Electronic Supplementary Material (ESI) for RSC Advances.

Predicting the Reducing Power of Organic Super Electron Donors

Supporting Information

1. Model 2 HOMO / LUMO / Spin Density Figures

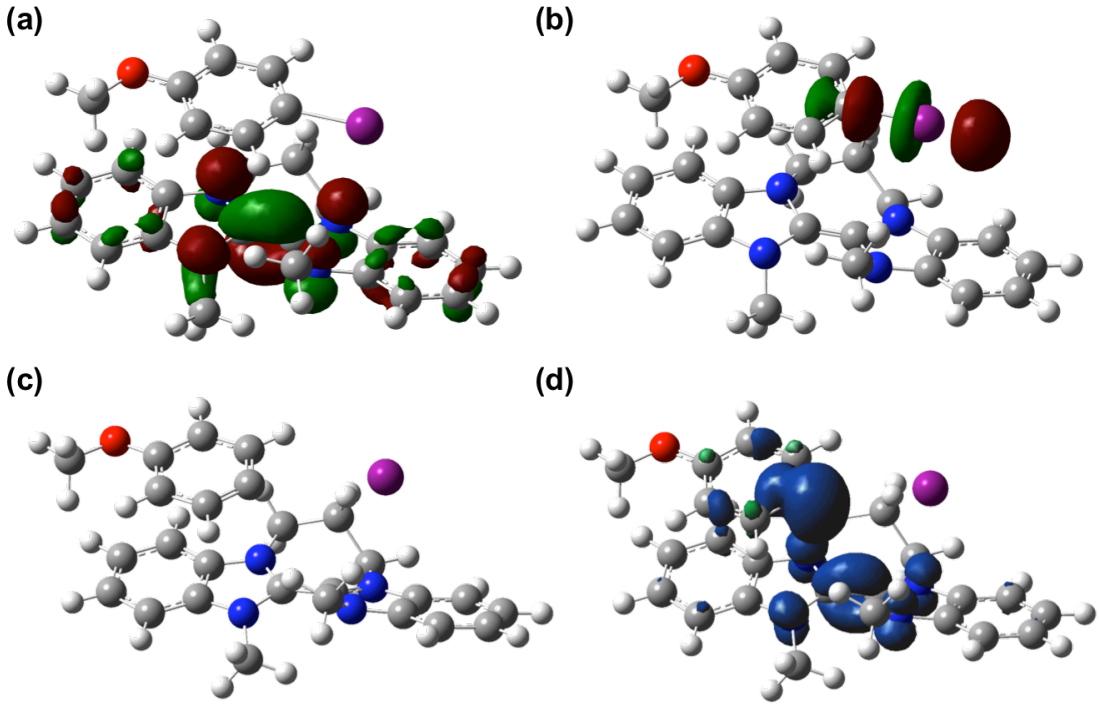


Figure S1. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **21** and 4-iodoanisole.

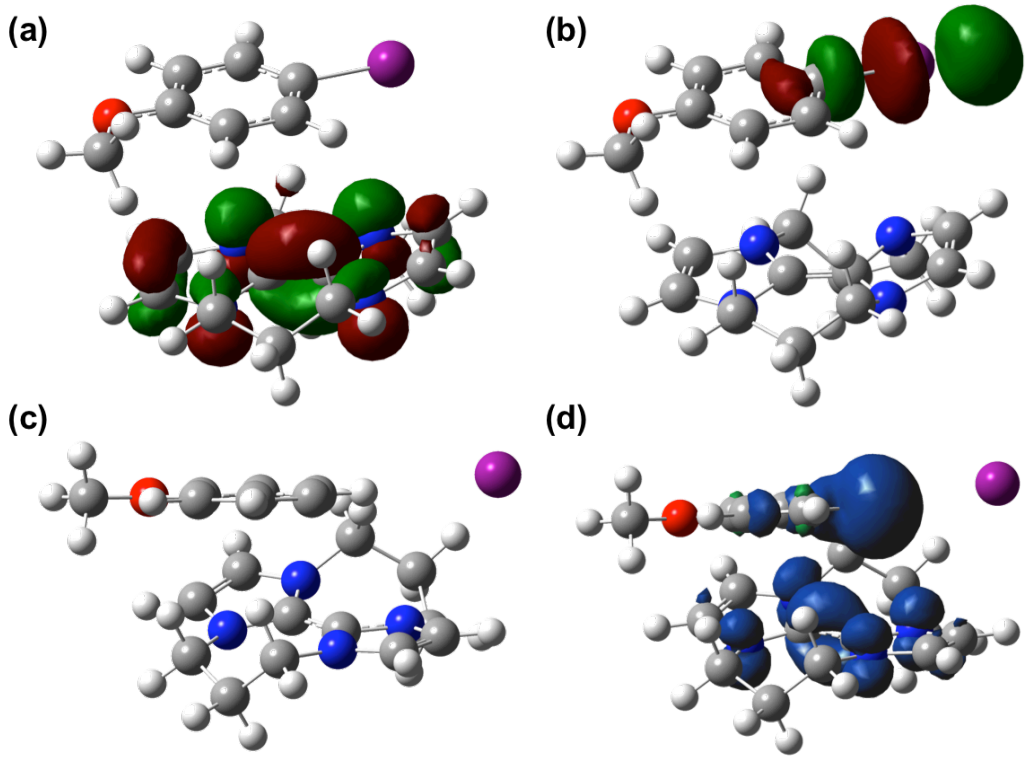


Figure S2. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **22** and 4-iodoanisole.

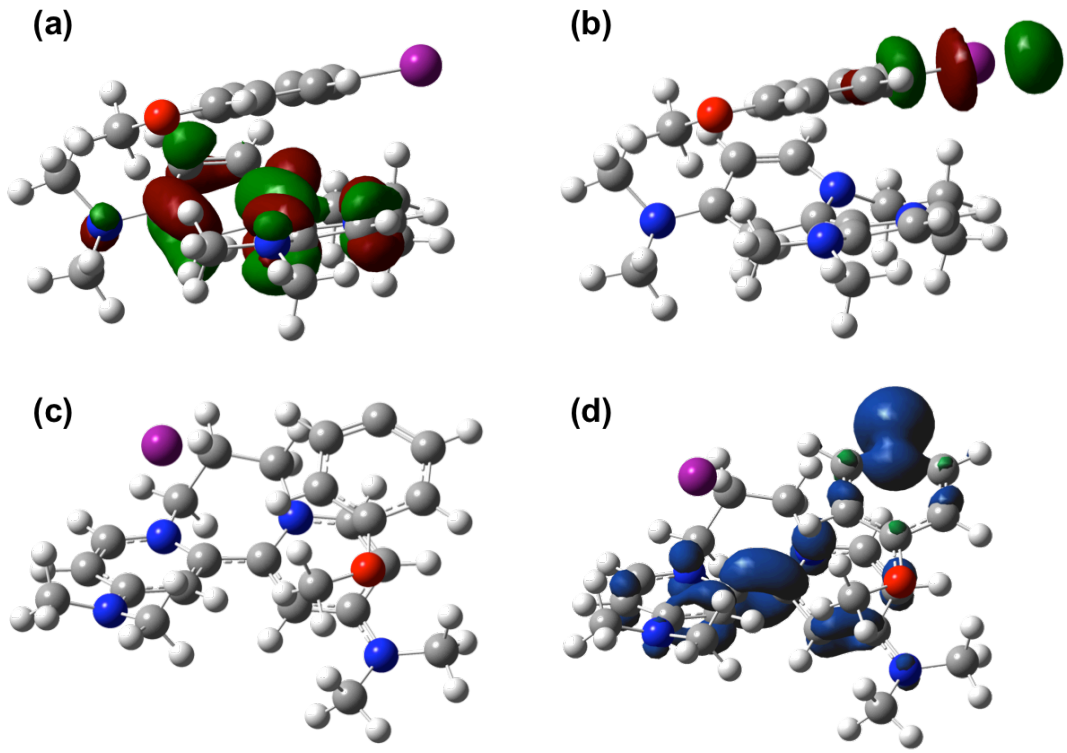


Figure S3. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **23** and 4-iodoanisole.

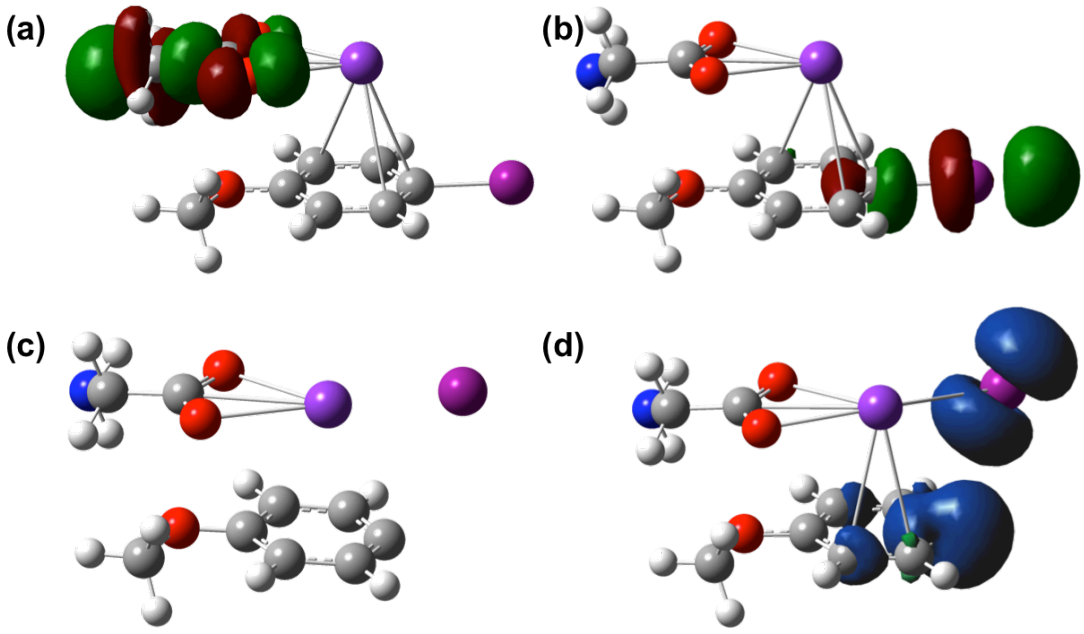


Figure S4. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **27** and 4-iodoanisole.

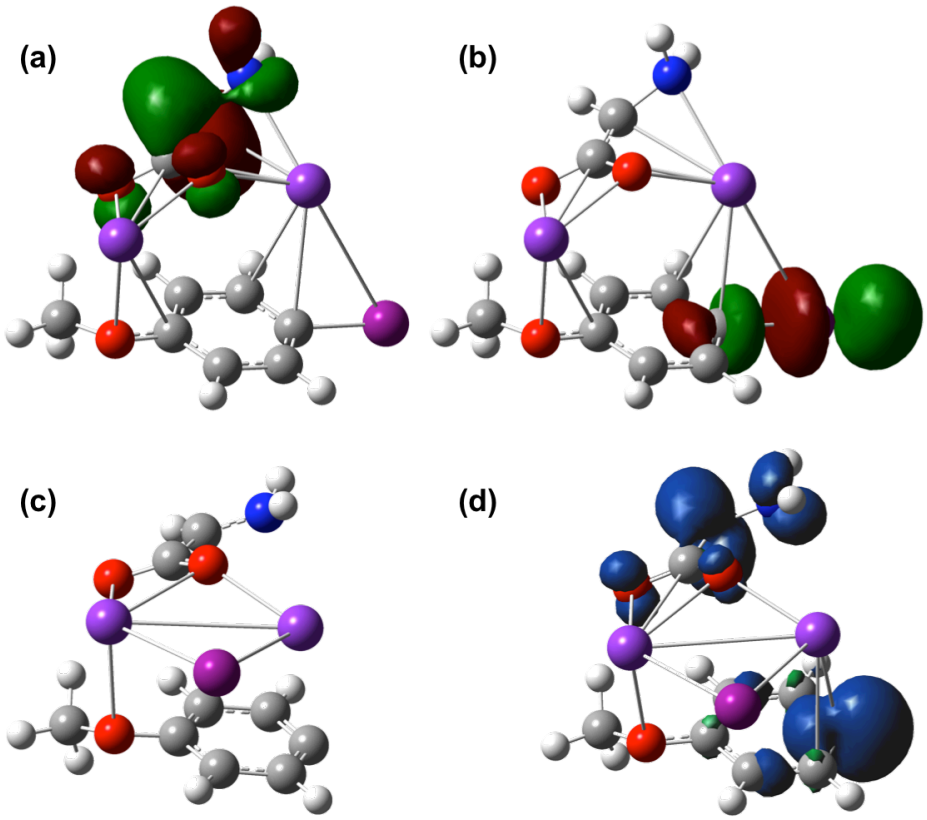


Figure S5. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **28** and 4-iodoanisole.

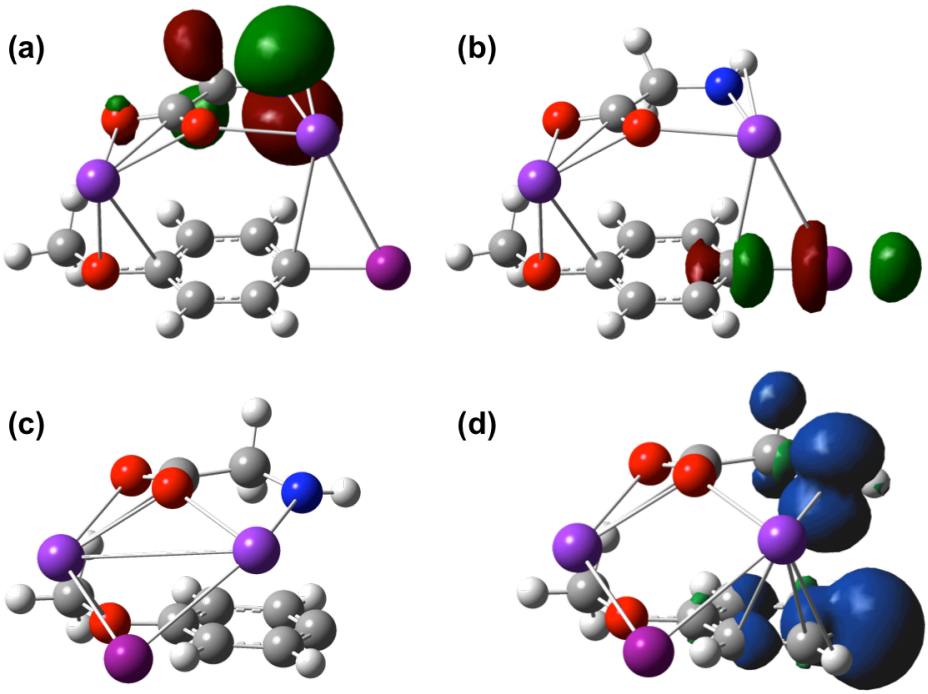


Figure S6. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **29** and 4-iodoanisole.

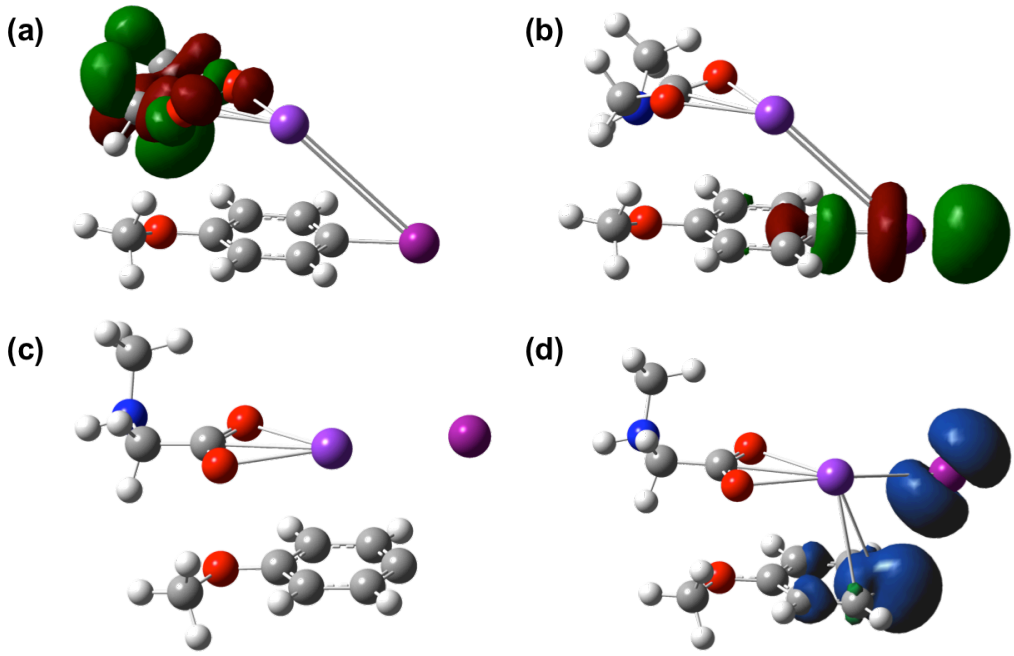


Figure S7. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **30** and 4-iodoanisole.

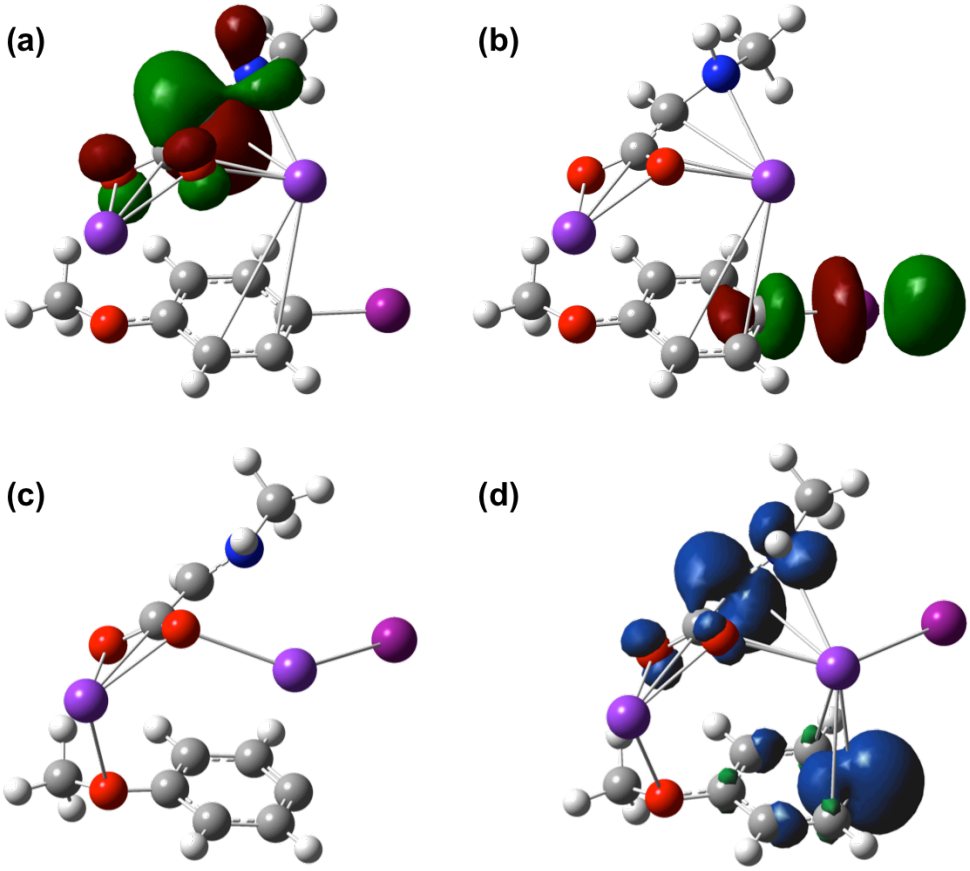


Figure S8. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **31** and 4-iodoanisole.

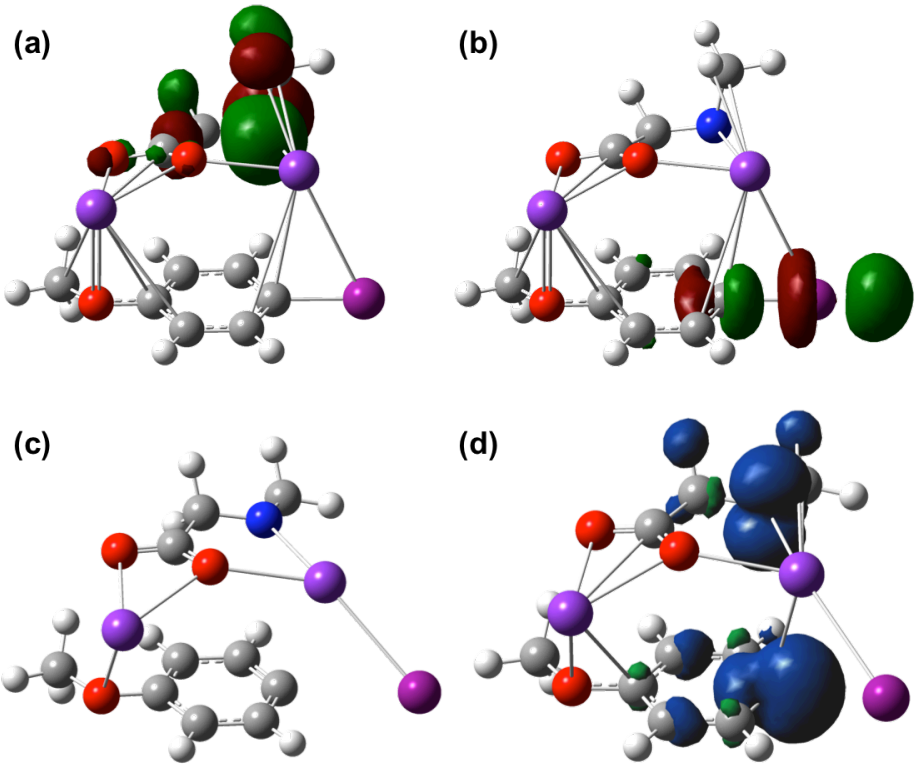


Figure S9. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **32** and 4-iodoanisole.

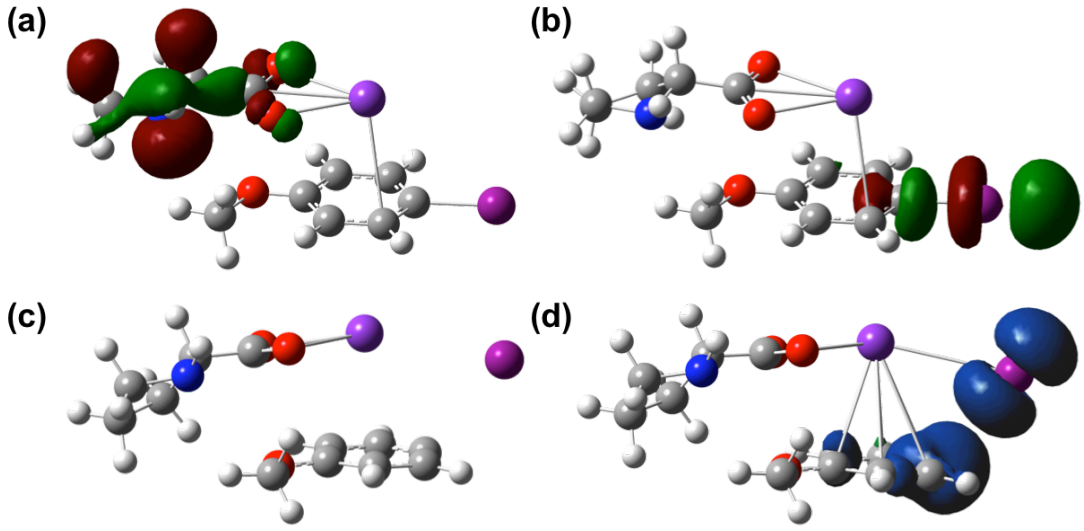


Figure S10. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **33** and 4-iodoanisole.

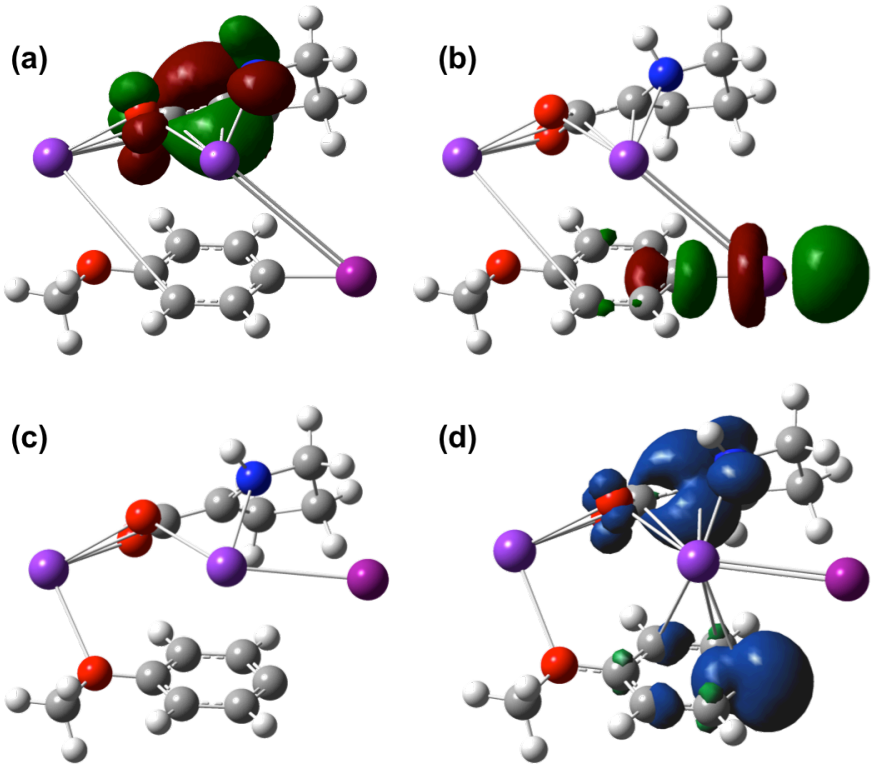


Figure S11. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **34** and 4-iodoanisole.

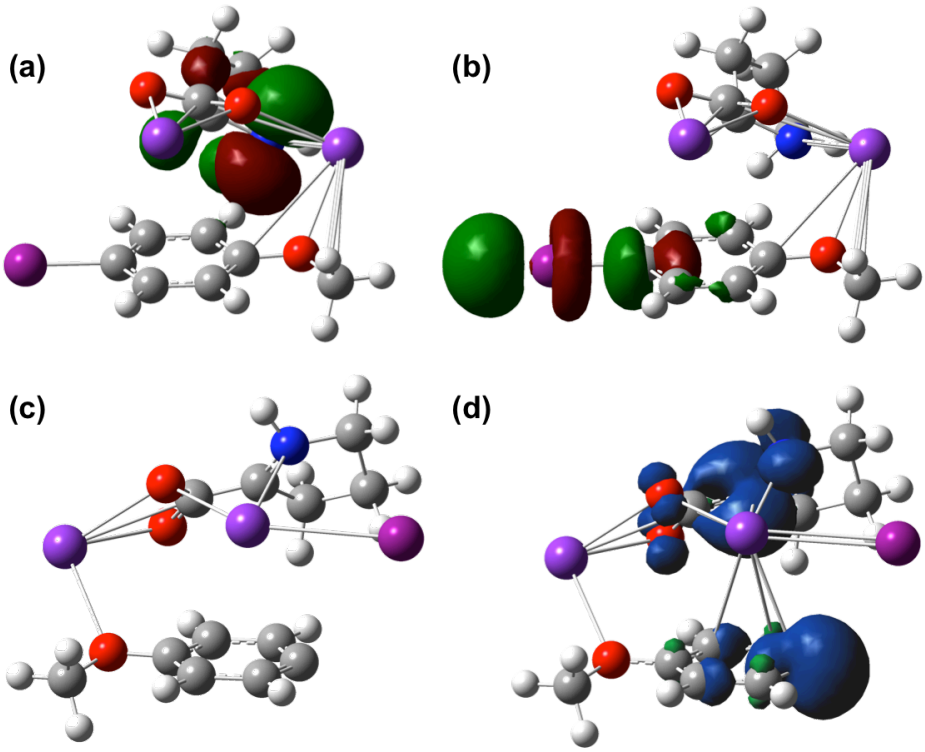


Figure S12. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **35** and 4-iodoanisole.

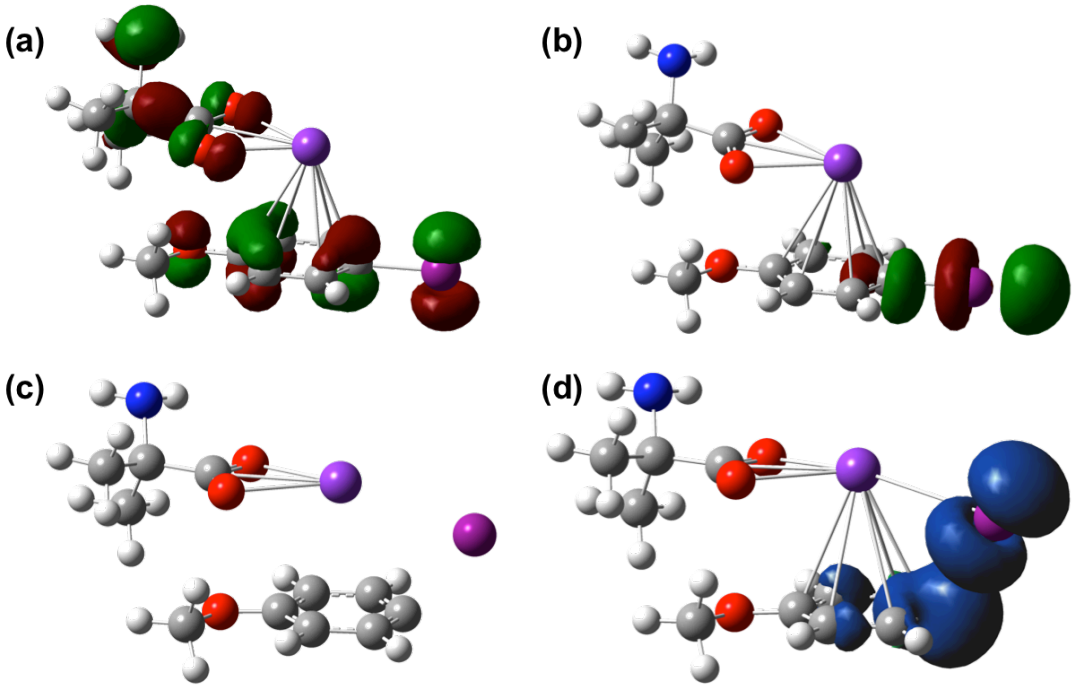


Figure S13. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **36** and 4-iodoanisole.

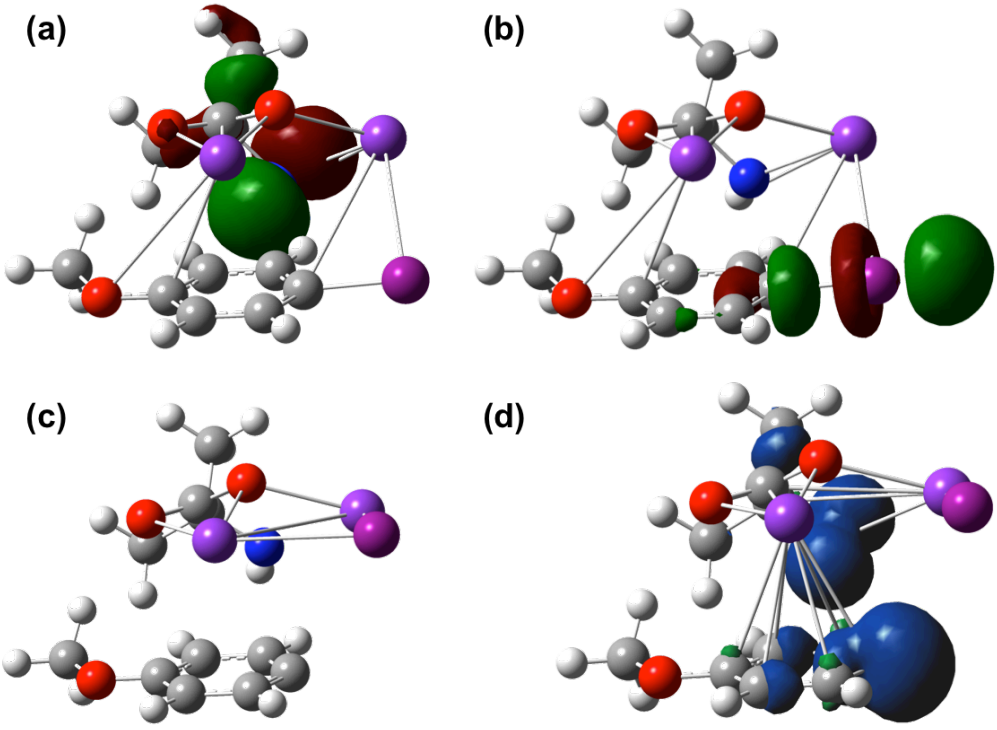


Figure S14. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **37** and 4-iodoanisole.

