.125561
26	8	0	-0.815629	-0.810913	2.003476
27	8	0	-7.395036	0.350460	0.289999
28	8	0	-7.305795	-1.105905	-1.279828
29	1	0	-5.419065	0.595000	1.634066
30	1	0	-3.049755	0.047289	2.258089
31	1	0	-2.889518	-2.836151	-0.892315
32	1	0	-5.237252	-2.300557	-1.516200
33	1	0	-1.441881	-2.757619	1.561033
34	6	0	0.355959	-3.064305	-0.317350
35	7	0	1.822342	-3.090563	0.088368
36	6	0	2.457382	-4.367239	-0.387305
37	6	0	3.863778	-4.472741	0.249056
38	7	0	4.299277	-3.165457	0.745698
39	6	0	4.081474	-2.171153	-0.311757
40	6	0	2.572555	-1.934159	-0.525780
41	6	0	1.974346	-3.028358	1.584383
42	6	0	3.470178	-2.801141	1.898647
43	1	0	2.496132	-4.308076	-1.475347
44	1	0	1.805756	-5.191019	-0.097243
45	1	0	4.574918	-4.836727	-0.492745
46	1	0	3.856292	-5.174300	1.084681
47	1	0	4.552462	-2.536199	-1.226235
48	1	0	4.552929	-1.229197	-0.034392
49	1	0	2.220135	-1.034527	-0.026652
50	1	0	2.286094	-1.876212	-1.573834
51	1	0	1.608640	-3.982130	1.969280
52	1	0	1.335770	-2.228220	1.957507
53	1	0	3.656062	-1.751099	2.131380
54	1	0	3.757768	-3.399654	2.763529
55	1	0	-1.224785	1.204937	1.405648
56	1	0	-0.097132	-3.908022	0.206258
57	1	0	0.361867	-3.272344	-1.389558
58	6	0	1.176963	5.160445	1.777966
59	1	0	0.792870	5.577053	2.706743
60	1	0	2.167093	4.735394	1.925273
61	1	0	1.218634	5.934786	1.016070
62	1	0	0.072567	-0.992478	0.989088
63	15	0	2.822169	1.825717	-0.683306
64	9	0	2.674433	2.984470	0.446534
65	9	0	1.951576	2.726232	-1.719470
66	9	0	1.451407	1.130749	-0.152637
67	9	0	2.976990	0.666548	-1.804606
68	9	0	3.676855	0.922704	0.366729
69	9	0	4.185631	2.520514	-1.210601

Structure 32 – Solvent: Methanol

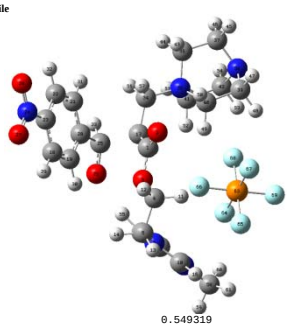


Zero-point correction= 0.549229
Thermal correction to Energy= 0.585213
Thermal correction to Enthalpy= 0.586157
Thermal correction to Gibbs Free Energy= 0.479854
Sum of electronic and zero-point Energies= -2446.011973
Sum of electronic and thermal Energies= -2445.975989
Sum of electronic and thermal Enthalpies= -2445.975045
Sum of electronic and thermal Free Energies= -2446.081347

