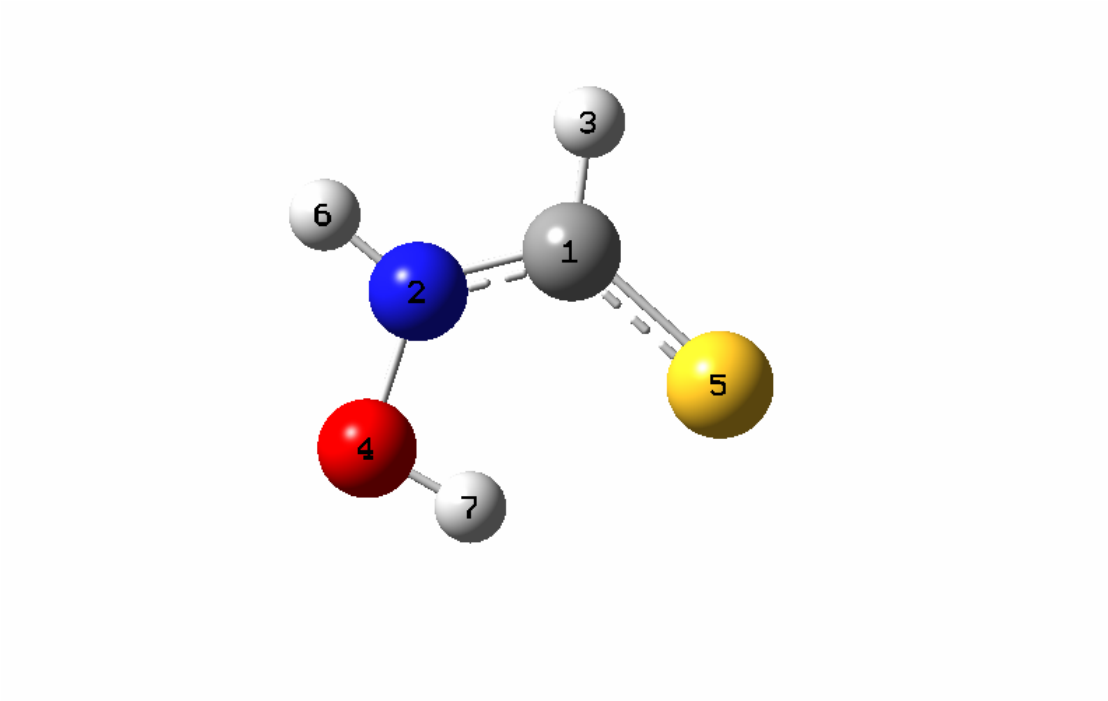
1Zc



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.140452	0.852177	0.000001
2	7	0	-1.144247	0.517986	-0.000001
3	1	0	0.288781	1.933335	-0.000001
4	8	0	-1.570802	-0.794170	0.000000
5	16	0	1.379817	-0.262046	0.000000
6	1	0	-1.925363	1.158501	-0.000001
7	1	0	-0.707060	-1.284693	0.000003

Zero-point correction= 0.047586 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.020073
E(RB+HF-LYP) = -568.116983527 A.U.

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7
1. C	0.0000						
2. N	1.3032	0.0000					
3. H	0.8661	0.0060	0.0000				
4. O	0.0767	1.0054	0.0190	0.0000			
5. S	1.6543	0.2525	0.0570	0.0440	0.0000		
6. H	0.0045	0.7884	0.0002	0.0048	0.0163	0.0000	
7. H	0.0009	0.0035	0.0017	0.7095	0.0359	0.0067	0.0000

Wiberg bond index, Totals by atom:

Atom	1
1. C	3.9057
2. N	3.3591

3. H 0.9500
4. O 1.8593
5. S 2.0600
6. H 0.8209
7. H 0.7583

Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.133972	0.837894	0.000319
2	7	0	-1.138536	0.514345	-0.000031
3	1	0	0.277823	1.922575	0.000135
4	8	0	-1.622358	-0.772268	-0.000170
5	16	0	1.412141	-0.263418	-0.000107
6	1	0	-1.909546	1.198684	-0.000619
7	1	0	-0.817751	-1.356216	0.001854

Total free energy in solution with all non electrostatic terms (a.u.) = -568.133414

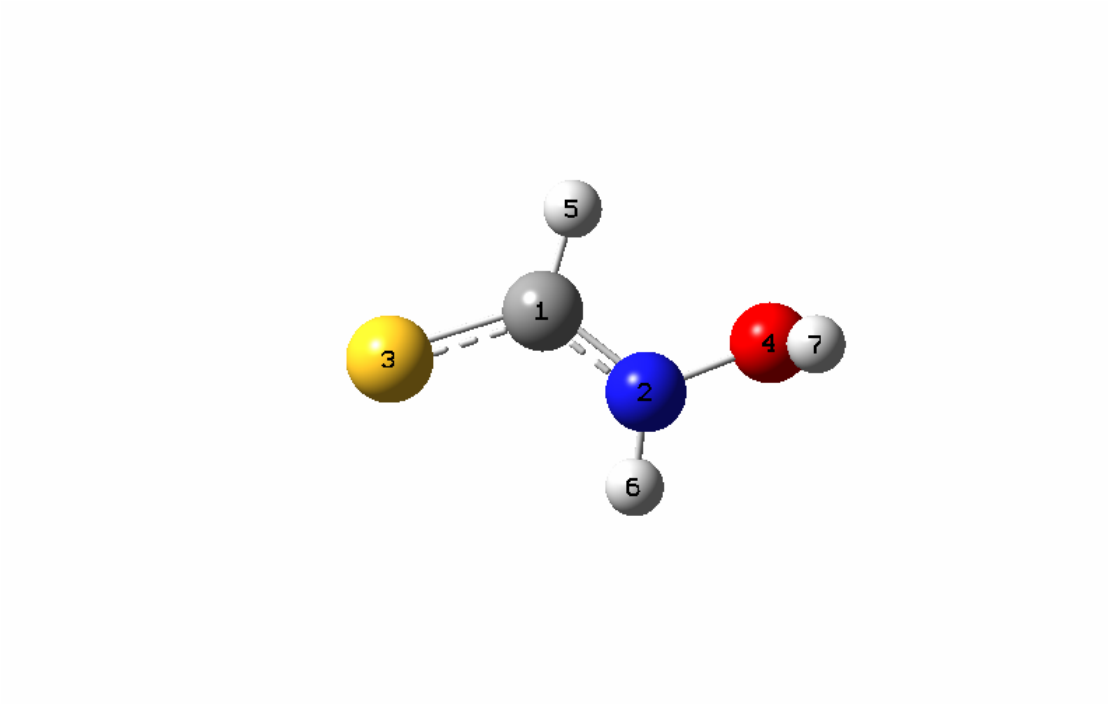
Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7
1. C	0.0000						
2. N	1.4342	0.0000					
3. H	0.8807	0.0080	0.0000				
4. O	0.1006	1.0189	0.0168	0.0000			
5. S	1.4767	0.2167	0.0417	0.0446	0.0000		
6. H	0.0063	0.7530	0.0018	0.0084	0.0193	0.0000	
7. H	0.0017	0.0050	0.0019	0.6915	0.0367	0.0072	0.0000

Wiberg bond index, Totals by atom:

Atom	1
1. C	3.9001
2. N	3.4358
3. H	0.9508
4. O	1.8807
5. S	1.8357
6. H	0.7959
7. H	0.7439

1Et



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.125149	0.436186	0.044877
2	7	0	0.933299	-0.395484	0.125436
3	16	0	-1.695413	-0.058179	-0.022152
4	8	0	2.208183	0.109141	-0.175444
5	1	0	0.181281	1.484359	0.072984
6	1	0	0.816773	-1.370622	-0.138353
7	1	0	2.680904	0.095277	0.676037

Zero-point correction= 0.047694 (Hartree/Particle)
E(RB+HF-LYP) = -568.110665707 A.U.

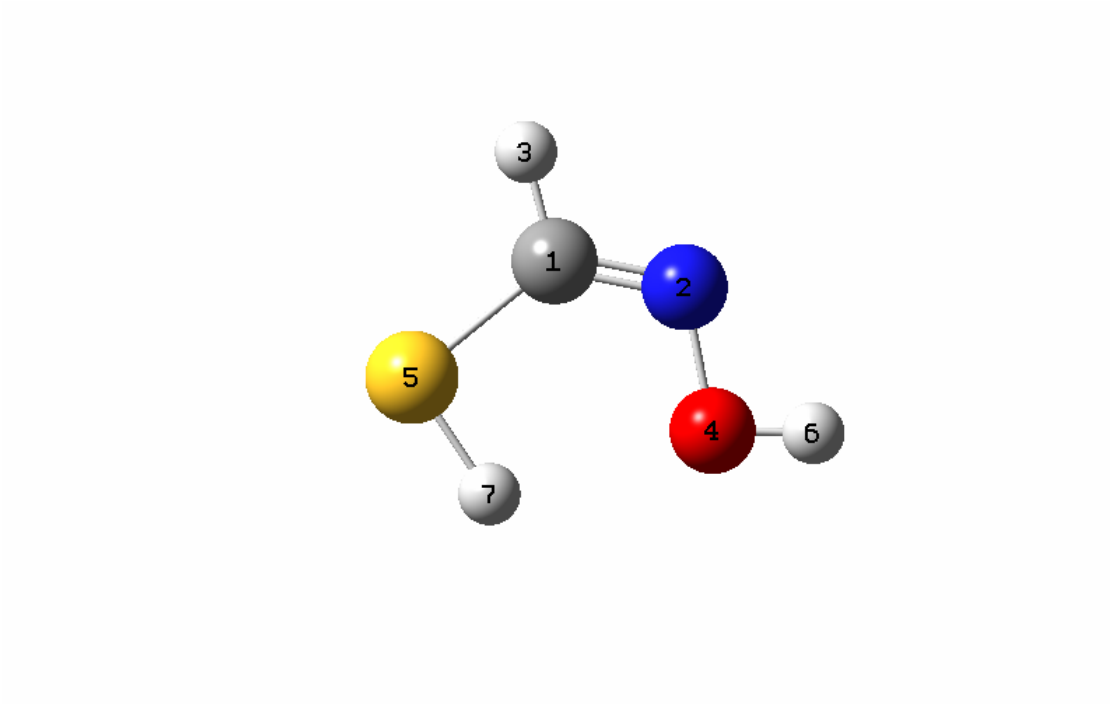
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.101849	0.430354	0.011978
2	7	0	0.933549	-0.385066	0.015260
3	16	0	-1.710074	-0.057299	0.000830
4	8	0	2.219918	0.118654	-0.117425
5	1	0	0.191348	1.485239	0.023756
6	1	0	0.849769	-1.411916	-0.057535
7	1	0	2.636972	0.007562	0.781211

Total free energy in solution with all non electrostatic terms a.u.)
= -568.132625

2Ztc



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.014828	0.888591	0.000000
2	7	0	1.238917	0.637851	0.000000
3	1	0	-0.289327	1.939225	0.000000
4	8	0	1.506321	-0.743071	0.000000
5	16	0	-1.386227	-0.229553	0.000000
6	1	0	2.475994	-0.765642	0.000000
7	1	0	-0.641064	-1.352667	0.000000

Zero-point correction= 0.044694 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.017073
E(RB+HF-LYP) = -568.114317993 A.U.

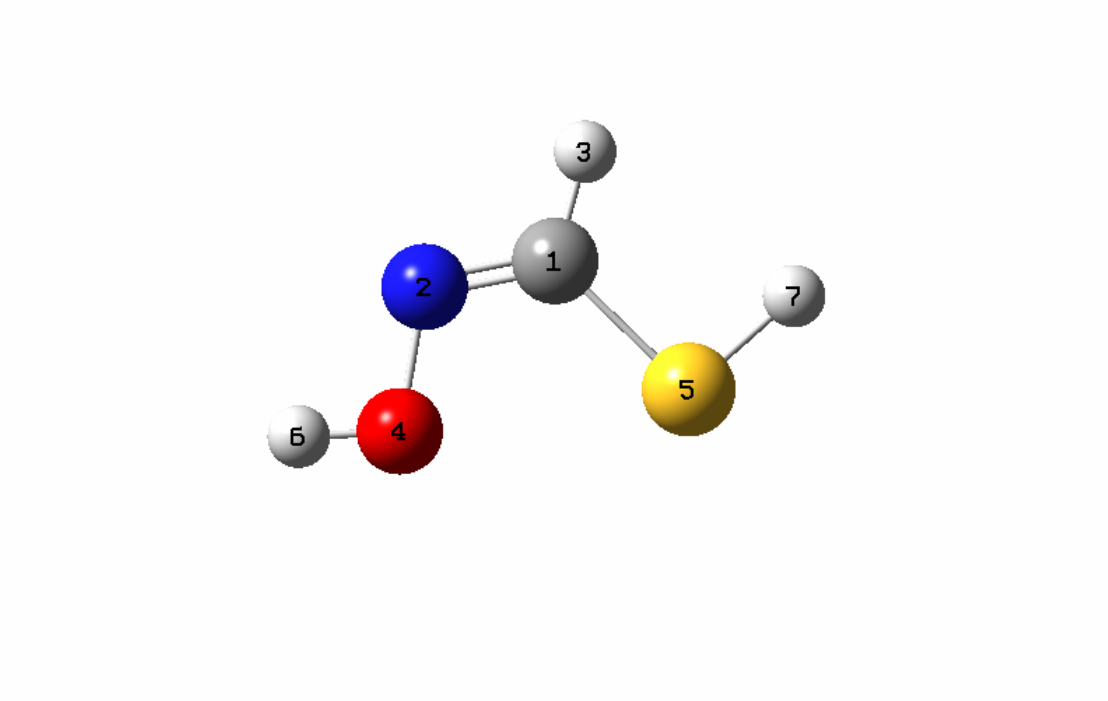
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.884074	0.000000
2	7	0	1.250921	0.613207	0.000000
3	1	0	-0.266787	1.941194	0.000000
4	8	0	1.514272	-0.761884	0.000000
5	16	0	-1.398775	-0.203610	0.000000
6	1	0	2.502622	-0.799984	0.000000
7	1	0	-0.726065	-1.385274	0.000000

Total free energy in solution with all non electrostatic terms (a.u.)
= -568.124861

2Ztt



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.002217	0.887305	-0.000058
2	7	0	-1.249032	0.637910	-0.000012
3	1	0	0.289494	1.933703	0.000159
4	8	0	-1.486845	-0.744899	0.000029
5	16	0	1.281264	-0.344873	-0.000018
6	1	0	-2.455424	-0.796124	0.000036
7	1	0	2.290383	0.550367	0.000285

Zero-point correction= 0.044872 (Hartree/Particle)
E(RB+HF-LYP) = -568.113220526 A.U.

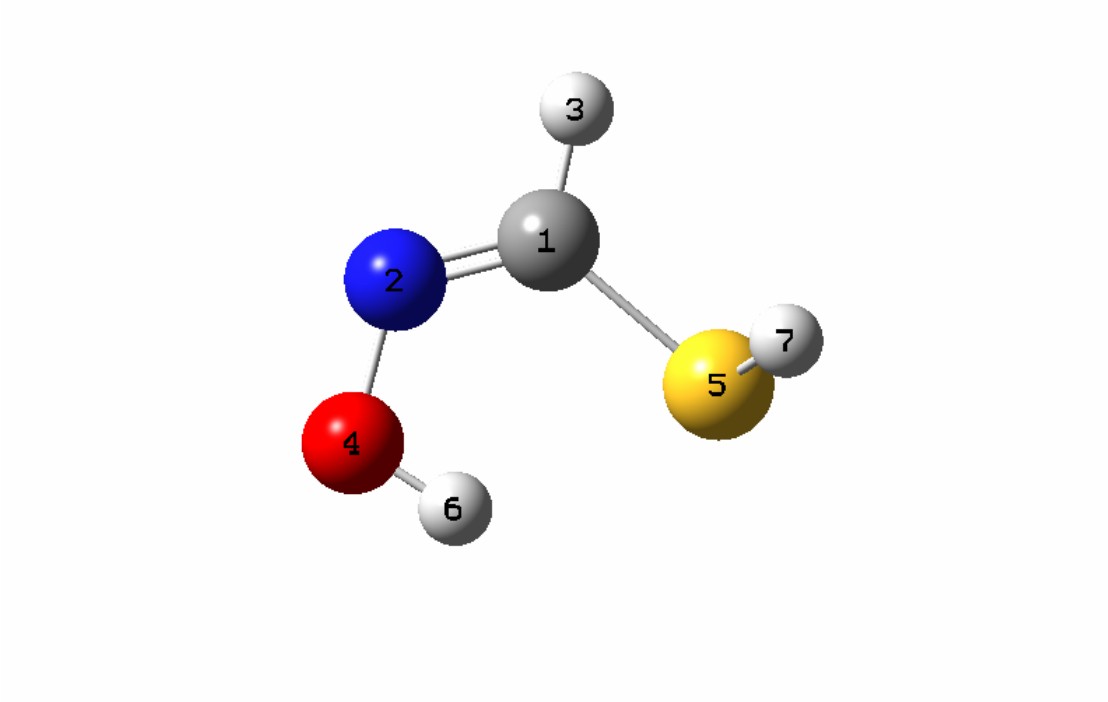
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.008417	0.888318	-0.000077
2	7	0	-1.245381	0.639898	-0.000005
3	1	0	0.310091	1.934966	-0.000209
4	8	0	-1.498144	-0.739561	0.000068
5	16	0	1.281948	-0.348695	-0.000106
6	1	0	-2.485413	-0.790875	0.000267
7	1	0	2.316475	0.542318	0.001586

Total free energy in solution with all non electrostatic terms (a.u.) = -568.127164

2Zct



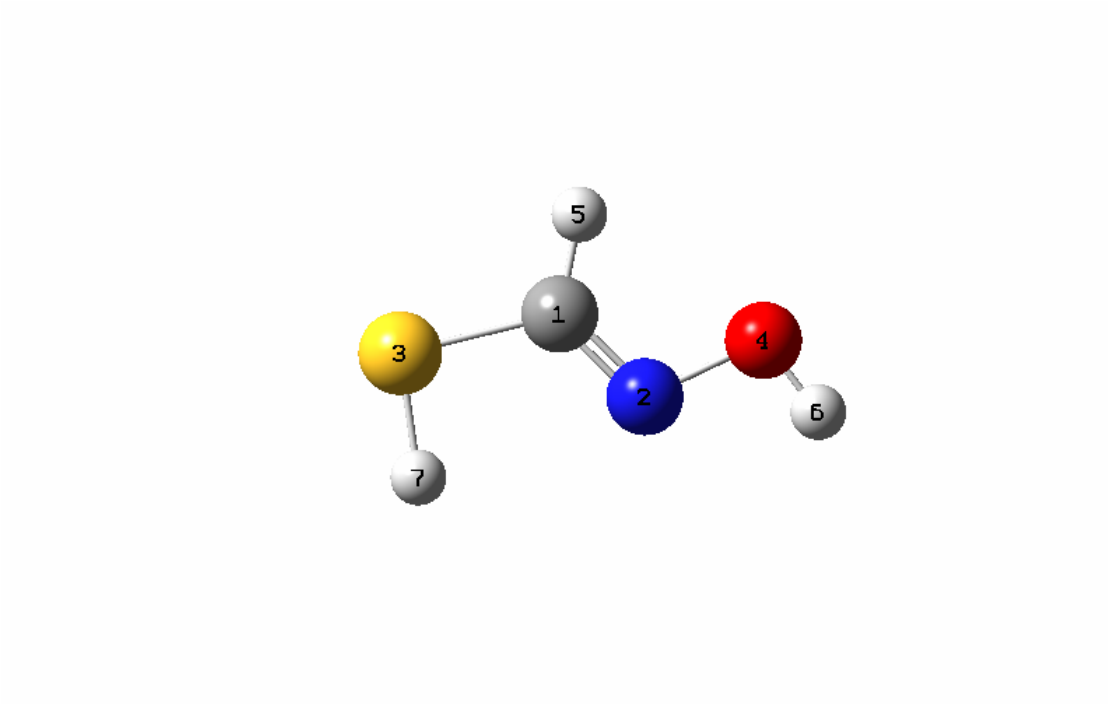
Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.053665	0.900231	-0.012252
2	7	0	-1.290252	0.578905	-0.004108
3	1	0	0.176116	1.960540	-0.036408
4	8	0	-1.634006	-0.740651	0.025005
5	16	0	1.324135	-0.269000	-0.079543
6	1	0	-0.806405	-1.272763	0.107486
7	1	0	1.869928	0.087705	1.103848

Zero-point correction= 0.044182 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.016288
E(RB+HF-LYP) = -568.103457332 A.U.