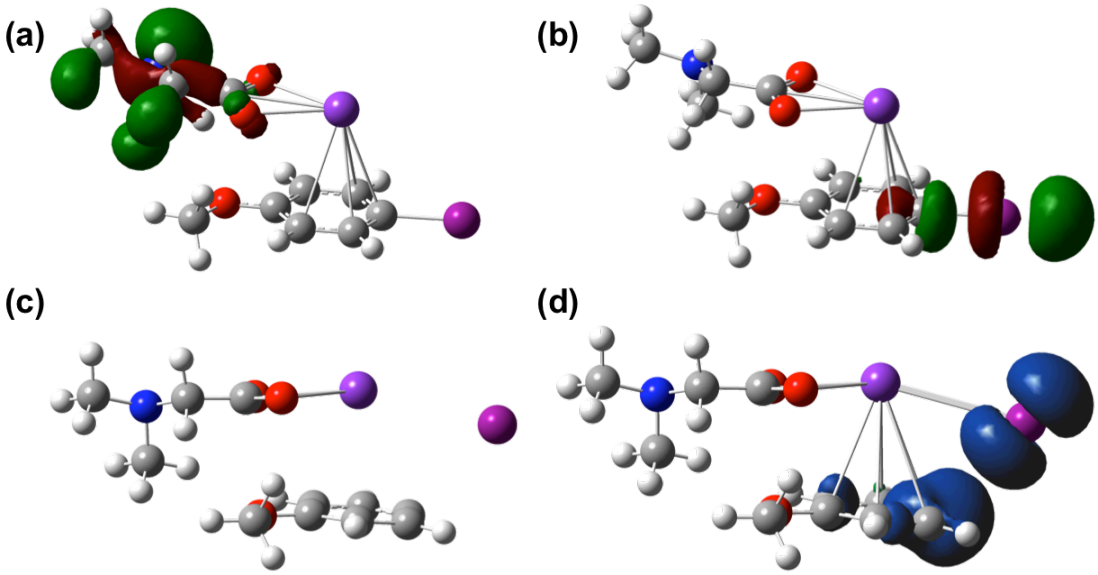


Figure S15. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **38** and 4-iodoanisole.

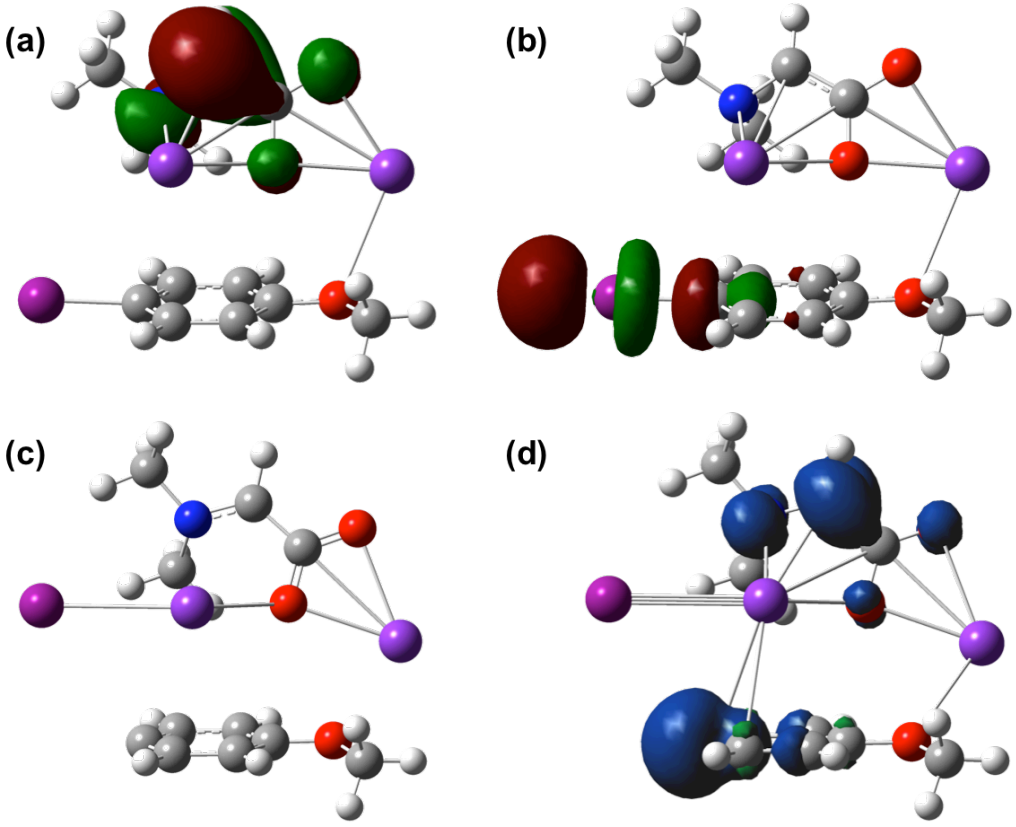


Figure S16. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **39** and 4-iodoanisole.

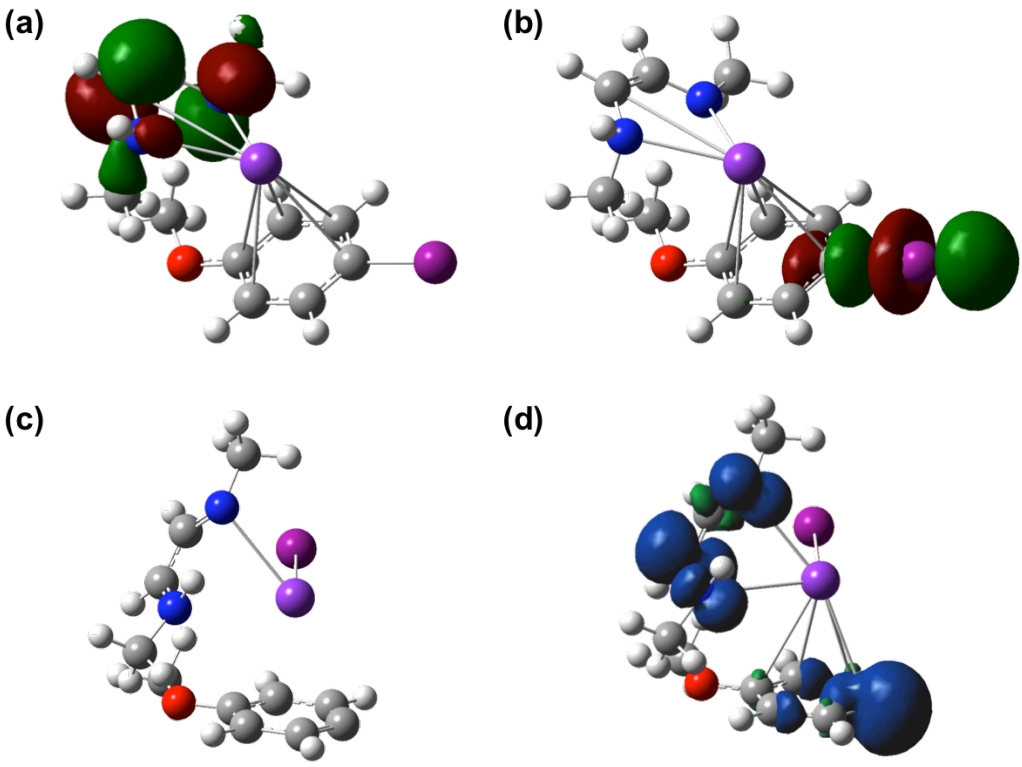


Figure S17. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **40** and 4-iodoanisole.

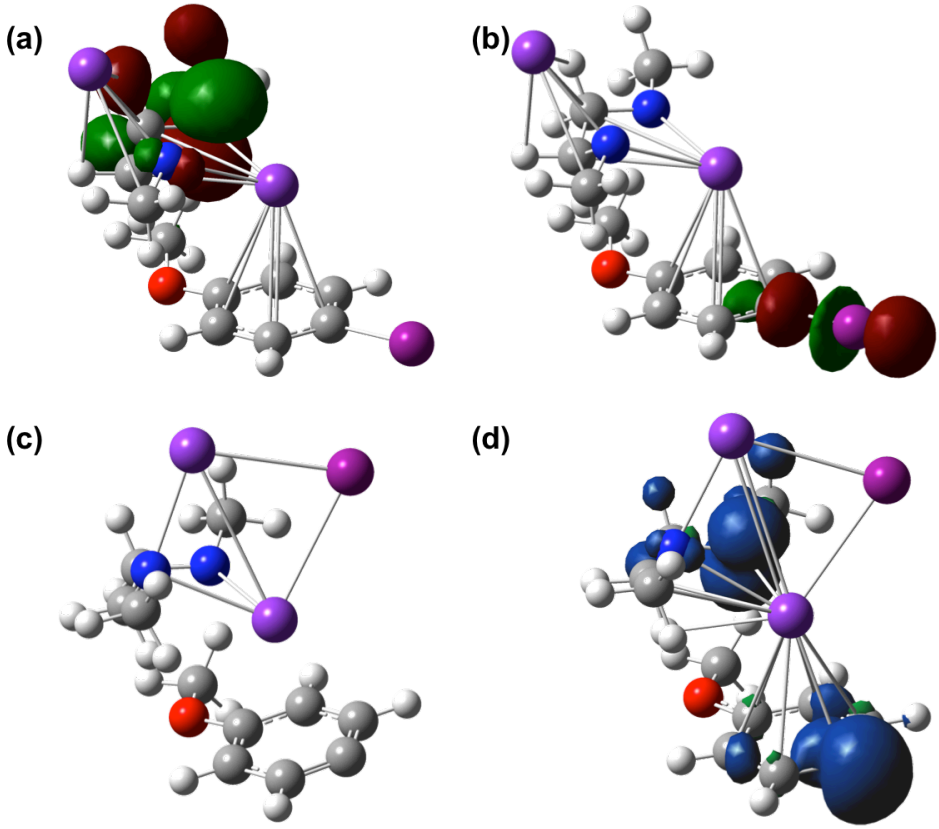


Figure S18. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **41** and 4-iodoanisole.

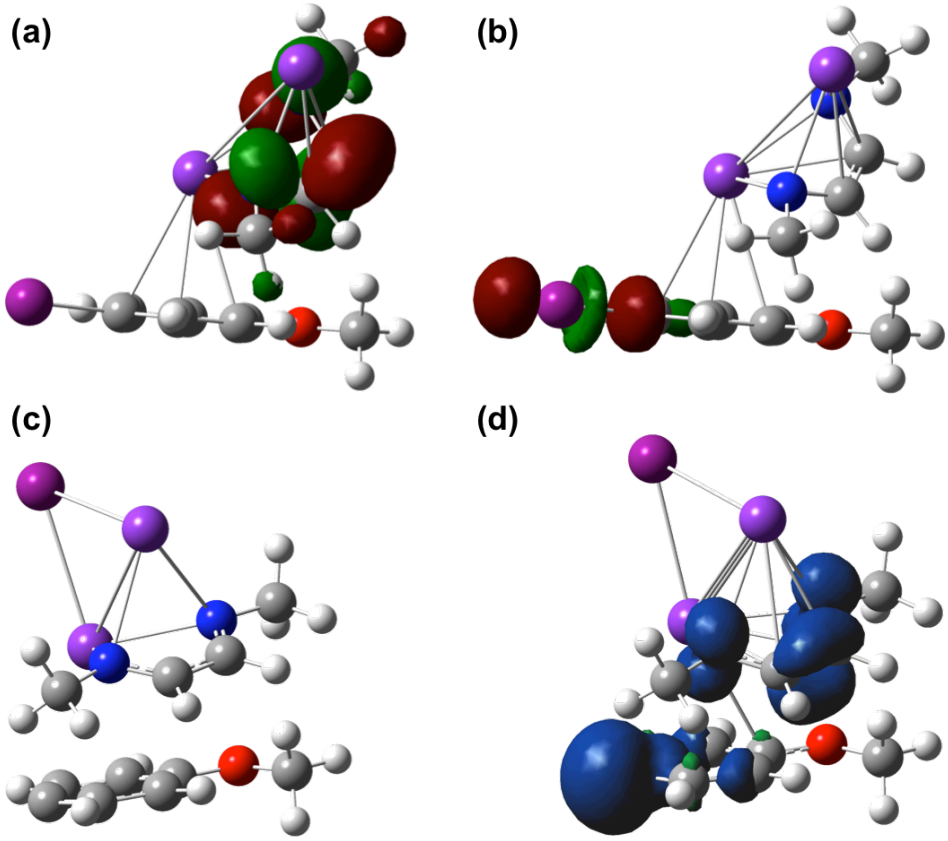


Figure S19. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **42** and 4-iodoanisole.

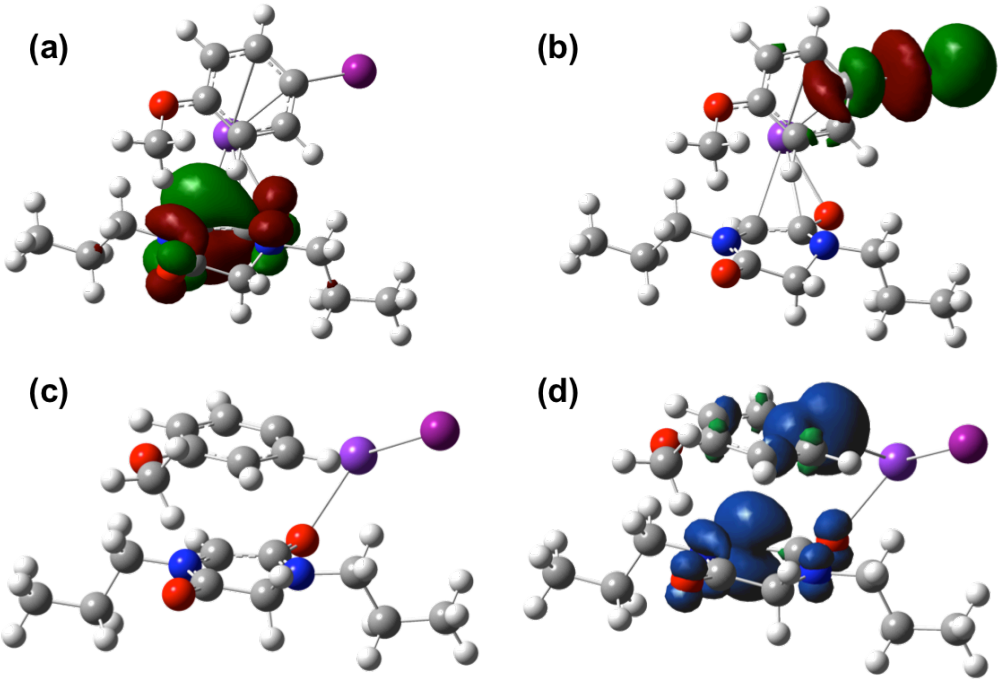


Figure S20. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **43** and 4-iodoanisole.

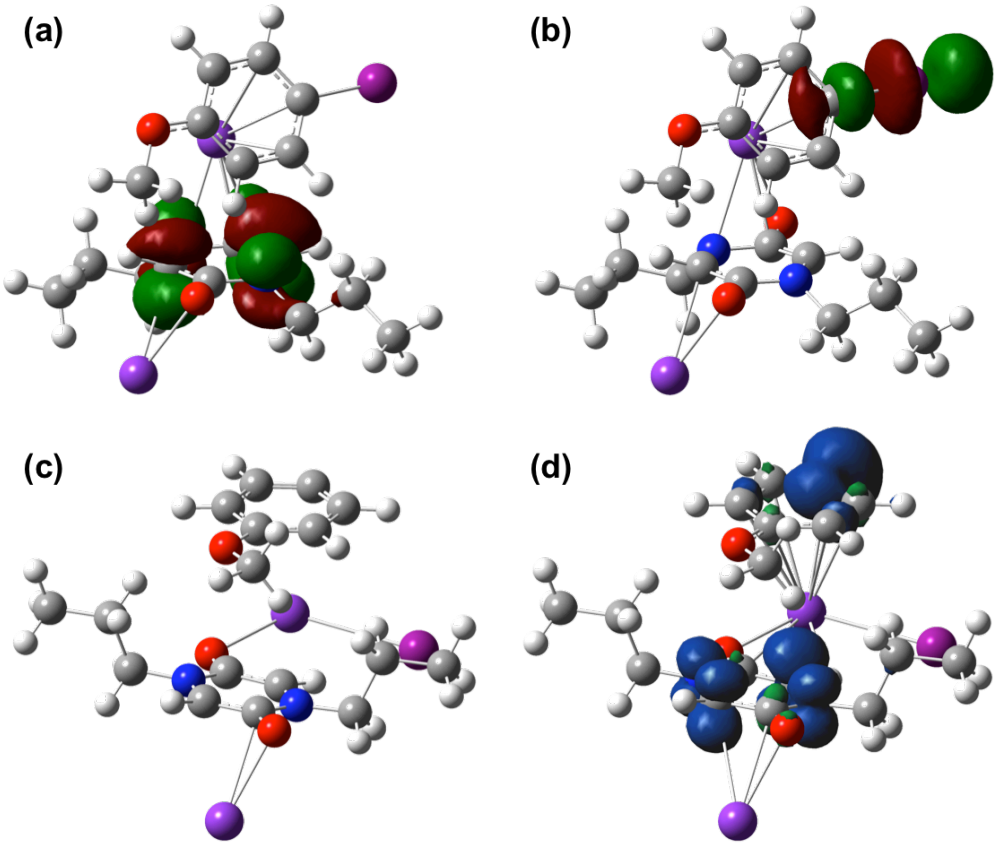
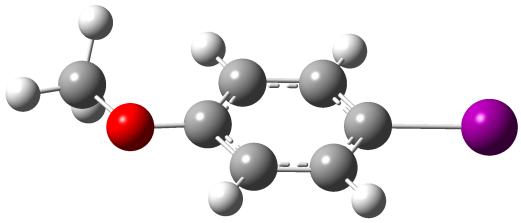


Figure S21. HOMO, LUMO and Spin Density Distribution for the electron transfer complex of **44** and 4-iodoanisole.

2. Model 1 Optimised Geometries and Coordinates

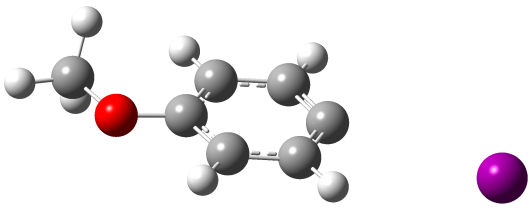
4-iodoanisole neutral



16
-641.6917422

C	-0.39875	1.33654	0.00007
C	0.20064	0.07456	0.00001
C	-0.57678	-1.07673	-0.00018
C	-1.97155	-0.97857	-0.00034
C	-2.57700	0.28105	-0.00025
C	-1.78328	1.43619	-0.00010
H	0.20938	2.23877	0.00018
H	-0.11031	-2.05986	-0.00028
H	-2.56172	-1.89062	-0.00056
H	-2.27189	2.40903	-0.00005
O	-3.91934	0.48453	-0.00022
C	-4.75155	-0.66465	0.00050
H	-5.77822	-0.29273	-0.00028
H	-4.57736	-1.27347	-0.89763
H	-4.57826	-1.27201	0.89979
I	2.30515	-0.07897	0.00004

4-iodoanisole radical anion

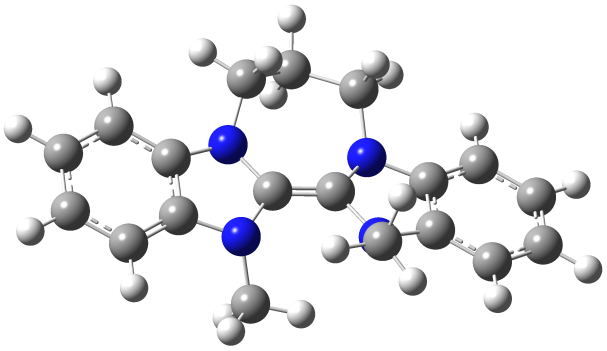


16
-641.7557501

C	0.81276	-0.83088	-0.00093
C	0.55146	0.52812	-0.00098
C	1.52727	1.49676	-0.00058
C	2.87306	1.08856	-0.00011
C	3.17302	-0.27650	-0.00007
C	2.14766	-1.23343	-0.00048

H	-0.00306	-1.55343	-0.00119
H	1.28099	2.55821	-0.00061
H	3.65767	1.84121	0.00024
H	2.41925	-2.28874	-0.00041
O	4.44806	-0.77953	0.00036
C	5.50703	0.15645	0.00080
H	6.42966	-0.42943	0.00106
H	5.47521	0.79171	-0.89630
H	5.47461	0.79156	0.89797
I	-3.01646	-0.01980	0.00020

21 neutral

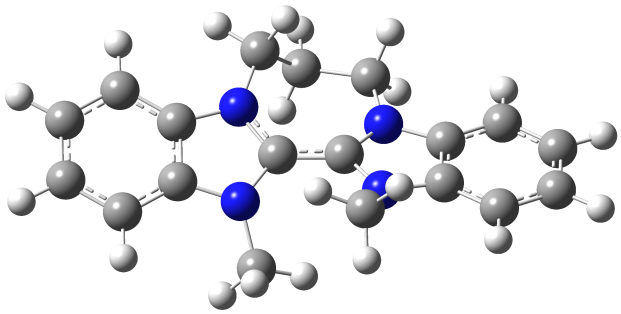


43
-954.7983378

C	-3.97779	-1.61609	-0.09040
C	-2.81886	-0.85763	-0.07068
C	-2.86334	0.54438	-0.04716
C	-4.07445	1.21846	0.00972
C	-5.25216	0.45225	0.01314
C	-5.20700	-0.93771	-0.04707
H	-3.94305	-2.70309	-0.12764
H	-4.12655	2.30468	0.03465
H	-6.21430	0.95988	0.05667
H	-6.13290	-1.50996	-0.05511
C	-0.68454	-0.08855	-0.07064
N	-1.55041	1.03037	-0.12716
N	-1.47657	-1.26863	-0.08605
C	0.66548	-0.06588	0.03435
C	2.79237	-0.85700	0.03335
C	2.84050	0.51676	-0.24950
C	3.94973	-1.61548	0.12226
C	4.05478	1.15861	-0.45366
C	5.17762	-0.97144	-0.09382
H	3.91291	-2.67777	0.35646
C	5.22767	0.39133	-0.37779
H	4.10830	2.22447	-0.66553
H	6.10025	-1.54639	-0.03598
H	6.18996	0.87352	-0.54121
N	1.53443	1.03127	-0.27150

N	1.45567	−1.24494	0.21628
C	1.32304	2.35284	0.30942
H	1.38850	2.29341	1.41164
H	2.13976	2.98887	−0.04474
C	−0.00279	2.98126	−0.08418
H	−0.10012	3.00736	−1.17699
H	0.00365	4.01587	0.28158
C	−1.21134	2.28368	0.52423
H	−2.08548	2.93405	0.43213
H	−1.02892	2.10249	1.60003
C	−1.12383	−2.35303	−0.99956
H	−0.06021	−2.58219	−0.90809
H	−1.70375	−3.24158	−0.73335
H	−1.34187	−2.07498	−2.04165
C	1.16522	−2.08518	1.37657
H	0.10661	−2.35926	1.37638
H	1.76437	−2.99861	1.31433
H	1.39908	−1.55668	2.31398

21 radical cation

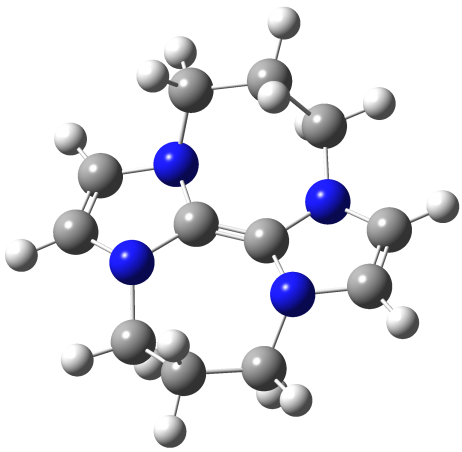


43
−954.6472359

C	−3.98421	−1.55966	−0.30475
C	−2.82188	−0.81704	−0.12825
C	−2.85598	0.54024	0.22421
C	−4.06195	1.20234	0.43968
C	−5.22940	0.45575	0.27590
C	−5.19364	−0.89624	−0.09317
H	−3.95437	−2.60986	−0.58726
H	−4.10550	2.25113	0.72308
H	−6.19158	0.93702	0.43850
H	−6.12799	−1.44035	−0.21435
C	−0.70460	−0.07624	−0.01135
N	−1.53987	0.97428	0.28050
N	−1.48948	−1.18052	−0.28542
C	0.69865	−0.06187	0.04948
C	2.81148	−0.83741	0.11831
C	2.85969	0.54140	−0.11725
C	3.96576	−1.60195	0.24370
C	4.07095	1.21547	−0.24710

C	5.18243	−0.93071	0.10624
H	3.92598	−2.67221	0.43396
C	5.23272	0.44854	−0.13645
H	4.12047	2.28767	−0.42029
H	6.11133	−1.49110	0.19040
H	6.20027	0.93583	−0.23796
N	1.55215	1.00470	−0.16682
N	1.47476	−1.19422	0.23370
C	1.29220	2.43782	−0.30385
H	1.66304	2.92338	0.61087
H	1.90271	2.79124	−1.14279
C	−0.15702	2.82695	−0.52805
H	−0.51796	2.47906	−1.50347
H	−0.18062	3.92190	−0.54292
C	−1.09684	2.32684	0.56567
H	−1.99540	2.94549	0.61001
H	−0.61358	2.35884	1.55342
C	−1.10991	−2.32323	−1.10964
H	−0.08842	−2.18947	−1.47066
H	−1.18506	−3.25505	−0.54046
H	−1.78613	−2.36814	−1.97027
C	1.08087	−2.38851	0.97607
H	0.06133	−2.26978	1.34735
H	1.14507	−3.27861	0.34269
H	1.75762	−2.50152	1.83011

22 neutral

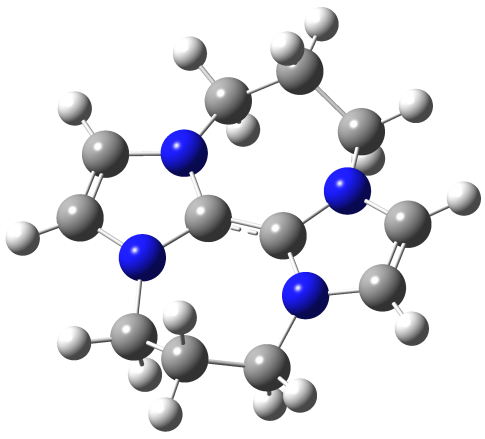


32
−685.6500854

C	−0.99771	−2.69086	−0.45527
C	−0.08440	−0.66677	−0.04778
C	0.27075	−2.88620	−0.08104
H	−1.74940	−3.42315	−0.72813
H	0.83423	−3.81138	−0.03273
C	0.08875	0.67313	−0.10659
C	−0.39351	2.88272	−0.26289

C	0.87846	2.78855	0.14870
H	-1.00000	3.76332	-0.43682
H	1.59792	3.56711	0.36774
N	0.88758	-1.66433	0.28542
N	-1.32799	-1.30802	-0.38920
N	-0.90854	1.60166	-0.48959
N	1.22384	1.42218	0.29907
C	-2.46761	-1.05481	0.51014
H	-3.35015	-1.48270	0.01552
H	-2.33191	-1.58366	1.47064
C	-2.68961	0.43678	0.77433
H	-3.74139	0.58715	1.04598
H	-2.08439	0.76494	1.62824
C	-2.34004	1.31654	-0.42406
H	-2.67513	0.84541	-1.35720
H	-2.84603	2.28438	-0.34013
C	2.55943	1.02196	-0.12287
H	3.24417	1.79933	0.23568
H	2.61877	0.99678	-1.22754
C	2.98909	-0.32849	0.42801
H	2.86209	-0.34920	1.51833
H	4.05795	-0.44794	0.20786
C	2.25391	-1.50230	-0.20109
H	2.78285	-2.43236	0.03769
H	2.25123	-1.37997	-1.30254

22 radical cation

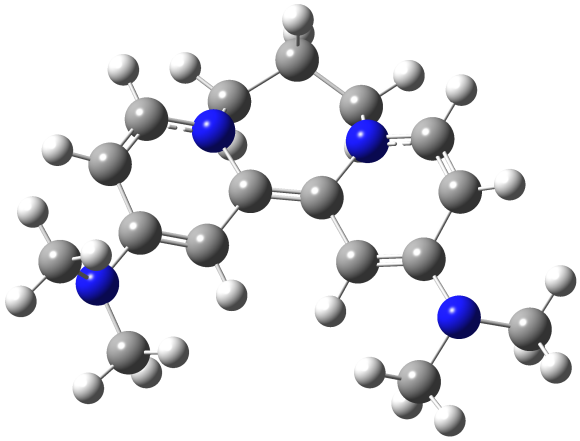


32
-685.5262611

C	-0.67378	-2.84896	0.15124
C	0.00006	-0.70500	-0.05358
C	0.67350	-2.84909	0.15120
H	-1.37704	-3.66645	0.23461
H	1.37663	-3.66668	0.23479
C	0.00013	0.70502	-0.05372
C	-0.67355	2.84901	0.15148
C	0.67373	2.84904	0.15131

H	-1.37671	3.66658	0.23492
H	1.37689	3.66661	0.23477
N	1.10673	-1.53834	0.03925
N	-1.10679	-1.53811	0.03934
N	-1.10669	1.53822	0.03934
N	1.10686	1.53828	0.03904
C	-2.49799	-1.25390	-0.29676
H	-2.59450	-1.17786	-1.39099
H	-3.06490	-2.12898	0.03217
C	-3.04389	0.00014	0.35411
H	-4.13039	0.00022	0.20902
H	-2.84649	0.00018	1.43308
C	-2.49781	1.25403	-0.29692
H	-2.59416	1.17777	-1.39116
H	-3.06474	2.12921	0.03170
C	2.49793	1.25386	-0.29696
H	3.06501	2.12893	0.03168
H	2.59450	1.17748	-1.39118
C	3.04371	-0.00006	0.35427
H	2.84596	0.00004	1.43318
H	4.13023	-0.00008	0.20948
C	2.49790	-1.25409	-0.29670
H	3.06486	-2.12914	0.03226
H	2.59454	-1.17804	-1.39093

23 neutral

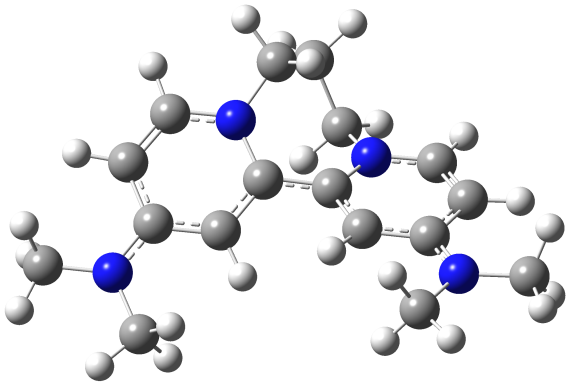


45
-880.9308864

C	-2.79001	-0.69727	-0.02424
C	-1.46364	-0.62290	-0.32664
C	-0.69617	0.61016	-0.17614
C	-2.79767	1.69009	0.31110
C	-3.46853	0.52248	0.39137
H	-0.92479	-1.51812	-0.60792
H	-3.30063	2.63755	0.49641
H	-4.51764	0.53790	0.66450

C	0.67257	0.59539	−0.12247
C	1.43615	−0.63692	−0.34091
C	2.63197	1.48386	0.94367
C	2.63383	−0.83552	0.27387
H	1.02223	−1.39440	−0.99737
C	3.19049	0.25939	1.05892
H	3.09520	2.36314	1.39116
H	4.06649	0.12322	1.68498
C	−1.10634	3.00878	−0.77770
H	−0.91938	2.72328	−1.82671
H	−1.98122	3.66641	−0.76504
C	1.39006	2.99561	−0.47198
H	1.50749	2.79385	−1.55030
H	2.24509	3.60279	−0.15536
C	0.09973	3.75673	−0.23958
H	−0.03239	3.96012	0.83123
H	0.16670	4.71786	−0.76775
N	−1.46663	1.80344	−0.03118
N	1.46096	1.73354	0.25845
N	−3.55390	−1.86726	−0.15743
N	3.36117	−2.03626	0.21194
C	−2.85094	−3.03046	−0.66122
H	−2.06518	−3.38151	0.03469
H	−3.57405	−3.83960	−0.80575
H	−2.38739	−2.79765	−1.62605
C	−4.40910	−2.20373	0.97588
H	−5.09579	−3.00227	0.67450
H	−3.81737	−2.55252	1.84140
H	−5.00488	−1.34359	1.28731
C	4.76876	−1.90671	−0.14866
H	5.27691	−2.85722	0.04885
H	4.88989	−1.65650	−1.21883
H	5.25214	−1.12733	0.44438
C	2.72554	−3.12660	−0.50052
H	2.62834	−2.92660	−1.58453
H	3.33111	−4.03001	−0.36990
H	1.72779	−3.30718	−0.08501

23 radical cation

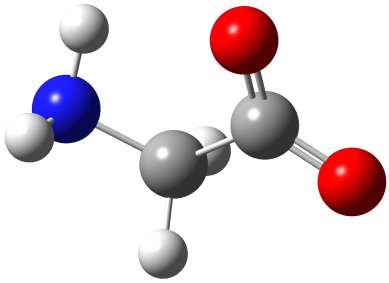


45
−880.8090837

C	2.87184	−0.71102	0.00235
C	1.48105	−0.70511	0.13936
C	0.70862	0.45413	−0.09655
C	2.72349	1.60824	−0.65563
C	3.50124	0.52550	−0.39106
H	0.96381	−1.57459	0.52789
H	3.15804	2.54745	−0.99036
H	4.57537	0.62050	−0.49618
C	−0.70859	0.45405	0.09694
C	−1.48092	−0.70525	−0.13894
C	−2.72361	1.60796	0.65600
C	−2.87173	−0.71128	−0.00201
H	−0.96360	−1.57476	−0.52732
C	−3.50127	0.52514	0.39139
H	−3.15827	2.54711	0.99079
H	−4.57540	0.62002	0.49661
C	0.59420	2.71967	−1.09793
H	1.25321	3.29719	−1.75085
H	−0.19941	2.28794	−1.71919
C	−0.59444	2.71999	1.09755
H	0.19957	2.28876	1.71863
H	−1.25334	3.29757	1.75053
C	−0.00053	3.59496	−0.00051
H	−0.77107	4.23903	−0.44086
H	0.76938	4.24007	0.43938
N	1.36789	1.60050	−0.55079
N	−1.36803	1.60038	0.55116
N	3.61825	−1.81091	0.25472
N	−3.61801	−1.81127	−0.25438
C	2.96267	−3.04019	0.66404
H	2.22343	−3.35160	−0.08681
H	3.71104	−3.82800	0.76176
H	2.45365	−2.91622	1.63127
C	5.07171	−1.74976	0.19083
H	5.47414	−2.73128	0.44647
H	5.41309	−1.49010	−0.81971

```
H                  5.47173     -1.01625      0.90354
C                 -5.07151     -1.74995     -0.19159
H                 -5.47386     -2.73145     -0.44745
H                 -5.41359     -1.49024      0.81869
H                 -5.47096     -1.01642     -0.90461
C                 -2.96233     -3.04034     -0.66423
H                 -2.22291     -3.35183      0.08639
H                 -3.71061     -3.82823     -0.76203
H                 -2.45351     -2.91599     -1.63153
```