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.236458	-1.083917	1.638153
2	8	0	-0.356769	-1.261032	2.708121
3	8	0	1.047413	0.044257	1.508930
4	6	0	0.921122	0.981216	2.561122
5	6	0	1.826803	2.148391	2.231534
6	7	0	1.403189	2.810216	0.994997
7	6	0	1.719545	2.393541	-0.276935
8	6	0	1.048011	3.202773	-1.135422
9	7	0	0.328784	4.092181	-0.369808
10	6	0	0.550889	3.827941	0.912004
11	1	0	-0.116937	1.314424	2.645243
12	1	0	1.229690	0.548039	3.514901
13	1	0	1.806291	2.885979	3.032882
14	1	0	2.853703	1.814270	2.085013
15	1	0	1.007127	3.217769	-2.210279
16	1	0	0.110549	4.350239	1.745381
17	6	0	0.208261	-1.874846	0.484693
18	6	0	4.555151	-0.487738	-1.498679
19	6	0	3.172607	-0.586766	-1.559047
20	6	0	2.462010	-1.354092	-0.630659
21	6	0	3.170645	-2.046608	0.353576
22	6	0	4.552752	-1.964110	0.431088
23	6	0	5.222530	-1.179410	-0.497523
24	7	0	6.685439	-1.079678	-0.420004
25	6	0	0.942496	-1.494233	-0.763347
26	8	0	0.419019	-0.331415	-1.427958
27	8	0	7.256378	-0.400573	-1.249309
28	8	0	7.252494	-1.681460	0.469323
29	1	0	5.112377	0.107564	-2.208661
30	1	0	2.626809	-0.055602	-2.328553
31	1	0	2.622870	-2.642932	1.072647
32	1	0	5.108918	-2.488074	1.196109
33	1	0	0.801869	-2.310938	-1.484241
34	6	0	-0.602175	-3.094878	0.538836
35	7	0	-2.097392	-2.944053	0.089053
36	6	0	-2.799062	-4.253259	0.255523
37	6	0	-4.263541	-4.103827	-0.233853
38	7	0	-4.542266	-2.726690	-0.638603
39	6	0	-4.273117	-1.831802	0.489937
40	6	0	-2.790994	-1.913327	0.928942
41	6	0	-2.168313	-2.530311	-1.349239
42	6	0	-3.657359	-2.366415	-1.747560
43	1	0	-2.740146	-4.511861	1.312969
44	1	0	-2.242348	-4.994245	-0.319017
45	1	0	-4.953817	-4.382335	0.563168
46	1	0	-4.446274	-4.759943	-1.085825
47	1	0	-4.928917	-2.112859	1.315505
48	1	0	-4.509310	-0.809975	0.193605
49	1	0	-2.260215	-0.977664	0.775396
50	1	0	-2.663645	-2.217047	1.966983
51	1	0	-1.670433	-3.313660	-1.923729
52	1	0	-1.607689	-1.600286	-1.439047
53	1	0	-3.854088	-1.330379	-2.021065
54	1	0	-3.891350	-3.002886	-2.602091
55	1	0	2.368629	1.552144	-0.447566
56	1	0	-0.235045	-3.890651	-0.115274
57	1	0	-0.695186	-3.473495	1.558816
58	6	0	-0.514648	5.170608	-0.882310
59	1	0	0.115337	5.978655	-1.249491
60	1	0	-1.132218	4.767776	-1.680157
61	1	0	-1.151498	5.521453	-0.075015
62	1	0	0.086981	0.254020	-0.734212
63	15	0	-2.577062	1.905129	-0.236234
64	9	0	-1.870202	2.548660	-1.548170
65	9	0	-2.405293	3.312190	0.551753
66	9	0	-1.109899	1.434545	0.314073
67	9	0	-3.264922	1.245318	1.075003
68	9	0	-2.724290	0.491316	-1.023875
69	9	0	-4.026402	2.369074	-0.777472

Structure 30 – Solvent: Acetonitrile



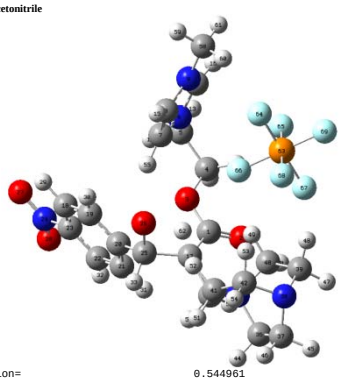
Zero-point correction= 0.549319
Thermal correction to Energy= 0.585178
Thermal correction to Enthalpy= 0.586122
Thermal correction to Gibbs Free Energy= 0.479350

Sum of electronic and zero-point Energies= -2445.987788
Sum of electronic and thermal Energies= -2445.951929
Sum of electronic and thermal Enthalpies= -2445.950985
Sum of electronic and thermal Free Energies= -2446.057757