2Etc



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.051087	0.423982	-0.000650
2	7	0	0.965823	-0.465155	-0.000509
3	16	0	-1.663643	0.003164	0.000233
4	8	0	2.240864	0.141223	0.000371
5	1	0	0.262085	1.494385	-0.000044
6	1	0	2.830127	-0.629469	0.001024
7	1	0	-1.468121	-1.333139	-0.000208

Zero-point correction= 0.044197 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.016718
E(RB+HF-LYP) = -568.109420251 A.U.

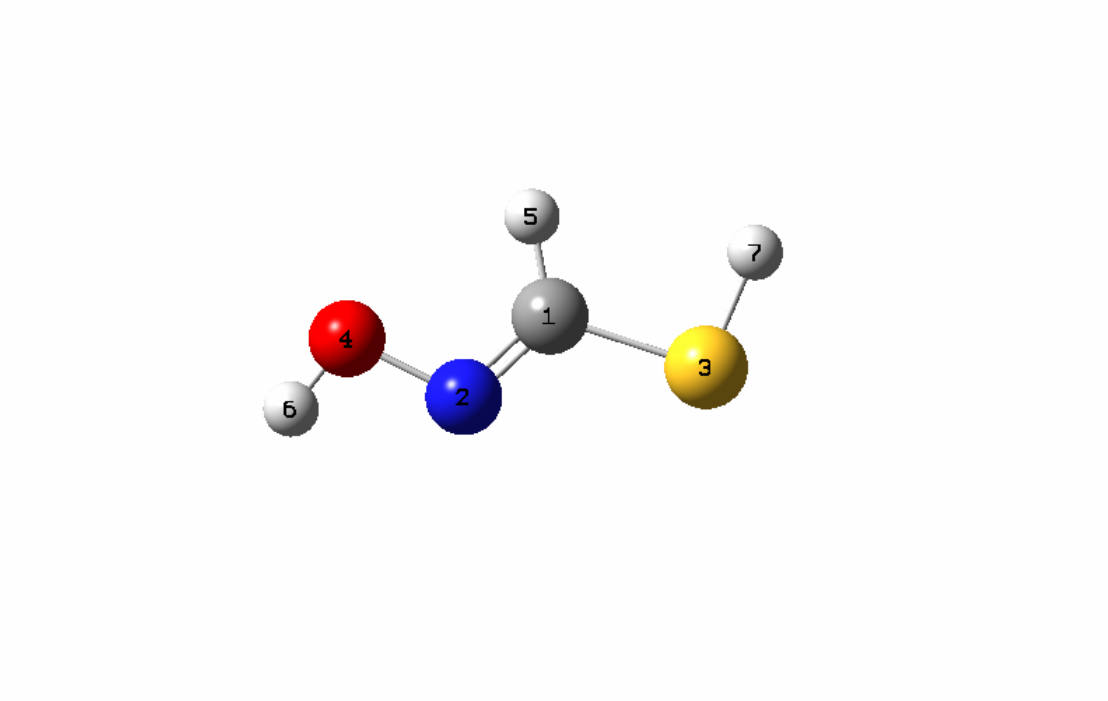
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.050269	0.422012	0.000623
2	7	0	-0.970384	-0.464643	0.000331
3	16	0	1.666154	0.004774	-0.000240
4	8	0	-2.244767	0.142107	-0.000225
5	1	0	-0.255184	1.497713	0.000046
6	1	0	-2.853286	-0.635638	-0.001261
7	1	0	1.502446	-1.354890	0.000810

Total free energy in solution with all non electrostatic terms a.u.)
= -568.121412

2Ett



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.053529	0.403397	-0.000259
2	7	0	-0.983503	-0.467787	0.001926
3	16	0	1.631191	-0.149767	-0.000881
4	8	0	-2.244591	0.160231	-0.001001
5	1	0	-0.247912	1.477076	-0.003104
6	1	0	-2.848709	-0.598894	0.002249
7	1	0	2.159992	1.090374	0.011039

Zero-point correction= 0.043868 (Hartree/Particle)
E(RB+HF-LYP) = -568.108035637 A.U.

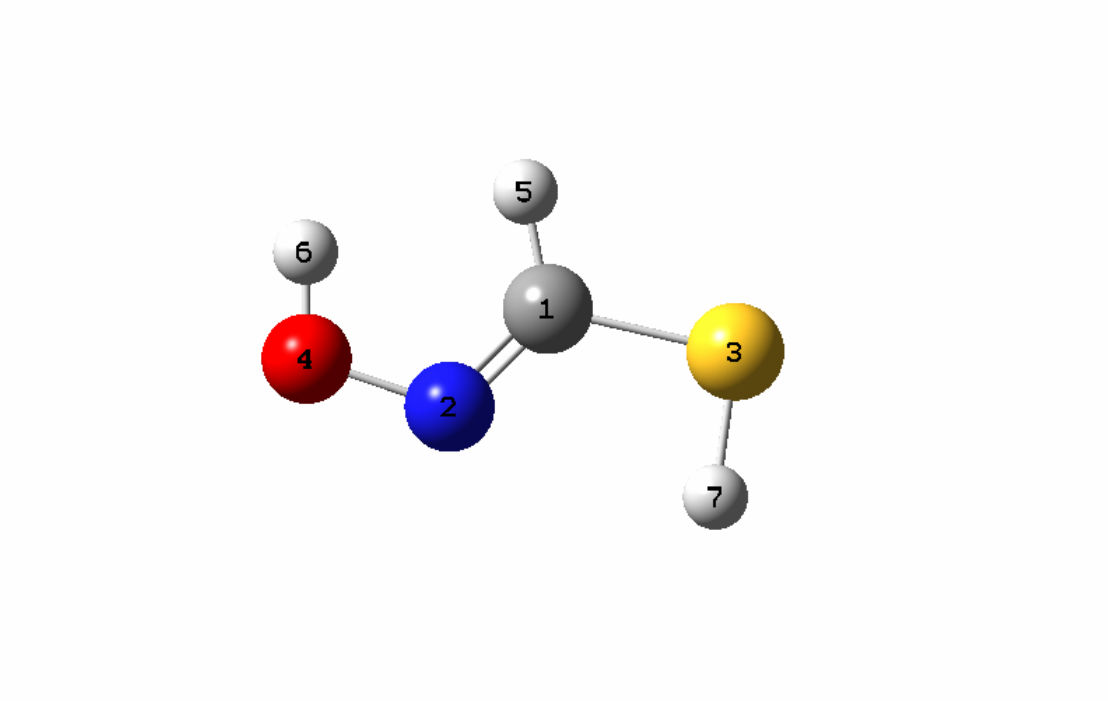
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.050769	0.405493	0.000103
2	7	0	-0.986054	-0.464016	0.001774
3	16	0	1.632064	-0.152645	-0.000823
4	8	0	-2.248585	0.160431	-0.001067
5	1	0	-0.232364	1.484967	-0.002628
6	1	0	-2.870045	-0.607132	0.002121
7	1	0	2.185058	1.096184	0.009177

Total free energy in solution with all non electrostatic terms (a.u.)
= -568.121245

2Ecc



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.065640	0.409817	-0.000049
2	7	0	-0.969375	-0.490233	-0.000045
3	16	0	1.659419	0.016483	0.000021
4	8	0	-2.285171	-0.048702	0.000025
5	1	0	-0.271329	1.486934	-0.000143
6	1	0	-2.294338	0.932742	0.000204
7	1	0	1.475802	-1.321068	0.000006

Zero-point correction= 0.043761 (Hartree/Particle)
E(RB+HF-LYP) = -568.100876963 A.U.

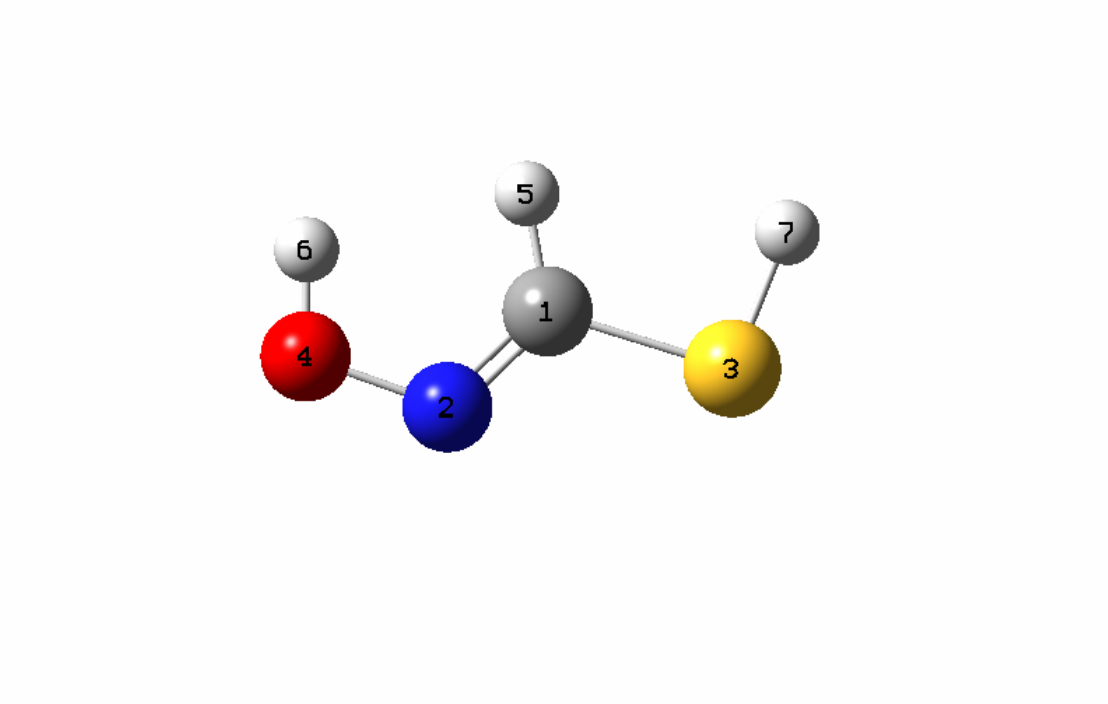
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.065351	0.406735	-0.000036
2	7	0	-0.969186	-0.496670	-0.000073
3	16	0	1.660821	0.020616	-0.000002
4	8	0	-2.290514	-0.048259	0.000027
5	1	0	-0.278678	1.484531	0.000068
6	1	0	-2.310873	0.949319	0.000170
7	1	0	1.516942	-1.341358	0.000309

Total free energy in solution with all non electrostatic terms (a.u.)
= -568.116787

2Ect



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.068044	0.388319	-0.000262
2	7	0	-0.987965	-0.493066	0.002743
3	16	0	1.628849	-0.137140	-0.001344
4	8	0	-2.291462	-0.027527	-0.000381
5	1	0	-0.258286	1.468756	-0.004132
6	1	0	-2.282009	0.954379	-0.005031
7	1	0	2.134424	1.112875	0.016096

Zero-point correction= 0.043259 (Hartree/Particle)
E(RB+HF-LYP) = -568.099137411 A.U.

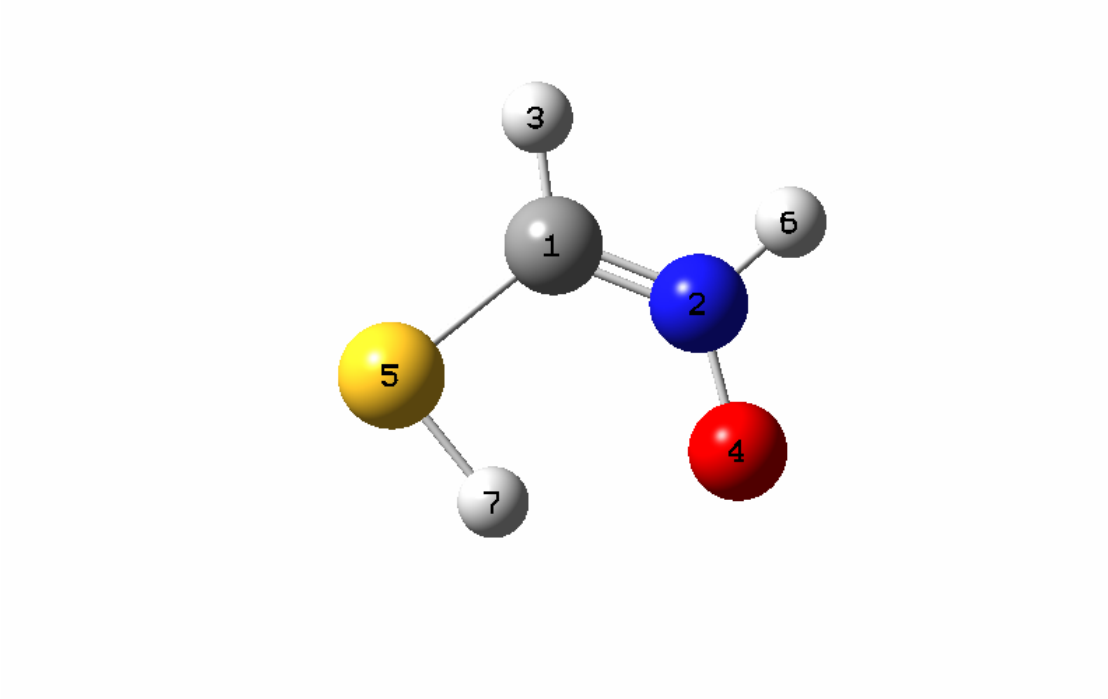
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.065706	0.388976	-0.000174
2	7	0	-0.986194	-0.496210	0.002513
3	16	0	1.629536	-0.137747	-0.001260
4	8	0	-2.297037	-0.027560	-0.000305
5	1	0	-0.255326	1.470801	-0.003662
6	1	0	-2.299943	0.970696	-0.005081
7	1	0	2.156586	1.122550	0.014795

Total free energy in solution with all non electrostatic terms (a.u.)
= -568.116602

3tc



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.012635	0.888093	0.000000
2	7	0	1.205900	0.402439	0.000000
3	1	0	-0.149929	1.960877	-0.000001
4	8	0	1.532641	-0.836763	0.000000
5	16	0	-1.370869	-0.201910	0.000000
6	1	0	1.976002	1.082598	0.000000
7	1	0	-0.518795	-1.264441	0.000002

Zero-point correction= 0.045197 (Hartree/Particle)
E(RB+HF-LYP) = -568.100550790 A.U.

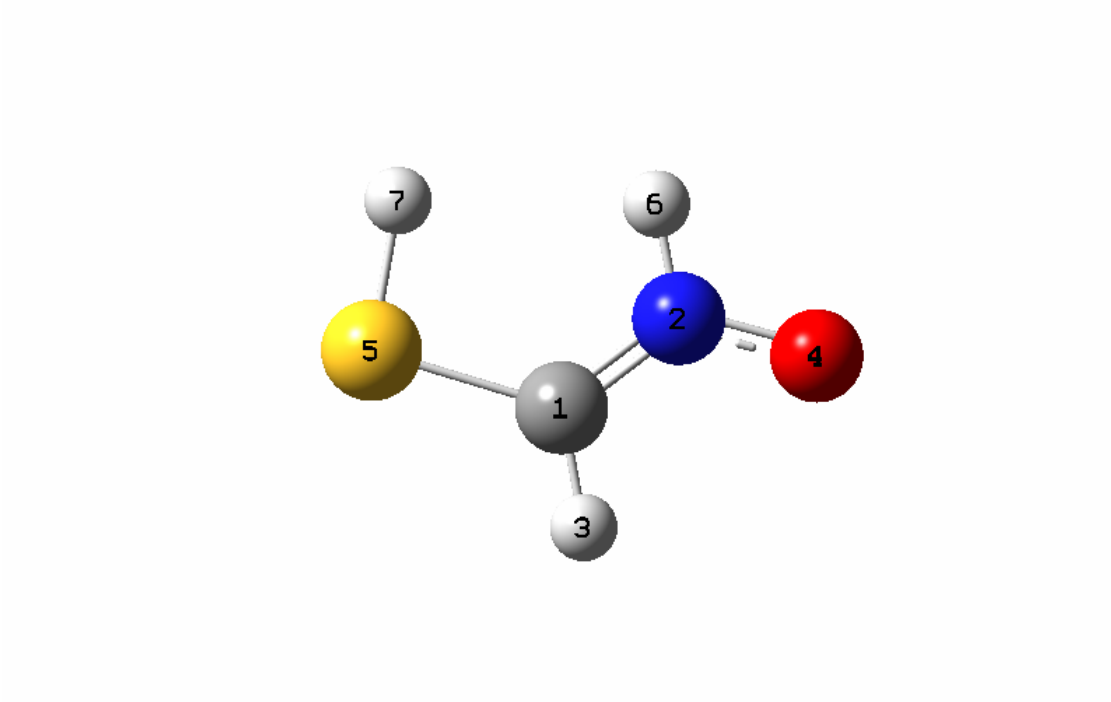
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.005184	0.867668	-0.000037
2	7	0	-1.215772	0.406878	0.000211
3	1	0	0.152570	1.944227	-0.000301
4	8	0	-1.571785	-0.835429	-0.000152
5	16	0	1.390107	-0.193684	-0.000024
6	1	0	-1.977987	1.116645	-0.000019
7	1	0	0.637281	-1.332654	0.000669

Total free energy in solution with all non electrostatic terms (a.u.)
= -568.117763

3cc



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.050420	-0.500163	0.000894
2	7	0	1.091444	0.294298	-0.000249
3	1	0	0.246782	-1.564883	0.001943
4	8	0	2.318151	-0.039112	-0.000137
5	16	0	-1.638994	0.010360	-0.000569
6	1	0	0.893624	1.310563	-0.002054
7	1	0	-1.404336	1.342342	0.006688

Zero-point correction= 0.044308 (Hartree/Particle)
E(RB+HF-LYP) = -568.088264611 A.U.

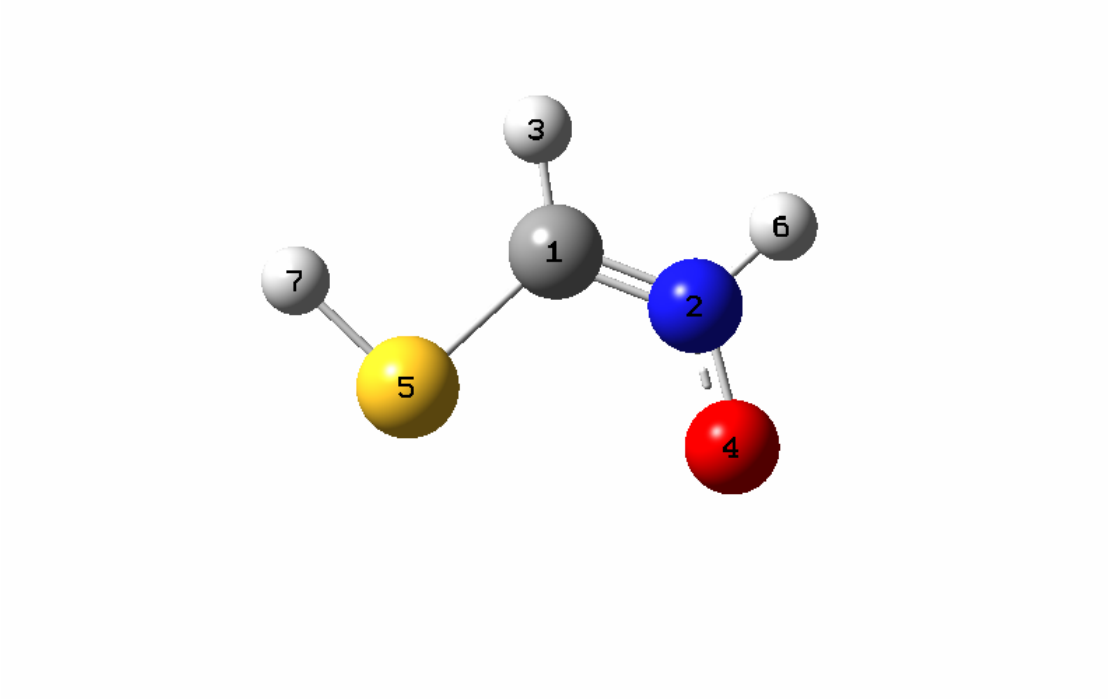
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.051235	-0.496183	0.000396
2	7	0	1.078601	0.305412	-0.000471
3	1	0	0.247094	-1.566745	0.001399
4	8	0	2.322246	-0.047250	0.000167
5	16	0	-1.634863	0.005748	-0.000317
6	1	0	0.887186	1.332247	-0.001615
7	1	0	-1.412062	1.359736	0.004870

Total free energy in solution with all non electrostatic terms (a.u.)
= -568.111607

3tt



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.007351	0.870078	-0.000038
2	7	0	1.226148	0.397801	-0.000211
3	1	0	-0.149946	1.940683	0.000554
4	8	0	1.546275	-0.834617	0.000149
5	16	0	-1.285846	-0.310994	-0.000045
6	1	0	1.991395	1.088039	0.000150
7	1	0	-2.265251	0.619051	0.000519

Zero-point correction= 0.045496 (Hartree/Particle)
E(RB+HF-LYP) = -568.096567498 A.U.