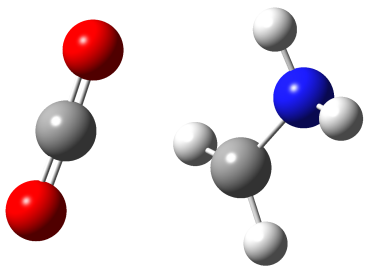
27 anion



```
9
-283.8693724

C                 -0.65061     -0.75280     -0.09480
H                 -0.62872     -1.53498      0.67465
H                 -0.63193     -1.27033     -1.06573
C                  0.66219      0.06505     -0.00063
O                  1.71684     -0.61418      0.06747
O                  0.55234      1.31663     -0.02825
N                 -1.89382      0.01648      0.01613
H                 -1.99825      0.29358      0.99060
H                 -1.70720      0.90330     -0.45369
```

27 radical

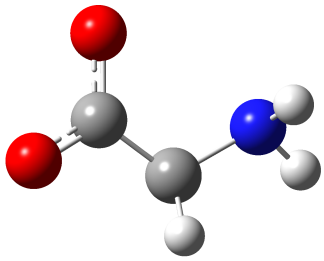


```
9
-283.7212725

C                  1.46749     -0.79229     -0.28053
H                  1.28163     -0.82214     -1.35126
```

H	1.65700	−1.72414	0.24514
C	−1.36877	0.14234	0.01356
O	−1.82161	−0.91374	0.17971
O	−0.95995	1.21834	−0.15041
N	2.10487	0.34156	0.20713
H	1.79569	1.22030	−0.19018
H	2.19176	0.39803	1.21382

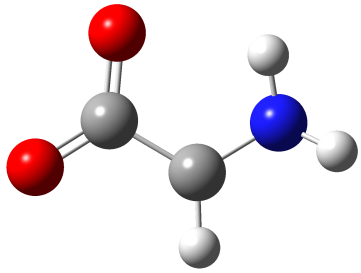
28 dianion



8
−283.1920040

C	0.66260	−0.67388	−0.22101
H	0.65445	−1.64341	0.30635
C	−0.61575	0.01516	−0.04471
O	−1.68388	−0.70635	0.08851
O	−0.67175	1.30185	−0.03396
N	1.88297	0.12769	0.01724
H	2.03052	0.33561	1.01326
H	2.69818	−0.39766	−0.28235

28 radical anion

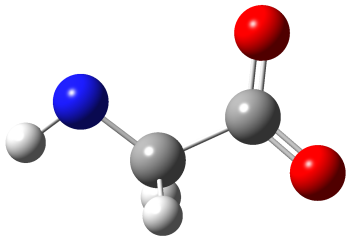


8
−283.2266551

C	0.64734	−0.70899	0.00960
H	0.69415	−1.79533	0.00634
C	−0.63212	0.03018	0.00248
O	−1.69653	−0.65239	−0.00049
O	−0.53526	1.29759	0.01015
N	1.82488	0.01060	−0.08777

H	1.65065	0.99765	0.08640
H	2.64404	−0.36526	0.37183

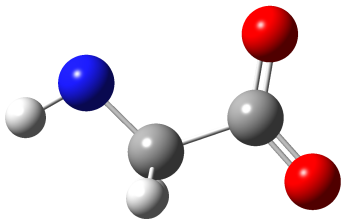
29 dianion



8
−283.2057930

C	−0.79022	−0.59123	−0.06711
H	−0.71974	−1.41516	0.68540
H	−0.74605	−1.13862	−1.04719
C	0.62435	0.05250	−0.00123
O	1.58922	−0.77971	0.05329
O	0.75993	1.30086	−0.02908
N	−1.93907	0.27841	0.08587
H	−2.75868	−0.33190	−0.02292

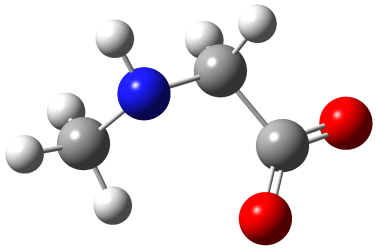
29 radical anion



8
−283.1977478

C	−0.75733	−0.60926	0.00014
H	−0.79994	−1.28709	0.87427
H	−0.79969	−1.28768	−0.87353
C	0.63908	0.06147	0.00019
O	1.58637	−0.76866	−0.00012
O	0.70165	1.30797	0.00006
N	−1.89603	0.26985	−0.00026
H	−2.72285	−0.34190	−0.00043

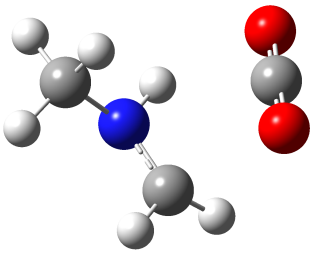
30 anion



12
−323.1499699

C	−0.08460	−0.92641	−0.09943
C	1.07147	0.10680	−0.03300
O	0.84252	1.28566	−0.38662
O	2.15524	−0.37666	0.38548
N	−1.37869	−0.40482	−0.52788
H	−1.99548	−1.19383	−0.69862
H	0.23272	−1.70365	−0.80748
C	−1.98723	0.45253	0.48095
H	−2.06313	−0.03631	1.47310
H	−1.37209	1.35209	0.58453
H	−2.99516	0.74625	0.16063
H	−0.13594	−1.40030	0.90099

30 radical

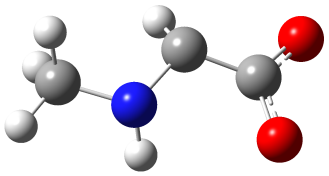


12
−323.0107602

C	−0.92681	−1.25978	−0.37255
C	1.68081	0.20058	−0.01143
O	1.23975	1.02839	−0.69904
O	2.16686	−0.59485	0.68114
N	−1.65826	−0.09345	−0.46044
H	−1.45242	0.47002	−1.27638
H	−0.68539	−1.76325	−1.30500
C	−1.86430	0.67775	0.75090
H	−2.31474	0.02841	1.51120
H	−0.92079	1.08341	1.15351
H	−2.55104	1.50548	0.54897

H	−1.05881	−1.84951	0.53244

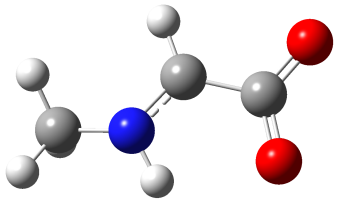
31 dianion



11
−322.4834831

C	−0.17397	−0.55287	−0.26832
C	1.17641	−0.03015	−0.04542
O	1.35485	1.24584	−0.00261
O	2.15266	−0.86122	0.10557
N	−1.24951	0.43623	−0.09128
H	−0.35203	−1.47171	0.32588
C	−2.53831	−0.18341	0.06308
H	−2.58244	−0.95093	0.87423
H	−3.31501	0.57101	0.27061
H	−2.79846	−0.70975	−0.87147
H	−1.05036	1.02938	0.71993

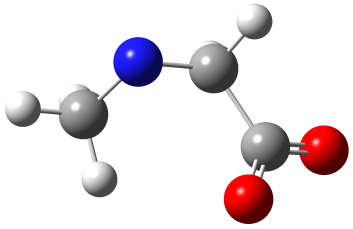
31 radical anion



11
−322.5145191

C	0.15428	−0.58014	0.09914
C	−1.20387	−0.00497	−0.01116
O	−1.26384	1.26409	−0.05459
O	−2.17286	−0.81529	−0.06031
N	1.22035	0.27198	0.26088
H	0.33415	−1.65201	0.16265
C	2.54536	−0.13492	−0.15157
H	2.62894	−0.27027	−1.24439
H	3.28109	0.61090	0.17035
H	2.79393	−1.09069	0.32845
H	0.93846	1.22793	0.05750

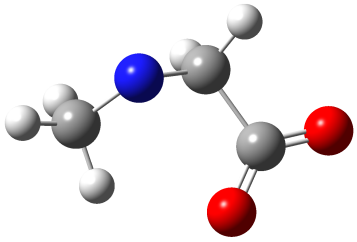
32 dianion



11
−322.5014565

C	−0.20500	−0.86034	−0.29426
C	1.03055	0.08151	−0.02983
O	0.97463	1.29438	−0.35698
O	2.04381	−0.48918	0.48447
N	−1.49023	−0.33767	−0.62396
H	0.15243	−1.53017	−1.10205
C	−2.01126	0.33837	0.52031
H	−2.08672	−0.32612	1.43984
H	−1.40892	1.21616	0.86856
H	−3.03569	0.71321	0.33224
H	−0.22273	−1.50827	0.63189

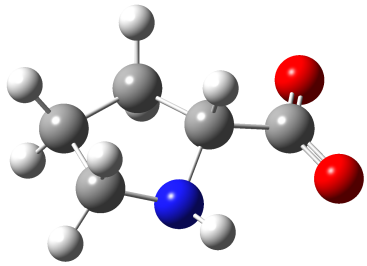
32 radical anion



11
−322.4998916

C	−0.11682	−0.95029	0.03895
C	1.04532	0.13850	−0.01212
O	0.71576	1.32967	−0.18316
O	2.18179	−0.35085	0.16180
N	−1.35378	−0.55768	−0.55043
H	0.27786	−1.83821	−0.46707
C	−2.08829	0.35608	0.28169
H	−2.18473	−0.02624	1.31547
H	−1.52860	1.30510	0.33863
H	−3.08726	0.53768	−0.13340
H	−0.22251	−1.17082	1.11910

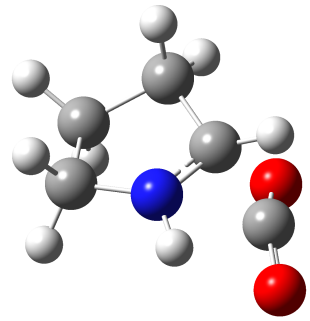
33 anion



16
−400.5540432

C	0.11859	−0.00471	0.38156
H	0.07122	−0.15198	1.48312
C	1.61833	0.00380	0.02225
O	2.15529	−1.13137	−0.04587
O	2.16330	1.12501	−0.12095
N	−0.61719	−1.07117	−0.30288
H	−0.25929	−1.98144	−0.03127
C	−0.70883	1.23301	0.02338
H	−0.62671	2.00896	0.79132
H	−0.32967	1.65259	−0.91437
C	−2.15271	0.68785	−0.13754
H	−2.85030	1.12098	0.58920
H	−2.53935	0.90342	−1.14057
C	−2.00765	−0.83584	0.06333
H	−2.69221	−1.42057	−0.56434
H	−2.20854	−1.08752	1.12371

33 radical

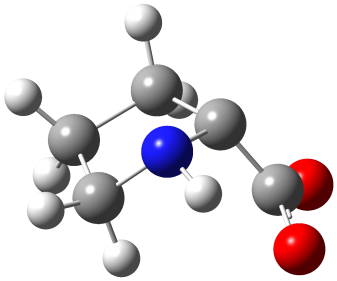


16
−400.4111134

C	−0.05494	−0.08045	0.92778
H	0.47735	−0.22145	1.87119
C	1.63965	0.04039	−0.13554
O	2.03287	−1.08899	−0.23949
O	1.81368	1.20440	−0.36630

N	−0.73191	−1.15560	0.43206
H	−0.31242	−2.07626	0.43830
C	−0.89752	1.13888	0.64977
H	−1.62228	1.28060	1.46476
H	−0.28972	2.04117	0.55305
C	−1.60068	0.73849	−0.65801
H	−2.56065	1.24208	−0.80033
H	−0.94924	0.98046	−1.50543
C	−1.76059	−0.78769	−0.54290
H	−1.59921	−1.30918	−1.49282
H	−2.74836	−1.06927	−0.15338

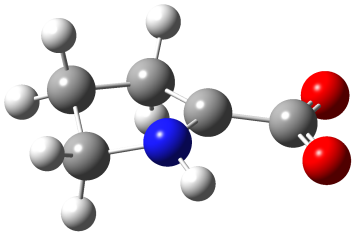
34 dianion



15
−399.8914677

C	−0.13324	0.15289	−0.80490
C	−1.37464	0.04793	−0.01682
O	−1.84747	−1.13155	0.22521
O	−1.98460	1.11620	0.36270
N	0.72218	−1.06223	−0.74896
H	0.06344	−1.83491	−0.65358
C	0.83009	1.25676	−0.41435
H	1.36199	1.71257	−1.27177
H	0.28764	2.05580	0.10669
C	1.89941	0.56078	0.50057
H	2.90828	0.64014	0.06334
H	1.93796	0.99352	1.51099
C	1.44409	−0.90741	0.53140
H	0.75887	−1.06134	1.38613
H	2.28886	−1.61305	0.62226

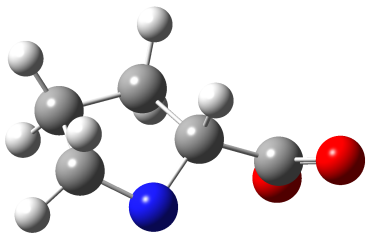
34 radical anion



15
−399.9188447

C	−0.14140	0.06877	−0.13155
C	−1.60645	0.01179	−0.00953
O	−2.12171	−1.15056	−0.00916
O	−2.21563	1.11766	0.09495
N	0.61619	−1.09293	−0.23164
H	0.11567	−1.92652	0.05990
C	0.76894	1.24941	0.03619
H	0.56433	2.05237	−0.68381
H	0.65103	1.68995	1.04039
C	2.17070	0.63043	−0.14394
H	2.46030	0.66912	−1.20195
H	2.94858	1.12519	0.44839
C	1.96359	−0.83478	0.26433
H	2.01701	−0.93329	1.36329
H	2.69622	−1.51681	−0.18411

35 dianion

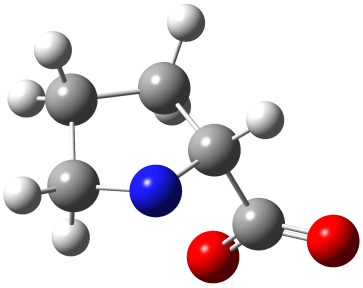


15
−399.9091035

C	−0.09578	−0.22372	−0.33436
H	−0.08305	−0.71258	−1.35207
C	−1.59086	0.00398	0.00899
O	−1.88110	0.93447	0.81168
O	−2.42756	−0.76436	−0.54852
N	0.60817	−1.02761	0.63572
C	0.73227	1.09059	−0.47108
H	0.67732	1.51334	−1.48806
H	0.32530	1.82410	0.23415
C	2.16368	0.64671	−0.08987

H	2.89746	0.82862	−0.89388
H	2.51334	1.16681	0.81415
C	1.95890	−0.87153	0.21081
H	2.68324	−1.25543	0.95162
H	2.18916	−1.40864	−0.76826

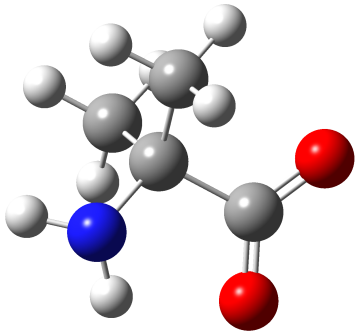
35 radical anion



15
−399.9035663

C	−0.14639	0.21404	−0.74688
H	−0.50101	0.46479	−1.75303
C	−1.46064	0.02542	0.14349
O	−1.25639	−0.05632	1.37438
O	−2.53416	−0.03004	−0.48931
N	0.51411	−1.06481	−0.77116
C	0.82554	1.25685	−0.14072
H	1.04172	2.06366	−0.85073
H	0.38342	1.69079	0.76156
C	2.08255	0.43808	0.21018
H	2.83952	0.52762	−0.58038
H	2.54062	0.74081	1.15929
C	1.54306	−0.99878	0.24709
H	1.05334	−1.18425	1.22085
H	2.30328	−1.77256	0.08098

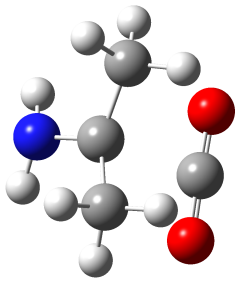
36 anion



```
15
-362.4700599

C                  0.53097     -0.03228     -0.04167
C                 -1.03176      0.05075     -0.04252
O                 -1.52526      1.19848      0.06038
O                 -1.64518     -1.04638     -0.08605
N                  0.94105     -1.28810     -0.68670
H                  1.80316     -1.63058     -0.26811
H                  0.20452     -1.96448     -0.48795
C                  1.14883      1.14312     -0.79419
H                  0.85297      2.09234     -0.33526
H                  2.24638      1.05851     -0.78176
H                  0.81395      1.13679     -1.83858
C                  0.96027      0.01245      1.43334
H                  0.52086     -0.83364      1.97848
H                  2.05702     -0.04970      1.51197
H                  0.62746      0.94641      1.90371
```

36 radical

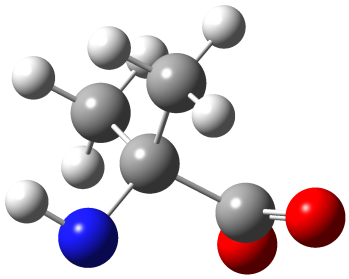


```
15
-362.3282860

C                  1.02790      0.00007     -0.03638
C                 -1.84193      0.00023      0.11051
O                 -1.87377      1.16225      0.10714
O                 -1.87187     -1.16185      0.10598
N                  0.99779     -0.00126     -1.43976
H                  0.60679      0.83563     -1.85807
```

H	0.60518	−0.83826	−1.85633
C	1.44423	1.29104	0.59016
H	1.26448	1.27025	1.67145
H	2.52067	1.49077	0.43123
H	0.88543	2.13688	0.16609
C	1.44229	−1.29038	0.59256
H	0.88286	−2.13625	0.16939
H	2.51863	−1.49150	0.43477
H	1.26171	−1.26767	1.67367

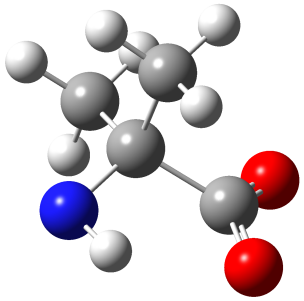
37 dianion



14
−361.8123220

C	−0.54164	−0.00004	−0.11312
C	1.02498	0.00007	−0.01304
O	1.60937	−1.11991	0.02670
O	1.60925	1.12011	0.02689
N	−0.91345	−0.00033	−1.51955
H	−1.94446	0.00015	−1.52428
C	−1.08136	−1.24296	0.63614
H	−0.79058	−1.26000	1.70254
H	−2.18274	−1.24342	0.57246
H	−0.69243	−2.14580	0.15484
C	−1.08161	1.24302	0.63573
H	−0.69289	2.14579	0.15417
H	−2.18300	1.24321	0.57203
H	−0.79087	1.26031	1.70211

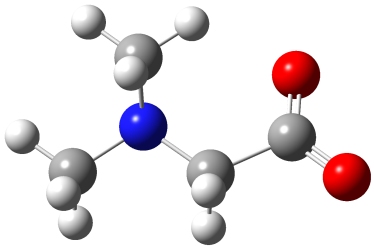
37 radical anion



14
−361.8092287

C	−0.55645	−0.07666	−0.09522
C	1.01433	0.12263	−0.02541
O	1.68931	−0.92800	−0.14630
O	1.41399	1.28686	0.18635
N	−0.88599	−1.10714	−1.04262
H	−0.16702	−1.82577	−0.87806
C	−0.96857	−0.56553	1.31152
H	−0.71770	0.20797	2.04910
H	−2.05003	−0.75498	1.34509
H	−0.43117	−1.48694	1.56475
C	−1.29421	1.21152	−0.44166
H	−0.98357	1.57092	−1.43020
H	−2.37685	1.02348	−0.45974
H	−1.06872	1.99270	0.29152

38 anion

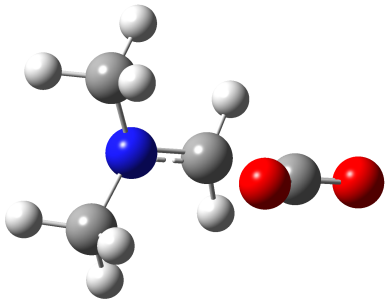


15
−362.4419395

C	0.06837	−0.72305	0.09008
H	−0.01574	−1.05457	1.14725
H	0.09380	−1.63391	−0.52469
C	1.45820	−0.05078	−0.07200
O	2.39800	−0.72244	0.42533
O	1.53008	1.04420	−0.67389
N	−1.09398	0.06159	−0.30311
C	−1.25776	1.21473	0.56530

H	-1.43497	0.90789	1.62010
H	-0.35465	1.82889	0.51718
H	-2.11941	1.80976	0.23402
C	-2.28699	-0.76096	-0.26685
H	-3.15898	-0.16806	-0.57377
H	-2.17946	-1.60686	-0.95774
H	-2.48819	-1.16793	0.74872

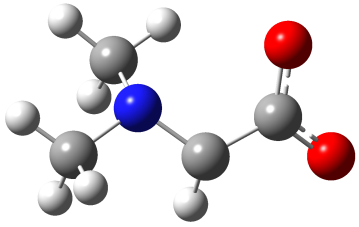
38 radical



15
-362.2998120

C	0.05099	0.00150	-1.06303
H	0.30567	-0.92331	-1.58154
H	0.30578	0.92765	-1.57907
C	1.49393	-0.00045	0.22291
O	2.50082	0.00085	-0.43657
O	1.02583	-0.00238	1.33291
N	-1.15486	0.00072	-0.43751
C	-1.62762	-1.22737	0.17360
H	-2.72099	-1.20375	0.23300
H	-1.31260	-2.08142	-0.43272
H	-1.20800	-1.32361	1.18653
C	-1.62717	1.22713	0.17732
H	-1.20725	1.32027	1.19041
H	-1.31204	2.08289	-0.42654
H	-2.72053	1.20363	0.23696

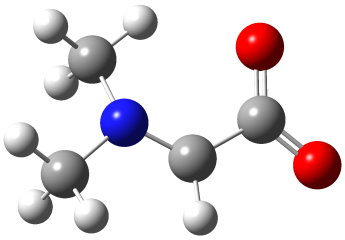
39 dianion



14
−361.7790759

C	−0.09167	−0.76414	−0.01907
H	0.03994	−1.36815	0.90550
C	−1.40200	−0.11507	−0.09081
O	−2.40110	−0.69224	0.49007
O	−1.54093	0.98776	−0.74132
N	1.08678	0.05658	−0.29193
C	1.24823	1.15372	0.64672
H	2.10274	1.79719	0.36414
H	0.32915	1.74954	0.63642
H	1.42456	0.77683	1.68429
C	2.28143	−0.74332	−0.30722
H	3.16934	−0.12288	−0.51832
H	2.45865	−1.25324	0.67485
H	2.18853	−1.52660	−1.07102

39 radical anion

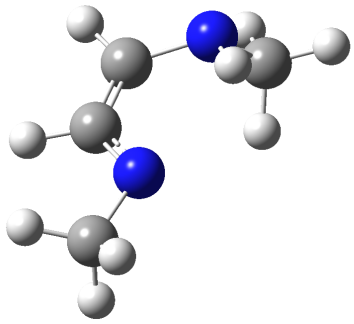


14
−361.7976113

C	−0.09982	−0.68892	0.01536
H	−0.05300	−1.77697	0.02360
C	−1.45196	−0.06957	−0.02185
O	−2.40139	−0.87314	0.21289
O	−1.56089	1.16434	−0.28662
N	1.10243	−0.04790	−0.22002
C	1.29638	1.31003	0.26559
H	2.13965	1.76603	−0.26949
H	0.37763	1.87400	0.09375
H	1.52941	1.30260	1.34799
C	2.28646	−0.86938	−0.08008

H	3.14067	−0.36521	−0.54907
H	2.53046	−1.05354	0.98411
H	2.13003	−1.83414	−0.57501

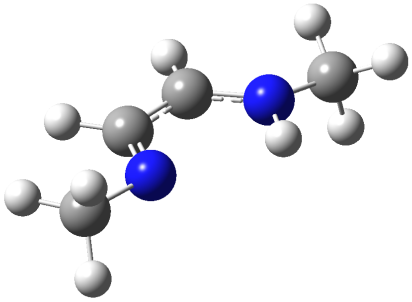
40 anion



15
−267.2627687

C	−0.68755	0.99393	0.01359
H	−1.09095	1.98705	0.20987
C	0.66028	0.73145	0.13146
H	1.26952	1.56744	0.53422
N	1.27890	−0.39819	−0.23577
N	−1.56466	0.03071	−0.59780
H	−0.94830	−0.65537	−1.03216
C	2.67754	−0.44607	0.10350
H	2.87440	−0.84469	1.12475
H	3.22743	−1.10523	−0.58866
H	3.17517	0.54894	0.06289
C	−2.41064	−0.67419	0.36411
H	−2.98406	−1.46303	−0.14614
H	−1.83382	−1.12763	1.19174
H	−3.12684	0.03415	0.80251

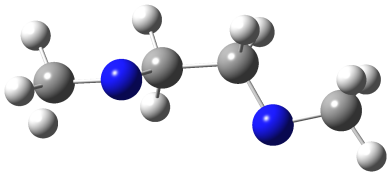
40 radical



15
−267.2013262

C	−0.64856	0.80430	−0.02925
H	−1.17761	1.75403	−0.00401
C	0.75982	0.74152	0.00873
H	1.30202	1.69698	0.05680
N	1.38209	−0.40878	−0.01221
N	−1.38915	−0.32119	−0.13381
H	−0.86285	−1.18554	−0.06960
C	2.82738	−0.36415	0.03101
H	3.19185	−0.94320	0.89184
H	3.24291	−0.83964	−0.86953
H	3.22971	0.66105	0.10226
C	−2.81957	−0.34653	0.07969
H	−3.25732	−1.19663	−0.45262
H	−3.07753	−0.42357	1.14642
H	−3.25616	0.57547	−0.32049

41 dianion

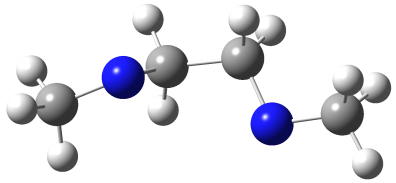


16
−267.7947450

C	−0.74208	0.54556	−0.20011
H	−0.76773	0.46645	−1.32640
H	−1.13416	1.59478	−0.00335
C	0.74215	0.54558	0.20009
H	1.13420	1.59477	0.00333
H	0.76784	0.46647	1.32642
N	1.56970	−0.42936	−0.43393
N	−1.56971	−0.42933	0.43393
C	2.88447	−0.27877	0.06336

H	2.98535	−0.41220	1.18593
H	3.58611	−0.99923	−0.39706
H	3.33610	0.75474	−0.10737
C	−2.88452	−0.27876	−0.06336
H	−3.58618	−0.99917	0.39711
H	−3.33607	0.75480	0.10733
H	−2.98540	−0.41224	−1.18588

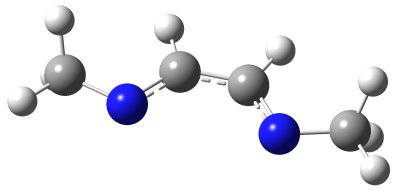
41 radical anion



16
−267.7933218

C	0.75269	0.70187	0.15931
H	0.78068	0.75910	1.28409
H	1.21478	1.67744	−0.17431
C	−0.71237	0.70991	−0.23896
H	−1.15739	1.71953	−0.10172
H	−0.77830	0.47871	−1.32182
N	−1.48646	−0.22003	0.53981
N	1.40358	−0.43908	−0.37621
C	−2.75632	−0.48633	−0.08284
H	−2.61275	−0.98104	−1.06149
H	−3.37620	−1.13173	0.55134
H	−3.30970	0.45166	−0.28602
C	2.76319	−0.43691	0.05960
H	3.31547	−1.30046	−0.34694
H	3.33539	0.48326	−0.24783
H	2.88506	−0.47392	1.17681

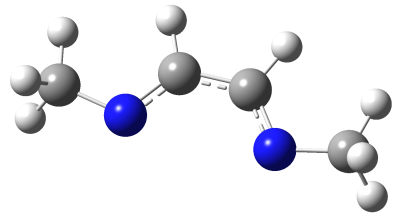
42 dianion



14
−266.6085801

C	−0.69921	0.51224	−0.00031
H	−1.13634	1.53310	−0.00032
C	0.69920	0.51224	−0.00031
H	1.13634	1.53311	−0.00031
N	1.55312	−0.55145	−0.00054
N	−1.55312	−0.55145	−0.00055
C	2.91224	−0.12796	0.00054
H	3.19946	0.50520	0.89056
H	3.60069	−0.99087	0.00001
H	3.20032	0.50701	−0.88787
C	−2.91224	−0.12796	0.00055
H	−3.60069	−0.99086	−0.00001
H	−3.19945	0.50518	0.89058
H	−3.20032	0.50703	−0.88785

42 radical anion

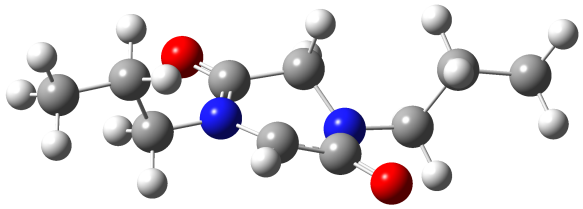


14
−266.6579070

C	−0.71093	0.57472	−0.00456
H	−1.16122	1.58565	−0.00073
C	0.71093	0.57472	−0.00455
H	1.16121	1.58565	−0.00074
N	1.50044	−0.48882	−0.01262
N	−1.50044	−0.48883	−0.01268
C	2.91420	−0.20149	0.01019
H	3.38243	−0.57563	0.93923
H	3.43391	−0.70865	−0.82108
H	3.14709	0.88100	−0.06276
C	−2.91420	−0.20149	0.01020
H	−3.43398	−0.70885	−0.82089
H	−3.38234	−0.57541	0.93938

H	−3.14710	0.88098	−0.06297

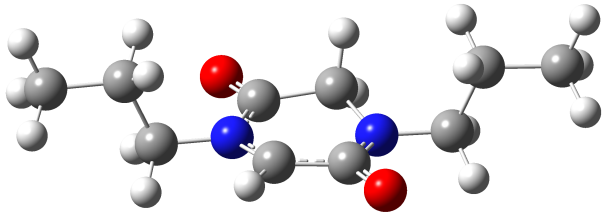
43 anion



31
−651.1624749

C	0.65717	1.20875	0.09754
C	−0.82682	1.22100	−0.20881
C	−0.56530	−1.18960	−0.08074
C	0.79839	−1.17638	−0.33613
H	1.07248	2.17206	−0.21896
H	0.75957	1.12758	1.20163
H	−1.11611	−2.11120	0.06217
N	−1.35583	−0.00615	−0.28671
N	1.33384	0.12922	−0.59770
O	1.57871	−2.17390	−0.37631
O	−1.46998	2.28090	−0.34198
C	2.78246	0.23031	−0.60438
H	3.05336	1.17538	−1.10174
C	−2.78043	−0.15688	−0.51745
H	−3.12561	0.72534	−1.06871
H	−2.92610	−1.04863	−1.14257
C	−3.56369	−0.29012	0.78722
H	−3.38257	0.61245	1.38623
H	−3.16794	−1.14321	1.35502
C	−5.05663	−0.46873	0.53181
H	−5.61491	−0.55763	1.47171
H	−5.46090	0.38856	−0.02364
H	−5.24571	−1.37382	−0.06156
C	3.43565	0.17191	0.77872
H	3.07303	−0.73321	1.28231
H	3.12270	1.03796	1.37899
C	4.95763	0.14769	0.67114
H	5.43332	0.12015	1.65966
H	5.28870	−0.73651	0.10989
H	5.32662	1.03870	0.14298
H	3.16345	−0.59905	−1.20963

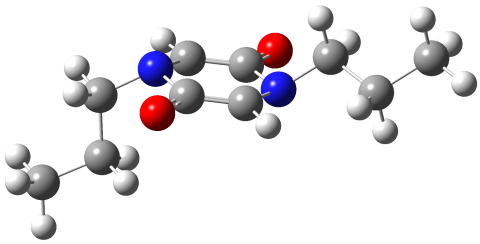
43 radical



31
-651.0673086

C	0.64891	1.25703	-0.18676
C	-0.84754	1.16617	-0.39309
C	-0.61708	-1.22394	-0.32211
C	0.82729	-1.18527	-0.38584
H	1.00080	2.08946	-0.80709
H	0.79507	1.55022	0.86797
H	-1.11719	-2.18411	-0.26603
N	-1.39285	-0.09891	-0.44140
N	1.39228	0.05804	-0.52135
O	1.49687	-2.22437	-0.37258
O	-1.53658	2.17004	-0.45719
C	2.84505	0.16563	-0.51553
H	3.11096	1.07769	-1.06732
C	-2.85320	-0.22785	-0.49110
H	-3.23234	0.59749	-1.10092
H	-3.07738	-1.17405	-0.99626
C	-3.46780	-0.19047	0.90371
H	-3.19170	0.75893	1.37998
H	-3.03337	-1.00064	1.50517
C	-4.98500	-0.33119	0.84062
H	-5.42114	-0.30369	1.84534
H	-5.42762	0.48530	0.25574
H	-5.27182	-1.28132	0.37123
C	3.44085	0.20087	0.89078
H	3.12623	-0.70764	1.42026
H	3.03636	1.06113	1.44200
C	4.96304	0.28852	0.84337
H	5.38849	0.32256	1.85274
H	5.38549	-0.58189	0.32500
H	5.28613	1.19162	0.30841
H	3.23758	-0.69715	-1.06321