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.948239	0.016011	-0.501099
2	8	0	1.273154	0.515435	-1.553841
3	8	0	0.691238	-1.280456	-0.367536
4	6	0	0.551073	-2.077436	-1.532356
5	6	0	0.313088	-3.475154	-0.993811
6	7	0	-0.805044	-3.472283	-0.048030
7	6	0	-0.772505	-2.969844	1.241485
8	6	0	-2.030592	-3.116105	1.731328
9	7	0	-2.801928	-3.684867	0.739715
10	6	0	-2.039436	-3.884194	-0.325677
11	1	0	-0.302425	-1.718568	-2.113552
12	1	0	1.454589	-2.048925	-2.143877
13	1	0	0.083079	-4.171924	-1.798061
14	1	0	1.194703	-3.828408	-0.459484
15	1	0	-2.454504	-2.838711	2.680444
16	1	0	-2.365613	-4.312889	-1.258837
17	6	0	0.831811	0.705354	0.825542
18	6	0	4.817458	-1.543226	0.061717
19	6	0	3.615592	-1.379912	0.733644
20	6	0	3.216186	-0.125180	1.196717
21	6	0	4.062154	0.970783	1.005633
22	6	0	5.271970	0.831688	0.340957
23	6	0	5.624455	-0.427939	-0.126129
24	7	0	6.902391	-0.587127	-0.830135
25	6	0	1.851805	-0.008414	1.902810
26	8	0	1.381218	-1.145048	2.377253
27	8	0	7.204555	-1.695786	-1.224304
28	8	0	7.596376	0.397698	-0.986577
29	1	0	5.139439	-2.507288	-0.307863
30	1	0	2.953537	-2.213298	0.934510
31	1	0	3.786258	1.945233	1.395492
32	1	0	5.938344	1.669295	0.189099
33	1	0	1.971615	0.805064	2.659087
34	6	0	1.050482	2.200068	0.698815
35	7	0	-0.164937	3.038721	0.361227
36	6	0	0.297606	4.465042	0.200670
37	6	0	-0.922261	5.362935	-0.124103
38	7	0	-2.147799	4.572791	-0.188624
39	6	0	-2.007811	3.551920	-1.225702
40	6	0	-0.821745	2.600495	-0.923603
41	6	0	-1.188058	2.985855	1.466453
42	6	0	-2.368128	3.923520	1.101167
43	1	0	1.036855	4.462610	-0.599656
44	1	0	0.785640	4.744931	1.133850
45	1	0	-0.774001	5.859879	-1.083017
46	1	0	-1.038414	6.128687	0.643153
47	1	0	-1.852077	4.049060	-2.183651
48	1	0	-2.928057	2.972251	-1.278920
49	1	0	-1.156722	1.576016	-0.776923
50	1	0	-0.049713	2.617070	-1.690860
51	1	0	-0.677926	3.284849	2.382069
52	1	0	-1.519608	1.953741	1.550098
53	1	0	-3.287119	3.342359	1.046350
54	1	0	-2.484939	4.693147	1.864635
55	1	0	0.105378	-2.462172	1.648692
56	1	0	1.416381	2.611111	1.641947
57	1	0	1.778842	2.409963	-0.085978
58	6	0	-4.225405	-3.996792	0.835191
59	1	0	-4.364318	-4.906522	1.416570
60	1	0	-4.724859	-3.155929	1.308898
61	1	0	-4.617706	-4.127534	-0.170250
62	1	0	-0.133218	0.447398	1.262175
63	15	0	-3.504452	-0.270828	-0.576044
64	9	0	-3.957647	-0.987067	0.805982
65	9	0	-3.667515	-1.675167	-1.369162
66	9	0	-1.949928	-0.630182	-0.256970
67	9	0	-3.036481	0.465101	-1.946438
68	9	0	-3.328347	1.138896	0.229075
69	9	0	-5.043819	0.101719	-0.896089

Structure 31 – Solvent: Acetonitrile

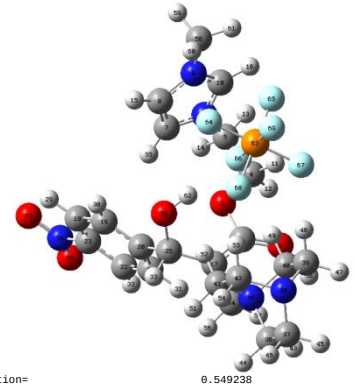


Zero-point correction= 0.544961
Thermal correction to Energy= 0.580636
Thermal correction to Enthalpy= 0.581580
Thermal correction to Gibbs Free Energy= 0.475009
Sum of electronic and zero-point Energies= -2445.952451
Sum of electronic and thermal Energies= -2445.916776
Sum of electronic and thermal Enthalpies= -2445.915832
Sum of electronic and thermal Free Energies= -2446.022403