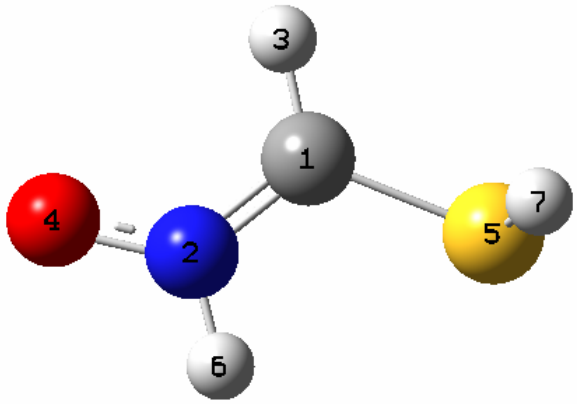
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.007886	0.864420	-0.000311
2	7	0	-1.226579	0.409337	-0.001128
3	1	0	0.163874	1.937403	0.002807
4	8	0	-1.553356	-0.841461	0.000494
5	16	0	1.287777	-0.311344	0.000022
6	1	0	-1.998914	1.107956	0.002460
7	1	0	2.290837	0.615958	0.000189

Total free energy in solution with all non electrostatic terms (a.u.)
= -568.119226

3ct



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.050104	0.544122	-0.005468
2	7	0	-1.075165	-0.280799	0.033735
3	1	0	-0.275087	1.600934	-0.087164
4	8	0	-2.298442	0.002533	-0.005432
5	16	0	1.582890	-0.112632	-0.084390
6	1	0	-0.824149	-1.284753	0.097163
7	1	0	1.987312	0.166529	1.180365

Zero-point correction= 0.045089 (Hartree/Particle)
E(RB+HF-LYP) = -568.092949466 A.U.

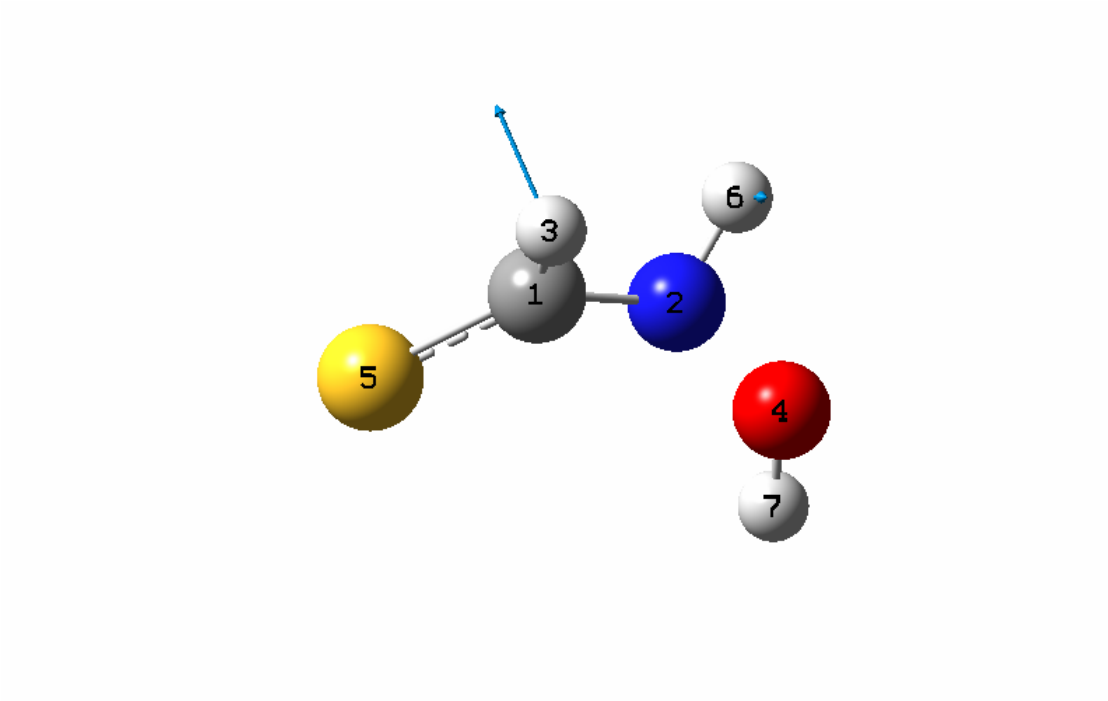
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.053981	0.517317	-0.027382
2	7	0	-1.076051	-0.292215	0.058883
3	1	0	-0.264743	1.577653	-0.153550
4	8	0	-2.311015	0.029255	-0.016287
5	16	0	1.586896	-0.131321	-0.073087
6	1	0	-0.865389	-1.309331	0.191067
7	1	0	2.084157	0.540377	1.014295

Total free energy in solution with all non electrostatic terms (a.u.)
= -568.110493

TS1



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.150747	0.500538	0.337709
2	7	0	1.022077	0.430362	-0.497682
3	1	0	-0.033268	1.033203	1.288565
4	8	0	1.906193	-0.478330	0.234187
5	16	0	-1.552004	-0.203274	-0.061631
6	1	0	1.530452	1.313917	-0.413034
7	1	0	1.835283	-1.283855	-0.305421

Zero-point correction= 0.046718 (Hartree/Particle)
E(RB+HF-LYP) = -568.078851753 A.U.

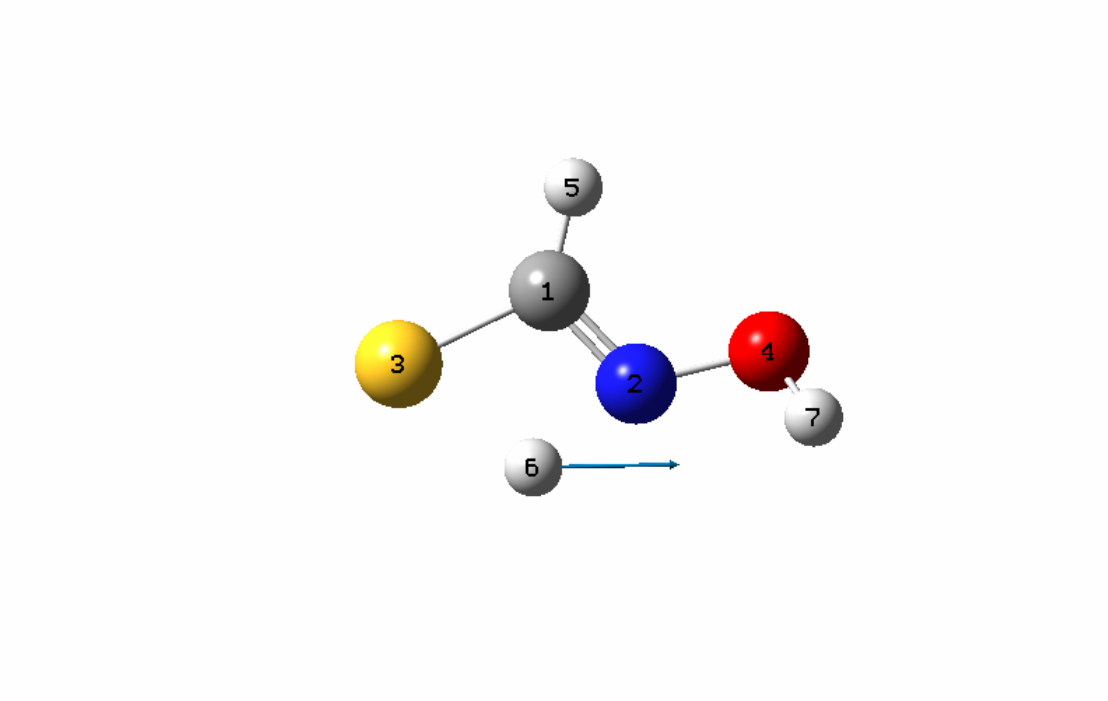
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.137416	0.509803	0.340295
2	7	0	1.027727	0.446791	-0.498992
3	1	0	-0.026119	1.044568	1.292918
4	8	0	1.881893	-0.498524	0.227876
5	16	0	-1.543113	-0.202410	-0.062799
6	1	0	1.551054	1.330032	-0.377569
7	1	0	1.740128	-1.334206	-0.282407

Total free energy in solution with all non electrostatic terms (a.u.)
= -568.093320

TS2



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.057087	0.642487	0.049201
2	7	0	0.831106	-0.308941	0.048687
3	16	0	-1.601658	-0.109003	-0.015559
4	8	0	2.192200	0.021434	-0.103958
5	1	0	0.187875	1.700561	0.071744
6	1	0	-0.222971	-1.166641	-0.054656
7	1	0	2.648808	-0.653684	0.427507

Zero-point correction= 0.040974 (Hartree/Particle)
E(RB+HF-LYP) = -568.055577584 A.U.

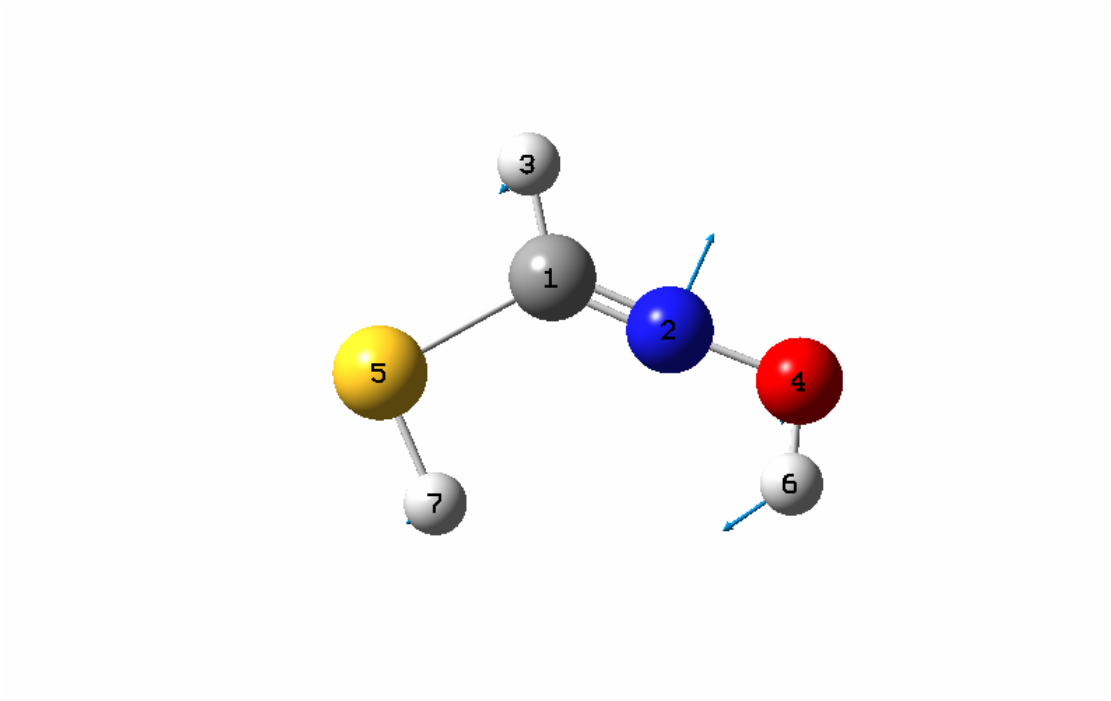
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.046941	0.658864	0.042344
2	7	0	0.827868	-0.297707	0.023972
3	16	0	-1.599076	-0.114185	-0.010229
4	8	0	2.189351	0.010546	-0.088105
5	1	0	0.186150	1.718916	0.065051
6	1	0	-0.256306	-1.155986	-0.048511
7	1	0	2.627130	-0.689581	0.430096

Total free energy in solution with all non electrostatic terms (a.u.)
= -568.058899

TS3



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.033357	0.722446	-0.000192
2	7	0	1.083792	0.223450	0.001855
3	1	0	-0.257532	1.800674	-0.001176
4	8	0	2.315849	-0.261935	-0.000993
5	16	0	-1.671775	-0.183479	-0.000292
6	1	0	2.239333	-1.240833	-0.000465
7	1	0	-1.146594	-1.427526	0.002428

Zero-point correction= 0.042368 (Hartree/Particle)
E(RB+HF-LYP) = -568.031848726 A.U.

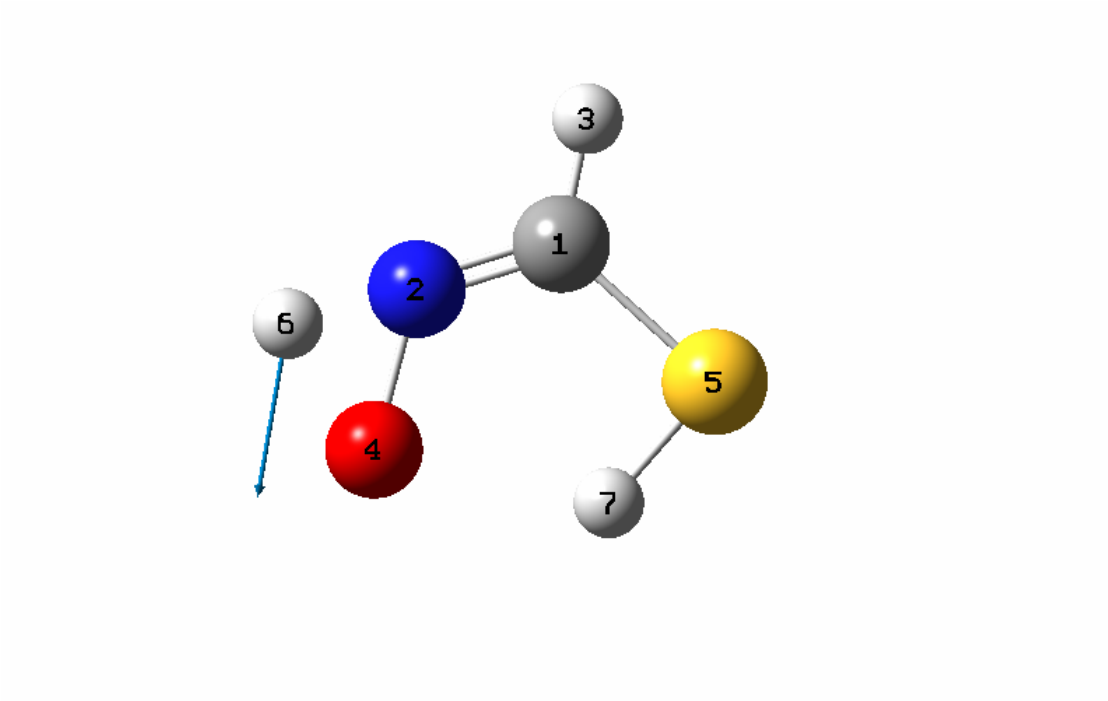
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.017256	0.736512	-0.000572
2	7	0	1.086715	0.218885	0.002841
3	1	0	-0.246940	1.811059	-0.002606
4	8	0	2.316692	-0.267441	-0.001552
5	16	0	-1.679393	-0.184199	-0.000134
6	1	0	2.240471	-1.246444	0.001079
7	1	0	-1.160242	-1.429175	-0.000365

Total free energy in solution with all non electrostatic terms (a.u.)
= -568.033953

TS4



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.053479	0.929602	0.000146
2	7	0	-1.171176	0.545784	-0.000199
3	1	0	0.276442	1.990364	0.000494
4	8	0	-1.534465	-0.814946	-0.000105
5	16	0	1.355359	-0.240998	-0.000105
6	1	0	-2.265792	0.253181	0.000728
7	1	0	0.456687	-1.266108	0.001825

Zero-point correction= 0.038399 (Hartree/Particle)
E(RB+HF-LYP) = -568.029000176 A.U.

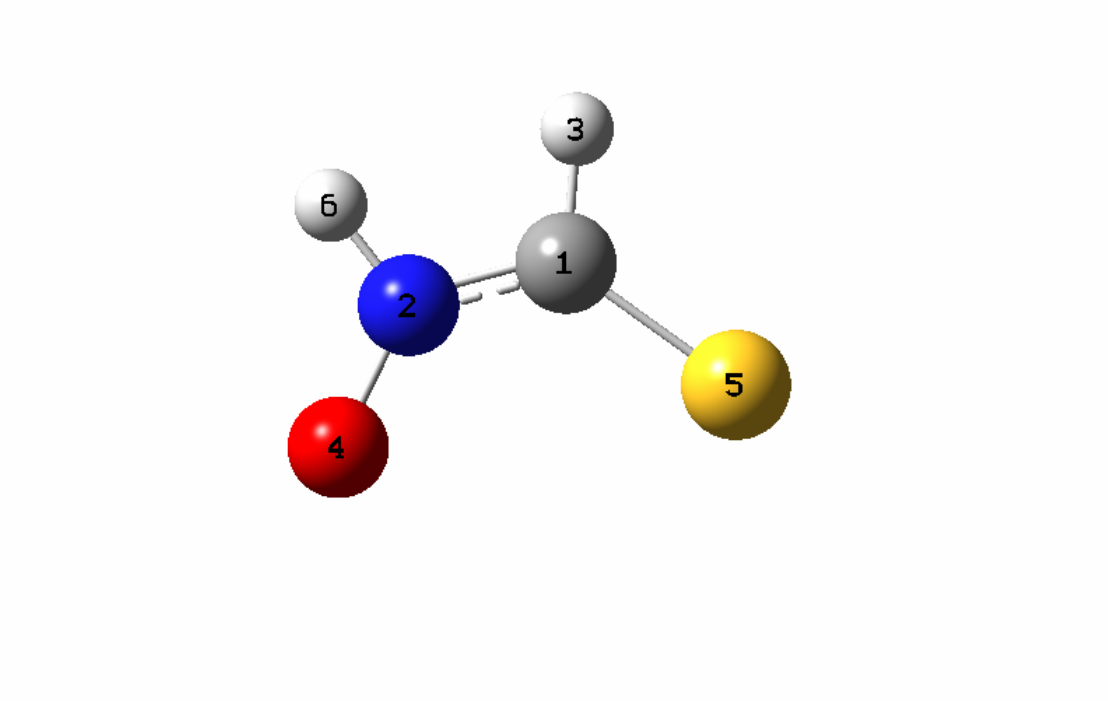
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.033651	0.913333	0.026495
2	7	0	-1.185211	0.528303	0.006987
3	1	0	0.249178	1.974154	0.081885
4	8	0	-1.578587	-0.815971	-0.034160
5	16	0	1.378574	-0.229471	-0.035637
6	1	0	-2.286854	0.289493	0.000940
7	1	0	0.703773	-1.242459	0.552766

Total free energy in solution with all non electrostatic terms a.u.)
= -568.030226

1Z-Oanion



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.089194	0.739298	0.000000
2	7	0	-1.195054	0.394433	0.000000
3	1	0	0.179958	1.833004	0.000001
4	8	0	-1.770113	-0.766743	0.000000
5	16	0	1.477576	-0.256666	0.000000
6	1	0	-1.830056	1.210779	0.000001

Zero-point correction= 0.035467 Hartree/Particle)
E(RB+HF-LYP) = -567.558703009 A.U.