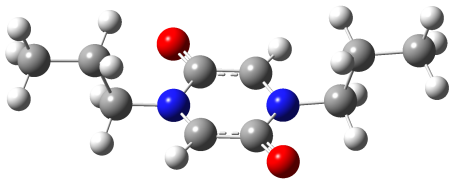
44 dianion



30
-650.5267276

C	-0.71867	1.26088	0.67098
C	0.53549	1.42679	0.13433
C	0.55413	-1.00794	-0.08060
C	-0.70406	-1.16605	0.46484
H	-1.26791	2.14746	0.98756
H	1.02985	-1.89177	-0.49944
N	1.24662	0.24439	-0.29596
N	-1.37066	0.00211	0.96131
O	-1.34506	-2.27953	0.55158
O	1.14434	2.55484	-0.01189
C	-2.79676	0.01031	0.67110
H	-3.24096	0.87209	1.19797
C	2.62638	0.22922	0.16137
H	2.98827	1.26341	0.11730
H	2.68185	-0.11955	1.21970
C	3.53258	-0.65851	-0.68815
H	3.45336	-0.32865	-1.73430
H	3.18278	-1.69918	-0.64930
C	4.98592	-0.59330	-0.22243
H	5.63732	-1.23403	-0.83242
H	5.36822	0.43563	-0.28103
H	5.07162	-0.92122	0.82326
C	-3.14458	0.09317	-0.81797
H	-2.66871	-0.76138	-1.31830
H	-2.70186	1.00706	-1.23637
C	-4.65250	0.07346	-1.05058
H	-4.90452	0.13347	-2.11864
H	-5.09402	-0.85168	-0.65208
H	-5.13902	0.91966	-0.54267
H	-3.22976	-0.90758	1.08649

44 radical anion

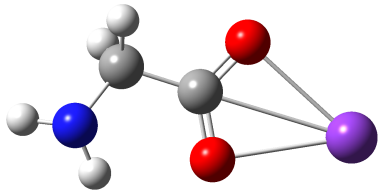


30
-650.5433453

C	0.60784	1.22198	-0.49767
C	-0.79260	1.22002	-0.49847
C	-0.60790	-1.22259	-0.49727
C	0.79255	-1.22063	-0.49778
H	1.14862	2.16204	-0.48613
H	-1.14867	-2.16266	-0.48552
N	-1.37114	-0.05381	-0.54357
N	1.37108	0.05318	-0.54328
O	1.53701	-2.24466	-0.46569
O	-1.53708	2.24406	-0.46698
C	2.81300	0.16327	-0.45227
H	3.11711	1.06892	-0.99624
C	-2.81306	-0.16382	-0.45231
H	-3.24424	0.71205	-0.94806
H	-3.11716	-1.07018	-0.99511
C	-3.30070	-0.22558	0.99477
H	-2.97255	0.69281	1.49847
H	-2.81127	-1.07110	1.49779
C	-4.81738	-0.36561	1.07126
H	-5.16323	-0.40486	2.11148
H	-5.31081	0.48472	0.58149
H	-5.15086	-1.28394	0.56818
C	3.30081	0.22684	0.99467
H	2.97269	-0.69089	1.49962
H	2.81149	1.07301	1.49672
C	4.81751	0.36689	1.07077
H	5.16354	0.40733	2.11090
H	5.31082	-0.48403	0.58191
H	5.15094	1.28461	0.56657
H	3.24407	-0.71326	-0.94692

3. Model 1K Optimised Geometries and Coordinates

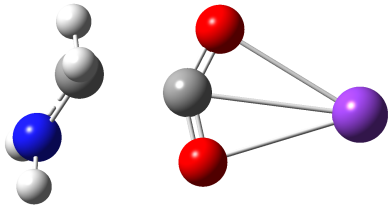
27 neutral



10
−883.7361013

C	2.03215	0.55563	0.06367
H	2.23635	0.98706	1.05872
H	2.23935	1.34145	−0.67352
C	0.52615	0.28289	0.03727
O	−0.23255	1.28879	−0.03145
O	0.13823	−0.91601	0.11711
N	2.81152	−0.64518	−0.22317
H	3.69900	−0.62711	0.26857
H	2.28111	−1.44331	0.12012
K	−2.35430	−0.19764	−0.02645

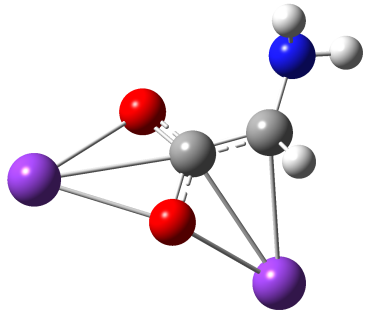
27 radical cation



10
−883.5046190

C	−2.24791	0.52091	0.19486
H	−2.34395	1.41110	−0.42448
H	−2.23846	0.68251	1.27560
C	−0.41556	0.21000	0.06716
O	0.13532	1.28129	−0.07865
O	−0.15334	−0.96718	0.18555
N	−2.96376	−0.54801	−0.21755
H	−3.21075	−0.65546	−1.19278
H	−3.01606	−1.38109	0.35508
K	2.50950	−0.16418	−0.04831

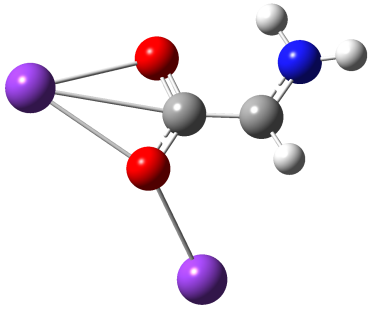
28 neutral



```
10
-1483.0112073

C                  1.23234      1.13149      0.38219
H                  1.63729      0.81062      1.35508
C                  0.00305      0.50975      0.03099
O                 -0.25813     -0.68898      0.55065
O                 -0.84025      1.02089     -0.79951
N                  1.48518      2.50011     -0.02637
H                  1.16693      3.18822      0.65497
H                  2.47186      2.67522     -0.17864
K                 -2.75307     -0.36302      0.05602
K                  2.00056     -1.56738     -0.16839
```

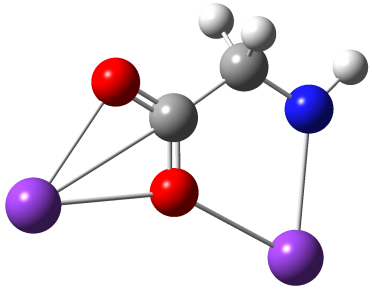
28 radical cation



```
10
-1482.9041927

C                  1.10309      1.48328      0.40709
H                  1.89652      1.16888      1.08045
C                 -0.05257      0.64949      0.10669
O                 -0.04665     -0.57503      0.51097
O                 -1.00215      1.17457     -0.54626
N                  1.14833      2.74193     -0.10334
H                  0.31292      3.06231     -0.57833
H                  1.79307      3.42999      0.25293
K                 -2.69272     -0.69963      0.02380
K                  2.16885     -1.63973     -0.17285
```

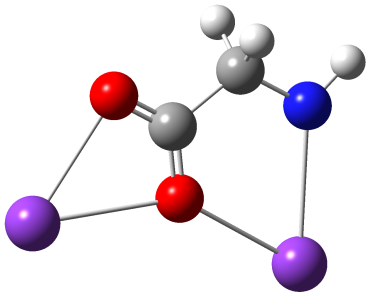
29 neutral



```
10
-1483.0221830

C                  0.90508      1.82431      0.00013
H                  0.70976      2.48667      0.87522
H                  0.70957      2.48719     -0.87449
C                 -0.31230      0.89334      0.00005
O                 -1.45364      1.44138     -0.00010
O                 -0.16313     -0.37595      0.00024
N                  2.19320      1.17167     -0.00021
H                  2.88674      1.92122     -0.00027
K                 -2.75849     -0.73519     -0.00005
K                  2.21738     -1.36619     -0.00001
```

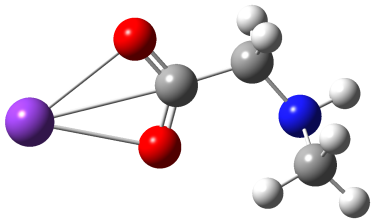
29 radical cation



```
10
-1482.8829437

C                  0.85654      1.90406      0.00016
H                  0.74199      2.57235      0.87280
H                  0.74163      2.57267     -0.87219
C                 -0.32019      0.92251      0.00027
O                 -1.45494      1.44787      0.00030
O                 -0.08581     -0.32411      0.00031
N                  2.15533      1.29697     -0.00016
H                  2.84398      2.05710     -0.00035
K                 -2.78016     -0.77492     -0.00032
K                  2.23768     -1.44772     -0.00002
```

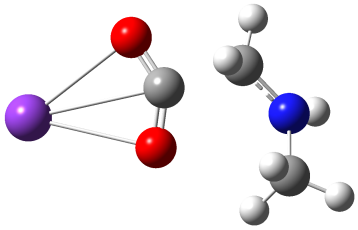
30 neutral



```
13
-923.0198855

C                  1.52777      0.96855     -0.10474
C                  0.08219      0.45523     -0.03250
O                 -0.18179     -0.72169     -0.39031
O                 -0.76461      1.29371      0.39356
N                  2.50435     -0.01536     -0.53909
H                  3.35991      0.47024     -0.78936
H                  1.52159      1.80737     -0.81287
C                  2.80140     -0.99846      0.49495
H                  3.12583     -0.53719      1.44753
H                  1.89937     -1.58977      0.68579
H                  3.59219     -1.67325      0.14686
H                  1.75572      1.39359      0.89214
K                 -2.72011     -0.36271      0.00165
```

30 radical cation

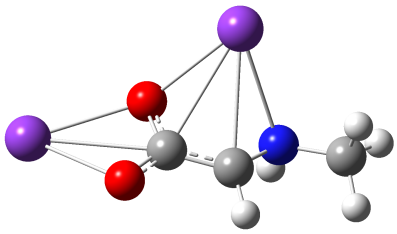


```
13
-922.8006572

C                  1.67985      1.02770      0.13992
C                  0.00760      0.44727      0.02591
O                 -0.08775     -0.76597     -0.07515
O                 -0.75370      1.39884      0.10514
N                  2.56375      0.14470     -0.40265
H                  2.76851      0.23247     -1.39258
H                  1.63132      1.98481     -0.37828
C                  2.90944     -1.10576      0.23325
H                  2.94391     -0.95734      1.31659
H                  2.14495     -1.86080     -0.00217
H                  3.88388     -1.44037     -0.13282
H                  1.73982      1.09540      1.23122
```

K	−2.83728	−0.38660	−0.02409

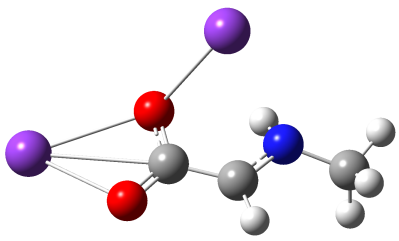
31 neutral



13
−1522.3087034

C	0.92407	−1.07198	0.36419
C	−0.38989	−0.55026	0.29081
O	−0.66616	0.46948	−0.50779
O	−1.33324	−1.03871	1.03591
N	1.91367	−0.74984	−0.65824
K	1.40582	1.73970	0.24310
K	−3.18167	0.01419	−0.29441
H	1.04301	−2.03968	0.86361
C	3.25468	−1.13761	−0.25092
H	3.32538	−2.19588	0.06523
H	3.96804	−0.97449	−1.07086
H	3.56445	−0.52994	0.61395
H	1.70659	−1.22207	−1.53883

31 radical cation

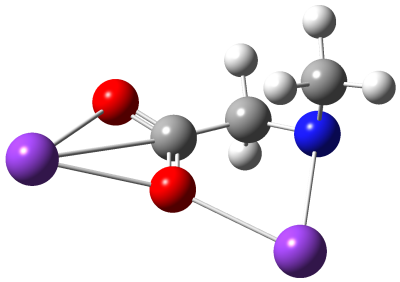


13
−1522.1923903

C	1.00518	−1.06621	0.52129
C	−0.34889	−0.54719	0.35615
O	−0.53750	0.29778	−0.60144
O	−1.24841	−0.93554	1.15026
N	1.97088	−0.75456	−0.40423
K	1.29720	2.03898	0.18424
K	−3.20041	−0.11646	−0.34159
H	1.27526	−1.69433	1.36617

C	3.20956	−1.52085	−0.43257
H	3.03898	−2.56082	−0.74477
H	3.91528	−1.05002	−1.12273
H	3.64869	−1.52309	0.57115
H	1.57884	−0.51021	−1.31044

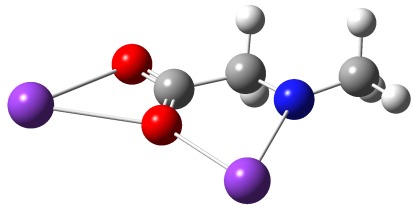
32 neutral



13
−1522.3070548

C	0.85165	1.51390	−0.68627
C	−0.47188	0.74518	−0.40400
O	−0.43713	−0.52206	−0.22116
O	−1.54891	1.40354	−0.40067
N	2.07201	0.97592	−0.17541
H	0.89033	1.57307	−1.79107
C	2.05254	1.08509	1.25559
H	1.87791	2.12529	1.62979
H	1.25296	0.47635	1.77279
H	3.01370	0.75971	1.69254
H	0.63226	2.55369	−0.34040
K	−3.00479	−0.55204	0.31241
K	1.90601	−1.62883	−0.19415

32 radical cation

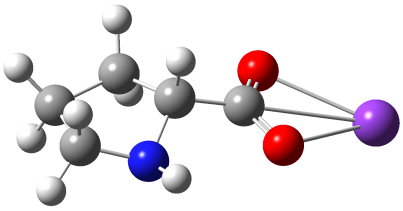


13
−1522.1791769

C	0.92926	1.48175	−0.08702
C	−0.45015	0.81324	−0.07914
O	−0.53029	−0.45181	−0.03259
O	−1.42301	1.59812	−0.12319

N	2.05104	0.59308	0.02487
H	1.00742	2.06152	-1.02553
C	3.28957	1.31817	0.14941
H	3.41685	2.02841	-0.68522
H	3.28506	1.91874	1.07531
H	4.14151	0.63223	0.17463
H	0.94355	2.23966	0.71626
K	-3.24936	-0.21695	0.08355
K	1.45266	-2.09261	-0.03528

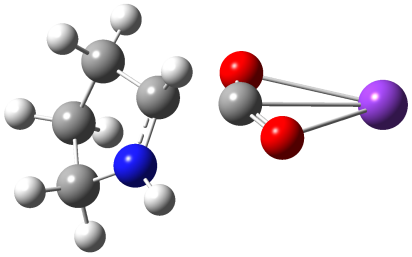
33 neutral



17
-1000.4232462

C	-0.98853	-0.00490	0.47115
H	-1.13034	-0.12800	1.56592
C	0.52348	0.00946	0.25183
O	1.09845	-1.11434	0.19336
O	1.10510	1.12751	0.18746
N	-1.64551	-1.08722	-0.26195
H	-1.34599	-1.99407	0.08211
C	-1.76956	1.23340	0.01415
H	-1.79705	1.99956	0.79524
H	-1.27730	1.67013	-0.86089
C	-3.17538	0.68290	-0.33998
H	-3.96982	1.14349	0.25737
H	-3.40255	0.86378	-1.39628
C	-3.07011	-0.83012	-0.07102
H	-3.67711	-1.43371	-0.75577
H	-3.39416	-1.04621	0.96490
K	3.40869	-0.00601	-0.20117

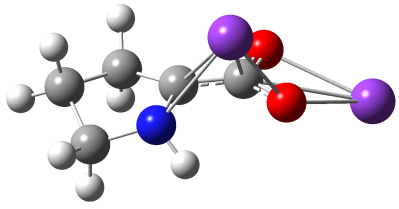
33 radical cation



17
−1000.2088008

C	−1.20295	−0.31136	0.88985
H	−0.98737	−0.75306	1.86885
C	0.46926	−0.13263	0.34967
O	1.04659	−1.21310	0.33534
O	0.76310	1.02709	0.10121
N	−1.79247	−1.16835	−0.00794
H	−1.53621	−2.14792	−0.06757
C	−1.97882	0.98934	0.79482
H	−2.81626	0.94905	1.50339
H	−1.35241	1.85283	1.02461
C	−2.47859	0.96916	−0.65751
H	−3.38729	1.55800	−0.80316
H	−1.69768	1.35447	−1.32195
C	−2.71286	−0.52142	−0.93820
H	−2.49736	−0.82956	−1.96670
H	−3.73707	−0.83378	−0.68682
K	3.34238	0.13463	−0.29575

34 neutral

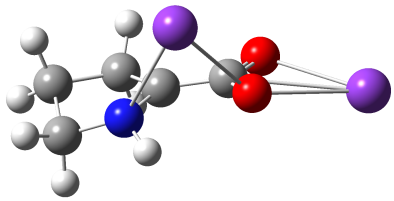


17
−1599.7073062

C	−0.80240	−0.47367	−0.13002
C	0.57450	−0.32324	−0.18861
O	1.15530	0.61686	0.57096
O	1.31759	−1.05373	−0.98229
N	−1.60844	0.24671	0.89112
H	−1.07468	0.26744	1.75921
C	−1.64535	−1.54805	−0.76650
H	−1.55417	−1.58569	−1.86056

H	−1.40689	−2.56513	−0.39834
C	−3.06483	−1.15939	−0.32104
H	−3.46626	−0.37969	−0.98465
H	−3.77258	−1.99698	−0.30212
C	−2.82166	−0.56768	1.06770
H	−2.65396	−1.39555	1.77897
H	−3.66114	0.03794	1.43500
K	3.41401	−0.55252	0.30308
K	−0.48643	2.33241	−0.42645

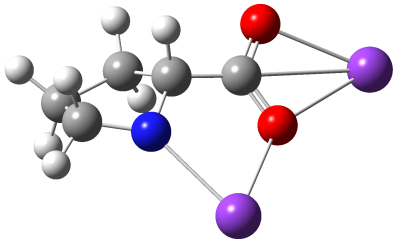
34 radical cation



17
−1599.6007890

C	−0.84758	−0.60460	−0.02691
C	0.59160	−0.41734	−0.11443
O	1.09535	0.58776	0.52351
O	1.26544	−1.23346	−0.80437
N	−1.62657	0.16693	0.82917
H	−1.15590	0.46648	1.67922
C	−1.68950	−1.64348	−0.70016
H	−1.48906	−1.72028	−1.77393
H	−1.48368	−2.63367	−0.26277
C	−3.11969	−1.18151	−0.36747
H	−3.46979	−0.46963	−1.12538
H	−3.83764	−2.00412	−0.30779
C	−2.95102	−0.46171	0.97422
H	−2.94057	−1.18402	1.80350
H	−3.72269	0.28974	1.16784
K	3.53032	−0.53800	0.24578
K	−0.44105	2.49087	−0.42102

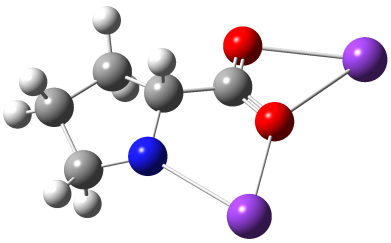
35 neutral



```
17
-1599.7151565

C                 -0.88227     -0.75230     -0.50864
H                 -0.97409     -1.23140     -1.51833
C                  0.61677     -0.51716     -0.33182
O                  1.05441      0.60920      0.08571
O                  1.38261     -1.48701     -0.59773
N                 -1.75629      0.37720     -0.35351
C                 -1.38675     -1.83380      0.50606
H                 -1.20803     -2.85430      0.14441
H                 -0.85867     -1.71676      1.46268
C                 -2.88549     -1.49000      0.64319
H                 -3.53522     -2.33234      0.36613
H                 -3.12879     -1.19940      1.67348
C                 -3.04205     -0.26831     -0.30894
H                 -3.84169      0.41554      0.01847
H                 -3.35791     -0.67599     -1.30594
K                  3.50172     -0.32214      0.19743
K                 -0.59745      2.59299      0.10419
```

35 radical cation

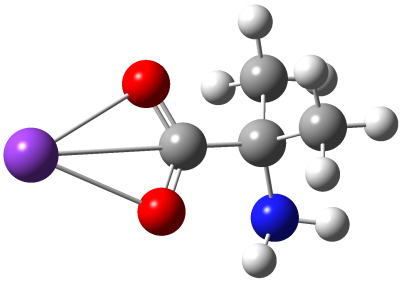


```
17
-1599.5862070

C                 -0.96209     -0.65964     -0.50410
H                 -1.01297     -0.59377     -1.61030
C                  0.54624     -0.55891     -0.18842
O                  1.06837      0.59617     -0.11960
O                  1.15983     -1.63890     -0.06432
N                 -1.73119      0.46337      0.00164
C                 -1.65479     -1.94867     -0.04299
```

H	-1.47068	-2.78477	-0.72247
H	-1.27976	-2.22699	0.94998
C	-3.11800	-1.51301	0.02487
H	-3.57061	-1.53452	-0.97504
H	-3.72829	-2.12780	0.69351
C	-2.98736	-0.06339	0.50811
H	-2.93001	-0.02514	1.61168
H	-3.81439	0.59762	0.21657
K	3.51320	-0.57153	0.17149
K	-0.29449	2.79550	-0.03932

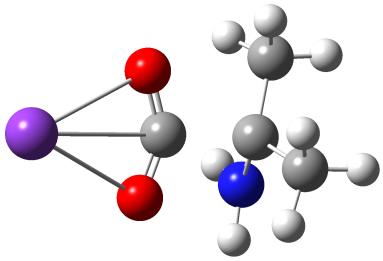
36 neutral



16
-962.3380344

C	1.54017	-0.00987	-0.04636
C	-0.00484	0.00377	-0.00467
O	-0.58225	1.11871	0.11026
O	-0.59298	-1.11496	-0.03160
N	1.96629	-1.16787	-0.84120
H	2.93716	-1.38865	-0.62954
H	1.40036	-1.96587	-0.56110
K	-2.92586	0.01539	-0.02083
C	2.09172	1.25890	-0.68806
H	1.80239	2.14282	-0.11079
H	3.18858	1.20164	-0.72918
H	1.71151	1.36317	-1.71070
C	2.00703	-0.10446	1.41688
H	1.63157	-1.02901	1.87377
H	3.10548	-0.11466	1.45562
H	1.64767	0.75326	1.99996

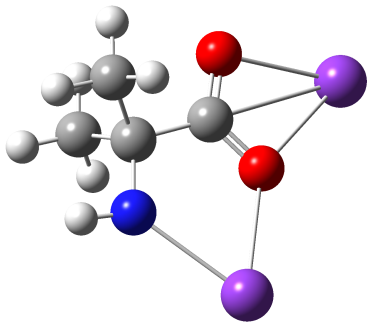
36 radical cation



16
-962.1138954

C	1.79719	-0.02814	-0.00239
C	-0.13642	0.01343	-0.10856
O	-0.53265	1.15363	-0.00158
O	-0.56392	-1.11573	-0.22930
N	2.17145	-0.86369	-1.00894
H	2.30529	-0.49837	-1.94341
H	1.96264	-1.85223	-0.94113
K	-3.08511	0.02373	0.02925
C	2.24859	1.40031	-0.17032
H	1.74962	2.04323	0.55793
H	3.33278	1.44024	-0.00178
H	2.03235	1.77343	-1.17750
C	1.91290	-0.61291	1.39009
H	1.52028	-1.63422	1.42675
H	2.97600	-0.62727	1.66717
H	1.37695	0.01072	2.11284

37 neutral

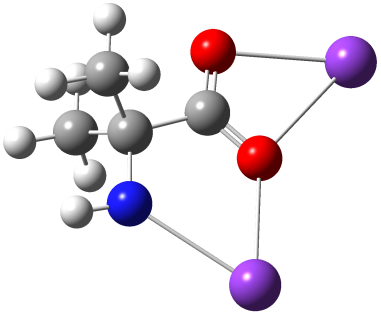


16
-1561.6231863

C	-1.12042	-1.09558	0.03110
C	0.30759	-0.51090	-0.13273
O	1.25715	-1.32993	-0.29828
O	0.50455	0.74951	-0.06253
N	-2.13356	-0.06443	0.03718

H	-3.02346	-0.56429	0.11507
K	3.09044	0.38866	0.06306
K	-1.48052	2.38420	-0.02765
C	-1.32550	-2.12080	-1.10829
H	-0.56408	-2.91168	-1.10472
H	-2.31888	-2.57704	-0.98907
H	-1.30451	-1.60481	-2.07762
C	-1.07561	-1.88999	1.36432
H	-0.88425	-1.20052	2.19838
H	-2.06057	-2.35090	1.52652
H	-0.30780	-2.67695	1.35826

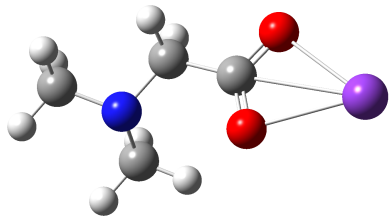
37 radical cation



16
-1561.4835723

C	-1.16905	-1.11198	-0.00001
C	0.27804	-0.55754	0.00013
O	1.18990	-1.41502	0.00023
O	0.46505	0.69827	0.00005
N	-2.14132	-0.04175	0.00029
H	-3.06325	-0.49627	0.00022
K	3.15980	0.24812	-0.00005
K	-1.31280	2.55871	0.00005
C	-1.36984	-1.97258	-1.26105
H	-0.60949	-2.75971	-1.27858
H	-2.36598	-2.43313	-1.24853
H	-1.27245	-1.36314	-2.16787
C	-1.36987	-1.97333	1.26052
H	-1.27239	-1.36442	2.16770
H	-2.36604	-2.43379	1.24776
H	-0.60956	-2.76051	1.27756

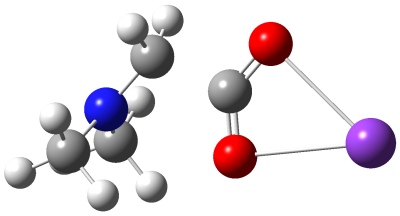
38 neutral



16
−962.3110000

C	−1.15649	−0.81012	0.09647
H	−1.36760	−1.19450	1.11608
H	−1.22669	−1.67164	−0.58256
C	0.31547	−0.37335	0.07180
O	1.12282	−1.18935	0.60259
O	0.63942	0.71201	−0.47597
N	−2.12330	0.18967	−0.31683
K	3.16587	0.22942	−0.12755
C	−2.19334	1.27450	0.64889
H	−2.53031	0.91423	1.64402
H	−1.20671	1.73576	0.75048
H	−2.90492	2.03276	0.29920
C	−3.43263	−0.41713	−0.48350
H	−4.15052	0.34179	−0.81851
H	−3.38320	−1.20793	−1.24198
H	−3.81431	−0.86187	0.45956

38 radical cation

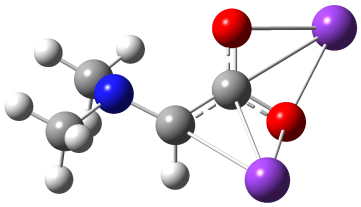


16
−962.0993494

C	−1.29193	1.13169	0.00622
H	−1.32222	1.73938	−0.90111
H	−1.32894	1.72838	0.92074
C	0.26898	0.50411	0.00675
O	1.09816	1.41320	−0.00151
O	0.36106	−0.72511	0.01531
N	−2.23773	0.11866	−0.00323
K	3.09301	−0.42658	−0.00311
C	−2.52650	−0.57488	−1.23879
H	−3.56048	−0.93371	−1.21877

H	−2.36936	0.09698	−2.08560
H	−1.84527	−1.43764	−1.31593
C	−2.53959	−0.58183	1.22521
H	−1.80348	−1.39330	1.34549
H	−2.46925	0.10694	2.07041
H	−3.54357	−1.01187	1.15966

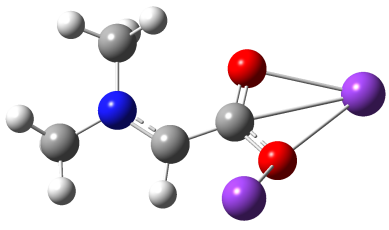
39 neutral



16
−1561.5925158

C	−1.09080	0.02995	0.22852
H	−1.31744	0.41334	1.24344
C	0.29545	−0.12213	−0.05681
O	1.15237	0.68741	0.55435
O	0.73929	−0.97104	−0.91849
N	−2.03163	−0.94820	−0.26320
K	3.06486	−0.94808	0.04111
K	−0.22682	2.73087	−0.05560
C	−1.91582	−2.22835	0.41819
H	−2.60401	−2.96605	−0.02279
H	−0.88874	−2.59212	0.30581
H	−2.14841	−2.13979	1.50304
C	−3.38947	−0.46216	−0.17885
H	−4.09262	−1.21314	−0.56686
H	−3.68975	−0.23098	0.86982
H	−3.48970	0.45833	−0.76809

39 radical cation

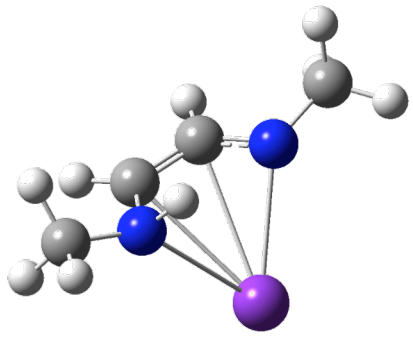


16
−1561.4775122

C	−1.16433	0.08834	0.42228
H	−1.32924	0.85592	1.17664

C	0.21593	−0.26338	0.09916
O	1.11777	0.58502	0.47650
O	0.49318	−1.34015	−0.50300
N	−2.28777	−0.56174	0.00918
K	2.98335	−1.31945	0.17609
K	0.34156	2.87406	−0.30424
C	−2.27916	−1.64014	−0.96437
H	−3.27580	−1.69585	−1.41679
H	−1.52732	−1.44824	−1.72978
H	−2.04779	−2.60513	−0.48990
C	−3.50532	−0.43146	0.78845
H	−4.37291	−0.41222	0.11902
H	−3.61809	−1.27701	1.48529
H	−3.47808	0.49802	1.36498

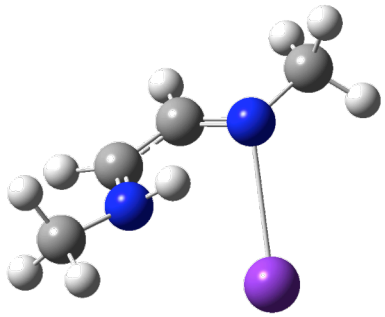
40 neutral



16
−867.1345481

C	−0.72355	−0.84205	0.74867
H	−1.27881	−1.18238	1.61887
C	0.64061	−0.95840	0.64682
H	1.14780	−1.44723	1.49771
N	1.37153	−0.49433	−0.38842
N	−1.48459	−0.28014	−0.34296
H	−1.01136	−0.56467	−1.20333
C	2.74530	−0.95071	−0.38527
H	2.86732	−1.97125	−0.79958
H	3.37300	−0.29003	−1.00140
H	3.19207	−0.97278	0.63120
C	−2.86995	−0.73343	−0.36394
H	−3.38278	−0.32725	−1.24359
H	−2.96035	−1.83356	−0.37239
H	−3.38395	−0.36091	0.53212
K	0.18284	1.85678	0.08328

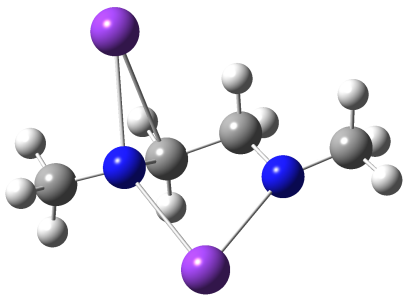
40 radical cation



16
−866.9935616

C	−0.83728	−1.04882	0.65715
H	−1.41591	−1.44222	1.48991
C	0.56054	−1.22821	0.58435
H	1.02034	−1.88666	1.33290
N	1.26658	−0.63811	−0.34950
N	−1.50748	−0.35755	−0.30749
H	−1.02204	−0.33193	−1.20071
C	2.67691	−0.97673	−0.41189
H	2.88342	−1.50250	−1.35441
H	3.28539	−0.06209	−0.42031
H	3.00299	−1.61458	0.42393
C	−2.96406	−0.39945	−0.36857
H	−3.32137	0.38419	−1.04200
H	−3.32617	−1.37255	−0.72551
H	−3.36745	−0.21410	0.63206
K	0.38581	1.94375	0.14194

41 neutral

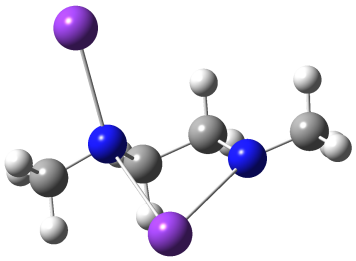


18
−1467.6082910

C	−0.35592	0.05792	1.10125
H	0.21502	0.60946	1.89524
H	−1.24822	−0.33438	1.68234
C	0.47962	−1.17224	0.71565

H	0.58835	−1.78185	1.65288
H	−0.16762	−1.84632	0.06049
N	1.73132	−0.89395	0.09981
N	−0.75956	0.90908	0.01274
C	2.42021	−2.13438	−0.08552
H	1.86993	−2.85787	−0.74684
H	3.40977	−1.98258	−0.54601
H	2.59170	−2.70372	0.86495
C	−1.64181	1.90875	0.53839
H	−1.96784	2.61450	−0.24321
H	−2.58668	1.49250	1.00299
H	−1.20429	2.52411	1.36573
K	1.78669	1.60414	−0.52037
K	−2.50854	−0.96203	−0.60568