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.460190	-0.870198	-1.143815
2	8	0	0.099530	-0.992126	-2.215831
3	8	0	-1.226437	0.208468	-0.879454
4	6	0	-1.156669	1.287297	-1.795147
5	6	0	-1.789206	2.469337	-1.094517
6	7	0	-0.994964	2.895510	0.062680
7	6	0	-0.845046	2.208246	1.250037
8	6	0	-0.045680	2.972627	2.037363
9	7	0	0.278596	4.103166	1.321018
10	6	0	-0.295131	4.026780	0.128511
11	1	0	-0.116359	1.492609	-2.049170
12	1	0	-1.717643	1.051555	-2.702083
13	1	0	-1.864667	3.317317	-1.773506
14	1	0	-2.786995	2.211409	-0.737513
15	1	0	0.338004	2.805308	3.028609
16	1	0	-0.218722	4.764727	-0.652648
17	6	0	-0.334685	-1.779701	0.001752
18	6	0	-4.849923	-0.150116	1.093093
19	6	0	-3.539981	-0.455687	1.434614
20	6	0	-2.820949	-1.413340	0.721188
21	6	0	-3.441640	-2.088275	-0.334527
22	6	0	-4.747236	-1.798329	-0.693623
23	6	0	-5.429681	-0.825357	0.028402
24	7	0	-6.811182	-0.505282	-0.347327
25	6	0	-1.397219	-1.742212	1.125166
26	8	0	-0.814388	-0.811035	2.002910
27	8	0	-7.394570	0.348263	0.290562
28	8	0	-7.305345	-1.108617	-1.278765
29	1	0	-5.418113	0.594105	1.633809
30	1	0	-3.048594	0.047203	2.257391
31	1	0	-2.888625	-2.837817	-0.891622
32	1	0	-5.236637	-2.303029	-1.515088
33	1	0	-1.440189	-2.757960	1.560737
34	6	0	0.357149	-3.064350	-0.318135
35	7	0	1.823428	-3.090604	0.087960
36	6	0	2.458760	-4.367013	-0.388085
37	6	0	3.864964	-4.472631	0.248650
38	7	0	4.300175	-3.165493	0.746025
39	6	0	4.082559	-2.170742	-0.311040
40	6	0	2.573675	-1.933900	-0.525512
41	6	0	1.974959	-3.029020	1.584043
42	6	0	3.470666	-2.801838	1.898901
43	1	0	2.497845	-4.307364	-1.476086
44	1	0	1.807160	-5.190990	-0.098561
45	1	0	4.576351	-4.836212	-0.493106
46	1	0	3.857280	-5.174540	1.083971
47	1	0	4.553938	-2.535285	-1.225516
48	1	0	4.553747	-1.228824	-0.033043
49	1	0	2.220960	-1.034467	-0.026227
50	1	0	2.287575	-1.875717	-1.573655
51	1	0	1.609206	-3.982972	1.968420
52	1	0	1.336208	-2.229075	1.957287
53	1	0	3.656408	-1.751905	2.132257
54	1	0	3.758611	-3.400795	2.763553
55	1	0	-1.224521	1.205214	1.405089
56	1	0	-0.096001	-3.908255	0.205106
57	1	0	0.363329	-3.272091	-1.390390
58	6	0	1.173187	5.163345	1.776183
59	1	0	0.789501	5.578914	2.705586
60	1	0	2.164101	4.739659	1.922237
61	1	0	1.212819	5.938151	1.014665
62	1	0	0.073588	-0.992520	0.988453
63	15	0	2.821493	1.826635	-0.682321
64	9	0	2.672320	2.984518	0.448166
65	9	0	1.950910	2.727150	-1.718450
66	9	0	1.451024	1.130331	-0.152869
67	9	0	2.977882	0.668306	-1.804295
68	9	0	3.676373	0.923566	0.367541
69	9	0	4.184808	2.522782	-1.208428