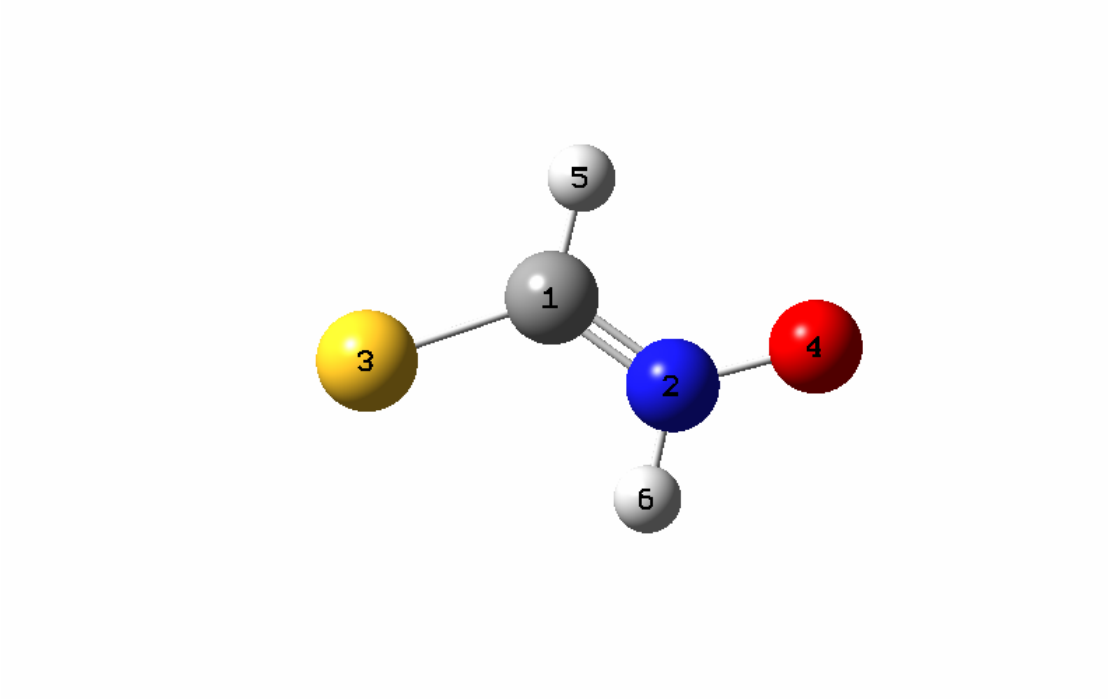
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.065154	0.784402	-0.000232
2	7	0	-1.194216	0.402315	0.000191
3	1	0	0.173884	1.870277	-0.000225
4	8	0	-1.678979	-0.808615	-0.000107
5	16	0	1.444821	-0.255926	0.000046
6	1	0	-1.890601	1.170843	0.000402

Total free energy in solution with all non electrostatic terms (a.u.)
= -567.665128

1E-Oanion



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.027464	0.474714	-0.000001
2	7	0	1.040261	-0.298528	0.000000
3	16	0	-1.663041	-0.082508	0.000000
4	8	0	2.304826	0.041524	0.000000
5	1	0	0.234332	1.534732	0.000001
6	1	0	0.818670	-1.305382	0.000000

Zero-point correction= 0.035566 (Hartree/Particle)
E(RB+HF-LYP) = -567.567237055 A.U.

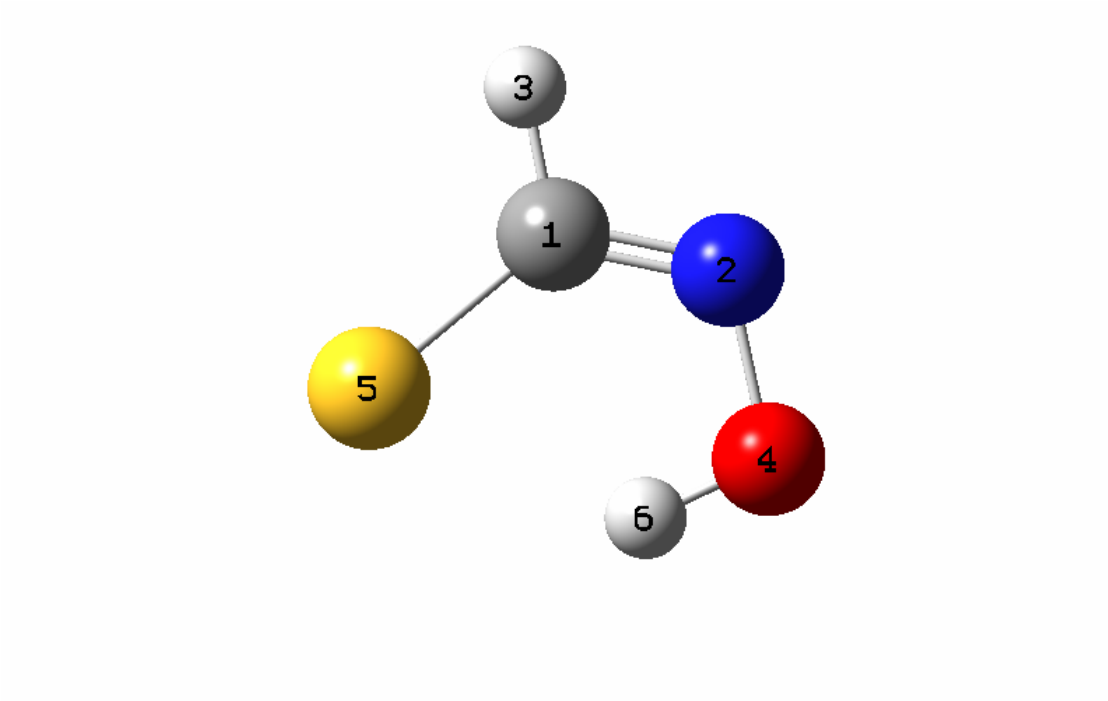
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.014527	0.470545	0.001047
2	7	0	-1.036382	-0.313374	0.000633
3	16	0	1.664197	-0.078637	-0.000331
4	8	0	-2.296726	0.053780	-0.000766
5	1	0	-0.237705	1.532932	-0.000244
6	1	0	-0.848131	-1.334638	0.000959

Total free energy in solution with all non electrostatic terms (a.u.)
= -567.662942

1Z-Nanion



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.010974	0.868428	0.000043
2	7	0	1.262086	0.610039	-0.000022
3	1	0	-0.218852	1.942764	-0.000019
4	8	0	1.558421	-0.770868	-0.000013
5	16	0	-1.354890	-0.253554	-0.000011
6	1	0	0.660953	-1.199785	0.000181

Zero-point correction= 0.035229 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.008268
E(RB+HF-LYP) = -567.581015618 A.U.
Wiberg bond index matrix in the NAO basis:

Atom		1	2	3	4	5	6
1.	C	0.0000	1.7268	0.9087	0.0933	1.2399	0.0018
2.	N	1.7268	0.0000	0.0157	1.0112	0.2336	0.0247
3.	H	0.9087	0.0157	0.0000	0.0234	0.0368	0.0021
4.	O	0.0933	1.0112	0.0234	0.0000	0.0510	0.6994
5.	S	1.2399	0.2336	0.0368	0.0510	0.0000	0.0695
6.	H	0.0018	0.0247	0.0021	0.6994	0.0695	0.0000

Wiberg bond index, Totals by atom:

Atom		1
1.	C	3.9705
2.	N	3.0119

```
   3.  H  0.9867
   4.  O  1.8783
   5.  S  1.6308
   6.  H  0.7975
```

Solution

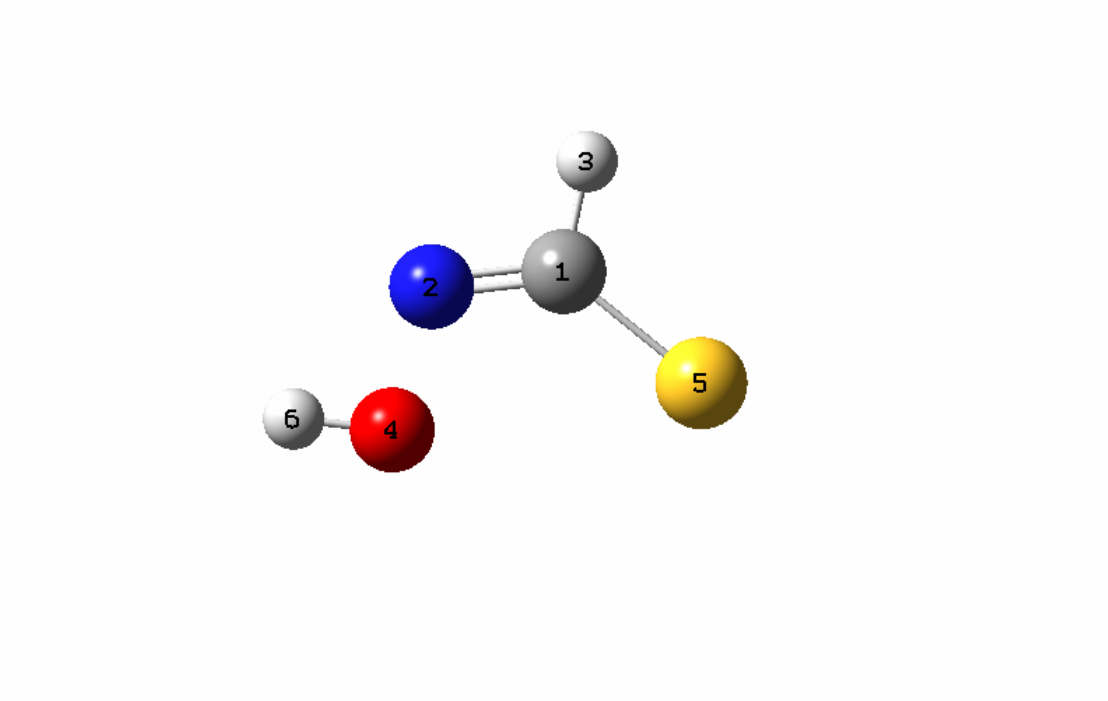
```
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0       -0.018125    0.873532    0.000615
   2          7             0        1.249856    0.611079   -0.000172
   3          1             0       -0.233690    1.945125   -0.000106
   4          8             0        1.578074   -0.757548   -0.000515
   5         16             0       -1.358976   -0.259987   -0.000205
   6          1             0        0.712476   -1.243689    0.005027
---------------------------------------------------------------------

Total free energy in solution with all non electrostatic terms (a.u.)
=    -567.669314
Wiberg bond index matrix in the NAO basis:

    Atom    1       2       3       4       5       6
    ---- ------  ------  ------  ------  ------  ------
  1.  C  0.0000  1.7320  0.8993  0.0952  1.2282  0.0017
  2.  N  1.7320  0.0000  0.0150  1.0092  0.2184  0.0225
  3.  H  0.8993  0.0150  0.0000  0.0222  0.0316  0.0017
  4.  O  0.0952  1.0092  0.0222  0.0000  0.0476  0.6945
  5.  S  1.2282  0.2184  0.0316  0.0476  0.0000  0.0626
  6.  H  0.0017  0.0225  0.0017  0.6945  0.0626  0.0000

Wiberg bond index, Totals by atom:
     Atom    1
    ---- ------
  1.  C  3.9565
  2.  N  2.9971
  3.  H  0.9699
  4.  O  1.8686
  5.  S  1.5883
  6.  H  0.7830
```

2Z-Sanion



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.086609	0.800575	0.000000
2	7	0	-1.205016	0.652429	0.000159
3	1	0	0.313938	1.875913	-0.000886
4	8	0	-1.590247	-0.746350	-0.000457
5	16	0	1.429811	-0.289769	0.000072
6	1	0	-2.553484	-0.639265	0.002284

Zero-point correction= 0.034871 (Hartree/Particle)
E(RB+HF-LYP) = -567.565725918 A.U.

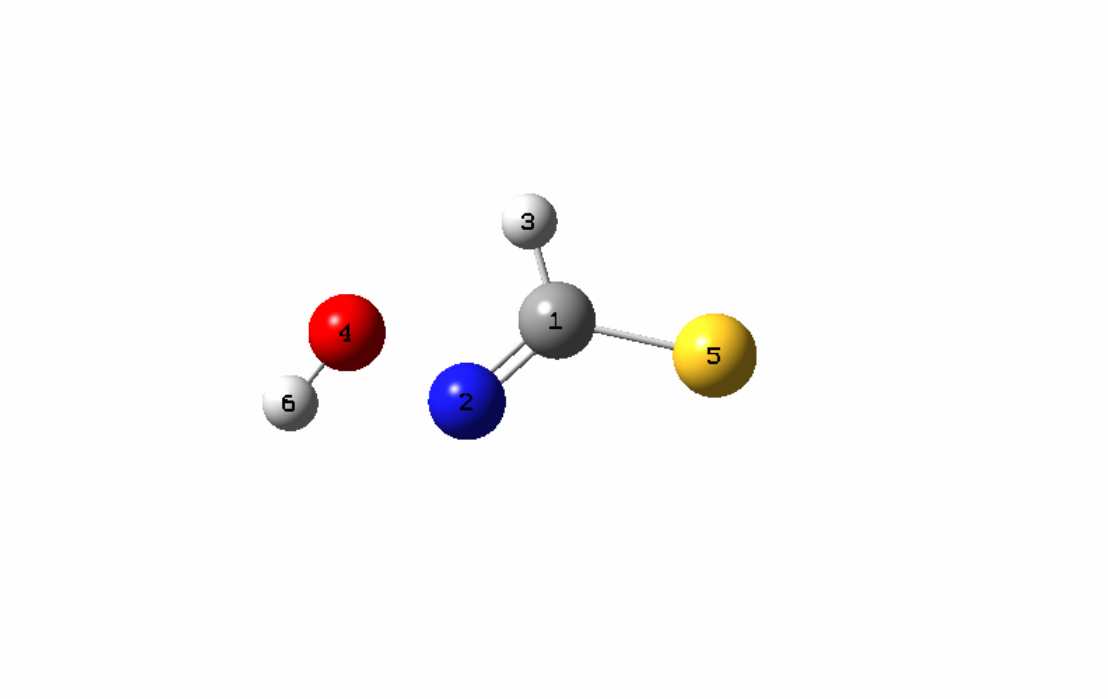
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.072011	0.827435	0.000017
2	7	0	-1.206334	0.635499	0.000008
3	1	0	0.309342	1.896022	-0.000102
4	8	0	-1.558908	-0.743518	-0.000038
5	16	0	1.419765	-0.291504	0.000004
6	1	0	-2.542056	-0.696921	0.000190

Total free energy in solution with all non electrostatic terms (a.u.)
= -567.667821

2E-Sanion



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.021446	0.331944	-0.000098
2	7	0	-0.941927	-0.536194	-0.000043
3	1	0	-0.275603	1.391869	0.000034
4	8	0	-2.228963	0.201204	0.000040
5	16	0	1.712962	-0.042900	0.000027
6	1	0	-2.835266	-0.553416	0.000104

Zero-point correction= 0.033989 (Hartree/Particle)
E(RB+HF-LYP) = -567.565408408 A.U.

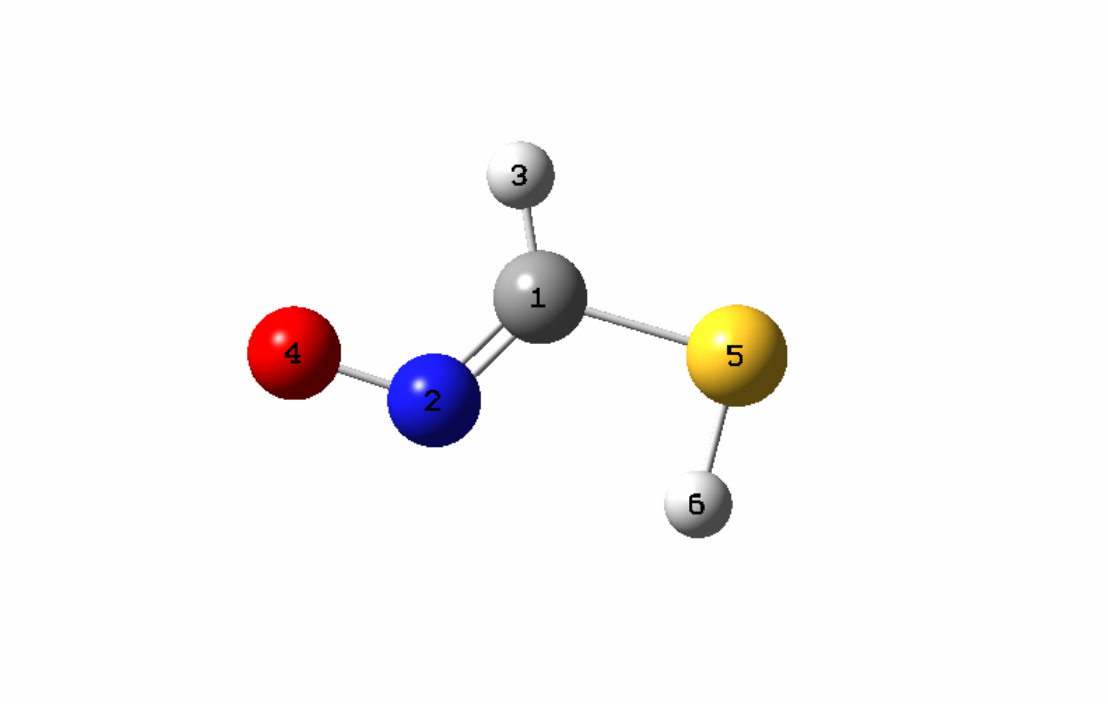
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.010593	0.368646	0.001423
2	7	0	-0.941119	-0.502489	-0.000400
3	1	0	-0.258209	1.433728	0.002840
4	8	0	-2.215219	0.172094	-0.001936
5	16	0	1.709278	-0.057567	-0.000228
6	1	0	-2.844214	-0.583865	0.010570

Total free energy in solution with all non electrostatic terms (a.u.)
= -567.551592

2E-Oanion



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.130265	0.497178	-0.000466
2	7	0	-1.068480	-0.415034	-0.000950
3	1	0	-0.303692	1.577633	0.001490
4	8	0	-2.307296	0.000871	0.000602
5	16	0	1.609672	-0.020505	0.000022
6	1	0	1.268257	-1.334356	0.002787

Zero-point correction= 0.029610 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.002012
E(RB+HF-LYP) = -567.528872557 A.U.