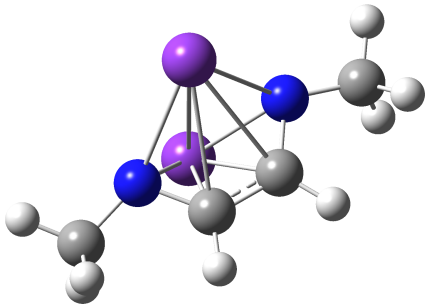
41 radical cation



18
−1467.4791864

C	0.12466	0.05264	1.42472
H	0.85090	0.86919	1.70449
H	−0.36567	−0.18667	2.39736
C	0.96335	−1.14575	1.00884
H	1.52976	−1.55220	1.86803
H	0.29980	−1.96386	0.66400
N	1.89001	−0.81213	−0.04623
N	−0.79957	0.43838	0.39816
C	2.70380	−1.93558	−0.42990
H	2.08146	−2.80600	−0.69991
H	3.35157	−1.67779	−1.27344
H	3.33535	−2.25089	0.41903
C	−1.47561	1.63784	0.82777
H	−2.23026	1.96461	0.09192
H	−1.99908	1.54012	1.80693
H	−0.79743	2.52178	0.97965
K	1.26588	1.79280	−0.77889
K	−2.71781	−1.02948	−0.66375

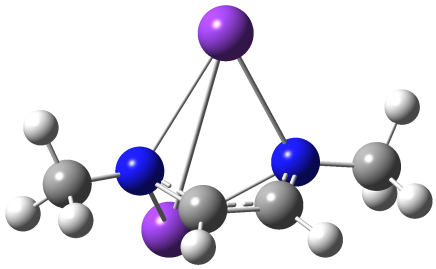
42 neutral



16
−1466.4425703

C	−0.69297	0.01963	1.16459
H	−1.16468	−0.00640	2.16135
C	0.69304	0.01931	1.16456
H	1.16478	−0.00695	2.16129
N	1.51220	0.10441	0.04513
N	−1.51215	0.10514	0.04518
C	2.87869	−0.23079	0.36465
H	3.03187	−1.30292	0.64450
H	3.53757	−0.03809	−0.49594
H	3.29120	0.34946	1.22119
C	−2.87869	−0.22981	0.36469
H	−3.53757	−0.03684	−0.49584
H	−3.03210	−1.30196	0.64439
H	−3.29104	0.35039	1.22134
K	0.00044	2.16504	−0.64021
K	−0.00048	−2.00417	−0.73060

42 radical cation

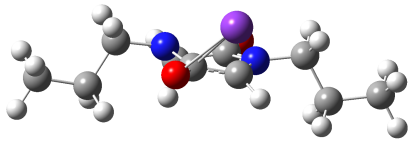


16
−1466.3442431

C	−0.71100	0.00221	1.28320
H	−1.18888	0.00218	2.27305
C	0.71099	0.00221	1.28321
H	1.18887	0.00217	2.27305
N	1.45661	0.00499	0.17716

N	-1.45660	0.00499	0.17716
C	2.89451	-0.01451	0.39018
H	3.33721	-0.94241	-0.00554
H	3.37954	0.81342	-0.14807
H	3.17269	0.06258	1.45424
C	-2.89451	-0.01450	0.39018
H	-3.37953	0.81342	-0.14808
H	-3.33720	-0.94242	-0.00552
H	-3.17267	0.06261	1.45424
K	0.00000	2.13840	-0.77906
K	-0.00000	-2.12755	-0.78452

43 neutral

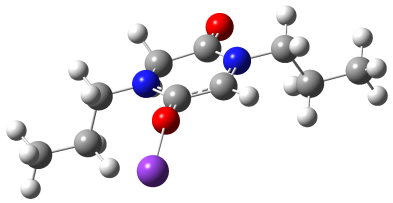


32
-1251.0190056

C	-0.59772	-1.75418	-0.27575
C	0.88873	-1.61475	-0.55182
C	0.61110	0.59285	0.43831
C	-0.76979	0.58537	0.29015
H	-0.99323	-2.49400	-0.97889
H	-0.70999	-2.15766	0.74992
H	1.09171	1.17995	1.21619
N	1.41007	-0.43509	-0.16646
N	-1.29823	-0.49240	-0.45289
O	-1.55671	1.51026	0.69941
O	1.54074	-2.52498	-1.07767
C	-2.74598	-0.59487	-0.54986
H	-2.97577	-1.24908	-1.40435
C	2.83036	-0.19018	-0.35477
H	3.16595	-0.80177	-1.19984
H	2.95467	0.87127	-0.61130
C	3.65016	-0.53398	0.88699
H	3.48774	-1.59455	1.11939
H	3.27578	0.04712	1.74140
C	5.13489	-0.25889	0.67262
H	5.71955	-0.51699	1.56310
H	5.52053	-0.84909	-0.16919
H	5.30919	0.80235	0.44888
C	-3.43259	-1.13005	0.70774
H	-3.12952	-0.50295	1.55573
H	-3.08926	-2.15380	0.91131
C	-4.95057	-1.12207	0.55446
H	-5.44512	-1.52326	1.44700
H	-5.31905	-0.10015	0.39310

H	−5.25966	−1.73159	−0.30584
H	−3.13572	0.40423	−0.77208
K	−0.25444	3.32130	−0.48691

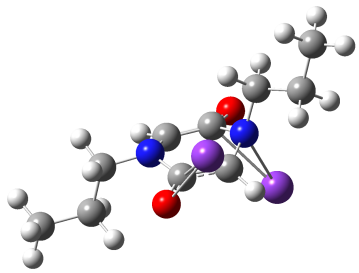
43 radical cation



32
−1250.8650650

C	0.37441	−1.92707	−0.35635
C	1.76662	−1.34021	−0.45263
C	0.78824	0.85134	−0.36711
C	−0.56019	0.35128	−0.38786
H	0.30193	−2.68864	−1.14304
H	0.32630	−2.45299	0.61020
H	0.95480	1.92132	−0.32235
N	1.88138	0.03722	−0.46254
N	−0.72698	−0.98934	−0.48664
O	−1.53531	1.13783	−0.34553
O	2.73997	−2.06546	−0.49381
C	−2.07139	−1.55499	−0.46857
H	−2.02558	−2.51925	−0.99074
C	3.23034	0.62035	−0.46333
H	3.85782	−0.01604	−1.09368
H	3.15216	1.61031	−0.92582
C	3.80474	0.71273	0.94627
H	3.82153	−0.29397	1.38234
H	3.13917	1.33137	1.56370
C	5.21052	1.30399	0.92438
H	5.61933	1.37105	1.93817
H	5.88499	0.67893	0.32603
H	5.20595	2.31297	0.49203
C	−2.61815	−1.74079	0.94554
H	−2.61432	−0.76557	1.45002
H	−1.94866	−2.40136	1.51268
C	−4.02632	−2.32638	0.91945
H	−4.42004	−2.45242	1.93374
H	−4.71249	−1.67134	0.36615
H	−4.03138	−3.30856	0.42976
H	−2.72283	−0.88812	−1.04289
K	−3.31051	2.87456	−0.02979

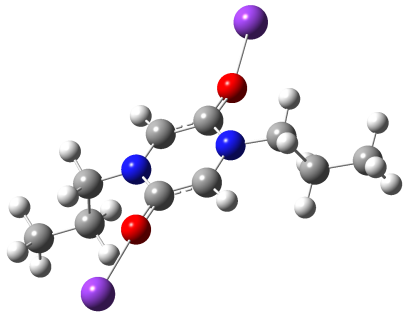
44 neutral



32
−1850.3110592

C	−0.89009	−1.16564	−1.06824
C	0.38889	−1.55464	−0.80282
C	0.44570	0.29300	0.79092
C	−0.83812	0.71289	0.44899
H	−1.57508	−1.81612	−1.60603
H	0.84260	0.54853	1.77525
N	1.21425	−0.61186	−0.03635
N	−1.40103	0.11882	−0.68618
O	−1.50350	1.62626	1.06917
O	0.95916	−2.67666	−1.10471
C	−2.81037	0.34659	−0.94039
H	−3.00721	0.09469	−1.99351
C	2.17408	0.04644	−0.93064
H	2.53555	−0.71074	−1.63959
H	1.66515	0.84225	−1.51317
C	3.36106	0.64360	−0.18664
H	3.88199	−0.16660	0.34339
H	2.99539	1.33922	0.58344
C	4.32518	1.36334	−1.12567
H	5.17554	1.79236	−0.58116
H	4.72096	0.67185	−1.88111
H	3.81665	2.17905	−1.65807
C	−3.74296	−0.45917	−0.03333
H	−3.49460	−0.21200	1.00703
H	−3.54699	−1.53097	−0.17452
C	−5.20962	−0.15195	−0.31925
H	−5.87712	−0.73984	0.32261
H	−5.42406	0.91155	−0.14635
H	−5.46040	−0.37952	−1.36468
H	−3.01396	1.41418	−0.80146
K	0.34384	3.29245	0.63187
K	1.14064	−2.91509	1.45616

44 radical cation

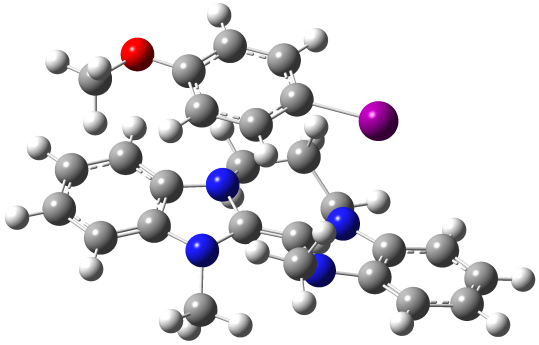


32
−1850.2100884

C	0.35233	−1.26107	−0.37378
C	1.41107	−0.35794	−0.38338
C	−0.27376	1.38649	−0.40812
C	−1.33221	0.48393	−0.40094
H	0.54366	−2.32787	−0.35451
H	−0.46627	2.45316	−0.41484
N	1.06031	0.98555	−0.43455
N	−0.98180	−0.86101	−0.41804
O	−2.56945	0.80589	−0.38432
O	2.64757	−0.68172	−0.35340
C	−2.01684	−1.87318	−0.28704
H	−1.65548	−2.78437	−0.78105
C	2.09496	2.00242	−0.32930
H	2.99440	1.61485	−0.81671
H	1.75062	2.88657	−0.88141
C	2.39800	2.36602	1.12293
H	2.70894	1.45294	1.64745
H	1.47232	2.71588	1.60014
C	3.48171	3.43441	1.21956
H	3.69346	3.68965	2.26408
H	4.41630	3.08596	0.75991
H	3.17407	4.35252	0.70196
C	−2.36038	−2.16005	1.17341
H	−2.68259	−1.22009	1.64057
H	−1.44851	−2.48430	1.69314
C	−3.44765	−3.22213	1.29733
H	−3.68743	−3.42284	2.34764
H	−4.36948	−2.90005	0.79428
H	−3.12720	−4.16638	0.83765
H	−2.90361	−1.51812	−0.82134
K	−4.85659	1.62402	−0.38542
K	4.67601	−2.04960	−0.35832

4. Model 2 Optimised Geometries and Coordinates

21 + 4-iodoanisole Reactant Complex

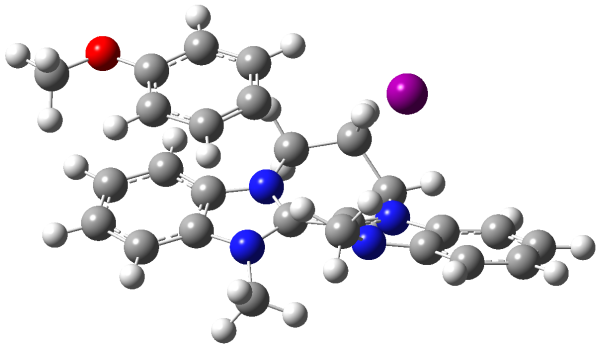


59
−1596.5101342

C	−4.08509	−1.85526	−1.30867
C	−2.92914	−1.64605	−0.57687
C	−2.97393	−1.24381	0.76953
C	−4.18524	−1.09520	1.42797
C	−5.36260	−1.33542	0.69588
C	−5.31685	−1.69649	−0.64655
H	−4.04718	−2.13796	−2.35879
H	−4.23937	−0.78585	2.46920
H	−6.32526	−1.22602	1.19214
H	−6.24278	−1.86149	−1.19428
C	−0.79050	−1.36256	0.14328
N	−1.66877	−1.00130	1.18575
N	−1.59121	−1.72804	−0.97113
C	0.56325	−1.44815	0.20193
C	2.70003	−1.81414	−0.49475
C	2.75092	−1.08513	0.70548
C	3.85313	−2.28166	−1.10384
C	3.96790	−0.80954	1.31723
C	5.08742	−2.00267	−0.48807
H	3.80987	−2.86999	−2.01807
C	5.13976	−1.27885	0.69869
H	4.02550	−0.26188	2.25444
H	6.00626	−2.36479	−0.94497
H	6.10219	−1.07266	1.16348
N	1.45202	−0.78917	1.10911
N	1.35736	−2.01574	−0.84970
C	1.21837	−0.59632	2.53116
H	1.38357	−1.54913	3.06923
H	1.97447	0.11776	2.87373
C	−0.15604	−0.06150	2.89030
H	−0.34700	0.89139	2.38272
H	−0.14986	0.12334	3.97145
C	−1.28450	−1.03381	2.57704
H	−2.17131	−0.76633	3.15718

H	-0.98427	-2.06009	2.86197
C	-1.25479	-1.32753	-2.33098
H	-0.16963	-1.28033	-2.43980
H	-1.64831	-2.06821	-3.03630
H	-1.69281	-0.34569	-2.56397
C	1.02140	-3.36854	-1.29542
H	-0.04910	-3.43937	-1.49786
H	1.56859	-3.58716	-2.21718
H	1.28895	-4.10939	-0.52643
C	0.69131	1.55564	-1.33164
C	2.08570	1.54170	-1.27819
C	2.74313	2.14153	-0.19932
C	1.99893	2.74993	0.81937
C	0.61039	2.76457	0.76061
C	-0.04004	2.16231	-0.31821
H	0.18678	1.09227	-2.17515
H	2.63698	1.05512	-2.07718
H	2.52703	3.22018	1.64677
H	0.04008	3.25062	1.54964
O	4.09164	2.18983	-0.06260
C	4.86055	1.59668	-1.09870
H	4.70678	2.13259	-2.04581
H	5.90367	1.68635	-0.78795
H	4.60347	0.53670	-1.21762
I	-2.14636	2.18647	-0.42852

21 + 4-iodoanisole Product Complex

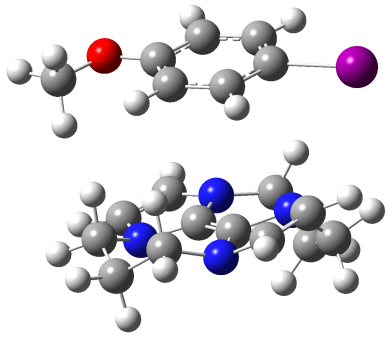


59
-1596.4764732

C	-4.42312	-1.12337	-1.53158
C	-3.29643	-1.18839	-0.72123
C	-3.38792	-1.15421	0.67741
C	-4.61991	-1.08438	1.32038
C	-5.75432	-1.03241	0.50900
C	-5.65978	-1.04666	-0.88933
H	-4.34380	-1.11708	-2.61590
H	-4.70781	-1.05539	2.40314
H	-6.73528	-0.97256	0.97533
H	-6.56791	-0.99070	-1.48541

C	−1.21889	−1.23898	0.11138
N	−2.09340	−1.18620	1.16623
N	−1.95145	−1.23314	−1.05840
C	0.17251	−1.41417	0.19922
C	2.28143	−1.93786	−0.40089
C	2.31993	−1.34157	0.86564
C	3.43278	−2.39990	−1.02654
C	3.51755	−1.16574	1.55185
C	4.63927	−2.22505	−0.33969
H	3.40197	−2.86826	−2.00729
C	4.68072	−1.61511	0.92079
H	3.55371	−0.69761	2.53192
H	5.56348	−2.57476	−0.79530
H	5.63711	−1.49059	1.42411
N	1.02080	−1.02844	1.22059
N	0.95514	−1.98128	−0.79656
C	0.75205	−0.38657	2.50506
H	1.01271	−1.11259	3.28911
H	1.44408	0.46201	2.58178
C	−0.67216	0.09829	2.69774
H	−0.91860	0.90728	1.99599
H	−0.72528	0.50675	3.71251
C	−1.71220	−1.00952	2.55657
H	−2.62527	−0.73922	3.09070
H	−1.34579	−1.96238	2.96650
C	−1.48406	−0.70345	−2.33652
H	−0.44238	−0.39229	−2.23395
H	−1.57760	−1.45697	−3.12516
H	−2.08083	0.18365	−2.57220
C	0.51137	−2.91917	−1.81798
H	−0.54709	−3.14206	−1.67767
H	0.67245	−2.50660	−2.81916
H	1.08703	−3.84507	−1.71082
C	2.20311	1.05149	−1.72647
C	3.56345	1.09797	−1.37529
C	3.93221	1.66127	−0.15218
C	2.96160	2.19811	0.70846
C	1.61310	2.16168	0.36016
C	1.28416	1.57640	−0.84882
H	1.90601	0.61237	−2.67846
H	4.30331	0.68206	−2.05333
H	3.29063	2.64248	1.64704
H	0.84579	2.57611	1.01295
O	5.21839	1.72745	0.29792
C	6.22532	1.25904	−0.58274
H	6.23657	1.84746	−1.51067
H	7.17178	1.38772	−0.05360
H	6.07078	0.19818	−0.82092
I	−2.22670	2.30935	−0.24498

22 + 4-iodoanisole Reactant Complex

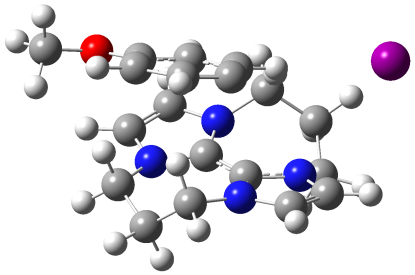


48
−1327.3585646

C	−0.67451	−2.85054	−0.71196
C	1.08126	−1.71175	0.13049
C	0.42122	−3.25073	−1.36746
H	−1.70373	−3.16608	−0.84137
H	0.50609	−3.92952	−2.20843
C	1.71122	−0.67105	0.72333
C	2.03387	1.16474	2.01527
C	3.20227	0.90153	1.41123
H	1.77911	1.95186	2.71355
H	4.15063	1.41911	1.46997
N	1.58694	−2.66982	−0.80930
N	−0.32430	−1.94552	0.32565
N	1.08615	0.22132	1.62190
N	3.07126	−0.28602	0.65004
C	−0.75762	−2.41453	1.65128
H	−1.85342	−2.33433	1.66155
H	−0.49358	−3.47662	1.80056
C	−0.16406	−1.57226	2.77937
H	−0.78566	−1.70408	3.67286
H	0.84445	−1.92369	3.02884
C	−0.09176	−0.08892	2.42838
H	−1.00764	0.22193	1.90923
H	−0.00718	0.50744	3.34370
C	3.82318	−0.38571	−0.58830
H	4.83339	−0.02213	−0.36754
H	3.38603	0.27561	−1.36103
C	3.89154	−1.79585	−1.15482
H	4.20313	−2.50604	−0.37793
H	4.65800	−1.79496	−1.94001
C	2.58158	−2.24756	−1.78421
H	2.76339	−3.10699	−2.43974
H	2.18052	−1.42071	−2.40682
C	−1.68783	1.24666	−0.44207
C	−0.57723	0.90116	−1.19847
C	0.53490	1.74845	−1.22719
C	0.53067	2.92377	−0.47339
C	−0.59159	3.25571	0.29760

C	-1.70306	2.42381	0.31055
H	-0.55342	-0.03536	-1.75206
H	1.39628	1.46039	-1.82273
H	-0.57680	4.17594	0.87846
H	-2.57302	2.68903	0.90748
O	1.56244	3.80762	-0.42204
C	2.71793	3.49668	-1.18118
H	3.41802	4.31817	-1.01517
H	3.16368	2.55376	-0.83512
H	2.47730	3.42714	-2.25113
I	-3.36485	-0.03249	-0.38905

22 + 4-iodoanisole Product Complex

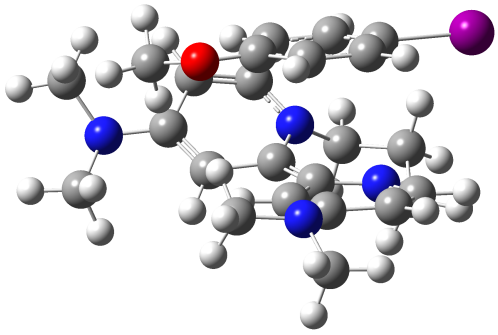


48
-1327.3486282

C	1.72081	-0.61874	2.19780
C	-0.10796	-1.21958	1.05334
C	0.64954	-0.06799	2.81608
H	2.77763	-0.53569	2.40980
H	0.59100	0.58327	3.67691
C	-0.89278	-1.70799	0.00715
C	-1.40234	-2.47295	-2.04080
C	-2.56034	-2.32139	-1.36038
H	-1.22339	-2.82285	-3.04847
H	-3.58106	-2.51630	-1.66012
N	-0.48937	-0.45790	2.12606
N	1.26413	-1.34631	1.11312
N	-0.35672	-2.10994	-1.20545
N	-2.26288	-1.86557	-0.08233
C	1.99907	-2.44764	0.48972
H	2.99214	-2.45300	0.94647
H	1.48365	-3.37464	0.77689
C	2.12276	-2.35906	-1.03553
H	3.02454	-1.79924	-1.30157
H	2.20500	-3.37868	-1.43047
C	0.95032	-1.63694	-1.67724
H	1.03066	-0.56211	-1.46095
H	0.96363	-1.76724	-2.76276
C	-3.30050	-1.35446	0.80804
H	-4.12533	-2.07397	0.76772
H	-3.66316	-0.39539	0.40845

C	−2.85254	−1.15639	2.24750
H	−2.45486	−2.08697	2.67209
H	−3.75136	−0.89220	2.81600
C	−1.84264	−0.02358	2.41550
H	−1.83540	0.33077	3.45016
H	−2.10883	0.82301	1.76585
C	−0.70519	2.83602	0.62838
C	−1.98537	3.31727	0.77383
C	−3.00086	2.73131	−0.00274
C	−2.67306	1.69960	−0.88908
C	−1.34833	1.25333	−1.01103
C	−0.33512	1.82473	−0.23904
H	−2.22454	4.12525	1.46332
H	−4.02058	3.09352	0.09382
H	−1.13747	0.46074	−1.72940
H	0.70396	1.49262	−0.32267
O	−3.58350	1.04871	−1.67249
C	−4.92656	1.49745	−1.61341
H	−5.48449	0.87371	−2.31507
H	−5.34015	1.37540	−0.60174
H	−5.00305	2.55085	−1.91471
I	3.67377	1.02602	−0.46015

23 + 4-iodoanisole Reactant Complex

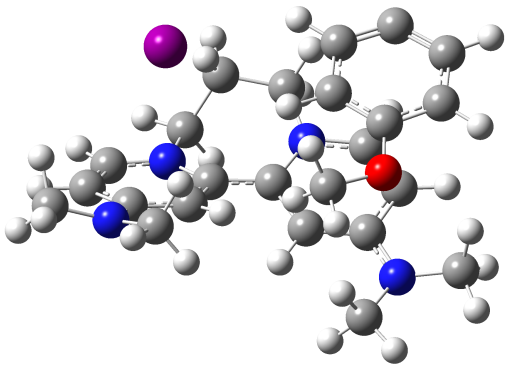


61
−1522.6443805

C	−3.47306	−1.34678	0.03694
C	−2.68284	−0.71330	0.94695
C	−1.28283	−1.10298	1.15798
C	−1.75827	−3.02900	−0.18933
C	−2.90523	−2.49293	−0.66862
H	−3.08018	0.09107	1.55646
H	−1.40284	−3.99323	−0.55124
H	−3.44255	−3.02764	−1.44277
C	−0.34120	−0.16493	1.50693
C	−0.66029	1.25517	1.42780
C	1.92179	0.53719	1.99489
C	0.28409	2.23410	1.51107
H	−1.67506	1.51185	1.15540

C	1.65287	1.84424	1.80233
H	2.92786	0.20402	2.23641
H	2.46490	2.56230	1.83090
C	-0.26899	-3.37932	1.67083
H	-0.79488	-3.43013	2.63946
H	-0.31834	-4.37335	1.21419
C	1.28371	-1.67604	2.66656
H	0.59871	-1.70331	3.53170
H	2.30122	-1.56390	3.05131
C	1.17439	-2.98529	1.90566
H	1.71577	-2.91250	0.95300
H	1.64864	-3.76864	2.51222
N	-0.97983	-2.46150	0.78831
N	0.99235	-0.47447	1.89001
N	-4.83524	-1.05696	-0.15128
N	0.02783	3.58149	1.22616
C	-5.37211	0.02925	0.64217
H	-4.90011	1.00146	0.40032
H	-6.44609	0.10815	0.44614
H	-5.22530	-0.17377	1.70827
C	-5.33800	-1.03139	-1.51867
H	-6.42728	-1.14898	-1.49967
H	-5.10583	-0.07939	-2.02890
H	-4.91875	-1.84808	-2.10833
C	0.54316	4.54750	2.18959
H	0.49811	5.54934	1.74902
H	-0.04976	4.54436	3.12212
H	1.58312	4.33095	2.44206
C	-1.32160	3.90413	0.80463
H	-2.06438	3.73377	1.60679
H	-1.35377	4.96192	0.52399
H	-1.59291	3.30138	-0.06915
C	-0.52525	0.07018	-1.84127
C	-0.54682	1.45602	-2.00397
C	0.63579	2.19808	-1.89119
C	1.83357	1.56069	-1.60036
C	1.84691	0.17305	-1.43318
C	0.68273	-0.57133	-1.55364
H	-1.43001	-0.52890	-1.89606
H	2.74746	2.14089	-1.49576
I	3.66424	-0.79654	-0.97303
O	-1.67468	2.17502	-2.26745
C	-2.90203	1.46502	-2.23779
H	-3.02830	0.95308	-1.27357
H	-3.68899	2.21051	-2.37544
H	-2.94940	0.72465	-3.04953
H	0.68865	-1.64845	-1.39934
H	0.59427	3.27922	-2.01001

23 + 4-iodoanisole Product Complex

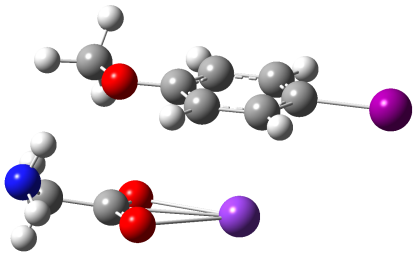


61
−1522.6179362

C	−2.59853	1.77323	0.66268
C	−1.25950	1.40959	0.76934
C	−0.80308	0.38105	1.62890
C	−3.06428	0.14115	2.35455
C	−3.52213	1.14480	1.56171
H	−0.55225	1.79450	0.05044
H	−3.73872	−0.41715	2.99752
H	−4.58020	1.37406	1.57371
C	0.60548	0.08681	1.65546
C	1.47314	1.17957	1.34753
C	2.57857	−1.25484	1.72613
C	2.84624	1.06599	1.19118
H	1.01178	2.15550	1.28657
C	3.41092	−0.24011	1.39082
H	2.97322	−2.25534	1.88446
H	4.46636	−0.45172	1.27454
C	−1.42356	−1.44811	3.16194
H	−0.67228	−1.18539	3.92124
H	−2.32750	−1.77670	3.67814
C	0.60423	−2.47591	2.12105
H	1.01976	−2.83015	3.07413
H	0.95259	−3.14695	1.32760
C	−0.90191	−2.51257	2.20583
H	−1.36832	−2.37379	1.22130
H	−1.17161	−3.51151	2.56522
N	−1.76693	−0.25501	2.40081
N	1.22483	−1.15433	1.86819
N	−3.03420	2.64432	−0.28682
N	3.64798	2.13361	0.90795
C	−2.10613	3.05500	−1.32734
H	−1.74625	2.18551	−1.90139
H	−2.61611	3.74550	−2.00183
H	−1.24915	3.58122	−0.88662
C	−4.46022	2.72170	−0.57500
H	−4.61448	3.44957	−1.37402
H	−4.85731	1.74760	−0.89706

H	-5.01429	3.06756	0.30475
C	4.99969	1.89734	0.42112
H	5.47864	2.86265	0.24465
H	5.59476	1.36251	1.16901
H	4.99559	1.32662	-0.51892
C	3.02469	3.40510	0.59352
H	2.41965	3.75257	1.43977
H	3.80473	4.14579	0.40755
H	2.37938	3.33393	-0.29609
C	1.36742	-0.89259	-1.56103
C	2.59081	-0.28071	-1.85067
C	3.77987	-1.02332	-1.86643
C	3.75705	-2.38578	-1.56358
C	2.53038	-2.94820	-1.26429
C	1.33590	-2.26424	-1.26853
H	0.42150	-0.35343	-1.56380
H	4.67547	-2.97079	-1.57719
I	-2.53505	-1.26405	-1.48817
O	2.71927	1.05140	-2.13330
C	1.51592	1.76173	-2.37715
H	0.90293	1.81620	-1.46724
H	1.81138	2.76826	-2.68270
H	0.93339	1.28330	-3.17561
H	0.37111	-2.73397	-1.07052
H	4.71173	-0.52272	-2.12572

27 + 4-iodoanisole Reactant Complex

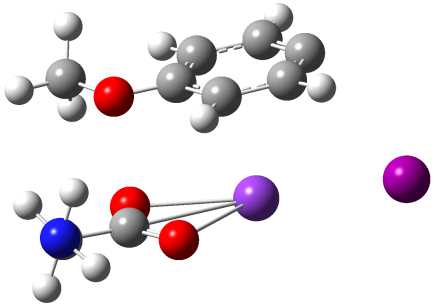


26
-1525.4457676

C	-4.63307	-0.55931	0.07747
C	-3.21391	-1.07627	-0.19152
O	-2.57126	-1.55511	0.78219
O	-2.78786	-1.00673	-1.38097
N	-4.88877	-0.08606	1.43416
H	-4.23069	0.66823	1.62598
H	-4.85820	0.23491	-0.64255
H	-5.32130	-1.38745	-0.14682
K	-0.42186	-1.84829	-0.66041
C	0.81342	0.44158	1.31632
C	-0.51916	0.83409	1.32150
C	-1.11439	1.34891	0.15952

C	-0.36234	1.45046	-1.01665
C	0.97989	1.05486	-1.02133
C	1.56188	0.55202	0.13850
H	1.26370	0.04636	2.22473
H	-1.12470	0.74088	2.22058
H	-0.80165	1.82804	-1.93517
H	1.55948	1.14071	-1.93852
I	3.57158	-0.09181	0.10964
O	-2.40579	1.72432	0.27190
C	-3.04033	2.24148	-0.89412
H	-3.06273	1.47275	-1.67767
H	-4.05704	2.49710	-0.58749
H	-2.52425	3.14595	-1.24275
H	-4.61217	-0.82849	2.07407

27 + 4-iodoanisole Product Complex

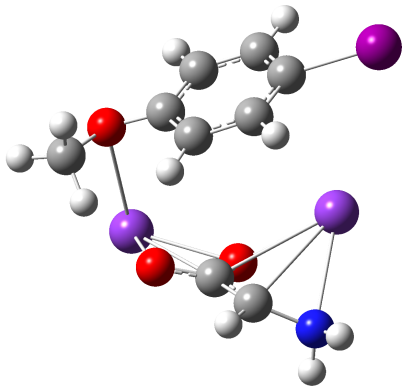


26
-1525.3450477

C	-3.83819	-1.70072	0.27967
C	-2.46321	-1.44409	-0.35081
O	-1.44216	-1.70115	0.34112
O	-2.44670	-1.01251	-1.54134
N	-3.88824	-1.65948	1.73706
H	-3.60111	-0.72603	2.02806
H	-4.55347	-0.98375	-0.13781
H	-4.16199	-2.69509	-0.06164
K	0.15016	-0.83918	-1.53403
C	0.78036	1.58710	1.23934
C	-0.56436	1.25506	1.40953
C	-1.49553	1.53616	0.39783
C	-1.07541	2.09993	-0.81894
C	0.27783	2.42269	-1.00495
C	1.15169	2.15336	0.02700
H	1.49260	1.43243	2.05061
H	-0.91900	0.79972	2.33230
H	-1.78576	2.29207	-1.61859
H	0.60971	2.88018	-1.93631
I	3.24367	-0.44849	0.23241
O	-2.78328	1.25317	0.69027

C	-3.77366	1.61955	-0.26735
H	-3.64278	1.03201	-1.18553
H	-4.73260	1.38128	0.19856
H	-3.72530	2.69718	-0.47347
H	-3.15036	-2.26948	2.08479

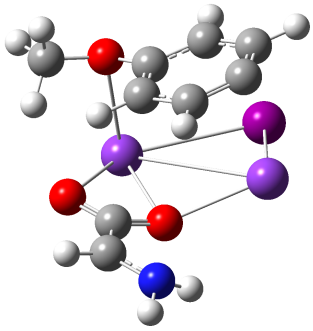
28 + 4-iodoanisole Reactant Complex



26
-2124.7332791

C	1.87055	2.51372	1.15473
C	2.42534	1.48878	0.35653
O	2.18560	1.42718	-0.93987
O	3.15623	0.55865	0.90206
N	1.32321	3.71962	0.51954
K	-0.28044	1.96329	-0.74737
K	3.72030	-0.58137	-1.29979
H	2.30479	2.63014	2.15020
H	2.05899	4.34710	0.19070
C	-0.69657	-0.54517	1.16903
C	0.60494	-1.04426	1.23042
C	1.04993	-1.92124	0.23768
C	0.20879	-2.26676	-0.82723
C	-1.08136	-1.75118	-0.90110
C	-1.52964	-0.89838	0.10841
H	-1.03940	0.13690	1.94515
H	1.27465	-0.69897	2.01228
H	0.57516	-2.95225	-1.58976
H	-1.73114	-2.02609	-1.72933
O	2.29206	-2.48132	0.22204
C	3.03045	-2.43762	1.45131
H	3.29122	-1.39980	1.69032
H	2.43502	-2.89318	2.25377
H	3.92527	-3.04074	1.27388
I	-3.48830	-0.10402	0.00947
H	0.80009	4.25295	1.20771