Structure 32 – Solvent: Acetonitrile



Zero-point correction= 0.549238
Thermal correction to Energy= 0.585219
Thermal correction to Enthalpy= 0.586163
Thermal correction to Gibbs Free Energy= 0.479874
Sum of electronic and zero-point Energies= -2446.012176
Sum of electronic and thermal Energies= -2445.976195
Sum of electronic and thermal Enthalpies= -2445.975251
Sum of electronic and thermal Free Energies= -2446.081540

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.237133	-1.082664	1.637634
2	8	0	-0.356062	-1.259268	2.707788
3	8	0	1.048044	0.045406	1.507819
4	6	0	0.922657	0.982488	2.560058
5	6	0	1.827796	2.149781	2.229480
6	7	0	1.402475	2.811867	0.993668
7	6	0	1.718420	2.396494	-0.278794
8	6	0	1.045412	3.205652	-1.136212
9	7	0	0.325907	4.093813	-0.369440
10	6	0	0.549130	3.828821	0.912034
11	1	0	-0.115363	1.315518	2.645202
12	1	0	1.232281	0.549454	3.513556
13	1	0	1.808318	2.887152	3.031047
14	1	0	2.854527	1.815805	2.081469
15	1	0	1.004145	3.221691	-2.211040
16	1	0	0.109067	4.350203	1.746135
17	6	0	0.208956	-1.874219	0.484640
18	6	0	4.555639	-0.485663	-1.497412
19	6	0	3.173104	-0.584823	-1.558113
20	6	0	2.462551	-1.353621	-0.630963
21	6	0	3.171213	-2.047688	0.352210
22	6	0	4.553270	-1.965135	0.429981
23	6	0	5.223023	-1.178810	-0.497310
24	7	0	6.685888	-1.078968	-0.419489
25	6	0	0.943062	-1.493867	-0.763599
26	8	0	0.419350	-0.331217	-1.428248
27	8	0	7.256869	-0.398872	-1.247955
28	8	0	7.252921	-1.681579	0.469298
29	1	0	5.112846	0.110900	-2.206356
30	1	0	2.627342	-0.052712	-2.326981
31	1	0	2.623424	-2.645288	1.070278
32	1	0	5.109464	-2.490245	1.194194
33	1	0	0.802411	-2.319720	-1.484317
34	6	0	-0.600872	-3.094695	0.539417
35	7	0	-2.096031	-2.944992	0.089536
36	6	0	-2.797014	-4.254529	0.256480
37	6	0	-4.261349	-4.106197	-0.233644
38	7	0	-4.541006	-2.729201	-0.638296
39	6	0	-4.272485	-1.834155	0.490266
40	6	0	-2.790253	-1.914420	0.929080
41	6	0	-2.167167	-2.531743	-1.348902
42	6	0	-3.656245	-2.368294	-1.747172
43	1	0	-2.738435	-4.512357	1.314130
44	1	0	-2.239652	-4.995603	-0.317305
45	1	0	-4.951814	-4.385533	0.562926
46	1	0	-4.443030	-4.762230	-1.085904
47	1	0	-4.927926	-2.115840	1.315904
48	1	0	-4.509562	-0.812504	0.194006
49	1	0	-2.260051	-0.978502	0.775123
50	1	0	-2.662587	-2.217661	1.967217
51	1	0	-1.669118	-3.315150	-1.923156
52	1	0	-1.606848	-1.601569	-1.438996
53	1	0	-3.853380	-1.332242	-2.020356
54	1	0	-3.889965	-3.004573	-2.601915
55	1	0	2.368432	1.556022	-0.450449
56	1	0	-0.233154	-3.890582	-0.114221
57	1	0	-0.693616	-3.472855	1.559595
58	6	0	-0.519091	5.171706	-0.880514
59	1	0	0.109759	5.980679	-1.247591
60	1	0	-1.136852	4.768840	-1.678173
61	1	0	-1.155633	5.521255	-0.072428
62	1	0	0.087928	0.254442	-0.734402
63	15	0	-2.577934	1.904063	-0.236068
64	9	0	-1.871587	2.548206	-1.547935
65	9	0	-2.407256	3.311117	0.552066
66	9	0	-1.110663	1.434360	0.314214
67	9	0	-3.265541	1.243665	1.075131
68	9	0	-2.724407	0.490308	-1.023910
69	9	0	-4.027755	2.367150	-0.777288