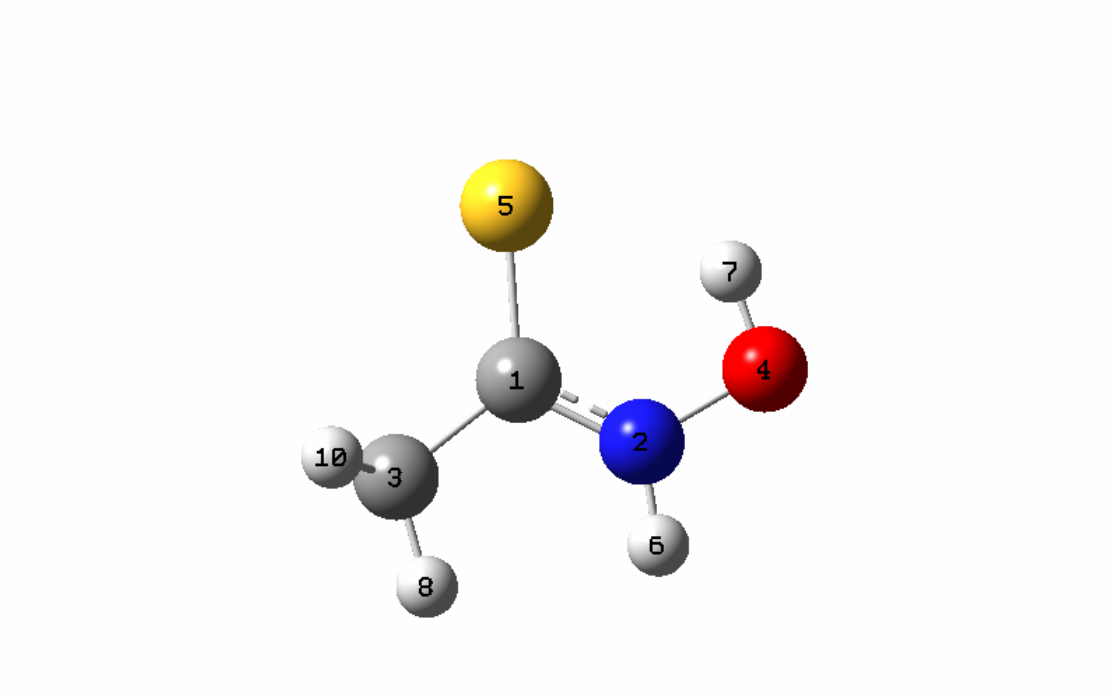
Solution

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.128567	0.457974	0.000599
2	7	0	1.072315	-0.432827	-0.000650
3	1	0	0.310380	1.538288	0.001772
4	8	0	2.325611	0.021640	0.000049
5	16	0	-1.612132	-0.004711	-0.000370
6	1	0	-1.398749	-1.354088	0.004709

Total free energy in solution: with all non electrostatic terms (a.u.)
= -567.630104

Thioacetohydroxamic acid
1Z



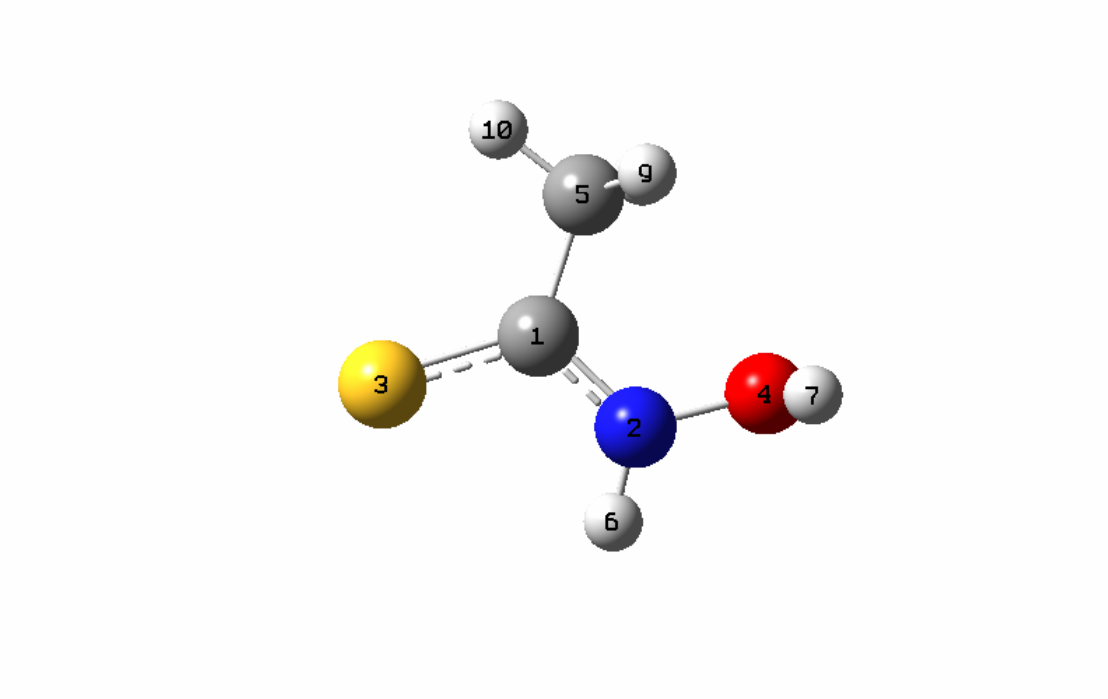
Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.361209	-0.287828	0.000013
2	7	0	0.827240	-0.884227	0.000156
3	6	0	-1.542625	-1.225201	-0.000030
4	8	0	2.015941	-0.185978	-0.000035
5	16	0	-0.475298	1.389423	-0.000003
6	1	0	0.987137	-1.881706	-0.000455
7	1	0	1.687038	0.755097	-0.000160
8	1	0	-1.245287	-2.281191	-0.000100
9	1	0	-2.159699	-1.033608	-0.882495
10	1	0	-2.159617	-1.033770	0.882535

Zero-point correction= 0.075644 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.045839
E(RB+HF-LYP) = -607.452786320 A.U.

1E

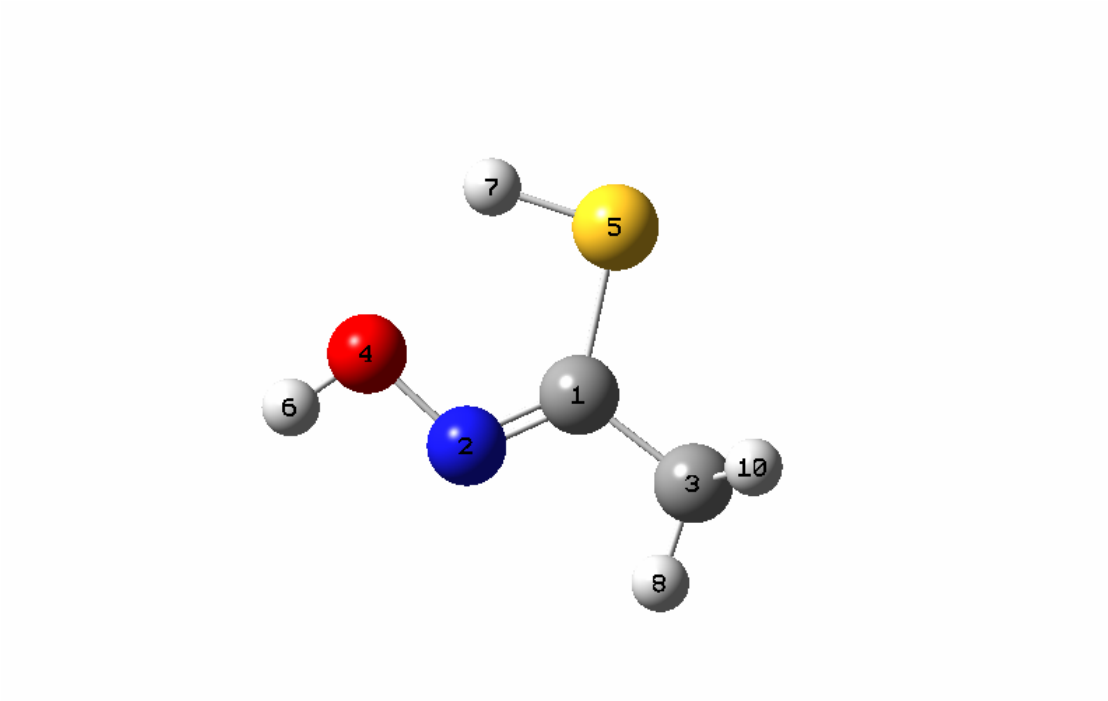


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.167473	0.157522	0.031771
2	7	0	0.817710	-0.771242	0.155725
3	16	0	-1.752569	-0.333397	-0.024913
4	8	0	2.139592	-0.429711	-0.190207
5	6	0	0.291184	1.591967	0.011105
6	1	0	0.591079	-1.730409	-0.091235
7	1	0	2.620434	-0.441872	0.656468
8	1	0	0.887158	1.782512	-0.889020
9	1	0	0.933976	1.810994	0.872310
10	1	0	-0.574515	2.252585	0.024409

Zero-point correction= 0.075952 (Hartree/Particle)
E(RB+HF-LYP) = -607.445643837 A.U.

2Z

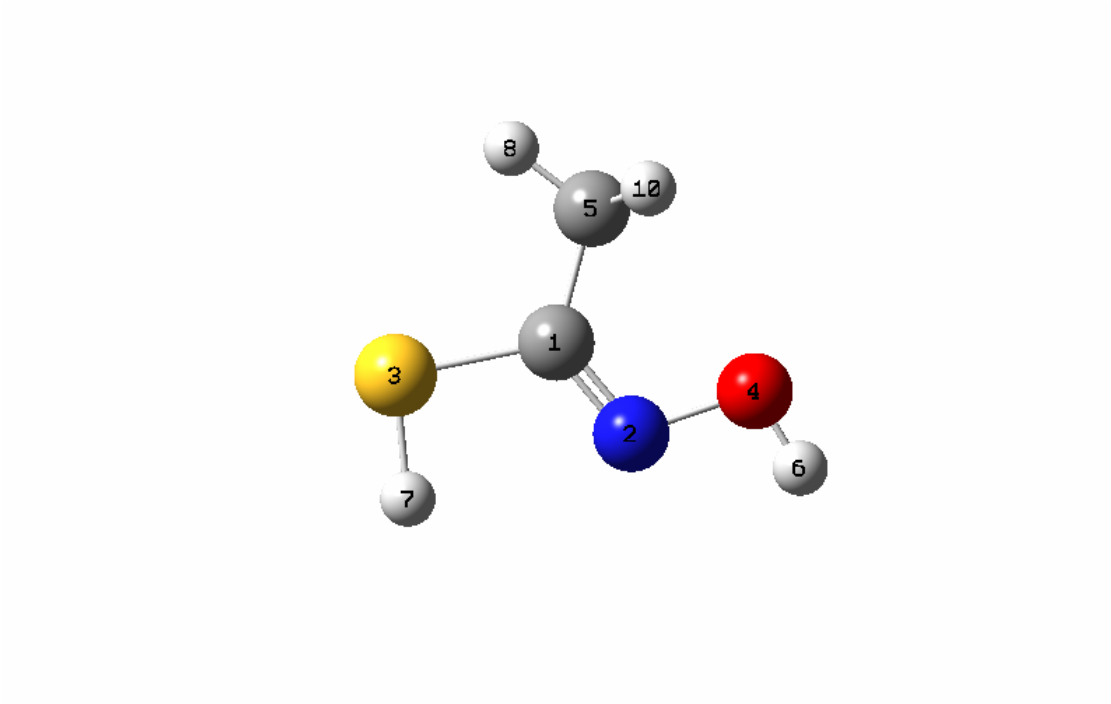


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.250810	-0.430185	-0.000354
2	7	0	-0.916407	-0.959182	-0.000023
3	6	0	1.439786	-1.350079	0.000111
4	8	0	-1.951586	-0.001833	0.000027
5	16	0	0.628905	1.311760	-0.000008
6	1	0	-2.744879	-0.559752	0.000225
7	1	0	-0.652500	1.729323	0.000583
8	1	0	1.093093	-2.386087	-0.000823
9	1	0	2.063673	-1.180000	-0.884914
10	1	0	2.062102	-1.181129	0.886469

Zero-point correction = 0.072674 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.042970
E(RB+HF-LYP) = -607.449739863 A.U.

2E

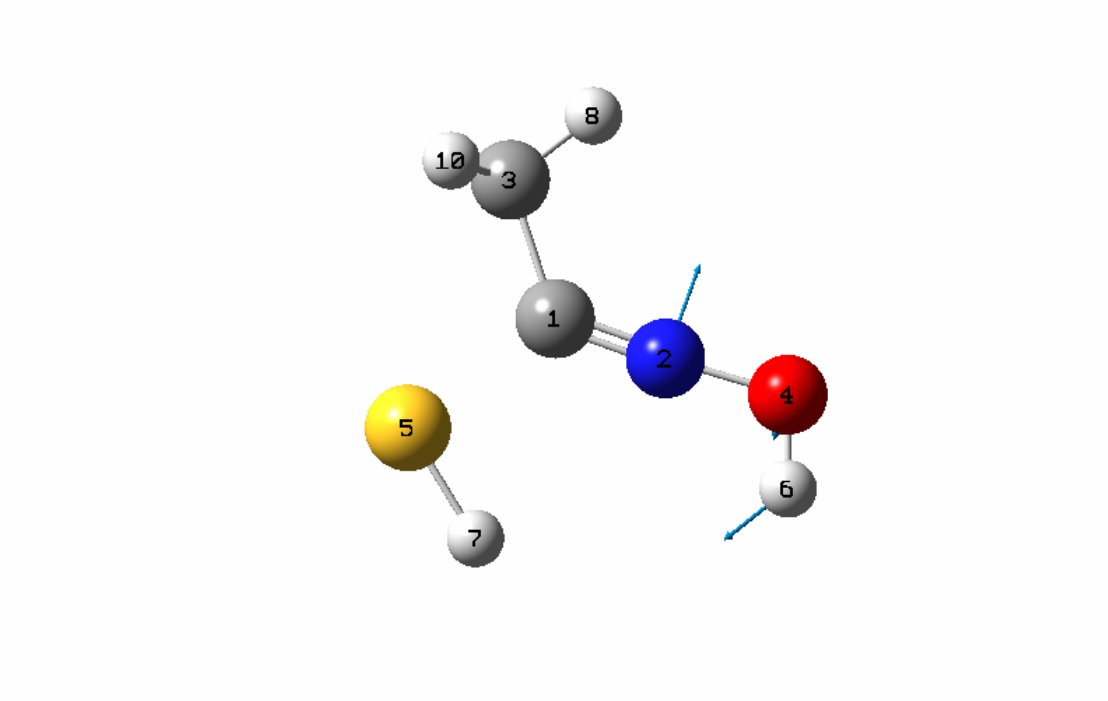


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.003120	0.118702	-0.000010
2	7	0	0.816574	-0.870418	-0.000006
3	16	0	-1.743272	-0.236145	-0.000023
4	8	0	2.157262	-0.408255	0.000041
5	6	0	0.389658	1.572946	-0.000008
6	1	0	2.650366	-1.243302	-0.000314
7	1	0	-1.608205	-1.579216	0.000350
8	1	0	-0.484984	2.227362	-0.001976
9	1	0	1.003893	1.790798	-0.880208
10	1	0	1.000503	1.791760	0.882335

Zero-point correction= 0.072381 (Hartree/Particle)
E(RB+HF-LYP) = -607.444575328 A.U.

TS3

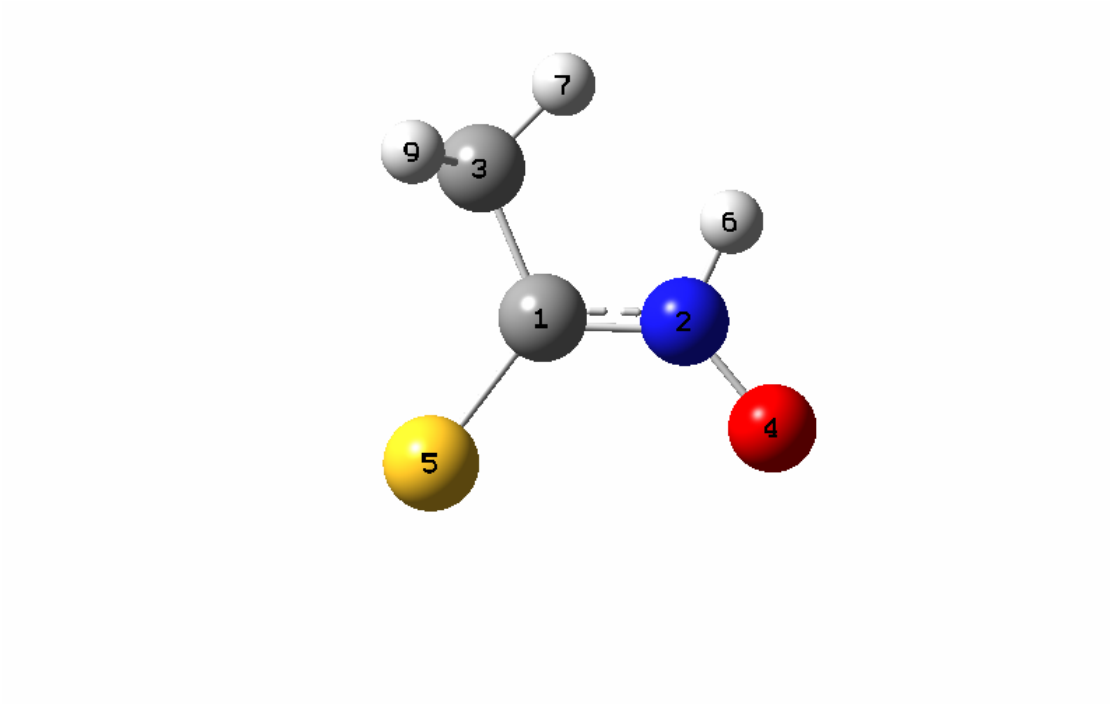


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.001092	0.363819	-0.000087
2	7	0	1.151644	-0.051813	-0.000717
3	6	0	-0.465288	1.809144	0.000120
4	8	0	2.424144	-0.429832	0.000373
5	16	0	-1.531763	-0.774773	0.000072
6	1	0	2.428604	-1.411392	0.000314
7	1	0	-0.828411	-1.925889	-0.000162
8	1	0	0.399472	2.476973	0.000155
9	1	0	-1.080535	2.010264	-0.884396
10	1	0	-1.080406	2.009982	0.884792

Zero-point correction= 0.070308 (Hartree/Particle)
E(RB+HF-LYP) = -607.366603548 A.U.

1Z-Oanion

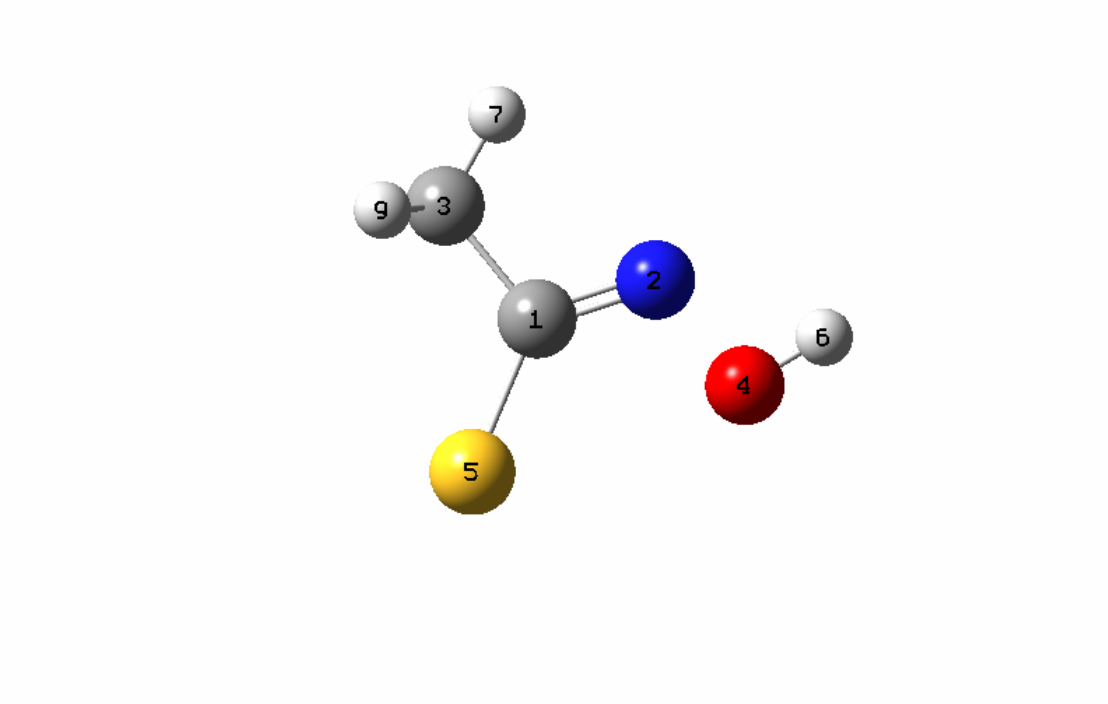


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.125065	0.334915	0.000068
2	7	0	1.205992	0.300291	0.000055
3	6	0	-0.703759	1.736339	-0.000030
4	8	0	2.027864	-0.700262	-0.000038
5	16	0	-1.170341	-1.028995	-0.000007
6	1	0	1.645770	1.234292	-0.000067
7	1	0	0.071220	2.522627	-0.000763
8	1	0	-1.342258	1.889456	-0.879923
9	1	0	-1.341179	1.890079	0.880552

Zero-point correction= 0.063620 (Hartree/Particle)
E(RB+HF-LYP) = -606.889124293 A.U.