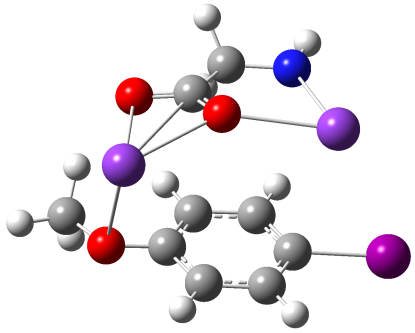
28 + 4-iodoanisole Product Complex



26
−2124.7525415

C	3.50209	−1.86217	−0.11637
C	2.27011	−1.50922	0.57208
O	1.16904	−1.69257	−0.06198
O	2.34639	−1.03945	1.74568
N	3.44665	−2.36931	−1.38845
K	−0.28198	−0.77903	−1.91334
K	−0.26664	−0.69389	2.04291
H	4.47264	−1.70909	0.34487
H	2.53787	−2.72659	−1.65793
C	2.34949	1.56920	−1.68892
C	2.22482	1.52860	−0.29279
C	1.01400	1.90210	0.30146
C	−0.07588	2.30960	−0.47896
C	0.04559	2.36922	−1.87115
C	1.25900	1.99541	−2.41742
H	3.28371	1.27033	−2.16266
H	3.05727	1.18112	0.31408
H	−1.00963	2.57750	0.01272
H	−0.79249	2.70215	−2.48252
O	0.80659	1.88056	1.65351
C	1.96856	1.99075	2.48209
H	2.55248	1.06416	2.45162
H	2.57469	2.84759	2.15936
H	1.59298	2.16857	3.49330
I	−2.98372	−0.31832	0.01670
H	4.24210	−2.88333	−1.73867

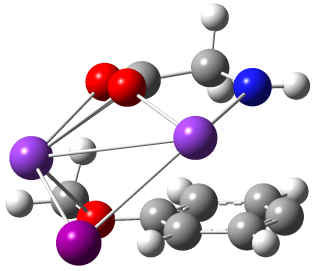
29 + 4-iodoanisole Reactant Complex



26
−2124.7352409

C	1.28863	2.29161	1.55464
C	2.07219	1.62674	0.41437
O	1.58980	1.57767	−0.76249
O	3.20609	1.13612	0.70427
N	−0.05355	2.70626	1.23384
H	1.37610	1.54815	2.38456
H	1.96971	3.11233	1.87838
K	3.48656	−0.03836	−1.57323
K	−0.90706	2.09031	−1.09080
C	−0.42126	−0.61996	1.23024
C	0.91236	−1.02352	1.30509
C	1.47987	−1.73910	0.24984
C	0.70878	−2.08390	−0.86568
C	−0.63026	−1.70829	−0.93053
C	−1.18371	−0.97840	0.12118
H	−0.83886	−0.00203	2.02113
H	1.50629	−0.72372	2.16219
H	1.16199	−2.66385	−1.66883
H	−1.23403	−1.99380	−1.78952
O	2.79291	−2.11407	0.20586
C	3.55433	−1.94043	1.40560
H	3.08009	−2.48700	2.23122
H	4.53492	−2.37497	1.19587
H	3.64566	−0.87297	1.64257
I	−3.22338	−0.42334	0.03365
H	−0.39419	3.21801	2.04913

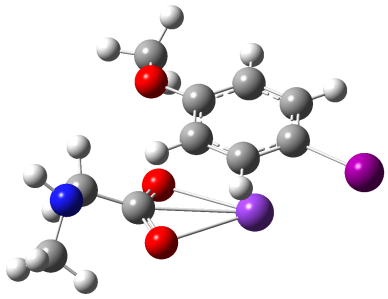
29 + 4-iodoanisole Product Complex



```
26
-2124.7283100

C                  2.35083     -1.44980      1.54935
C                  1.36725     -0.32267      1.89413
O                  0.14036     -0.61459      1.96430
O                  1.85960      0.81285      2.08417
N                  1.73803     -2.58124      0.90657
H                  3.18206     -1.03430      0.96068
H                  2.79846     -1.78603      2.50531
K                 -0.56032      1.84217      1.29587
K                 -1.04748     -2.36559      0.54695
C                  3.72597     -0.62011     -1.70642
C                  3.31574      0.62425     -1.19950
C                  1.95017      0.90079     -1.07972
C                  0.98993     -0.04888     -1.45469
C                  1.39298     -1.28750     -1.95633
C                  2.75148     -1.52447     -2.05764
H                  4.78705     -0.84365     -1.80809
H                  4.06804      1.34983     -0.90320
H                 -0.07051      0.19880     -1.36925
H                  0.65323     -2.02190     -2.27571
O                  1.45319      2.08775     -0.62284
C                  2.39479      3.02234     -0.10709
H                  3.08381      3.35343     -0.89518
H                  1.81086      3.88057      0.23693
H                  2.94109      2.57584      0.73307
I                 -2.95152      0.21613     -0.56196
H                  2.49861     -3.16570      0.54202
```

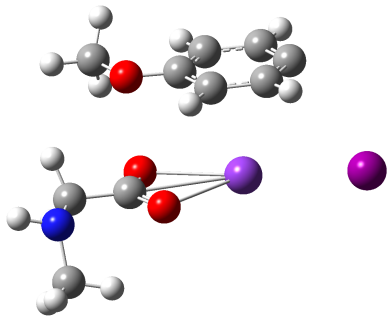
30 + 4-iodoanisole Reactant Complex



29
−1564.7262813

C	4.02709	0.46334	0.12192
C	2.85863	0.53404	−0.86877
O	2.12352	1.55530	−0.87507
O	2.71827	−0.46614	−1.63180
N	3.88508	1.33550	1.28206
H	4.49446	0.98387	2.01375
H	4.09129	−0.57488	0.46035
C	4.24360	2.72294	1.00305
H	5.25944	2.82216	0.57577
H	3.52606	3.13420	0.28772
H	4.19606	3.30802	1.92905
H	4.94553	0.68100	−0.45929
K	0.23159	0.23930	−2.07046
C	−0.63622	0.36238	1.08036
C	0.62463	−0.19998	1.23597
C	0.87655	−1.50270	0.78115
C	−0.13435	−2.22456	0.13425
C	−1.40499	−1.65699	−0.01947
C	−1.65077	−0.37178	0.45535
H	−0.81982	1.37799	1.42492
H	1.44820	0.37243	1.66606
H	0.04372	−3.22850	−0.24176
H	−2.19139	−2.22631	−0.51174
I	−3.55300	0.50239	0.18349
O	2.11456	−1.98327	1.02378
C	2.53952	−3.10602	0.26278
H	2.42530	−2.89039	−0.80738
H	3.59739	−3.24300	0.49925
H	1.98374	−4.00942	0.54770

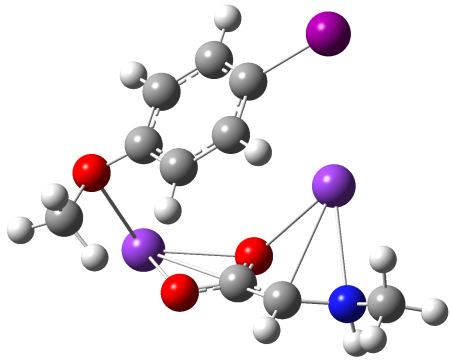
30 + 4-iodoanisole Product Complex



29
−1564.6266311

C	4.03294	−0.90555	0.17378
C	2.56143	−0.76332	0.58728
O	1.66905	−1.34447	−0.07768
O	2.35735	−0.04400	1.61157
N	4.26718	−1.77707	−0.96467
H	5.21183	−1.61896	−1.30080
H	4.38274	0.10449	−0.07243
C	4.11338	−3.18706	−0.62811
H	4.73252	−3.49252	0.23705
H	3.06226	−3.37735	−0.38755
H	4.39054	−3.80405	−1.49062
H	4.58197	−1.22359	1.08122
K	−0.22498	−0.37757	1.41928
C	−1.19130	1.34708	−1.40607
C	0.19740	1.26572	−1.52646
C	1.02702	1.93223	−0.60982
C	0.46772	2.63652	0.47071
C	−0.92716	2.70842	0.60792
C	−1.70212	2.06258	−0.33221
H	−1.83439	0.88665	−2.15708
H	0.66235	0.71030	−2.33858
H	1.10110	3.12811	1.20406
H	−1.36865	3.26660	1.43264
I	−3.44760	−0.84620	−0.12554
O	2.34987	1.86442	−0.86168
C	3.22438	2.55556	0.02462
H	3.17432	2.10284	1.02362
H	4.22497	2.43429	−0.39611
H	2.97341	3.62438	0.05690

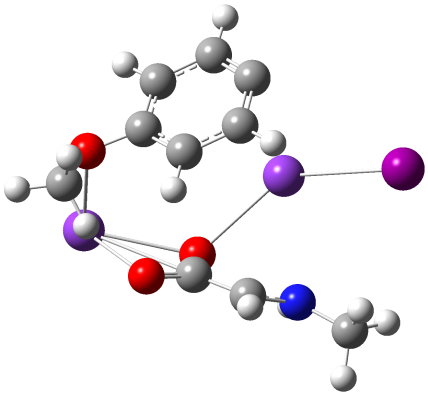
31 + 4-iodoanisole Reactant Complex



29
−2164.0218953

C	1.76838	2.41007	0.83381
C	2.37534	1.34639	0.12721
O	2.14646	1.15936	−1.15835
O	3.13991	0.50166	0.75589
N	1.17586	3.53981	0.13223
K	−0.33014	1.66352	−1.07057
K	3.68431	−0.87758	−1.30283
H	2.15553	2.61597	1.83811
C	0.28139	4.30658	0.98600
H	0.74806	4.61547	1.94042
H	−0.06472	5.20984	0.46394
H	−0.59465	3.69184	1.24805
H	1.89184	4.17641	−0.21804
C	−0.66614	−0.60198	1.18378
C	0.63540	−1.09079	1.30137
C	1.08085	−2.07587	0.41615
C	0.23847	−2.54477	−0.59975
C	−1.05311	−2.04420	−0.72926
C	−1.50033	−1.07905	0.17437
H	−1.00740	0.16713	1.87421
H	1.30462	−0.65272	2.03575
H	0.60508	−3.31157	−1.28027
H	−1.70584	−2.41494	−1.51661
O	2.32667	−2.62730	0.46016
C	3.07580	−2.41994	1.66553
H	3.32659	−1.35736	1.76892
H	2.49315	−2.77372	2.52656
H	3.97599	−3.03134	1.55800
I	−3.46055	−0.30481	−0.01296

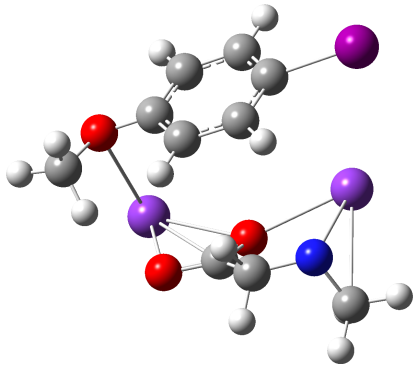
31 + 4-iodoanisole Product Complex



29
-2164.0287780

C	0.13872	2.22534	0.84547
C	1.41191	1.85760	0.24430
O	1.45188	1.77616	-1.04252
O	2.40433	1.62958	0.99904
N	-0.88689	2.65096	0.05386
K	-0.59590	0.08028	-1.38638
K	3.99669	1.09598	-0.99760
H	-0.02213	2.17130	1.91854
C	-2.10530	3.19041	0.62861
H	-1.93969	4.18081	1.07851
H	-2.86986	3.26464	-0.14957
H	-2.47186	2.49511	1.39123
H	-0.60134	2.99021	-0.85847
C	0.02589	-1.88438	1.06962
C	1.31475	-1.37070	1.27023
C	2.32399	-1.66089	0.34404
C	2.05487	-2.43174	-0.79317
C	0.77010	-2.94933	-0.99985
C	-0.18923	-2.66264	-0.04887
H	-0.78272	-1.64888	1.76018
H	1.51440	-0.72949	2.12481
H	2.86346	-2.64405	-1.49174
H	0.55413	-3.56596	-1.87156
O	3.61564	-1.22092	0.47850
C	4.03586	-0.87352	1.80167
H	3.56266	0.06129	2.12005
H	3.79535	-1.68962	2.49519
H	5.12147	-0.75189	1.74542
I	-3.50179	-0.43695	0.09441

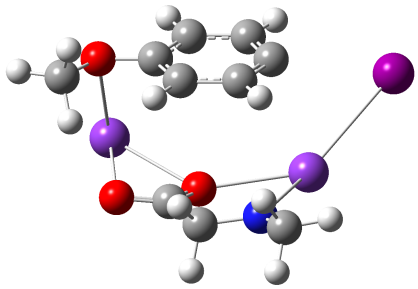
32 + 4-iodoanisole Reactant Complex



29
-2164.0186157

C	1.33279	2.22234	1.39239
C	2.13940	1.48010	0.28928
O	1.66212	1.36700	-0.88720
O	3.25091	0.97422	0.62685
N	0.04239	2.74760	1.09225
H	1.27668	1.48173	2.21186
C	0.18619	4.01468	0.43114
H	0.81245	4.74906	0.99424
H	0.67116	3.98354	-0.58875
H	-0.79648	4.49900	0.28689
H	2.05334	2.99111	1.76910
K	3.48046	-0.40751	-1.54577
K	-0.84820	1.82637	-1.22542
C	-0.42631	-0.66160	1.19967
C	0.89632	-1.09772	1.29310
C	1.40787	-1.97471	0.33629
C	0.59216	-2.44305	-0.69997
C	-0.73523	-2.03407	-0.77943
C	-1.23466	-1.14550	0.17475
H	-0.79729	0.07743	1.90754
H	1.52986	-0.69930	2.07926
H	1.00229	-3.14169	-1.42771
H	-1.37521	-2.41440	-1.57275
O	2.70940	-2.39026	0.30959
C	3.49219	-2.13288	1.48142
H	3.00276	-2.57185	2.36047
H	4.45015	-2.62928	1.30887
H	3.63435	-1.05303	1.61444
I	-3.25769	-0.53655	0.05580

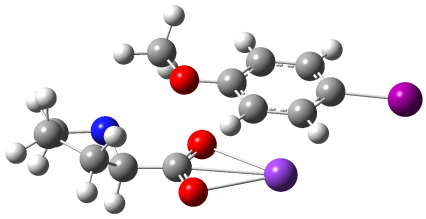
32 + 4-iodoanisole Product Complex



29
−2164.0143464

C	−2.18720	2.51468	0.28782
C	−2.29874	1.16946	1.01796
O	−1.25481	0.64658	1.49419
O	−3.45810	0.69224	1.09955
N	−0.85232	2.88848	−0.08518
H	−2.87219	2.50405	−0.57670
C	−0.84823	3.99421	−1.00818
H	−1.45170	3.76559	−1.90328
H	−1.30672	4.88286	−0.53980
H	0.17423	4.23954	−1.31173
H	−2.59093	3.28291	0.97559
K	−2.55205	−1.63686	1.95656
K	1.21147	1.24898	0.87161
C	−0.77456	0.39216	−2.13984
C	−2.01270	−0.18359	−1.81683
C	−2.03950	−1.41128	−1.15036
C	−0.85089	−2.08070	−0.82790
C	0.38485	−1.51054	−1.13783
C	0.36757	−0.28686	−1.77926
H	−0.73547	1.34856	−2.66001
H	−2.93044	0.33915	−2.07178
H	−0.90752	−3.05920	−0.34920
H	1.32197	−2.00351	−0.88113
O	−3.19052	−2.03140	−0.73887
C	−4.42479	−1.44155	−1.14436
H	−4.47837	−1.38910	−2.23977
H	−5.20720	−2.10773	−0.77314
H	−4.53239	−0.44462	−0.69938
I	3.92993	−0.48308	0.06123

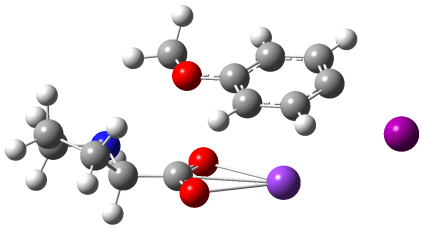
33 + 4-iodoanisole Reactant Complex



33
−1642.1327465

C	−4.05036	−0.92648	0.08999
H	−4.50485	−1.92165	0.27347
C	−2.54449	−1.18396	0.01828
O	−1.98291	−1.14177	−1.11143
O	−1.97495	−1.48330	1.10460
N	−4.61584	−0.30628	−1.10601
H	−4.57180	−0.93101	−1.90465
C	−4.50301	0.01975	1.21845
H	−4.69725	−0.53554	2.14058
H	−3.71264	0.74671	1.43131
C	−5.77437	0.70256	0.65435
H	−6.64687	0.57006	1.30330
H	−5.61197	1.77960	0.53088
C	−5.98064	0.04148	−0.71922
H	−6.44240	0.71025	−1.45524
H	−6.62435	−0.85191	−0.60825
K	0.30525	−1.90163	−0.07387
C	0.30514	1.25754	−0.99138
C	1.64596	0.87081	−1.07764
C	2.35843	0.56105	0.07821
C	1.74119	0.63581	1.33170
C	0.40828	1.02084	1.41837
C	−0.31839	1.34326	0.26040
H	−0.24150	1.47489	−1.90379
H	2.12242	0.80779	−2.05413
H	2.29585	0.39402	2.23611
H	−0.09499	1.07689	2.38155
I	4.37105	−0.05994	−0.06285
O	−1.59208	1.73044	0.44941
C	−2.34767	2.10462	−0.70264
H	−2.47206	1.24589	−1.37194
H	−3.32657	2.40817	−0.32530
H	−1.86608	2.95108	−1.21107

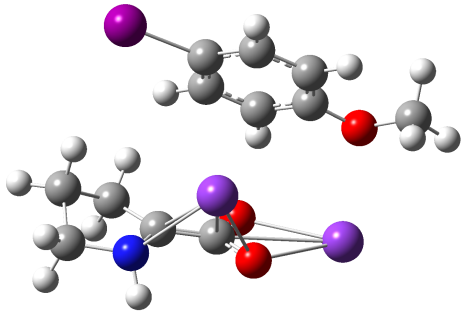
33 + 4-iodoanisole Product Complex



33
−1642.0329822

C	−3.71940	−1.11988	0.26443
H	−4.06319	−2.07173	0.72012
C	−2.19862	−1.12493	0.42198
O	−1.49106	−1.36096	−0.59621
O	−1.75530	−0.94568	1.59082
N	−4.18239	−1.00425	−1.11570
H	−3.93012	−1.82078	−1.66325
C	−4.45142	0.03815	0.96778
H	−4.68513	−0.21691	2.00544
H	−3.80885	0.92393	0.97649
C	−5.71948	0.26374	0.10574
H	−6.64519	0.16858	0.68355
H	−5.70719	1.26421	−0.34188
C	−5.62444	−0.80759	−0.99509
H	−6.06186	−0.48688	−1.94821
H	−6.14597	−1.72606	−0.66458
K	0.71283	−1.26939	0.79634
C	0.51964	1.76734	−0.96443
C	1.86440	1.88522	−0.56778
C	2.14177	1.91779	0.78516
C	1.17600	1.87440	1.78127
C	−0.15382	1.78226	1.38155
C	−0.48676	1.74625	0.00894
H	0.27855	1.73458	−2.02291
H	2.64585	1.99271	−1.32032
H	1.43585	1.91099	2.83828
H	−0.96293	1.71973	2.10687
I	4.03422	−0.58541	−0.34106
O	−1.80266	1.72351	−0.26294
C	−2.19618	1.58250	−1.62563
H	−1.79949	0.64324	−2.02904
H	−3.28516	1.52165	−1.61123
H	−1.86399	2.45109	−2.21045

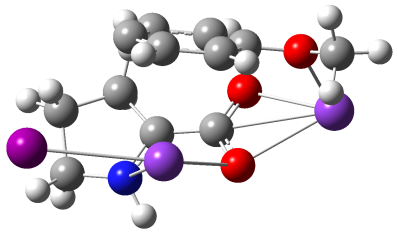
34 + 4-iodoanisole Reactant Complex



33
−2241.4175999

C	1.00340	2.43635	0.15623
C	2.13286	1.63576	0.18827
O	2.64947	1.15005	−0.94275
O	2.68399	1.30278	1.33529
N	0.40184	2.93978	−1.10178
H	1.11159	3.43041	−1.64248
C	0.25888	3.00478	1.32990
H	0.14843	2.27781	2.14683
H	0.73040	3.90199	1.77759
C	−1.08126	3.40088	0.69192
H	−1.71968	2.51111	0.57885
H	−1.64123	4.16242	1.24836
C	−0.64150	3.89711	−0.68682
H	−0.23376	4.91620	−0.57923
H	−1.46318	3.93318	−1.41480
K	4.38240	−0.25405	0.31678
K	0.37904	0.35819	−1.81153
I	−3.45850	−0.58378	0.15499
C	−1.46921	−1.28476	0.26832
C	−0.52617	−0.57356	1.01722
C	−1.10084	−2.42627	−0.43837
C	0.79557	−1.00814	1.04989
H	−0.80058	0.33154	1.55578
C	0.22678	−2.86781	−0.40718
H	−1.83620	−2.98069	−1.01767
C	1.17297	−2.14768	0.33232
H	1.54950	−0.39881	1.56054
H	0.49363	−3.76116	−0.96472
O	2.49979	−2.48089	0.39331
C	2.89237	−3.68852	−0.24252
H	2.72851	−3.63422	−1.32763
H	3.95946	−3.80701	−0.03918
H	2.34440	−4.54429	0.17382

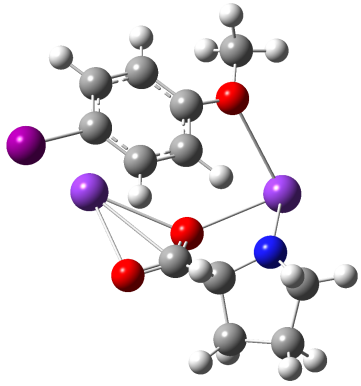
34 + 4-iodoanisole Product Complex



33
−2241.4365705

C	0.19018	2.43866	0.17350
C	1.54444	2.06427	−0.18096
O	1.72077	1.47073	−1.31312
O	2.47778	2.30701	0.64701
N	−0.84879	2.35517	−0.73277
H	−0.63110	2.53344	−1.70714
C	−0.32865	2.91961	1.49401
H	0.11840	2.38624	2.34019
H	−0.09813	3.98905	1.63026
C	−1.84587	2.70036	1.34323
H	−2.10597	1.66554	1.60058
H	−2.44709	3.38002	1.95415
C	−2.08339	2.89979	−0.15696
H	−2.18775	3.96762	−0.40359
H	−2.95187	2.34389	−0.52462
K	4.23937	0.97152	−0.69807
K	−0.23405	−0.39692	−1.27626
I	−3.38125	−0.85421	−0.28499
C	−0.40994	−1.93197	1.49984
C	0.29746	−0.79074	1.83155
C	0.10687	−2.97173	0.76023
C	1.62455	−0.69793	1.40333
H	−0.15821	0.02255	2.39522
C	1.44169	−2.87751	0.32933
H	−0.49339	−3.84200	0.49923
C	2.18807	−1.73937	0.65456
H	2.21431	0.19241	1.62241
H	1.86973	−3.69058	−0.25156
O	3.49401	−1.55437	0.26124
C	4.16248	−2.67910	−0.29541
H	3.73395	−2.95290	−1.26916
H	5.20631	−2.38149	−0.42594
H	4.10998	−3.53694	0.38739

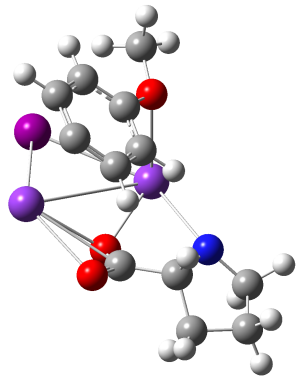
35 + 4-iodoanisole Reactant Complex



33
−2241.4259377

C	−2.36545	−1.66169	−0.12052
H	−1.53887	−2.10687	−0.73838
C	−1.64936	−1.06558	1.09175
O	−1.97644	0.08687	1.53101
O	−0.71786	−1.74984	1.60088
N	−3.20488	−0.78383	−0.88749
C	−3.26308	−2.87184	0.29104
H	−2.68570	−3.79906	0.39551
H	−3.74251	−2.66062	1.25646
C	−4.29764	−2.92111	−0.85496
H	−4.28298	−3.88056	−1.39078
H	−5.31445	−2.76418	−0.47233
C	−3.86943	−1.72394	−1.75448
H	−4.72311	−1.27160	−2.28390
H	−3.18863	−2.14054	−2.54336
K	0.53544	0.36288	2.32455
K	−3.60341	1.53399	0.15048
O	−1.23011	2.83124	−0.72268
C	−1.08854	4.23434	−0.54954
H	−0.37740	4.64522	−1.27782
H	−2.07776	4.66435	−0.72306
H	−0.75691	4.47364	0.47021
C	−0.09379	2.07586	−0.64186
C	−0.24025	0.71718	−0.95274
C	1.14874	2.58888	−0.25986
C	0.86029	−0.12867	−0.87266
H	−1.22991	0.32065	−1.22189
C	2.25574	1.73251	−0.18772
H	1.28541	3.64040	−0.02345
C	2.10652	0.38400	−0.49209
H	0.73572	−1.18805	−1.08705
H	3.22500	2.13278	0.10343
I	3.76925	−0.90802	−0.35337

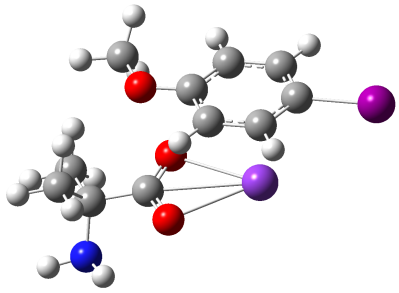
35 + 4-iodoanisole Product Complex



33
−2241.4309810

C	−3.29641	−0.15939	0.16108
H	−3.40768	−1.15860	−0.29964
C	−2.14148	−0.25947	1.17609
O	−1.28089	0.66507	1.17116
O	−2.14715	−1.25204	1.93645
N	−3.03175	0.77623	−0.92015
C	−4.63316	0.24979	0.80587
H	−5.13739	−0.59539	1.28198
H	−4.44898	1.02081	1.56655
C	−5.38721	0.84298	−0.38414
H	−5.82658	0.04232	−0.99294
H	−6.18286	1.53776	−0.09609
C	−4.25256	1.52907	−1.15649
H	−4.08157	2.54847	−0.76334
H	−4.42461	1.63462	−2.23584
K	0.59094	−0.99194	2.06636
K	−0.31553	1.75523	−0.95377
O	0.94471	−0.30976	−2.36445
C	2.21635	−0.06541	−2.96314
H	2.52359	−0.93417	−3.56052
H	2.07634	0.79938	−3.61631
H	2.96494	0.16633	−2.19615
C	0.83673	−1.40778	−1.56007
C	−0.46450	−1.72743	−1.14868
C	1.92866	−2.17969	−1.14684
C	−0.69010	−2.83267	−0.32325
H	−1.29254	−1.10391	−1.48948
C	1.70954	−3.29371	−0.32247
H	2.94302	−1.92237	−1.43822
C	0.41347	−3.57376	0.05276
H	−1.69532	−3.07374	0.01777
H	2.55071	−3.90532	0.00109
I	2.67659	1.31031	0.64214

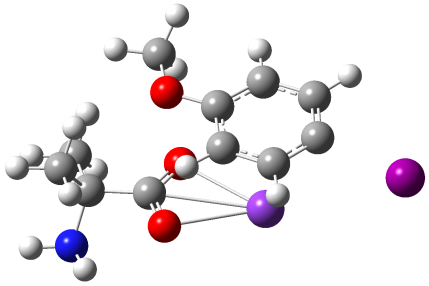
36 + 4-iodoanisole Reactant Complex



32
-1604.0449253

C	-4.40278	-0.56391	0.11918
C	-2.89856	-0.81522	-0.15018
O	-2.28591	-1.48536	0.72903
O	-2.37686	-0.35642	-1.20191
N	-4.99355	-1.89123	0.36467
H	-5.93517	-1.77653	0.73630
K	-0.11998	-1.60482	-0.69976
C	1.41996	0.37972	1.36471
C	0.13373	0.90017	1.44664
C	-0.43955	1.56072	0.34849
C	0.28390	1.67032	-0.84594
C	1.57743	1.14528	-0.92810
C	2.14135	0.50480	0.17226
H	1.85646	-0.12322	2.22537
H	-0.44976	0.80501	2.36029
H	-0.14457	2.15406	-1.71849
H	2.13424	1.23861	-1.85862
I	4.08302	-0.31054	0.03134
O	-1.67043	2.07034	0.54211
C	-2.29638	2.70600	-0.56804
H	-2.42434	1.98405	-1.38356
H	-3.27101	3.04208	-0.20623
H	-1.70964	3.57606	-0.89216
H	-4.44188	-2.34574	1.08989
C	-4.52352	0.35084	1.34640
H	-4.04396	1.32138	1.17065
H	-5.58459	0.52161	1.57573
H	-4.04305	-0.12192	2.21068
C	-5.09818	0.06453	-1.08045
H	-4.96912	-0.56182	-1.96899
H	-6.17236	0.16954	-0.87271
H	-4.68549	1.05775	-1.29018

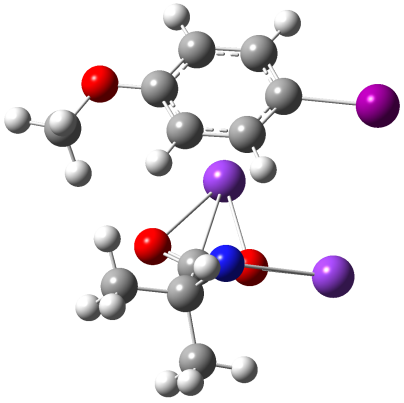
36 + 4-iodoanisole Product Complex



32
−1603.9450161

C	−4.11418	−0.94045	−0.05705
C	−2.57082	−0.92287	0.06739
O	−2.11072	−1.01444	1.24100
O	−1.87160	−0.82936	−0.97696
N	−4.55584	−2.16287	0.63733
H	−5.56766	−2.13651	0.75271
K	0.33935	−1.17764	0.37086
C	0.85008	1.64318	1.99055
C	−0.44914	1.74898	1.50187
C	−0.67925	1.94185	0.12273
C	0.39484	1.99188	−0.77454
C	1.71176	1.91101	−0.28414
C	1.88719	1.72556	1.07247
H	1.03211	1.50253	3.05494
H	−1.31046	1.67529	2.16321
H	0.23182	2.13122	−1.83932
H	2.55287	2.03633	−0.96702
I	3.82370	−0.69057	−0.26629
O	−1.96863	2.10307	−0.22915
C	−2.26685	2.18591	−1.61822
H	−1.94834	1.26460	−2.12123
H	−3.35294	2.28573	−1.68241
H	−1.79440	3.07209	−2.06288
H	−4.15032	−2.15182	1.57124
C	−4.67026	0.32552	0.61042
H	−4.31387	1.23338	0.10925
H	−5.76837	0.31011	0.56859
H	−4.35351	0.36312	1.65928
C	−4.56397	−1.01664	−1.50940
H	−4.13536	−1.89953	−1.99427
H	−5.66024	−1.08250	−1.55542
H	−4.24310	−0.12654	−2.06259

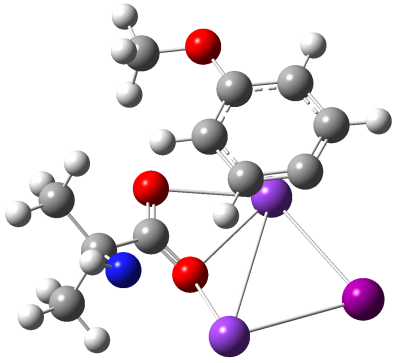
37 + 4-iodoanisole Reactant Complex



32
-2203.3381221

C	-2.87617	1.46204	-0.42033
C	-2.20120	0.70609	0.75198
O	-1.20297	1.26886	1.31937
O	-2.63423	-0.42344	1.10795
N	-1.84122	1.79780	-1.39493
K	-0.34842	-1.03595	2.20237
K	-0.00579	3.09482	-0.05788
C	0.38253	-0.51636	-0.93153
C	-0.66247	-1.43656	-1.00607
C	-0.47902	-2.74645	-0.55262
C	0.77365	-3.13811	-0.05236
C	1.81992	-2.22067	0.02349
C	1.60904	-0.90745	-0.40705
H	0.13699	0.49568	-1.26171
H	-1.61339	-1.06356	-1.37713
H	0.91076	-4.16450	0.28419
H	2.78452	-2.53095	0.42094
O	-1.45582	-3.68330	-0.53363
C	-2.76788	-3.24171	-0.89029
H	-2.80531	-2.97509	-1.95535
H	-3.42537	-4.09299	-0.70188
H	-3.06079	-2.37954	-0.27525
I	3.15150	0.52594	-0.20214
H	-2.32600	1.91908	-2.28688
C	-3.99804	0.60180	-1.01844
H	-3.58977	-0.31838	-1.45429
H	-4.75475	0.32250	-0.27326
H	-4.48751	1.16985	-1.82246
C	-3.55004	2.71264	0.20778
H	-2.79384	3.35788	0.67338
H	-4.04687	3.28196	-0.58996
H	-4.29748	2.45179	0.97536

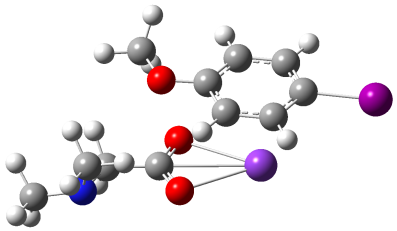
37 + 4-iodoanisole Product Complex



32
-2203.3251070

C	-2.49094	2.18281	-0.08463
C	-1.64283	1.29260	0.87572
O	-0.41854	1.59068	0.95628
O	-2.21001	0.36099	1.48408
N	-1.77629	2.26433	-1.34499
K	0.26840	-0.89179	1.56101
K	1.09227	2.33064	-0.96520
C	-0.43514	-0.97933	-1.65967
C	-1.64730	-1.38010	-1.07767
C	-1.72158	-2.60596	-0.40495
C	-0.59175	-3.43687	-0.32397
C	0.61860	-3.03885	-0.89803
C	0.64963	-1.82015	-1.55143
H	-0.38550	-0.02298	-2.17881
H	-2.50694	-0.72046	-1.13597
H	-0.68017	-4.38824	0.19928
H	1.50332	-3.66967	-0.82141
O	-2.84164	-3.06750	0.20992
C	-3.97914	-2.21007	0.21178
H	-4.34464	-2.05411	-0.81392
H	-4.74271	-2.73359	0.79115
H	-3.73344	-1.24775	0.68150
I	3.28526	0.03531	0.17015
H	-2.47301	2.46352	-2.07426
C	-3.92288	1.67702	-0.24851
H	-3.94974	0.71074	-0.76543
H	-4.39149	1.54692	0.73168
H	-4.50815	2.39831	-0.83409
C	-2.50559	3.60899	0.51237
H	-1.48400	3.97508	0.65077
H	-3.05611	4.29002	-0.14879
H	-3.00991	3.57851	1.48645

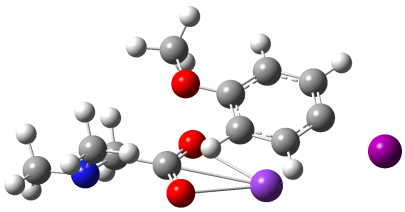
38 + 4-iodoanisole Reactant Complex



32
-1604.0200949

C	4.22074	-0.56507	0.51635
C	2.73329	-0.93845	0.58601
O	2.17556	-1.47253	-0.40443
O	2.17421	-0.69952	1.69720
N	4.83688	-0.64618	-0.79384
H	4.33244	0.44476	0.96273
H	4.73683	-1.26111	1.19295
K	-0.08055	-1.74133	0.86403
C	-1.28047	0.37665	-1.28264
C	0.03247	0.82377	-1.20935
C	0.51858	1.42125	-0.03552
C	-0.32313	1.54246	1.07722
C	-1.64573	1.09199	1.00290
C	-2.11964	0.51254	-0.17058
H	-1.64691	-0.07875	-2.20048
H	0.70784	0.71159	-2.05466
H	0.03439	1.97640	2.00644
H	-2.29580	1.19370	1.86975
I	-4.10600	-0.19624	-0.26680
O	1.79437	1.84960	-0.07897
C	2.33238	2.43434	1.10250
H	2.33917	1.69422	1.91299
H	3.35496	2.72089	0.84729
H	1.75995	3.32808	1.38485
C	4.30589	0.37517	-1.68164
H	4.77212	0.28056	-2.66990
H	3.22472	0.24692	-1.77898
H	4.50777	1.39734	-1.29564
C	6.27841	-0.51198	-0.67990
H	6.67835	-1.30802	-0.04000
H	6.73691	-0.60022	-1.67256
H	6.57779	0.46612	-0.24651

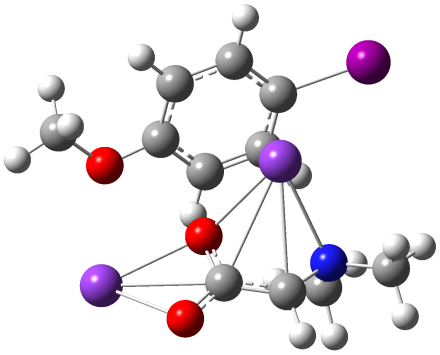
38 + 4-iodoanisole Product Complex



32
−1603.9201811

C	−3.83752	−1.08857	−0.66084
C	−2.35711	−1.12146	−0.25620
O	−2.04178	−1.15967	0.95923
O	−1.54015	−1.14258	−1.22368
N	−4.78857	−0.87322	0.41308
H	−3.94475	−0.33001	−1.46372
H	−4.04340	−2.06305	−1.12584
K	0.49352	−1.36084	0.39685
C	0.77782	1.55177	1.93209
C	−0.49959	1.54904	1.37966
C	−0.67920	1.74224	−0.00720
C	0.42810	1.89403	−0.85013
C	1.72160	1.92033	−0.29605
C	1.84736	1.73516	1.06672
H	0.91932	1.41569	3.00327
H	−1.38247	1.38718	1.99523
H	0.30577	2.02976	−1.92087
H	2.58123	2.12750	−0.93443
I	3.92602	−0.56483	−0.17059
O	−1.96068	1.79744	−0.41627
C	−2.20195	1.90416	−1.81479
H	−1.80096	1.01976	−2.32679
H	−3.28814	1.93865	−1.92235
H	−1.76606	2.83007	−2.21326
C	−4.67819	0.47675	0.94075
H	−5.39307	0.60930	1.76182
H	−3.66402	0.64153	1.31353
H	−4.89674	1.23885	0.16214
C	−6.14026	−1.11955	−0.05723
H	−6.22928	−2.15340	−0.41251
H	−6.85029	−0.97187	0.76576
H	−6.42859	−0.44019	−0.88762

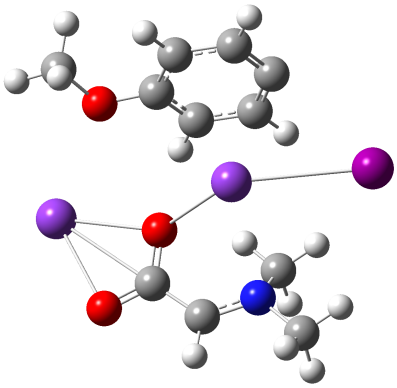
39 + 4-iodoanisole Reactant Complex



32
-2203.3033271

C	1.75017	-2.77663	-0.33784
C	2.59497	-1.63482	-0.36527
O	2.06794	-0.43416	-0.21751
O	3.87034	-1.74269	-0.56188
N	0.42895	-2.67862	0.27458
K	0.05716	-0.88437	-1.70104
K	4.29232	0.56411	0.46564
H	2.23965	-3.75370	-0.23304
C	-0.81201	0.75855	1.29771
C	0.45479	1.31486	1.36781
C	0.89656	2.19866	0.37676
C	0.05128	2.54450	-0.67823
C	-1.23446	1.98960	-0.74653
C	-1.65220	1.09449	0.23043
H	-1.13449	0.05004	2.05642
H	1.13516	1.04018	2.17015
H	0.36291	3.23483	-1.45674
H	-1.89327	2.26290	-1.56835
O	2.17135	2.66284	0.51642
C	2.62765	3.58679	-0.46062
H	2.64696	3.12242	-1.45653
H	1.99317	4.48260	-0.48036
H	3.64056	3.87018	-0.16349
I	-3.55235	0.18791	0.08374
C	-0.35527	-3.86571	-0.00907
H	0.12941	-4.78586	0.38045
H	-1.35185	-3.78779	0.44808
H	-0.46350	-3.98927	-1.09532
C	0.49574	-2.46672	1.71594
H	-0.51687	-2.36300	2.13858
H	1.00343	-3.31047	2.22585
H	1.06004	-1.54661	1.90409

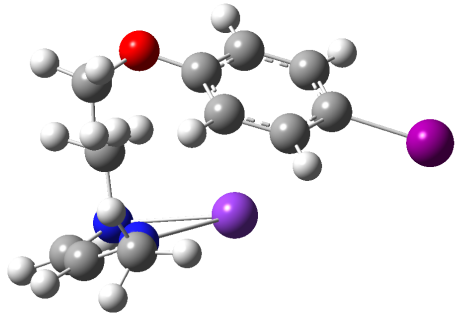
39 + 4-iodoanisole Product Complex



32
-2203.3117751

C	-0.47265	3.12779	-0.27368
C	-1.74062	2.39708	-0.24773
O	-1.72728	1.14866	0.06261
O	-2.79493	3.02487	-0.56103
N	0.70943	2.63171	0.22341
K	0.36107	-0.02395	-1.00727
K	-4.30133	0.96860	0.12100
H	-0.42742	4.06244	-0.82922
C	-0.06837	-1.73178	1.70587
C	-1.41121	-1.46943	1.43579
C	-2.03803	-2.07315	0.33648
C	-1.33050	-2.94053	-0.50084
C	0.02566	-3.20779	-0.23285
C	0.59931	-2.59978	0.85878
H	0.43327	-1.25532	2.54688
H	-1.98098	-0.77742	2.05241
H	-1.80356	-3.41567	-1.35624
H	0.59130	-3.87340	-0.88306
O	-3.35894	-1.74728	0.14752
C	-4.06746	-2.49729	-0.83020
H	-3.68989	-2.28798	-1.84019
H	-3.99447	-3.57273	-0.62334
H	-5.11308	-2.18640	-0.75777
I	3.53236	-0.47336	-0.15174
C	1.90737	3.42172	-0.02403
H	1.96674	4.27762	0.66874
H	2.78566	2.78143	0.11551
H	1.89598	3.79222	-1.05356
C	0.73487	1.96480	1.52681
H	1.63168	1.33618	1.58413
H	0.77174	2.72005	2.32916
H	-0.16404	1.35690	1.64478

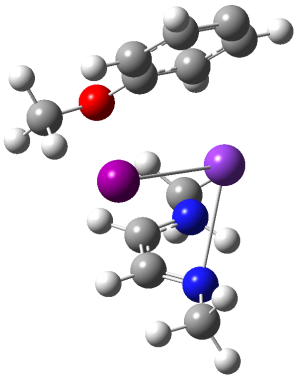
40 + 4-iodoanisole Reactant Complex



32
-1508.8416879

C	-4.25818	-1.52653	-0.35068
H	-5.31301	-1.74451	-0.51918
C	-3.81214	-1.24440	0.91679
H	-4.60127	-1.30034	1.68942
N	-2.56437	-0.91811	1.30120
N	-3.38412	-1.44566	-1.49887
H	-3.72576	-2.06700	-2.22486
C	-2.45091	-0.60629	2.70841
H	-3.06773	-1.26003	3.35428
H	-1.40862	-0.71620	3.04730
H	-2.74932	0.43771	2.95839
C	-3.29176	-0.08720	-2.04872
H	-2.62750	-0.07469	-2.92644
H	-4.27035	0.32856	-2.34090
H	-2.86867	0.57077	-1.27987
K	-0.77299	-1.42326	-0.57221
C	-0.27641	1.37189	1.03298
C	-0.71066	1.91113	-0.18442
C	0.09436	1.78579	-1.32580
C	1.32200	1.13311	-1.25609
C	1.74909	0.60054	-0.03722
C	0.95836	0.72353	1.10399
H	-0.89706	1.42472	1.92233
H	-0.26042	2.20534	-2.26573
H	1.93929	1.04233	-2.14754
H	1.28777	0.30528	2.05350
O	-1.88296	2.56063	-0.35222
C	-2.84231	2.46022	0.70357
H	-3.75371	2.91872	0.31439
H	-3.01456	1.40184	0.94742
H	-2.50151	3.01532	1.58767
I	3.59120	-0.42482	0.06276

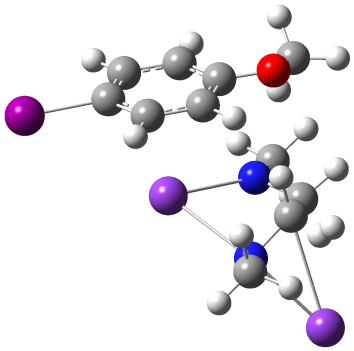
40 + 4-iodoanisole Product Complex



32
−1508.8350980

C	0.84231	2.25226	0.87309
H	1.12007	1.95922	1.88124
C	−0.50337	2.48636	0.51196
H	−1.26191	2.38930	1.29753
N	−0.81544	2.78133	−0.72342
N	1.84148	2.36899	−0.04387
H	1.57160	2.89051	−0.87292
C	−2.22013	3.02284	−0.99336
H	−2.33969	4.01676	−1.44618
H	−2.59414	2.28682	−1.71994
H	−2.84750	2.95761	−0.09143
C	3.22488	2.48752	0.38741
H	3.88958	2.29656	−0.46061
H	3.43982	3.48639	0.79226
H	3.41203	1.73832	1.16361
K	0.10903	0.23893	−1.54611
C	1.08533	−2.12075	0.38501
C	2.09735	−1.17671	0.59872
C	3.01947	−0.87904	−0.41903
C	2.94036	−1.52831	−1.65314
C	1.92727	−2.45664	−1.81897
C	1.00025	−2.77787	−0.85423
H	0.33564	−2.33411	1.14137
H	3.80097	−0.14746	−0.22313
H	3.65834	−1.30788	−2.44202
H	0.20522	−3.50207	−1.02628
O	2.25995	−0.49149	1.76161
C	1.26920	−0.68452	2.76805
H	1.53965	−0.01054	3.58453
H	0.26951	−0.43505	2.38313
H	1.28100	−1.72057	3.13057
I	−2.47002	−0.81084	0.28018

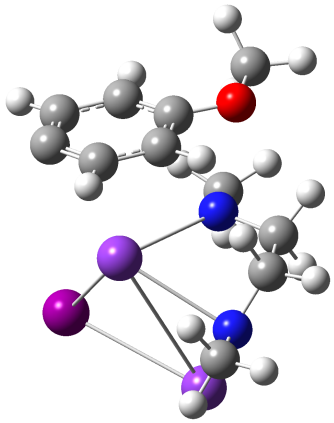
41 + 4-iodoanisole Reactant Complex



34
-2109.3174384

C	-2.97240	-0.26259	-0.70890
H	-2.18639	0.27158	-1.29732
H	-3.82750	-0.32332	-1.45432
C	-3.43947	0.69457	0.39743
H	-3.83452	1.60830	-0.12948
H	-4.38017	0.26281	0.87079
N	-2.46256	1.02010	1.38095
N	-2.55032	-1.56742	-0.27037
C	-3.03450	1.98274	2.26888
H	-3.95694	1.62101	2.79509
H	-2.32227	2.28478	3.05417
H	-3.37089	2.92929	1.75952
C	-2.26067	-2.35062	-1.43470
H	-1.89396	-3.35522	-1.16717
H	-3.14950	-2.50965	-2.11815
H	-1.49529	-1.89900	-2.11696
K	-0.43792	-0.58784	1.06334
K	-5.09311	-2.13488	0.07327
C	0.14614	1.87150	-1.12708
C	0.85713	2.22006	0.02951
C	1.97201	1.46991	0.41448
C	2.36191	0.36344	-0.33697
C	1.65338	0.00256	-1.48671
C	0.55452	0.75845	-1.87876
H	0.54741	3.06176	0.64233
H	2.52329	1.75131	1.30953
H	1.94946	-0.86612	-2.07130
H	-0.01842	0.48882	-2.76369
O	-0.91963	2.54562	-1.59809
C	-1.57773	3.43889	-0.69513
H	-2.47796	3.76811	-1.21871
H	-1.83572	2.88404	0.22029
H	-0.94301	4.30989	-0.48269
I	4.01221	-0.79668	0.28171

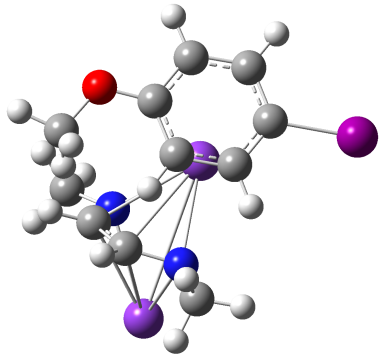
41 + 4-iodoanisole Product Complex



34
−2109.3236182

C	0.87405	2.55788	−0.33008
H	1.72953	1.90083	−0.64869
H	1.27926	3.59214	−0.44638
C	0.65286	2.28969	1.14989
H	1.54061	2.58317	1.74390
H	−0.18856	2.90579	1.52460
N	0.40629	0.88867	1.39108
N	−0.32603	2.32465	−1.07579
C	−0.14444	0.64165	2.69790
H	−1.20384	0.95244	2.71622
H	−0.11006	−0.42711	2.93652
H	0.37286	1.22273	3.48156
C	−0.03092	2.49336	−2.47187
H	−0.92654	2.33524	−3.09466
H	0.36900	3.50111	−2.73433
H	0.75324	1.78379	−2.86083
K	0.24651	−0.40101	−1.06677
K	−2.79096	1.96239	−0.24369
C	3.33862	−0.40969	0.20087
C	2.80358	−1.61380	0.67702
C	2.50928	−2.64822	−0.22786
C	2.75909	−2.42589	−1.56323
C	3.27727	−1.25049	−2.07737
C	3.56816	−0.22694	−1.17317
H	2.60526	−1.76227	1.73487
H	2.09245	−3.58705	0.13378
H	3.45982	−1.11476	−3.14237
H	3.97760	0.72328	−1.51205
O	3.66338	0.64376	0.99142
C	3.54154	0.46773	2.39433
H	3.86195	1.41034	2.84325
H	2.50163	0.25639	2.67300
H	4.19150	−0.34727	2.74091
I	−2.76839	−1.36774	0.20778

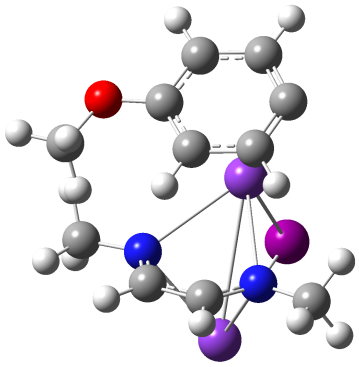
42 + 4-iodoanisole Reactant Complex



32
−2108.1510597

C	−3.30908	0.30280	−0.06281
H	−3.90209	1.21890	0.09534
C	−2.54286	−0.09684	1.02284
H	−2.62471	0.54666	1.91485
N	−1.67960	−1.18153	1.07064
N	−3.37163	−0.31959	−1.29823
C	−1.23110	−1.43594	2.41543
H	−2.03390	−1.79056	3.10616
H	−0.44553	−2.20749	2.42554
H	−0.80441	−0.53741	2.92418
C	−4.40118	0.25478	−2.13289
H	−4.37825	−0.19406	−3.13735
H	−5.43612	0.10480	−1.74259
H	−4.29941	1.35448	−2.27157
K	−0.70938	−0.25583	−1.25381
K	−3.89094	−2.49583	0.22234
C	0.28420	2.61583	0.21002
C	0.29298	1.59726	1.16841
C	1.22280	0.55680	1.07041
C	2.14533	0.54819	0.02707
C	2.14620	1.56406	−0.93254
C	1.21498	2.59334	−0.84122
H	−0.43767	1.57032	1.97106
H	1.19703	−0.24507	1.80520
H	2.86526	1.55391	−1.74917
H	1.19648	3.39577	−1.57650
O	−0.58145	3.65662	0.20758
C	−1.56169	3.69212	1.23958
H	−1.08177	3.78782	2.22323
H	−2.16927	4.57693	1.03877
H	−2.18481	2.78817	1.20634
I	3.51683	−1.04795	−0.14734

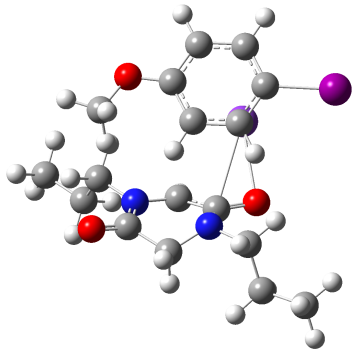
42 + 4-iodoanisole Product Complex



32
−2108.1893508

C	0.99403	2.40229	−0.13598
H	1.60137	3.26140	−0.45989
C	0.85005	2.23028	1.26730
H	1.38529	2.95169	1.90259
N	0.13164	1.25578	1.81451
N	0.44936	1.58630	−1.03377
C	0.12870	1.20696	3.26306
H	−0.88094	1.39014	3.66402
H	0.42196	0.20508	3.61428
H	0.81349	1.94134	3.72196
C	0.70216	1.90690	−2.42528
H	1.24816	1.08735	−2.91969
H	−0.24371	2.02671	−2.97551
H	1.28973	2.83306	−2.55676
K	0.09115	−0.94159	0.09622
K	−2.02252	2.08213	0.21596
C	3.31521	−0.87923	−0.57740
C	3.23223	−0.12618	0.60025
C	2.87051	−0.75621	1.80231
C	2.61912	−2.10905	1.77041
C	2.69198	−2.89170	0.63155
C	3.04438	−2.25822	−0.56271
H	3.41129	0.94475	0.59964
H	2.78506	−0.16965	2.71617
H	2.48751	−3.96127	0.64977
H	3.12188	−2.81749	−1.49387
O	3.64067	−0.35766	−1.78903
C	4.01910	1.01211	−1.82321
H	4.91346	1.17939	−1.20763
H	4.24244	1.23455	−2.86867
H	3.20004	1.65196	−1.47180
I	−3.26600	−0.96019	−0.39360

43 + 4-iodoanisole Reactant Complex

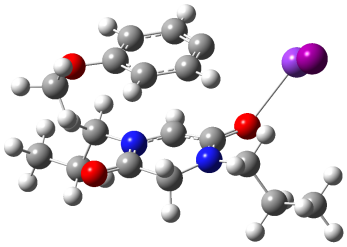


48
−1892.7323847

C	−2.33677	2.22137	−0.98959
C	−3.22320	0.98803	−0.95203
C	−2.06195	0.53690	1.13454
C	−0.99693	1.37478	0.83551
H	−2.25379	2.53771	−2.03416
H	−2.86178	3.01796	−0.42699
H	−2.28731	0.25258	2.15670
N	−3.06450	0.23681	0.15464
N	−1.01049	1.95421	−0.45491
O	0.00434	1.58814	1.60183
O	−4.02043	0.73132	−1.86459
C	−0.02540	2.99443	−0.71841
H	0.08371	3.08526	−1.80973
C	−3.91331	−0.92249	0.38471
H	−4.42982	−1.14191	−0.55468
H	−3.26525	−1.77440	0.64273
C	−4.94343	−0.68635	1.48695
H	−5.55931	0.17670	1.20183
H	−4.43425	−0.42468	2.42362
C	−5.81914	−1.91801	1.69576
H	−6.56235	−1.74654	2.48252
H	−6.35469	−2.17579	0.77294
H	−5.21119	−2.78500	1.98686
C	−0.36452	4.35838	−0.11517
H	−0.54629	4.22011	0.95846
H	−1.28964	4.74600	−0.56238
C	0.76901	5.35496	−0.33814
H	0.52484	6.33833	0.08003
H	1.69324	5.00284	0.13850
H	0.97003	5.48454	−1.41031
H	0.92897	2.65718	−0.30092
K	0.43049	−0.89316	2.05577
C	0.05148	−1.00899	−1.29290
C	−0.12551	−2.38405	−1.10494
C	0.90867	−3.14875	−0.54214
C	2.11880	−2.55258	−0.19999

C	2.29488	−1.18042	−0.41091
C	1.26609	−0.41107	−0.94766
H	−0.73980	−0.37632	−1.68550
H	0.75513	−4.21680	−0.39920
H	2.92085	−3.15635	0.22010
H	1.38113	0.66101	−1.08627
I	4.11369	−0.26044	0.13323
O	−1.25778	−3.05113	−1.42635
C	−2.20085	−2.36250	−2.24667
H	−1.73351	−2.07497	−3.19750
H	−3.01172	−3.07045	−2.42709
H	−2.59362	−1.46954	−1.74910

43 + 4-iodoanisole Product Complex

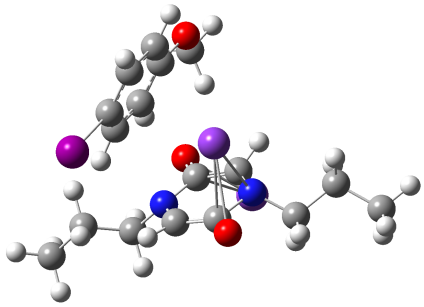


48
−1892.7076789

C	−1.29186	1.52059	−1.53199
C	−2.62078	0.97631	−1.05422
C	−1.80265	1.11660	1.19418
C	−0.46161	1.45019	0.78377
H	−0.97949	0.86719	−2.35683
H	−1.49140	2.51470	−1.96277
H	−2.01874	1.00590	2.24952
N	−2.79689	0.82337	0.30003
N	−0.23428	1.58142	−0.54411
O	0.44843	1.57071	1.63122
O	−3.50183	0.70927	−1.85529
C	1.12112	1.81876	−1.02732
H	1.17351	1.42864	−2.05211
C	−4.09258	0.33421	0.78399
H	−4.44208	−0.41604	0.06784
H	−3.90647	−0.15949	1.74414
C	−5.10471	1.46442	0.93294
H	−5.22743	1.95281	−0.04144
H	−4.70345	2.21185	1.63058
C	−6.44448	0.93487	1.43385
H	−7.17003	1.74818	1.54194
H	−6.85862	0.20056	0.73154
H	−6.33311	0.44688	2.41077
C	1.52204	3.29058	−0.99707
H	1.42472	3.65337	0.03383

H	0.82617	3.87224	−1.61766
C	2.95365	3.46998	−1.49380
H	3.25284	4.52362	−1.46310
H	3.65222	2.89228	−0.87522
H	3.05557	3.11623	−2.52793
H	1.81231	1.22208	−0.42216
K	2.44898	0.13925	2.40602
C	−1.03052	−1.87537	−1.18778
C	−2.10520	−2.26888	−0.37980
C	−1.95127	−2.37060	1.01114
C	−0.72515	−2.06698	1.60448
C	0.30519	−1.67581	0.76966
C	0.20786	−1.57188	−0.59800
H	−1.13676	−1.80932	−2.26746
H	−2.80182	−2.69380	1.60947
H	−0.60279	−2.14681	2.68381
H	1.06423	−1.27333	−1.20289
I	4.11824	−0.83771	−0.25100
O	−3.34362	−2.57086	−0.85487
C	−3.51921	−2.57429	−2.26617
H	−2.84158	−3.29957	−2.73658
H	−4.55492	−2.87615	−2.43514
H	−3.35463	−1.57180	−2.68054

44 + 4-iodoanisole Reactant Complex

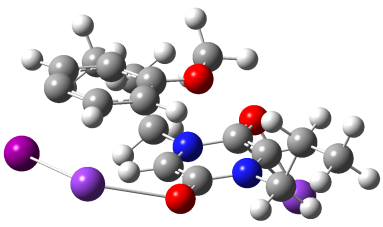


48
−2492.0257644

C	0.62836	0.71898	−1.55963
C	1.11305	−0.53371	−1.82921
C	2.50634	−0.24084	0.16258
C	2.05316	1.05287	0.36601
H	−0.23663	1.07710	−2.11268
H	2.96905	−0.75233	1.00727
N	2.11982	−1.08483	−0.94425
N	1.11468	1.58109	−0.52469
O	2.43545	1.79178	1.35885
O	0.64265	−1.35504	−2.70185
C	1.15432	3.00108	−0.82403
H	1.57736	3.15603	−1.83510
C	3.24128	−1.67708	−1.66857

H	2.82517	−2.16293	−2.55851
H	3.93988	−0.87898	−2.00204
C	4.01169	−2.70097	−0.84387
H	3.30179	−3.45695	−0.47815
H	4.44921	−2.21883	0.04195
C	5.11423	−3.36879	−1.66157
H	5.67254	−4.09942	−1.06368
H	4.69095	−3.89129	−2.52946
H	5.82799	−2.62347	−2.03805
C	−0.22084	3.66056	−0.74753
H	−0.60359	3.53406	0.27504
H	−0.91713	3.14225	−1.42233
C	−0.16215	5.14182	−1.10761
H	−1.15028	5.61091	−1.03243
H	0.51980	5.67844	−0.43391
H	0.20154	5.27957	−2.13446
H	1.81495	3.47268	−0.08776
K	4.86391	1.58791	0.66573
K	−0.42947	−2.21704	−0.40386
C	−0.71357	0.33263	1.81773
C	−1.69533	0.51348	0.83878
C	−2.76650	−0.37138	0.75083
C	−2.86880	−1.45359	1.63152
C	−1.88662	−1.64361	2.59904
C	−0.80692	−0.75109	2.69815
H	0.11948	1.03199	1.85459
H	−1.58806	1.34051	0.14073
H	−3.70629	−2.14554	1.56532
H	−1.94786	−2.47711	3.29662
O	0.10169	−1.02050	3.66464
C	1.17299	−0.08933	3.81501
H	0.78274	0.89279	4.11529
H	1.80543	−0.49510	4.60763
H	1.73984	0.02359	2.88179
I	−4.22019	−0.10254	−0.75377

44 + 4-iodoanisole Product Complex



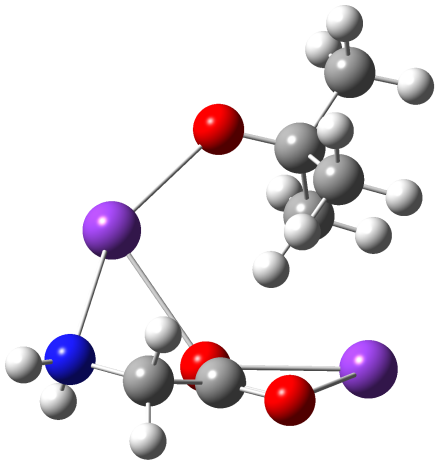
48
−2492.0430259

C	−0.59566	−0.62303	−0.66522
C	−1.20098	0.58184	−1.06867
C	−3.21360	−0.27864	−0.01058

C	−2.59617	−1.44726	0.43087
H	0.43592	−0.84799	−0.91686
H	−4.21936	−0.03982	0.32024
N	−2.53177	0.72619	−0.71018
N	−1.26296	−1.60254	0.05211
O	−3.17838	−2.37941	1.08807
O	−0.60565	1.49244	−1.72087
C	−0.49062	−2.74491	0.52868
H	0.22748	−3.01189	−0.25737
C	−3.27363	1.91679	−1.09203
H	−2.67983	2.43256	−1.85113
H	−4.22341	1.59372	−1.54594
C	−3.55151	2.85007	0.08491
H	−2.59106	3.15965	0.51256
H	−4.09384	2.29912	0.86626
C	−4.36398	4.06389	−0.35534
H	−4.55986	4.73510	0.48858
H	−3.82584	4.63386	−1.12399
H	−5.33096	3.75927	−0.77740
C	0.26385	−2.42767	1.81732
H	−0.46315	−2.14287	2.59048
H	0.92248	−1.56971	1.62470
C	1.10040	−3.61861	2.27009
H	1.64205	−3.38985	3.19496
H	0.46637	−4.49625	2.45402
H	1.83879	−3.87492	1.49961
H	−1.18659	−3.57259	0.68984
K	−4.76166	−2.99966	−0.78799
K	1.98418	1.37690	−1.62167
C	1.70673	1.54181	1.64011
C	3.06088	1.80218	1.36285
C	3.37135	2.98797	0.73828
C	2.44022	3.93590	0.34682
C	1.09775	3.66692	0.61701
C	0.73257	2.47993	1.27678
H	1.43728	0.60870	2.12720
H	3.81757	1.06279	1.61970
H	2.72958	4.86036	−0.15132
H	0.31398	4.36743	0.33339
O	−0.59165	2.33672	1.52290
C	−1.00814	1.20253	2.27099
H	−0.56435	1.21968	3.27569
H	−2.09594	1.27435	2.34033
H	−0.73737	0.27240	1.75805
I	3.32461	−1.57175	−0.69735

5. Donor Formation Optimised Geometries & coordinates

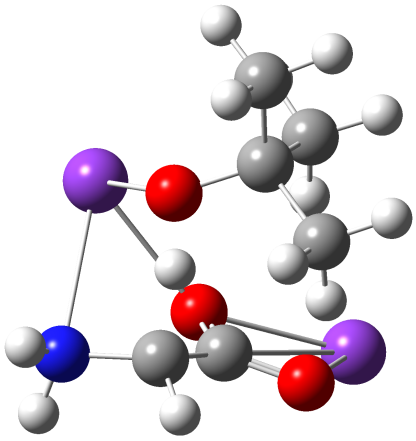
27 → 28 starting complex geometry



25
−1716.6727291

C	3.17980	−0.23302	0.73983
H	4.12801	0.32617	0.72717
C	2.10304	0.72087	0.21271
O	1.99885	1.82320	0.80356
O	1.39905	0.34639	−0.77031
N	3.22544	−1.49601	−0.00317
K	−0.15395	2.53048	−0.50289
K	0.46582	−2.17067	−0.43863
H	2.94555	−0.44145	1.79152
O	−1.90396	−1.68831	0.16766
C	−2.44196	−0.43366	0.24143
C	−2.31675	0.28347	−1.12713
H	−1.26148	0.27371	−1.44340
H	−2.88674	−0.27659	−1.87969
H	−2.70208	1.31876	−1.11652
C	−3.93638	−0.47305	0.62128
H	−4.04885	−0.97347	1.59236
H	−4.38759	0.52984	0.68741
H	−4.48482	−1.05712	−0.13002
C	−1.69793	0.40769	1.30790
H	−2.07070	1.44433	1.38693
H	−1.82426	−0.06639	2.28958
H	−0.61878	0.41080	1.08626
H	4.01387	−2.05049	0.31965
H	3.40390	−1.28657	−0.98347

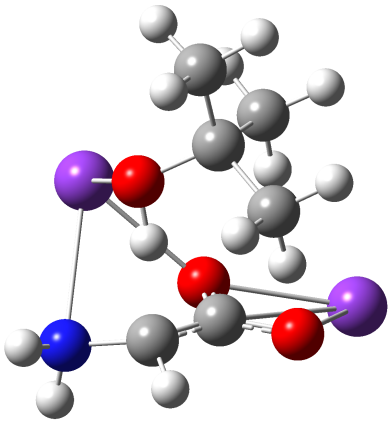
27 → 28 transition state geometry



25
−1716.6455406

C	−0.20805	1.01258	1.51965
H	−0.18652	0.71872	2.57724
C	−1.22464	0.25096	0.79345
O	−1.54847	−0.90649	1.22897
O	−1.70759	0.70110	−0.32364
N	−0.19783	2.47007	1.28514
K	−3.33105	−1.30116	−0.53120
K	0.38422	1.88344	−1.33075
H	1.03686	0.59543	0.85294
O	2.01186	0.45121	0.19867
C	2.21685	−0.92556	−0.02135
C	1.26356	−1.42479	−1.11968
H	0.22376	−1.23827	−0.81568
H	1.46893	−0.89683	−2.06336
H	1.38570	−2.50145	−1.30278
C	3.66534	−1.12570	−0.46806
H	4.34650	−0.77894	0.31945
H	3.87772	−2.18348	−0.67822
H	3.86348	−0.54062	−1.37656
C	1.95191	−1.71624	1.26712
H	2.17336	−2.78331	1.12522
H	2.59066	−1.33011	2.07226
H	0.90056	−1.60808	1.56467
H	0.63939	2.86179	1.70881
H	−0.98205	2.93725	1.73840