1E-Oanion

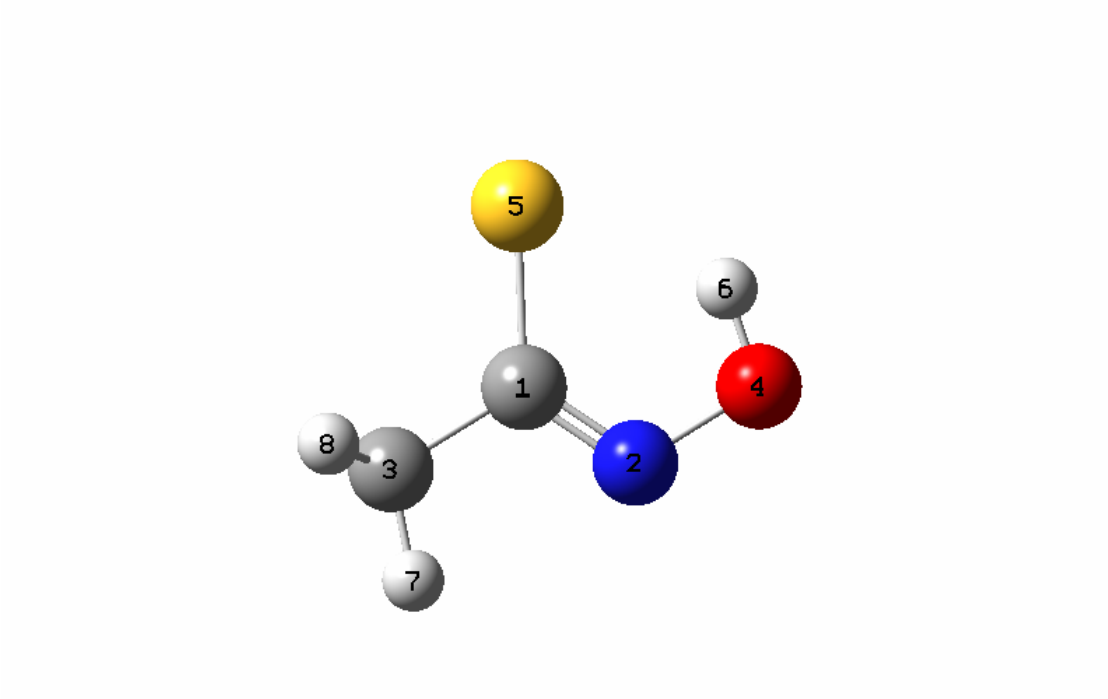


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.186913	0.362946	-0.000190
2	7	0	1.050491	0.769350	0.000648
3	6	0	-1.149737	1.543890	-0.000169
4	8	0	1.985443	-0.332701	-0.000056
5	16	0	-0.863673	-1.239594	0.000032
6	1	0	2.814475	0.170381	-0.001928
7	1	0	-0.607774	2.499308	-0.000666
8	1	0	-1.802782	1.499053	-0.880810
9	1	0	-1.802232	1.499901	0.880958

Zero-point correction= 0.062894 (Hartree/Particle)
E(RB+HF-LYP) = -606.897474336 A.U.

1Z-Nanion

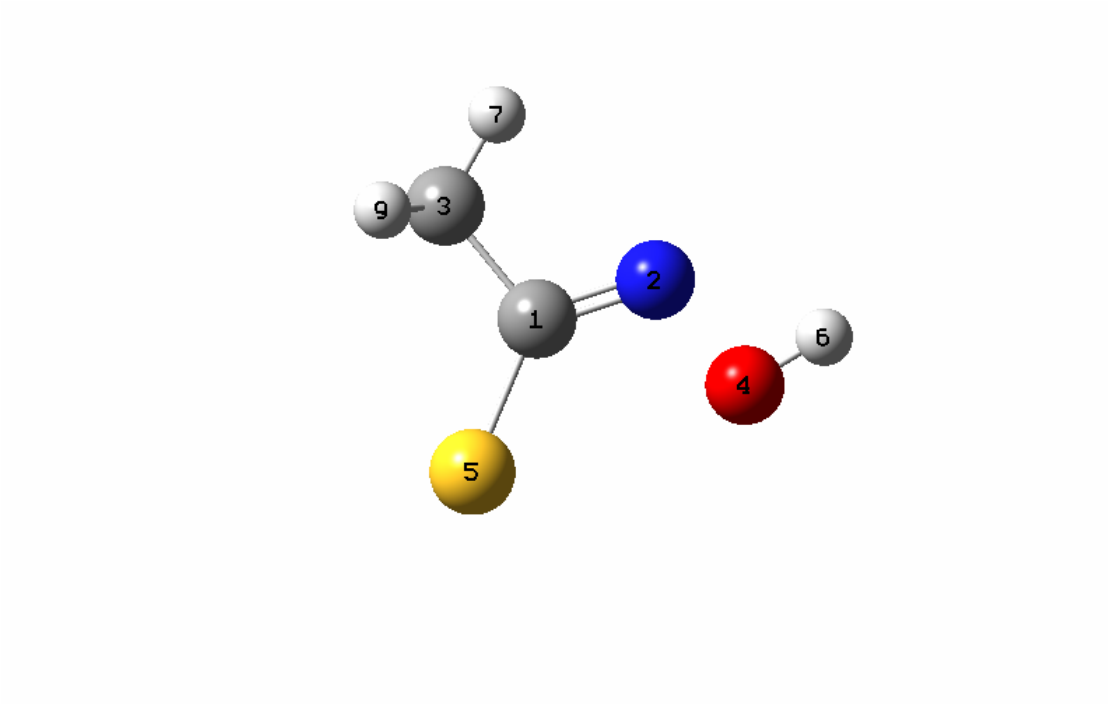


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.298803	-0.347928	-0.000074
2	7	0	0.778307	-1.077962	-0.000128
3	6	0	-1.587283	-1.140216	0.000045
4	8	0	1.975146	-0.338695	0.000079
5	16	0	-0.364626	1.411243	-0.000011
6	1	0	1.661449	0.608353	0.000223
7	1	0	-1.372922	-2.216674	-0.001386
8	1	0	-2.192917	-0.894823	0.882521
9	1	0	-2.194400	-0.892585	-0.880747

Zero-point correction= 0.063228 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.034303
E(RB+HF-LYP) = -606.914371239 A.U.

2Z-Sanion

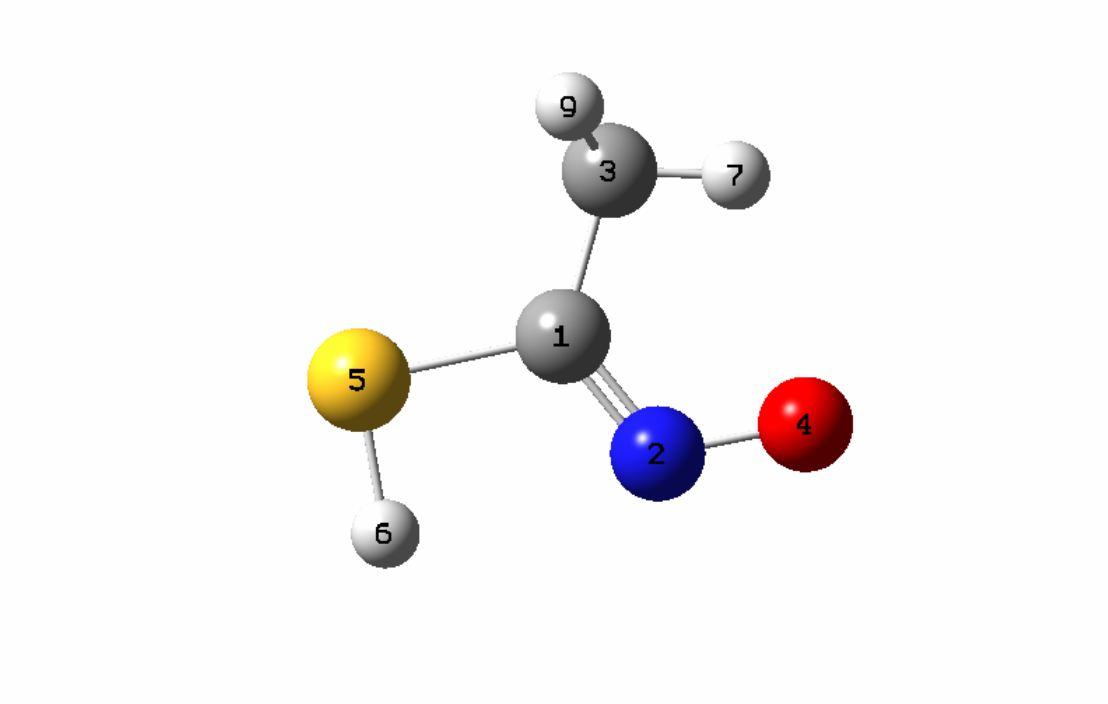


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.187290	0.362344	0.000030
2	7	0	1.050039	0.769473	0.000078
3	6	0	-1.150192	1.543533	-0.000037
4	8	0	1.985667	-0.332047	-0.000065
5	16	0	-0.863208	-1.239614	0.000006
6	1	0	2.814504	0.171486	0.000058
7	1	0	-0.608123	2.498857	-0.000147
8	1	0	-1.802938	1.499053	-0.880925
9	1	0	-1.802841	1.499225	0.880932

Zero-point correction = 0.062897 (Hartree/Particle)
E(RB+HF-LYP) = -606.897480118 A.U.

2E-Oanion

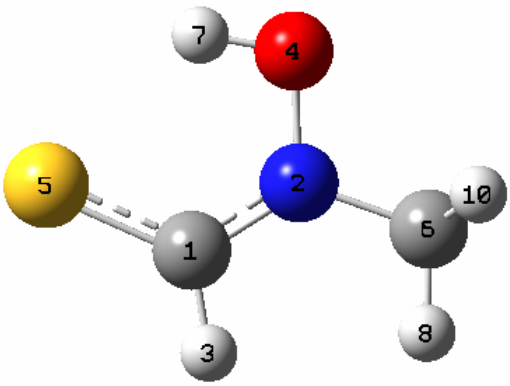


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.069400	0.150836	-0.000045
2	7	0	0.894414	-0.871283	-0.000155
3	6	0	0.474758	1.591289	-0.000031
4	8	0	2.180202	-0.616738	0.000121
5	16	0	-1.707524	-0.231107	0.000046
6	1	0	-1.475642	-1.569355	-0.000105
7	1	0	1.572925	1.549470	-0.000735
8	1	0	0.127184	2.149051	-0.886311
9	1	0	0.128446	2.148681	0.886989

Zero-point correction= 0.058221 (Hartree/Particle)
E(RB+HF-LYP) = -606.861793851 A.U.

***N*-methylthioformohydroxamic acid**
1Z

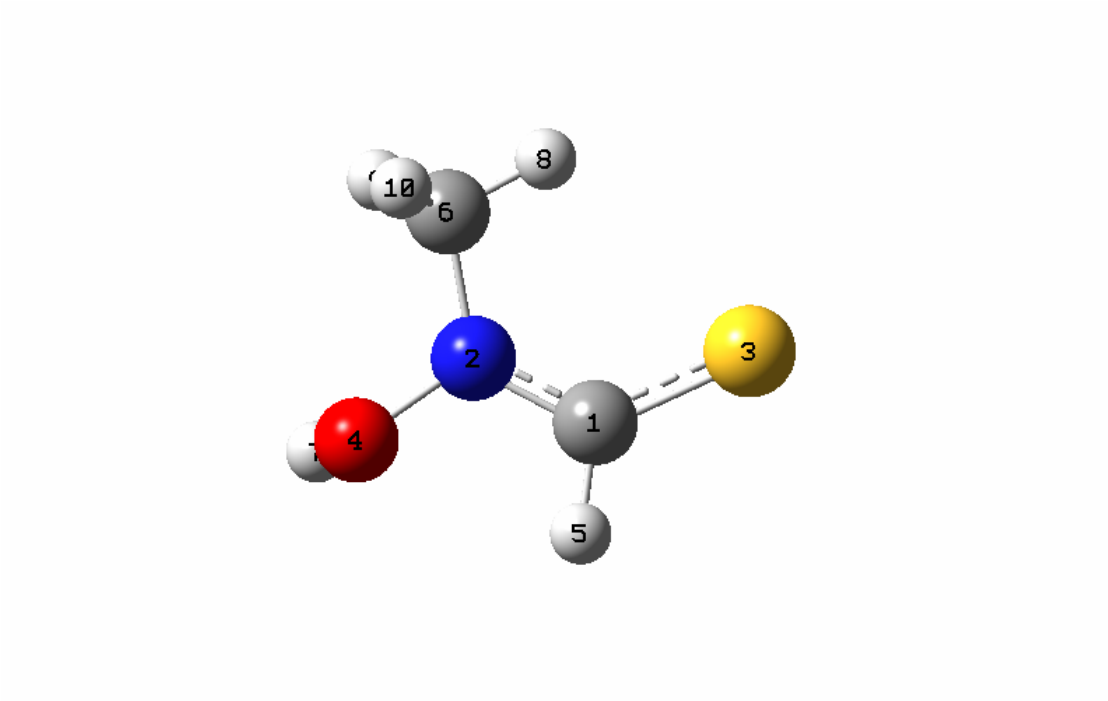


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.326882	-0.737136	-0.000065
2	7	0	0.797530	-0.030380	-0.000135
3	1	0	-0.147884	-1.812798	-0.000166
4	8	0	0.743752	1.351989	-0.000030
5	16	0	-1.852718	-0.056233	0.000043
6	6	0	2.159798	-0.513432	0.000098
7	1	0	-0.238664	1.518147	0.000137
8	1	0	2.139763	-1.604749	-0.001505
9	1	0	2.680510	-0.149075	-0.891177
10	1	0	2.679542	-0.151648	0.893007

Zero-point correction= 0.076290 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.046874
E(RB+HF-LYP) = -607.445515090 A.U.

1E

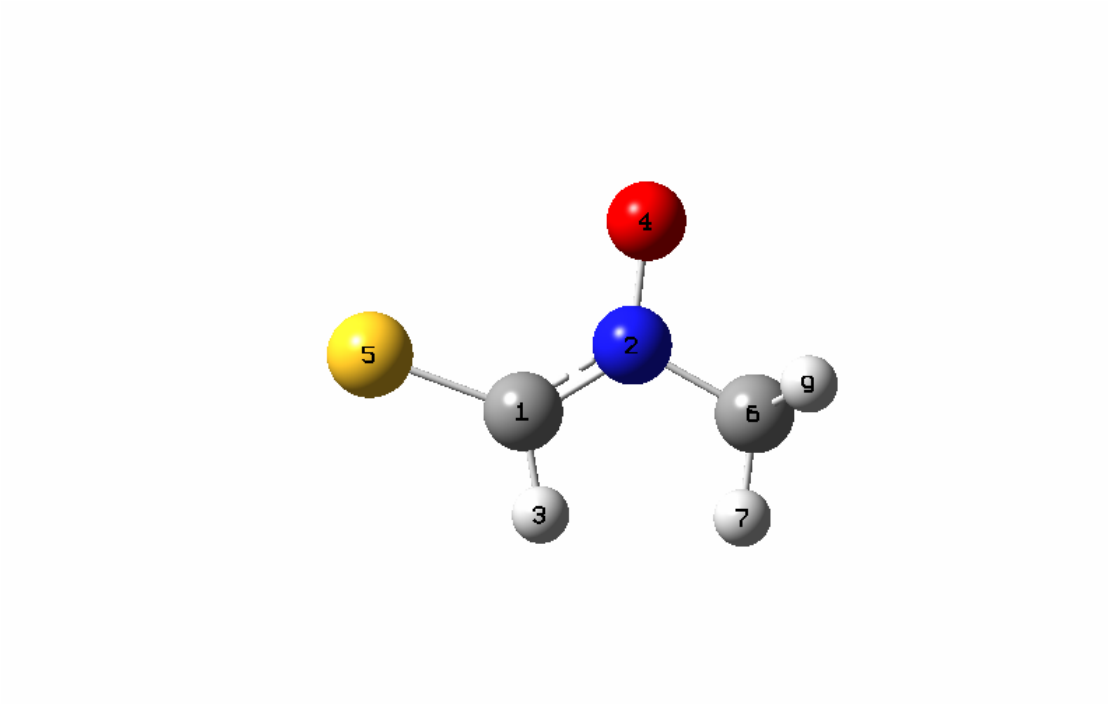


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.392576	-0.672233	0.006036
2	7	0	-0.793711	-0.046059	-0.077399
3	16	0	1.895507	0.021590	-0.001653
4	8	0	-1.933503	-0.843143	0.126555
5	1	0	0.249877	-1.752876	0.065877
6	6	0	-1.046030	1.378705	0.016528
7	1	0	-2.319880	-0.957708	-0.761812
8	1	0	-0.089681	1.892509	-0.084856
9	1	0	-1.724854	1.689526	-0.784892
10	1	0	-1.498848	1.611835	0.986106

Zero-point correction= 0.075813 (Hartree/Particle)
E(RB+HF-LYP) = -607.436340181 A.U.

1Z-Oanion

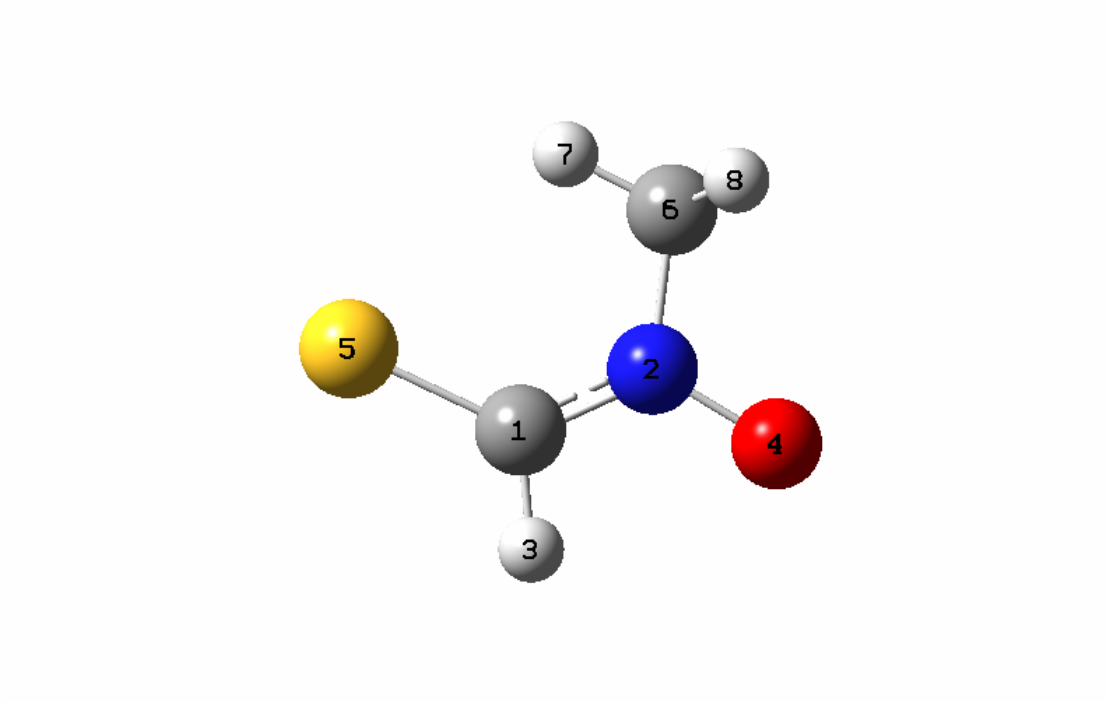


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.332188	-0.606301	0.000089
2	7	0	0.806130	0.086502	0.000094
3	1	0	-0.150760	-1.684056	-0.000056
4	8	0	0.955271	1.381724	-0.000014
5	16	0	-1.931887	-0.013121	-0.000029
6	6	0	2.084282	-0.628445	-0.000056
7	1	0	1.955920	-1.717026	-0.000242
8	1	0	2.653709	-0.319739	-0.886195
9	1	0	2.653680	-0.320075	0.886216

Zero-point correction= 0.063766 (Hartree/Particle)
E(RB+HF-LYP) = -606.882509095 A.U.

1E-Oanion

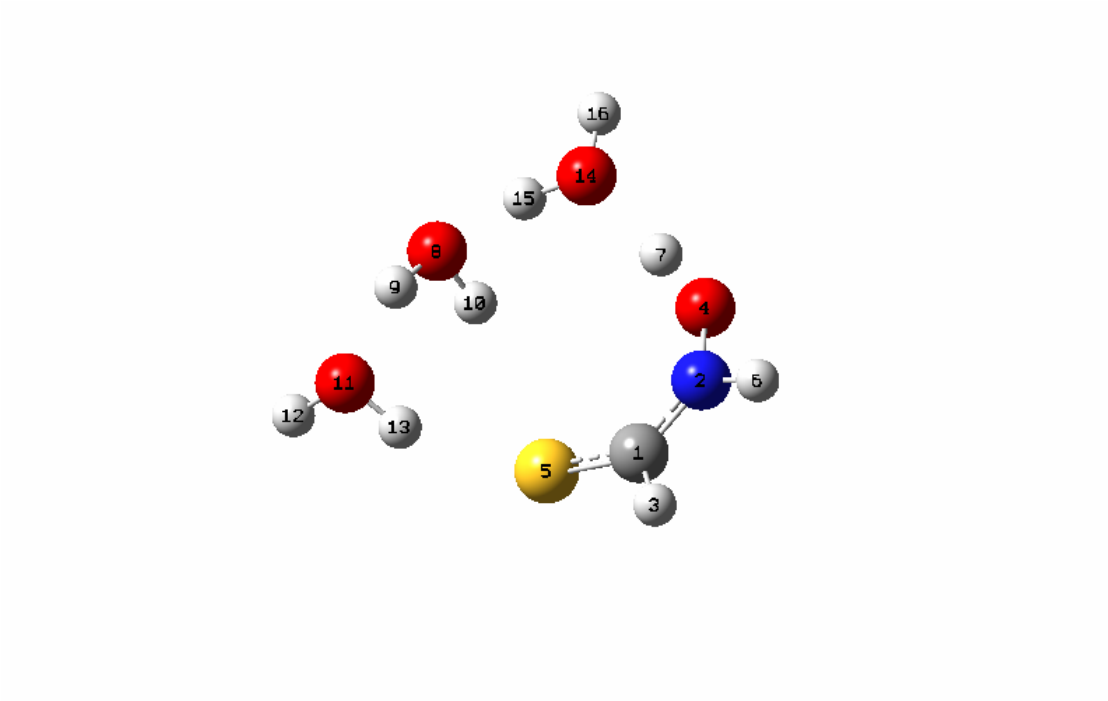


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.314764	-0.697129	0.000176
2	7	0	0.886898	-0.140651	-0.000004
3	1	0	-0.216915	-1.783739	-0.000295
4	8	0	2.016469	-0.821437	-0.000030
5	16	0	-1.876209	0.043928	-0.000028
6	6	0	1.064724	1.308722	-0.000007
7	1	0	0.097038	1.813462	-0.000205
8	1	0	1.649525	1.577033	0.887818
9	1	0	1.649906	1.576891	-0.887614

Zero-point correction= 0.063814 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.034675
E(RB+HF-LYP) = -606.890846258 A.U.

1Z.3H$_2$O



Gas

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.160890	-1.375945	0.469546
2	7	0	2.023757	-0.369991	0.499985
3	1	0	1.381141	-2.092391	1.265721
4	8	0	2.079053	0.632615	-0.429377
5	16	0	-0.112236	-1.625548	-0.581239
6	1	0	2.802647	-0.373646	1.151169
7	1	0	1.467246	1.366573	-0.077084
8	8	0	-1.628688	1.413230	-0.822570
9	1	0	-2.201779	0.917162	-0.191107
10	1	0	-1.099825	0.698960	-1.226672
11	8	0	-2.902975	-0.408805	0.869365
12	1	0	-3.616950	-0.857304	0.389947
13	1	0	-2.143733	-1.018642	0.788323
14	8	0	0.438217	2.456995	0.477079
15	1	0	-0.421344	2.144497	0.061966
16	1	0	0.611886	3.316888	0.064412

Zero-point correction= 0.123840 (Hartree/Particle)
E(RB+HF-LYP) = -797.292849764 A.U.

Solution

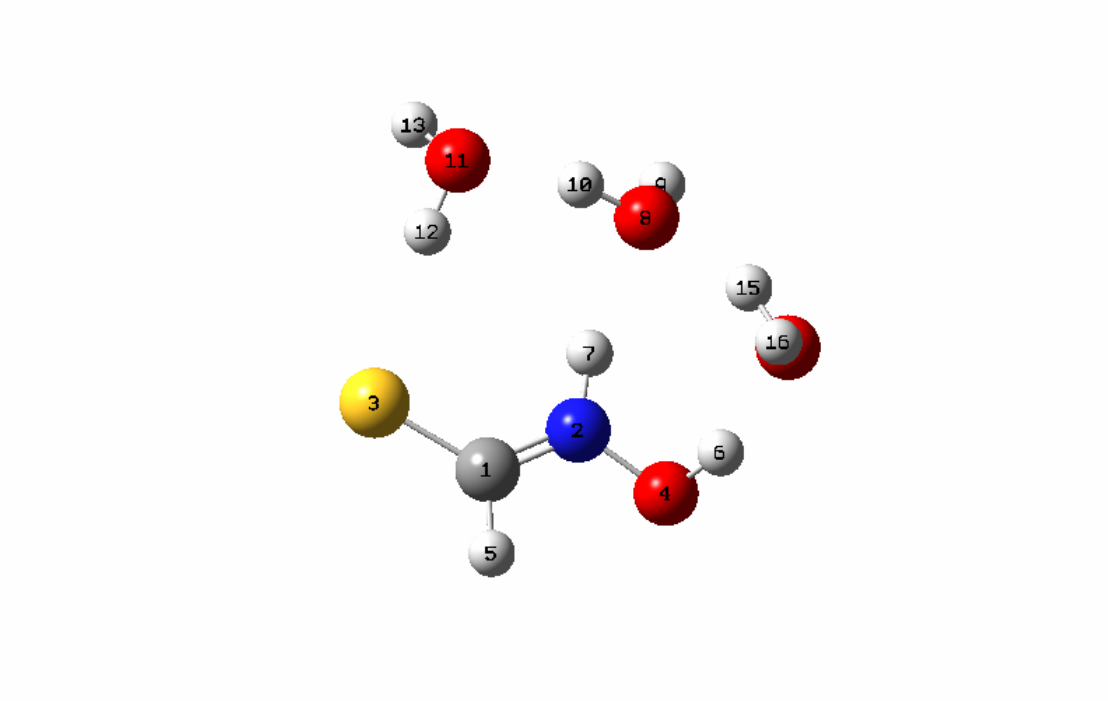
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.160890	-1.375945	0.469546
2	7	0	2.023757	-0.369991	0.499985

3	1	0	1.381141	-2.092391	1.265721
4	8	0	2.079053	0.632615	-0.429377
5	16	0	-0.112236	-1.625548	-0.581239
6	1	0	2.802647	-0.373646	1.151169
7	1	0	1.467246	1.366573	-0.077084
8	8	0	-1.628688	1.413230	-0.822570
9	1	0	-2.201779	0.917162	-0.191107
10	1	0	-1.099825	0.698960	-1.226672
11	8	0	-2.902975	-0.408805	0.869365
12	1	0	-3.616950	-0.857304	0.389947
13	1	0	-2.143733	-1.018642	0.788323
14	8	0	0.438217	2.456995	0.477079
15	1	0	-0.421344	2.144497	0.061966
16	1	0	0.611886	3.316888	0.064412

Total free energy in solution with all non electrostatic terms a.u.)
= -797.311244

1E.3H_2O

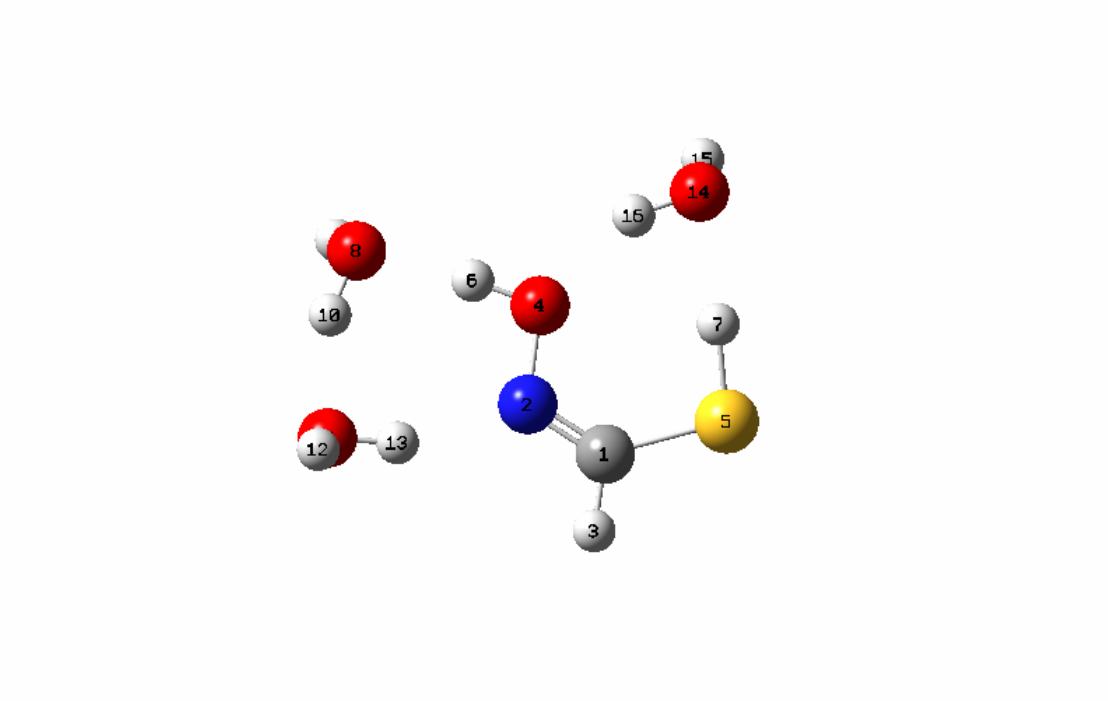


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.861825	-1.485013	0.028571
2	7	0	0.297558	-0.979149	-0.331525
3	16	0	-2.304619	-0.632015	0.170758
4	8	0	1.418889	-1.788004	-0.458530
5	1	0	-0.809645	-2.554386	0.237305
6	1	0	2.116486	-1.266242	0.030679
7	1	0	0.444121	0.002800	-0.599174
8	8	0	1.171432	1.734593	-0.583095
9	1	0	1.367724	2.153547	-1.433985
10	1	0	0.328827	2.157913	-0.244678
11	8	0	-1.241394	2.466723	0.262387
12	1	0	-1.628036	1.555137	0.314940
13	1	0	-1.799189	2.919323	-0.389131
14	8	0	2.976583	0.076923	0.715095
15	1	0	2.478830	0.838414	0.339963
16	1	0	2.858748	0.147974	1.674340

Zero-point correction= 0.124147 (Hartree/Particle)
E(RB+HF-LYP) = -797.299609068 A.U.

2Ztc.3H_2O

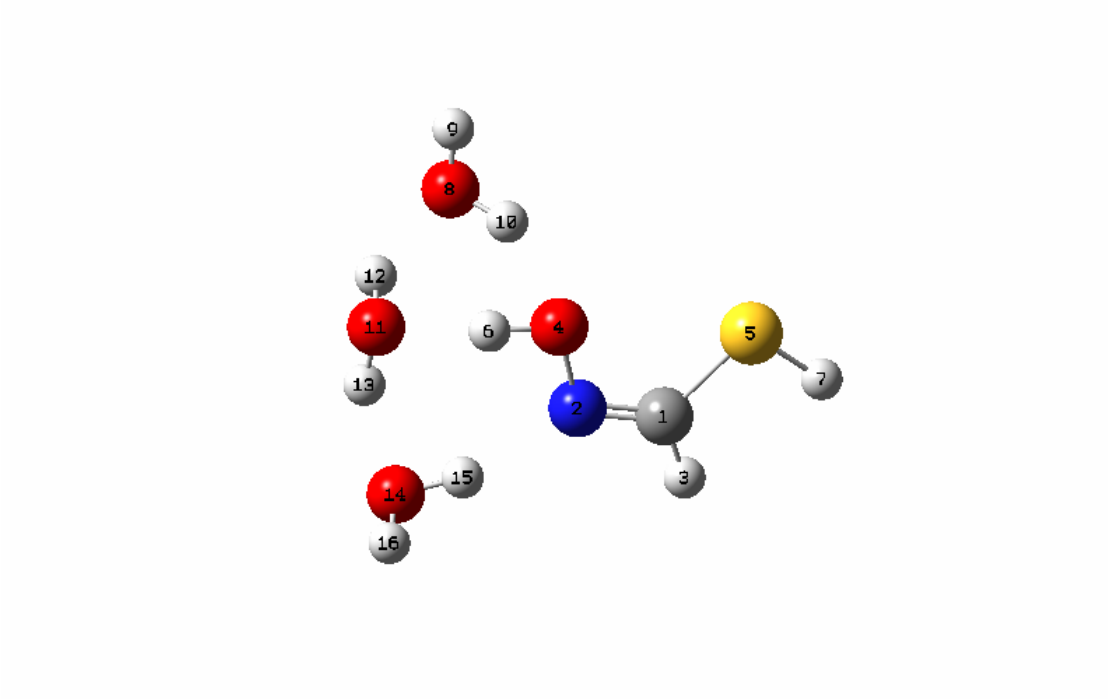


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.700125	-1.401044	-0.043734
2	7	0	-0.379307	-0.709952	-0.058248
3	1	0	0.546643	-2.475245	0.023172
4	8	0	-0.206415	0.668882	-0.174892
5	16	0	2.396674	-0.946860	-0.124884
6	1	0	-1.145450	1.018524	-0.207952
7	1	0	2.276028	0.407837	0.032727
8	8	0	-2.767773	1.431684	-0.247485
9	1	0	-3.048054	1.579702	-1.163702
10	1	0	-3.138244	0.539249	-0.014719
11	8	0	-3.174714	-1.179345	0.290063
12	1	0	-3.301989	-1.338284	1.238070
13	1	0	-2.197684	-1.245341	0.156806
14	8	0	2.018198	2.254633	0.448411
15	1	0	2.062478	2.709425	-0.407159
16	1	0	1.099519	1.922989	0.482270

Zero-point correction= 0.121007 (Hartree/Particle)
E(RB+HF-LYP) = -797.288848465 A.U.

2Ztt.H_2O

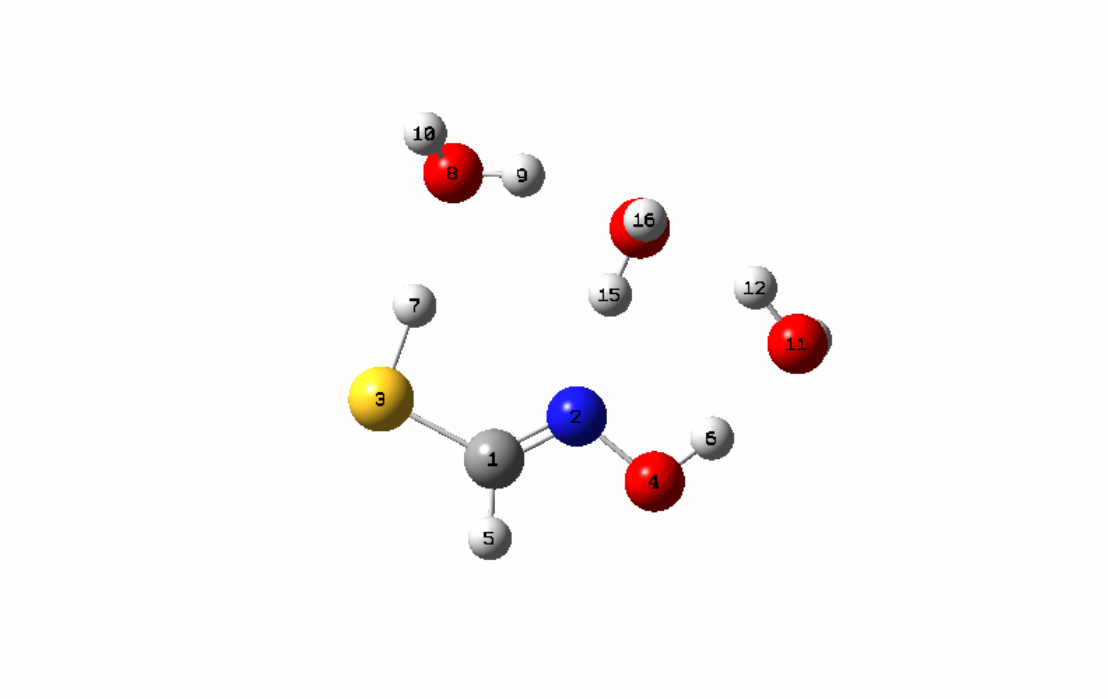


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.554715	-0.921711	-0.334241
2	7	0	0.321244	-0.806224	-0.022448
3	1	0	1.843639	-1.795239	-0.909456
4	8	0	0.061096	0.350978	0.700318
5	16	0	2.793668	0.258982	0.118203
6	1	0	-0.931638	0.290780	0.915566
7	1	0	3.795576	-0.392968	-0.507905
8	8	0	-1.488153	2.313177	-0.837410
9	1	0	-1.446295	3.168233	-0.382517
10	1	0	-0.680945	1.847263	-0.545458
11	8	0	-2.546109	0.348414	0.841511
12	1	0	-2.550461	1.076465	0.181513
13	1	0	-2.712635	-0.474806	0.321540
14	8	0	-2.266976	-2.033534	-0.513663
15	1	0	-1.313276	-1.794743	-0.485673
16	1	0	-2.358510	-2.727139	0.157684

Zero-point correction= 0.121608 (Hartree/Particle)
E(RB+HF-LYP) = -797.291345229 A.U.

2E.3H_2O

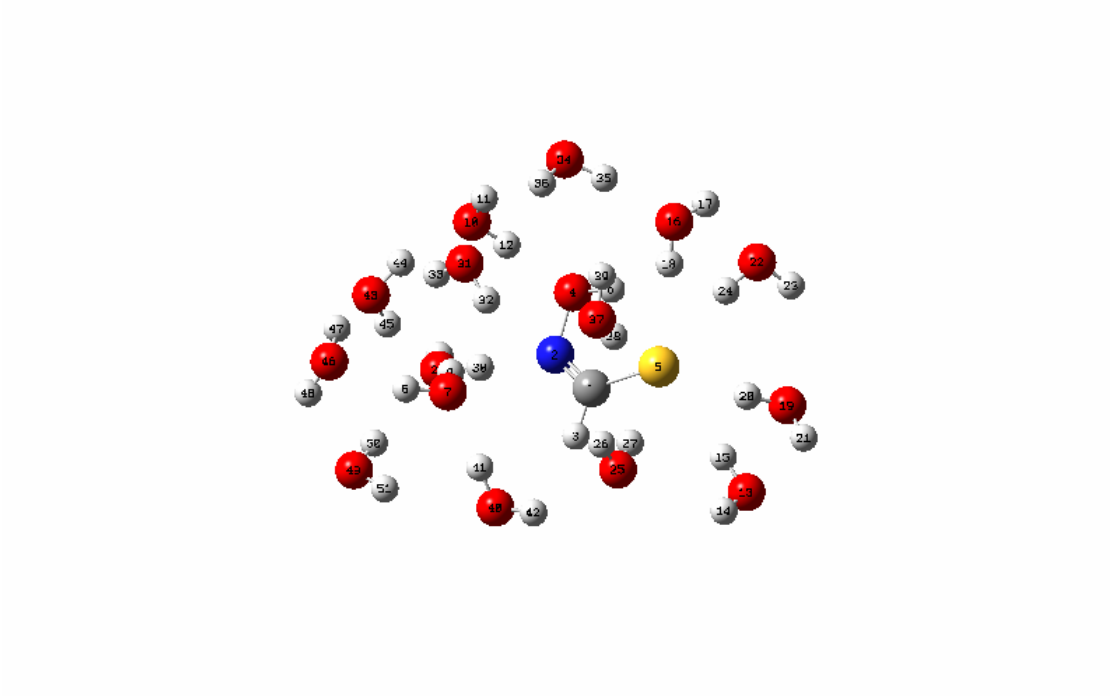


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.835820	-1.479623	0.026787
2	7	0	0.299710	-0.890534	0.063929
3	16	0	-2.387444	-0.654908	-0.012383
4	8	0	1.369418	-1.787634	0.075406
5	1	0	-0.894013	-2.568387	0.012145
6	1	0	2.158668	-1.191985	-0.015075
7	1	0	-1.924744	0.629967	-0.159784
8	8	0	-1.397948	2.452939	-0.373533
9	1	0	-0.438418	2.420578	-0.165281
10	1	0	-1.784084	2.995208	0.330808
11	8	0	3.330322	0.103859	-0.262182
12	1	0	2.753771	0.877974	-0.069870
13	1	0	3.505811	0.158202	-1.214079
14	8	0	1.165267	1.691274	0.450625
15	1	0	0.759727	0.778456	0.336900
16	1	0	1.242872	1.806483	1.411615

Zero-point correction= 0.120938 (Hartree/Particle)
E(RB+HF-LYP) = -797.287289373 A.U.

1ZN-anion.15H_2O



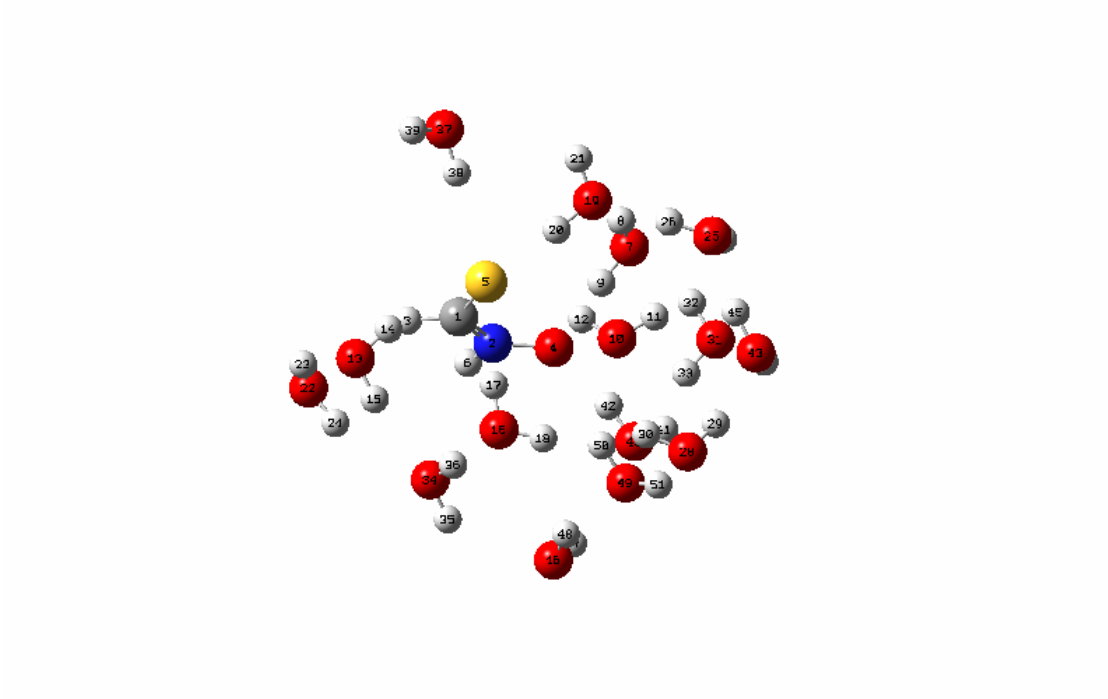
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.775630	-0.866463	-0.935847
2	7	0	-0.015397	-0.136289	-1.653155
3	1	0	0.436616	-1.908376	-0.854348
4	8	0	0.368515	1.222031	-1.766693
5	16	0	2.242938	-0.397058	-0.082649
6	1	0	1.208753	1.292414	-1.243401
7	8	0	-2.352078	-0.943365	0.919144
8	1	0	-3.268527	-0.880514	1.219598
9	1	0	-2.295314	-0.522828	0.063993
10	8	0	-1.829977	2.759030	-1.036410
11	1	0	-1.562850	3.265687	-0.274191
12	1	0	-1.068608	2.257670	-1.345012
13	8	0	4.149724	-3.132668	0.694925
14	1	0	3.661800	-3.544593	1.400336
15	1	0	3.644188	-2.366708	0.406924
16	8	0	2.577608	2.760822	1.040230
17	1	0	3.263446	3.154539	0.509531
18	1	0	2.474519	1.844594	0.758343
19	8	0	5.038885	-1.239534	-1.876248
20	1	0	4.170547	-1.037098	-1.516647
21	1	0	5.402562	-1.947915	-1.355310
22	8	0	4.386188	1.880123	-1.478495
23	1	0	5.123565	1.370850	-1.798966
24	1	0	3.706518	1.257654	-1.205075
25	8	0	1.349030	-2.636646	2.342027
26	1	0	0.994197	-2.083917	3.030475
27	1	0	1.618004	-2.061207	1.618962
28	8	0	-2.554516	-0.462625	-2.686199
29	1	0	-2.530774	-0.150356	-3.583385

30	1	0	-1.652095	-0.413947	-2.325156
31	8	0	-1.984672	1.850901	2.091449
32	1	0	-1.514709	1.057896	2.337076
33	1	0	-2.599658	1.620727	1.399757
34	8	0	0.188619	4.116186	1.196251
35	1	0	1.055043	3.712078	1.095929
36	1	0	-0.301155	3.601642	1.830530
37	8	0	0.891063	0.633463	2.897737
38	1	0	1.264544	0.268393	2.090418
39	1	0	1.002425	1.578574	2.865045
40	8	0	-1.317853	-3.466683	0.557971
41	1	0	-1.657839	-2.593516	0.776902
42	1	0	-0.487410	-3.575583	1.010327
43	8	0	-4.025233	1.161737	-1.060680
44	1	0	-3.379531	1.867765	-0.951675
45	1	0	-3.671714	0.533831	-1.700254
46	8	0	-4.937533	-0.280402	1.008268
47	1	0	-4.770223	0.435967	0.383316
48	1	0	-5.399248	-0.972857	0.543762
49	8	0	-4.399135	-2.652104	-0.936003
50	1	0	-3.961541	-2.062826	-1.543974
51	1	0	-3.727610	-3.054440	-0.392472

Zero-point correction= 0.410771 (Hartree/Particle)
E(RB+HF-LYP) = -567.580591429 A.U.

1Z-Oanion.15H_2O



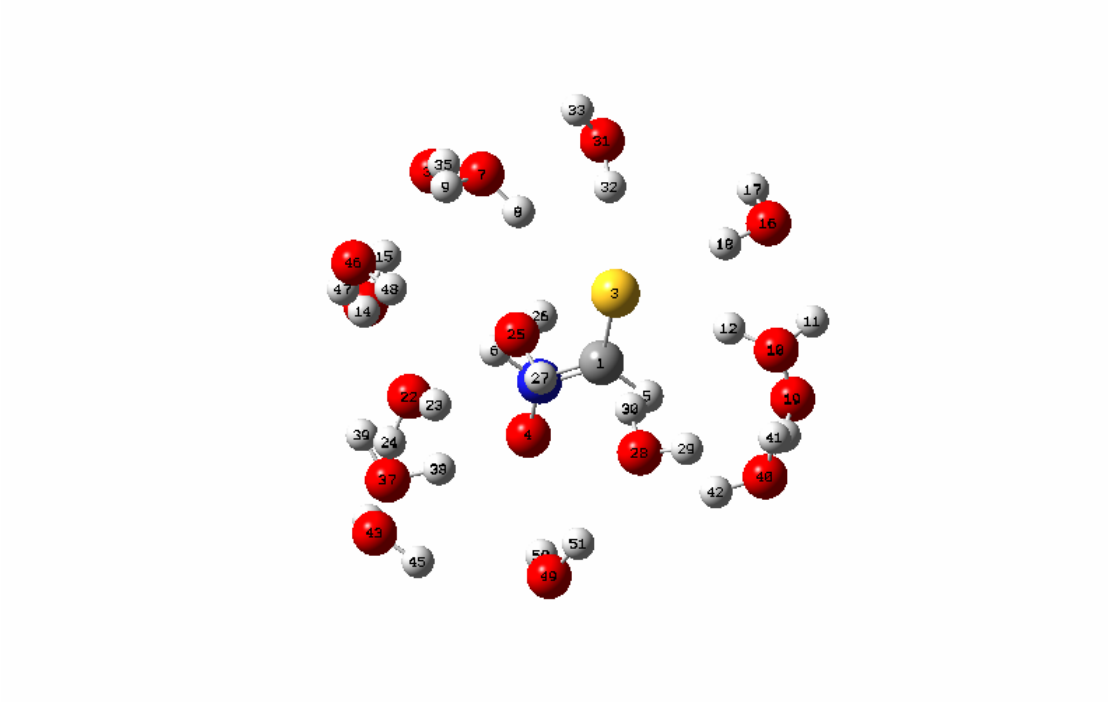
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.038619	0.733200	-0.832453
2	7	0	-1.318487	0.174433	-1.781617
3	1	0	-3.119016	0.655114	-1.025980
4	8	0	-0.019870	0.082664	-1.837519
5	16	0	-1.459550	1.473854	0.623047
6	1	0	-1.842928	-0.240725	-2.562323
7	8	0	1.583392	2.218601	-2.435519
8	1	0	1.408847	2.774708	-1.668491
9	1	0	0.985087	1.463131	-2.386416
10	8	0	1.316707	0.275056	2.063671
11	1	0	2.113944	0.745838	1.832747
12	1	0	0.573556	0.689059	1.612581
13	8	0	-4.226744	-0.147482	1.776910
14	1	0	-3.530454	0.478725	1.557144
15	1	0	-3.824479	-1.008400	1.840629
16	8	0	-1.183408	-1.654446	1.849131
17	1	0	-1.291646	-0.709087	1.686776
18	1	0	-0.248149	-1.843117	1.861386
19	8	0	0.794271	3.198416	-0.031548
20	1	0	0.036010	2.578929	0.172494
21	1	0	0.496972	4.091943	0.095671
22	8	0	-5.221417	-0.776027	-1.139660
23	1	0	-5.338590	-0.272323	-0.338506
24	1	0	-4.654910	-1.513216	-0.930629
25	8	0	3.336061	2.446754	0.482102
26	1	0	2.420538	2.747449	0.536419
27	1	0	3.561984	2.377672	-0.442147
28	8	0	2.810679	-2.124156	3.335660
29	1	0	3.405925	-1.527992	2.889600

30	1	0	1.935257	-1.753234	3.271461
31	8	0	3.400995	0.253565	-1.983149
32	1	0	2.898906	1.033754	-2.253016
33	1	0	2.777963	-0.456451	-1.856895
34	8	0	-2.644124	-2.720337	-0.226542
35	1	0	-2.270433	-3.558096	-0.479665
36	1	0	-2.159159	-2.403070	0.543101
37	8	0	-2.344708	4.706277	0.685724
38	1	0	-2.084384	3.792971	0.525515
39	1	0	-3.007991	4.693712	1.366661
40	8	0	1.680661	-1.910575	0.066318
41	1	0	2.317453	-1.654870	0.729783
42	1	0	1.140857	-1.148393	-0.134884
43	8	0	4.257930	-0.029362	1.093147
44	1	0	4.438193	-0.216808	0.177248
45	1	0	3.828806	0.835066	1.134798
46	8	0	-0.032276	-4.420075	-0.223303
47	1	0	0.382973	-4.069891	-1.006871
48	1	0	0.230547	-3.868250	0.508286
49	8	0	1.497738	-2.786264	-2.838133
50	1	0	0.995707	-1.992134	-2.673906
51	1	0	2.189459	-2.824771	-2.183607

Zero-point correction= 0.410379 (Hartree/Particle)
E(RB+HF-LYP) = -567.557435289 A.U.

1E-Oanion.15H_2O



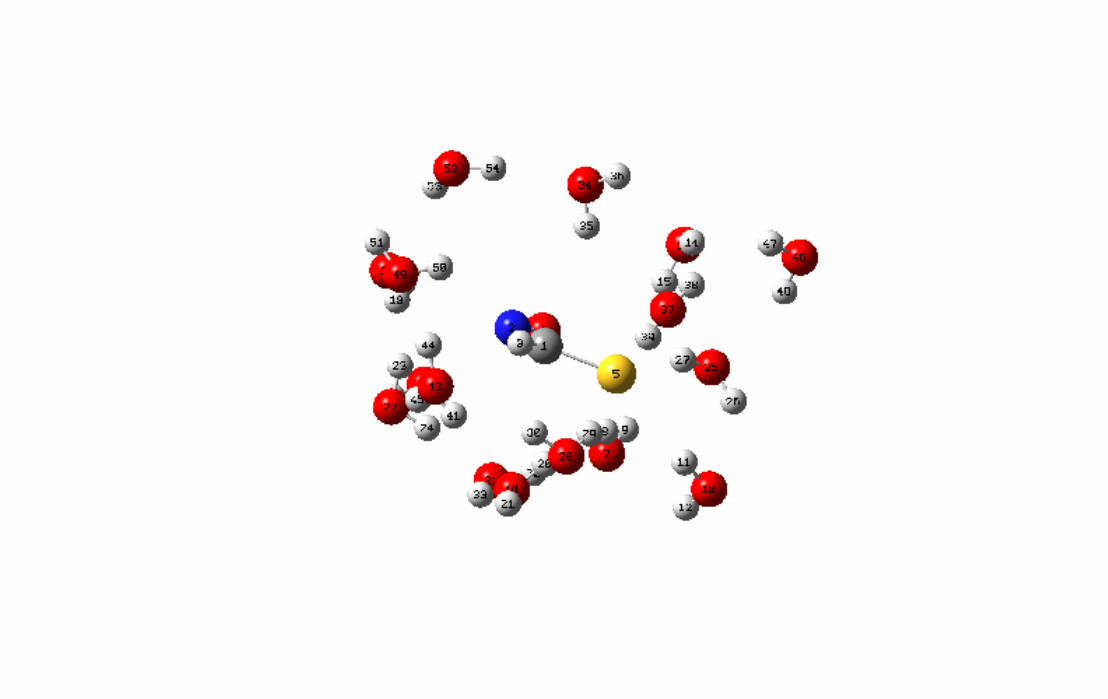
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.855642	-0.205447	-0.615345
2	7	0	-0.284470	-0.549468	-1.168344
3	16	0	1.107955	1.068513	0.556865
4	8	0	-0.488645	-1.535131	-1.987141
5	1	0	1.692535	-0.821665	-0.962929
6	1	0	-1.094680	0.021238	-0.878628
7	8	0	-1.342637	3.256949	0.901010
8	1	0	-0.666933	2.566095	0.884447
9	1	0	-1.993426	3.027301	1.557861
10	8	0	4.065350	0.026880	1.539434
11	1	0	4.727263	0.553864	1.102260
12	1	0	3.201600	0.423730	1.353870
13	8	0	-3.477254	0.867473	-1.704068
14	1	0	-3.511373	0.737167	-0.761553
15	1	0	-3.121229	1.746489	-1.867833
16	8	0	3.919971	2.350247	-0.774531
17	1	0	3.637152	2.976721	-1.431659
18	1	0	3.127651	1.976435	-0.372805
19	8	0	4.361570	-0.871696	-2.136655
20	1	0	4.139224	-0.027792	-1.755741
21	1	0	4.214011	-1.544190	-1.464801
22	8	0	-2.668711	-0.827924	1.042594
23	1	0	-2.202236	-0.978444	1.858476
24	1	0	-3.034536	-1.668542	0.742565
25	8	0	-0.701096	0.313932	3.308435
26	1	0	-0.257564	0.645425	2.520236
27	1	0	-0.259623	-0.487206	3.571185
28	8	0	1.557094	-1.860982	2.299294
29	1	0	2.419260	-1.786421	2.695724

30	1	0	1.392250	-1.052561	1.804076
31	8	0	0.865670	3.873263	-1.310328
32	1	0	1.007481	3.024157	-0.878560
33	1	0	0.410372	4.434381	-0.690565
34	8	0	-2.253924	3.304115	-1.665452
35	1	0	-2.035460	3.430063	-0.734251
36	1	0	-1.444122	3.361464	-2.164349
37	8	0	-3.070659	-2.359933	-2.323611
38	1	0	-2.125599	-2.157902	-2.328860
39	1	0	-3.540753	-1.536617	-2.418064
40	8	0	3.858976	-2.300111	0.137937
41	1	0	4.033382	-1.588136	0.765721
42	1	0	2.955395	-2.581179	0.252757
43	8	0	-3.307976	-3.334243	0.186987
44	1	0	-3.415914	-3.099836	-0.744082
45	1	0	-2.516351	-3.858922	0.266711
46	8	0	-3.694268	1.629928	2.490014
47	1	0	-3.890493	1.144713	1.693172
48	1	0	-3.016687	1.148892	2.957401
49	8	0	-0.109135	-4.129526	-0.128606
50	1	0	-0.244306	-3.743938	-0.990393
51	1	0	0.429260	-3.527957	0.376751

Zero-point correction= 0.410482 (Hartree/Particle)
E(RB+HF-LYP) = -567.566269021 A.U.

2Z-Sanion.15H_2O



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.234180	0.123580	0.725732
2	7	0	-0.964270	0.532744	-0.252706
3	1	0	-0.788151	0.187934	1.675558
4	8	0	-0.283320	0.471009	-1.510562
5	16	0	1.401896	-0.512419	0.802056
6	1	0	-1.019839	0.668878	-2.113970
7	8	0	1.185567	-2.322528	-2.052680
8	1	0	1.149992	-1.816068	-1.230022
9	1	0	1.611398	-1.776545	-2.707486
10	8	0	3.509074	-3.133121	-0.132827
11	1	0	2.944454	-2.520147	0.339416
12	1	0	2.977930	-3.546833	-0.806503
13	8	0	2.936073	2.426946	0.612501
14	1	0	3.120213	2.477569	1.547092
15	1	0	2.496932	1.582886	0.451757
16	8	0	-3.807537	1.842655	-1.628997
17	1	0	-3.461960	1.558603	-2.469903
18	1	0	-3.592798	1.167455	-0.985772
19	8	0	-0.977480	-3.155508	0.718157
20	1	0	-0.227960	-2.557137	0.687696
21	1	0	-1.063922	-3.460269	1.616345
22	8	0	-3.727046	-1.257390	-0.012700
23	1	0	-3.523768	-0.322555	0.004875
24	1	0	-2.902202	-1.736676	-0.014604
25	8	0	3.571320	-0.364207	-1.802576
26	1	0	4.064104	-1.132475	-1.530144
27	1	0	2.911187	-0.188578	-1.124665
28	8	0	0.262600	-2.384867	3.409582
29	1	0	0.789870	-1.864374	2.796839

30	1	0	-0.469238	-1.844600	3.690445
31	8	0	-1.436647	-2.938277	-2.516378
32	1	0	-0.487597	-2.767418	-2.492814
33	1	0	-1.694841	-3.253949	-1.654974
34	8	0	0.692180	3.790008	-1.058101
35	1	0	0.722883	2.854428	-1.237255
36	1	0	1.429287	3.994644	-0.490379
37	8	0	2.566836	0.950852	3.590584
38	1	0	3.108197	1.513194	3.042002
39	1	0	2.119653	0.333274	3.003875
40	8	0	-2.959397	-0.750668	-3.045223
41	1	0	-2.301836	-1.454457	-3.012679
42	1	0	-3.701277	-1.027618	-2.516036
43	8	0	-2.719666	-0.797485	3.247104
44	1	0	-2.870329	0.140335	3.314159
45	1	0	-3.114670	-1.094246	2.431998
46	8	0	5.573600	2.142285	-1.404558
47	1	0	4.904772	2.460130	-0.805226
48	1	0	5.221517	1.369282	-1.836373
49	8	0	-3.515445	1.752478	1.562097
50	1	0	-2.615401	1.913814	1.288397
51	1	0	-4.041038	2.486549	1.259692
52	8	0	-2.351141	4.158608	0.154635
53	1	0	-2.723412	3.767312	-0.630673
54	1	0	-1.404078	4.169333	0.050526

Zero-point correction= 0.426999 (Hartree/Particle)
E(RB+HF-LYP) = -567.564888695 A.U.