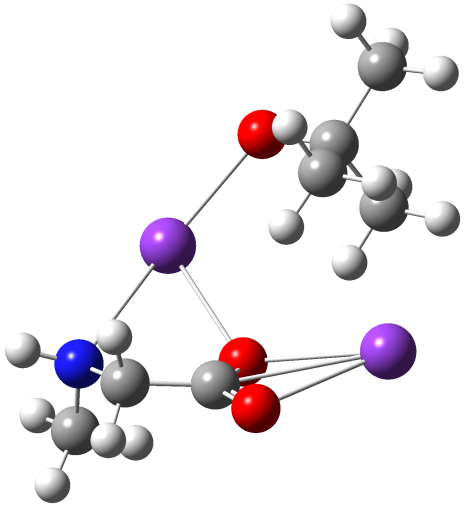
27 → 28 product complex geometry



25
−1716.6469373

C	−0.33814	1.07471	1.53102
H	−0.28393	0.78768	2.58680
C	−1.20718	0.23156	0.76111
O	−1.44918	−0.96784	1.16964
O	−1.69191	0.63440	−0.38807
N	−0.35487	2.52185	1.25815
K	−3.29117	−1.37333	−0.50839
K	0.34559	1.90731	−1.30737
H	1.20964	0.60163	0.79246
O	2.07315	0.47871	0.23132
C	2.24702	−0.91543	−0.00891
C	1.29295	−1.36378	−1.12183
H	0.25503	−1.16623	−0.82011
H	1.51910	−0.82439	−2.05374
H	1.39908	−2.43846	−1.32181
C	3.69590	−1.11012	−0.44122
H	4.37205	−0.79305	0.36239
H	3.89483	−2.16445	−0.67470
H	3.91087	−0.50684	−1.33329
C	1.94906	−1.70194	1.26910
H	2.14342	−2.77202	1.11506
H	2.59177	−1.34338	2.08335
H	0.89593	−1.56678	1.55115
H	0.43370	2.95856	1.72774
H	−1.18545	2.97690	1.63823

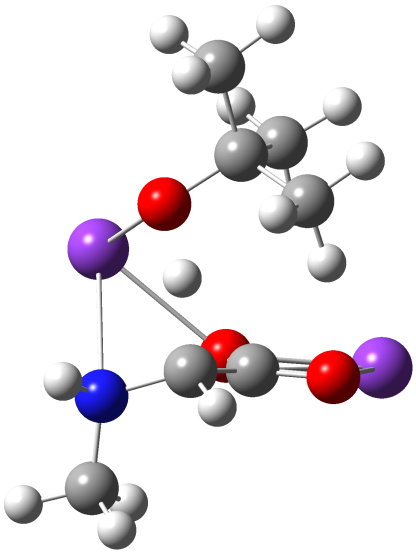
30 → 31 starting complex geometry



28
−1755.9594689

C	2.79778	0.22920	1.05299
H	3.72237	0.83058	1.10411
C	1.75779	1.06988	0.29628
O	1.64016	2.26084	0.67724
O	1.07445	0.52618	−0.61816
N	3.01808	−1.10108	0.49424
K	−0.66134	2.56800	−0.54119
K	0.44745	−2.05302	−0.36481
C	3.80256	−1.05184	−0.73935
H	4.00126	−2.07029	−1.09409
H	3.22460	−0.52061	−1.50419
H	4.76760	−0.53130	−0.61109
H	2.42108	0.12786	2.07927
O	−1.96981	−1.83469	0.22536
C	−2.64255	−0.64427	0.21022
C	−2.51060	0.02775	−1.18063
H	−1.44267	0.13518	−1.42799
H	−2.95806	−0.62807	−1.93871
H	−3.01633	1.00769	−1.24414
C	−4.14460	−0.83375	0.50551
H	−4.26354	−1.29253	1.49625
H	−4.70822	0.11246	0.48493
H	−4.57433	−1.51650	−0.23981
C	−2.06093	0.31776	1.27615
H	−2.55276	1.30672	1.28908
H	−2.18871	−0.13036	2.26971
H	−0.97854	0.43498	1.10850
H	3.52847	−1.64981	1.18011

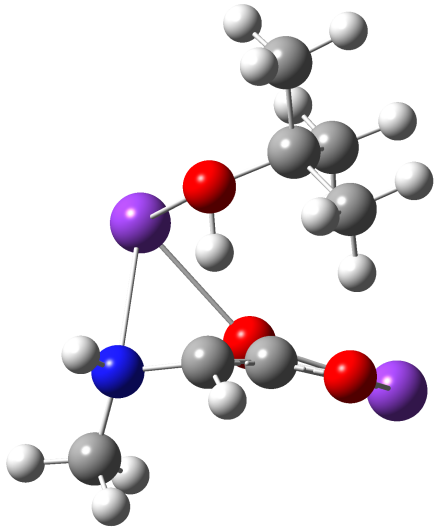
30 → 31 transition state geometry



28
−1755.9338955

C	0.41285	1.11361	−1.12820
H	0.44400	1.12336	−2.22939
C	1.17741	−0.02491	−0.60596
O	1.30220	−1.06590	−1.33467
O	1.61977	−0.00579	0.61293
N	0.71637	2.41506	−0.52284
K	2.66892	−2.36256	0.36611
K	−0.24122	1.33817	1.83051
C	2.01434	2.95538	−0.91919
H	2.15849	3.96170	−0.50096
H	2.79906	2.29927	−0.52158
H	2.13559	3.00694	−2.01642
H	−0.94675	0.82724	−0.63916
O	−1.98162	0.72463	−0.07303
C	−2.47199	−0.58728	−0.23064
C	−1.74176	−1.53679	0.73372
H	−0.66055	−1.49293	0.54095
H	−1.93921	−1.24219	1.77582
H	−2.07786	−2.57571	0.60948
C	−3.96667	−0.57916	0.09285
H	−4.49436	0.08025	−0.60802
H	−4.39861	−1.58745	0.02142
H	−4.12792	−0.19879	1.11067
C	−2.25059	−1.07083	−1.67026
H	−2.70312	−2.06039	−1.82512
H	−2.71178	−0.36152	−2.36983
H	−1.17592	−1.13379	−1.88633
H	−0.00637	3.06845	−0.81314

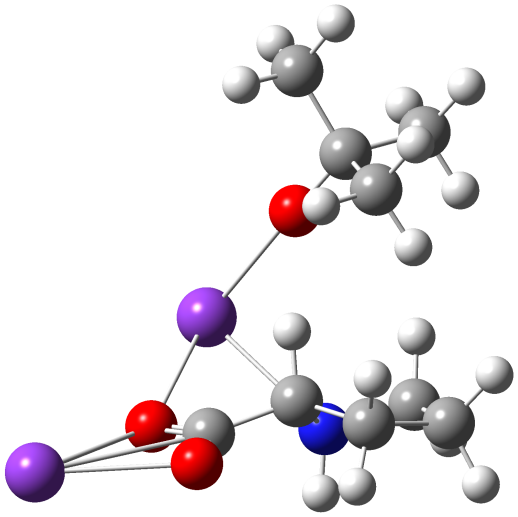
30 → 31 product complex geometry



28
−1755.9354102

C	−0.52467	−1.07774	−1.15450
H	−0.51075	−1.04838	−2.25317
C	−1.13064	0.09127	−0.57189
O	−1.14721	1.19488	−1.23547
O	−1.58480	0.06439	0.65543
N	−0.86670	−2.37824	−0.57806
K	−2.71388	2.36250	0.36720
K	0.21051	−1.40904	1.75535
C	−2.20751	−2.84373	−0.93215
H	−2.38768	−3.85091	−0.52768
H	−2.93892	−2.15522	−0.49123
H	−2.37360	−2.86481	−2.02446
H	1.15604	−0.82979	−0.61228
O	2.07278	−0.78702	−0.13095
C	2.55480	0.55192	−0.21712
C	1.80483	1.42937	0.79162
H	0.72877	1.41005	0.57021
H	1.98137	1.06439	1.81466
H	2.15217	2.47014	0.74260
C	4.04082	0.50697	0.12042
H	4.57414	−0.11137	−0.61216
H	4.47304	1.51645	0.11173
H	4.18955	0.06994	1.11674
C	2.33244	1.08975	−1.63183
H	2.76990	2.09184	−1.73691
H	2.80955	0.42146	−2.36015
H	1.25596	1.14576	−1.84318
H	−0.19525	−3.06236	−0.91618

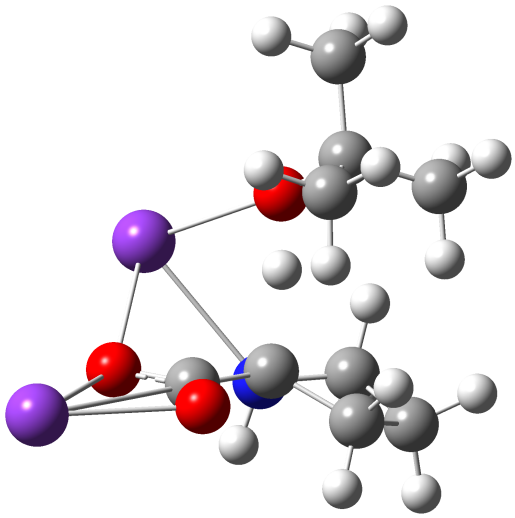
33 → 34 starting complex geometry



32
−1833.3598921

C	−0.55942	1.03975	−0.08022
C	−1.92018	0.35186	−0.18611
O	−2.17653	−0.55599	0.66903
O	−2.69002	0.68081	−1.12295
N	−0.23436	1.44258	1.30618
H	−0.99889	2.02802	1.64487
C	−0.35132	2.28983	−0.94815
H	−0.02283	2.02224	−1.95831
H	−1.29849	2.83300	−1.04050
C	0.70742	3.11166	−0.17353
H	1.63390	3.24196	−0.74454
H	0.32458	4.11063	0.06759
C	0.95229	2.29332	1.11621
H	1.12689	2.91322	2.00242
H	1.80494	1.61503	0.97882
K	−4.34504	−1.24735	−0.65522
K	0.14019	−1.25726	1.90634
O	1.96741	−1.07087	0.33386
C	2.95557	−0.91899	−0.60630
C	4.22402	−0.30578	0.02443
H	3.97745	0.67221	0.46169
H	4.58300	−0.96072	0.83048
H	5.03616	−0.16796	−0.70589
C	3.33522	−2.27975	−1.22661
H	2.44591	−2.72529	−1.69429
H	4.12777	−2.19519	−1.98610
H	3.68020	−2.95661	−0.43251
C	2.49197	0.01579	−1.74614
H	1.57920	−0.39143	−2.20480
H	2.25535	1.00831	−1.33673
H	3.25473	0.13697	−2.52946
H	0.20257	0.28726	−0.34840

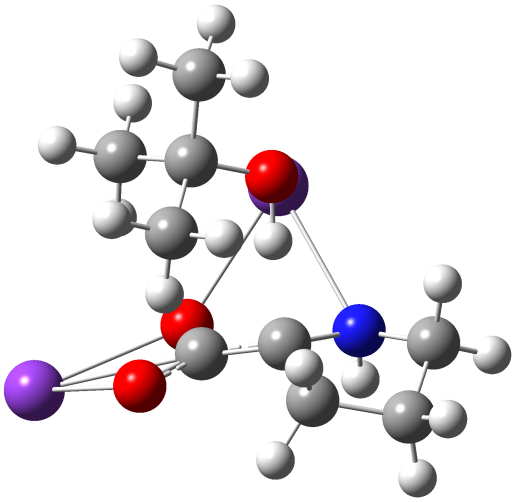
33 → 34 transition state geometry



32
−1833.3356245

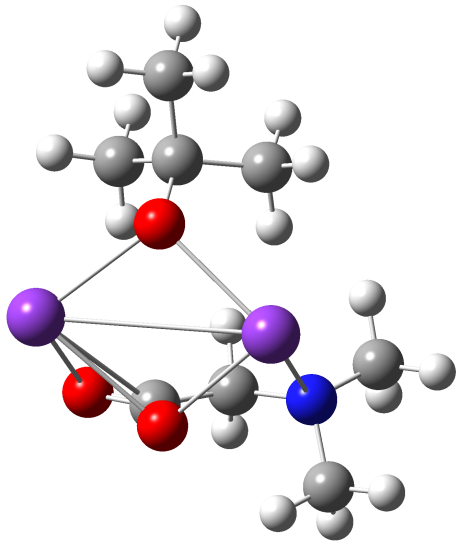
C	−0.15172	1.06022	−0.29986
C	−1.42536	0.36134	−0.34386
O	−2.07428	0.12504	0.76001
O	−1.84905	−0.07871	−1.46690
N	0.06266	1.99726	0.83251
H	−0.65632	2.72710	0.80869
C	0.31550	1.78301	−1.56731
H	0.78346	1.10215	−2.29087
H	−0.52572	2.26019	−2.09724
C	1.30993	2.85268	−1.04908
H	2.30986	2.75754	−1.49119
H	0.94702	3.86341	−1.27577
C	1.33938	2.62999	0.47928
H	1.48938	3.55453	1.05083
H	2.14159	1.92364	0.73360
K	−3.99896	−1.04130	−0.52196
K	−0.15066	−0.15702	2.50408
O	1.44973	−0.85561	0.63079
C	2.24931	−1.46974	−0.35397
C	3.01547	−2.61558	0.30564
H	3.64652	−2.22816	1.11622
H	2.30963	−3.34142	0.73004
H	3.65650	−3.13357	−0.42089
C	1.35555	−2.01242	−1.47669
H	0.75214	−1.20093	−1.90396
H	1.95317	−2.47560	−2.27346
H	0.66814	−2.76622	−1.07004
C	3.23849	−0.44746	−0.92896
H	2.69066	0.38399	−1.38976
H	3.86792	−0.04504	−0.12445
H	3.88697	−0.90294	−1.68944
H	0.79274	−0.06926	0.11754

33 → 34 product complex geometry



```
32
-1833.3369396
C                -0.01093     -1.28048     -0.31835
C                 1.15962     -0.46958     -0.27063
O                 1.74718     -0.22856      0.88047
O                 1.60044      0.08323     -1.34983
N                -0.27043     -2.20377      0.81762
H                 0.55455     -2.79388      0.96118
C                -0.44362     -1.95804     -1.62230
H                -1.21983     -1.38676     -2.15579
H                 0.39565     -2.07235     -2.32416
C                -1.00468     -3.31975     -1.16431
H                -1.86747     -3.65881     -1.75076
H                -0.22636     -4.09363     -1.22499
C                -1.34120     -3.06981      0.31338
H                -1.41841     -3.98623      0.91187
H                -2.29196     -2.52054      0.38738
K                 3.70347      0.99346     -0.28120
K                -0.35703      0.01289      2.38484
O                -1.95942      0.62820      0.27800
C                -1.74611      1.85346     -0.41736
C                -3.00427      2.69325     -0.22756
H                -3.86888      2.17614     -0.66113
H                -3.19607      2.85303      0.84158
H                -2.89701      3.67134     -0.71466
C                -0.52945      2.57340      0.17775
H                 0.35957      1.93368      0.08889
H                -0.33389      3.51628     -0.34999
H                -0.71164      2.81287      1.23599
C                -1.49913      1.56847     -1.89984
H                -0.57752      0.98248     -2.01857
H                -2.34424      1.00304     -2.31306
H                -1.39851      2.50728     -2.46075
H                -1.23441     -0.04648     -0.03939
```

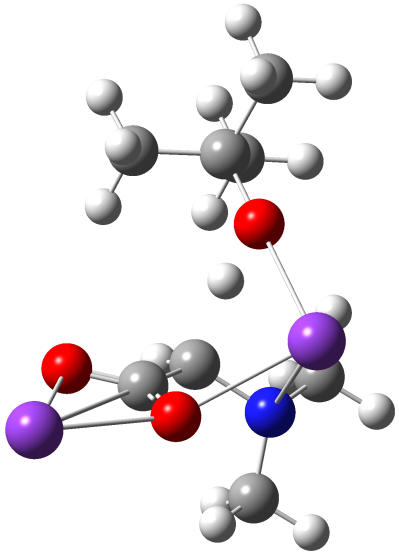
38 → 39 starting complex geometry



31
−1795.2680132

C	−1.88962	0.27819	−1.16992
H	−2.66323	0.69552	−1.84386
C	−1.15403	1.45717	−0.51000
O	−0.61240	2.25887	−1.30713
O	−1.09610	1.52268	0.75063
N	−2.45206	−0.71001	−0.25406
K	1.50304	2.26863	0.34806
K	−0.44462	−0.77134	1.81080
C	−3.63049	−0.17197	0.42042
H	−4.02016	−0.91234	1.13075
H	−3.35837	0.73908	0.96086
H	−4.43372	0.06654	−0.30434
C	−2.81834	−1.91531	−0.98867
H	−3.24320	−2.65307	−0.29693
H	−3.56835	−1.70836	−1.77693
H	−1.93034	−2.35056	−1.46244
H	−1.15107	−0.21820	−1.81336
O	1.82249	−0.23839	0.76281
C	2.21725	−1.03590	−0.29418
C	2.30391	−0.21142	−1.59630
H	1.33102	0.25976	−1.80437
H	3.06259	0.57824	−1.48331
H	2.58608	−0.82031	−2.46693
C	3.59297	−1.67201	−0.02398
H	3.54333	−2.27761	0.89132
H	3.93068	−2.31300	−0.85229
H	4.33781	−0.87981	0.13230
C	1.19738	−2.17303	−0.53013
H	1.46513	−2.81604	−1.38026
H	1.13469	−2.80779	0.36700
H	0.20561	−1.74009	−0.73092

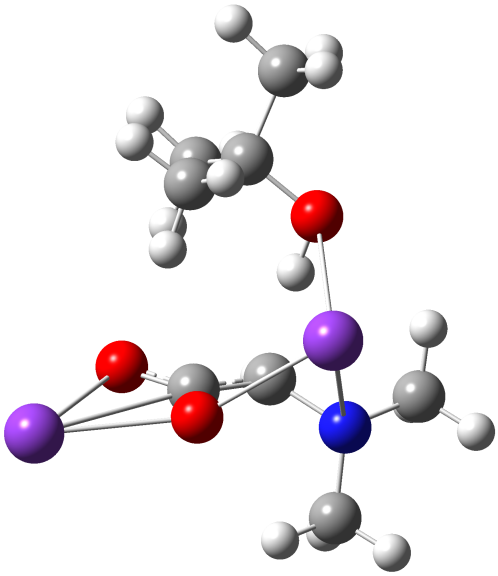
38 → 39 transition state geometry



31
−1795.2255402

C	0.19819	0.77721	−0.89578
H	0.01608	0.78085	−1.98595
C	1.34716	−0.06370	−0.55448
O	1.66319	−1.02350	−1.33445
O	1.96545	0.11465	0.57350
N	0.18582	2.13138	−0.32973
K	3.67049	−1.75627	0.02391
K	−0.01866	0.83308	2.10757
C	1.27432	2.95433	−0.83958
H	1.25160	3.95342	−0.37868
H	2.22906	2.47389	−0.59849
H	1.20593	3.07626	−1.93999
C	−1.08912	2.76928	−0.61816
H	−1.11967	3.77623	−0.17859
H	−1.25999	2.86931	−1.71093
H	−1.90591	2.16573	−0.20431
H	−0.91610	0.07802	−0.15429
O	−1.70807	−0.33078	0.58427
C	−2.61830	−1.12204	−0.14461
C	−1.86257	−2.25969	−0.84332
H	−1.08902	−1.84666	−1.50368
H	−1.36761	−2.88964	−0.09195
H	−2.54317	−2.88768	−1.43478
C	−3.63979	−1.69608	0.83629
H	−4.17152	−0.88026	1.34362
H	−4.37591	−2.32698	0.31902
H	−3.12909	−2.30341	1.59519
C	−3.33413	−0.25769	−1.19137
H	−4.06500	−0.84686	−1.76200
H	−3.86118	0.56785	−0.69461
H	−2.60310	0.16838	−1.89017

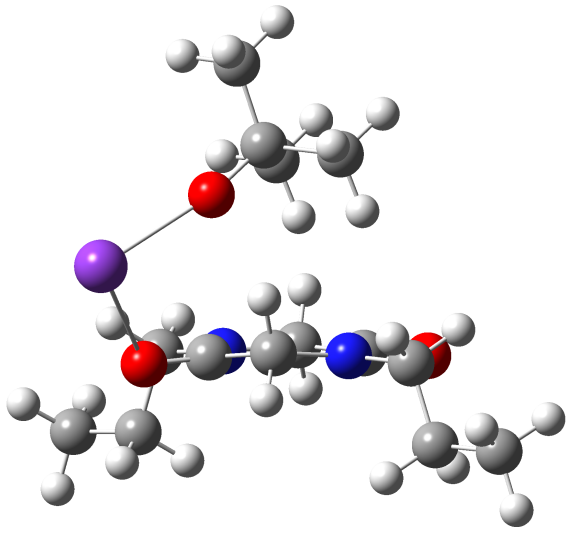
38 → 39 product complex geometry



31
−1795.2271704

C	0.50408	0.99628	−0.98589
H	0.46152	1.09493	−2.08244
C	1.14145	−0.21260	−0.53743
O	1.16751	−1.24138	−1.31078
O	1.61486	−0.29958	0.68002
N	0.82162	2.24574	−0.29617
K	2.76646	−2.54874	0.14912
K	−0.21420	1.01677	1.92937
C	2.19713	2.67339	−0.52408
H	2.41578	3.59451	0.03812
H	2.87378	1.88127	−0.18530
H	2.38625	2.86702	−1.59965
C	−0.09342	3.29451	−0.71601
H	0.13005	4.23229	−0.18783
H	−0.02104	3.49190	−1.80612
H	−1.12757	2.99558	−0.50144
H	−1.17396	0.64892	−0.46940
O	−2.08605	0.53223	0.00656
C	−2.53281	−0.80369	−0.21399
C	−1.76791	−1.75560	0.71263
H	−0.68931	−1.67055	0.51976
H	−1.97977	−1.51289	1.76460
H	−2.06967	−2.79767	0.54171
C	−4.02203	−0.82797	0.11131
H	−4.56588	−0.15894	−0.56708
H	−4.42814	−1.84256	0.00639
H	−4.18985	−0.48781	1.14185
C	−2.28596	−1.19756	−1.67146
H	−2.70000	−2.19479	−1.87348
H	−2.77324	−0.47458	−2.33799
H	−1.20691	−1.21008	−1.87673

26 → 43 starting complex geometry

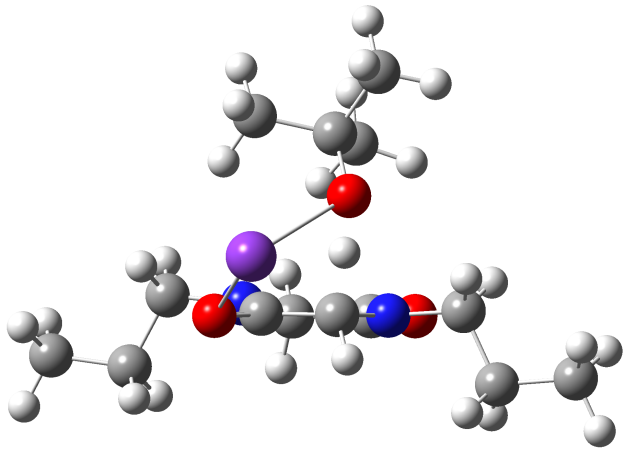


47
−1484.6405124

C	−0.76828	−1.64249	−1.41382
C	0.69278	−1.88825	−1.09227
C	0.47504	−0.41548	0.88675
C	−1.01391	−0.35251	0.67513
H	−0.79619	−1.11042	−2.37552
H	−1.22273	−2.62912	−1.56864
H	0.63244	−0.75055	1.92037
H	0.80865	0.63737	0.78376
N	1.21721	−1.28077	−0.01371
N	−1.53806	−0.90752	−0.42571
O	−1.70564	0.24163	1.51562
O	1.34073	−2.62032	−1.83748
C	−2.97474	−0.80617	−0.66553
H	−3.12623	−0.83634	−1.75221
C	2.62422	−1.50167	0.30688
H	3.18190	−1.55302	−0.63452
H	2.96998	−0.62425	0.86825
C	2.83850	−2.77724	1.11617
H	2.47423	−3.62517	0.52285
H	2.23146	−2.73022	2.03121
C	4.30945	−2.96830	1.47116
H	4.45977	−3.88920	2.04579
H	4.92241	−3.03107	0.56278
H	4.67973	−2.12743	2.07246
C	−3.75521	−1.92572	0.01742
H	−3.55885	−1.87229	1.09566
H	−3.37997	−2.89554	−0.33727
C	−5.25069	−1.80931	−0.25833
H	−5.80475	−2.61477	0.23647
H	−5.64062	−0.85203	0.11138
H	−5.45680	−1.86679	−1.33510
H	−3.31031	0.16889	−0.29752

O	0.48857	2.63151	0.24046
C	1.09051	2.71585	−0.99536
C	0.37047	1.80320	−2.01075
H	0.80041	1.86965	−3.02070
H	0.44949	0.76075	−1.67454
H	−0.69411	2.07211	−2.05816
C	1.04678	4.16253	−1.52312
H	0.00107	4.49365	−1.59202
H	1.57049	4.82327	−0.81821
H	1.51345	4.26655	−2.51411
C	2.56487	2.26827	−0.92167
H	3.09517	2.87882	−0.17883
H	2.61759	1.21592	−0.60669
H	3.08003	2.36000	−1.88917
K	−0.98630	2.71476	2.13544

26 → 43 transition state geometry

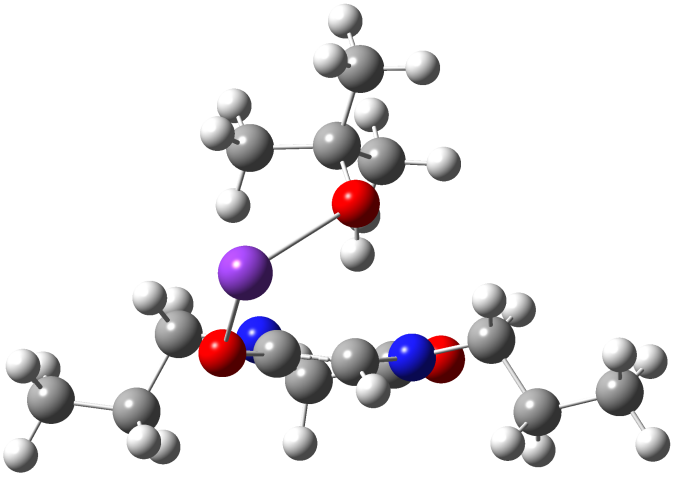


47
−1484.6317713

C	1.102684	−2.023961	0.908056
C	−0.400103	−2.208267	0.796819
C	−0.458715	−0.338593	−0.825684
C	0.984662	−0.153978	−0.688962
H	1.327266	−2.004556	1.982341
H	1.569181	−2.932630	0.496748
H	−0.713276	−0.464437	−1.886180
H	−0.939309	0.857653	−0.405737
N	−1.066636	−1.393209	−0.029278
N	1.645926	−0.828984	0.285838
O	1.578349	0.703611	−1.385160
O	−0.930760	−3.093896	1.475346
C	3.057803	−0.558851	0.517050
H	3.264381	−0.768060	1.575926
C	−2.518931	−1.494138	−0.096807
H	−2.876706	−1.861338	0.871366
H	−2.902981	−0.478029	−0.257631
C	−2.983850	−2.429155	−1.210342

H	−2.551236	−3.421807	−1.030413
H	−2.590890	−2.069204	−2.171411
C	−4.505719	−2.514744	−1.265287
H	−4.837365	−3.181913	−2.069239
H	−4.905716	−2.899799	−0.318201
H	−4.947043	−1.524548	−1.440773
C	3.982816	−1.384795	−0.374983
H	3.733009	−1.166047	−1.420846
H	3.796199	−2.454226	−0.207840
C	5.448909	−1.066254	−0.099149
H	6.109996	−1.659404	−0.741029
H	5.657618	−0.004500	−0.285135
H	5.706530	−1.284120	0.945870
H	3.225834	0.507574	0.336202
O	−1.362014	2.014468	−0.073570
C	−1.070168	2.335976	1.262285
C	−1.015474	1.071840	2.135544
H	−0.914534	1.333876	3.196754
H	−1.933947	0.485283	2.004058
H	−0.157472	0.445593	1.857510
C	0.292950	3.043460	1.340455
H	1.071138	2.390354	0.917314
H	0.264692	3.985408	0.772063
H	0.572005	3.286124	2.374772
C	−2.163623	3.267621	1.793210
H	−2.227802	4.164188	1.162287
H	−3.132904	2.753802	1.759928
H	−1.964200	3.579144	2.828195
K	0.148644	2.793270	−1.997881

26 → 43 product complex geometry

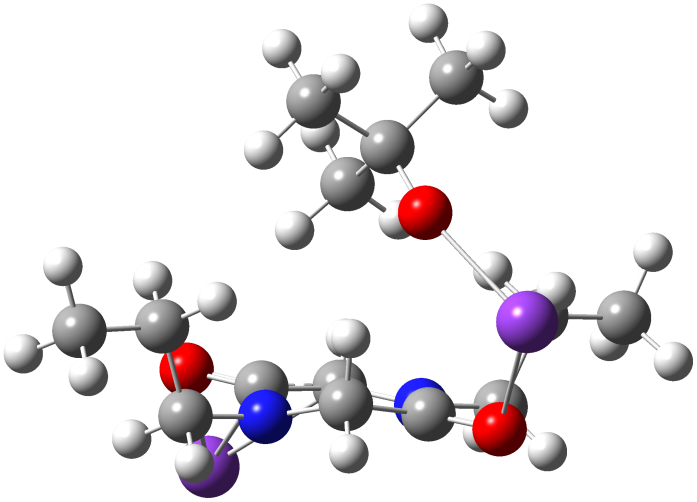


47
−1484.6407058

C	−0.57363	−2.34278	−0.71290
C	0.92703	−2.12301	−0.79131

C	0.54524	−0.51188	1.00145
C	−0.82873	−0.45613	0.77429
H	−0.90192	−2.70003	−1.69414
H	−0.76100	−3.14544	0.02568
H	0.94831	−0.33780	1.99558
H	0.73100	1.34676	0.31123
N	1.40003	−1.22429	0.09165
N	−1.28098	−1.11468	−0.38362
O	−1.66261	0.20151	1.48306
O	1.62812	−2.73156	−1.60785
C	−2.71285	−1.13228	−0.63889
H	−2.85617	−1.35355	−1.70702
C	2.81777	−0.89388	0.08313
H	3.20035	−1.08830	−0.92543
H	2.90675	0.18057	0.29573
C	3.60961	−1.70611	1.10448
H	3.49275	−2.77041	0.86198
H	3.17639	−1.55002	2.10212
C	5.08469	−1.31861	1.10393
H	5.65126	−1.90884	1.83337
H	5.52949	−1.48492	0.11399
H	5.20974	−0.25681	1.35559
C	−3.49500	−2.13717	0.20782
H	−3.27251	−1.93853	1.26377
H	−3.15441	−3.15686	−0.01841
C	−4.99453	−2.02821	−0.05086
H	−5.55779	−2.75423	0.54708
H	−5.35930	−1.02386	0.20282
H	−5.22368	−2.21274	−1.10927
H	−3.09924	−0.12548	−0.44656
O	0.78926	2.31231	0.09117
C	0.38172	2.48604	−1.27578
C	−1.14483	2.43727	−1.35360
H	−1.48429	2.52528	−2.39320
H	−1.51194	1.48575	−0.94766
H	−1.58636	3.26944	−0.78680
C	0.90366	3.85154	−1.70067
H	0.51059	4.63106	−1.03524
H	1.99885	3.87023	−1.65079
H	0.59213	4.07937	−2.72754
C	0.98655	1.37595	−2.13113
H	2.07718	1.36061	−2.01373
H	0.58071	0.40079	−1.83137
H	0.75018	1.53772	−3.18960
K	−0.97362	2.53845	2.11373

43 → 44 starting complex geometry

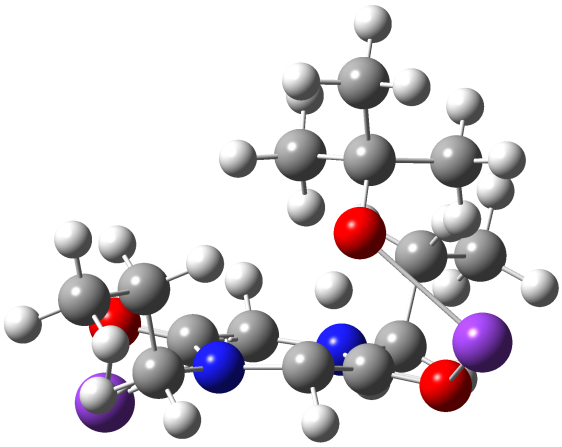


47
−2083.9510724

C	−0.13194	−0.54270	−1.44316
C	0.10796	0.94877	−1.39640
C	−1.67907	1.08993	0.26808
C	−2.01180	−0.26340	0.11259
H	−0.03648	−0.84333	−2.49578
H	0.70568	−0.99304	−0.87522
H	−1.69735	1.49418	1.27872
N	−0.65161	1.66242	−0.56680
N	−1.44342	−0.94908	−0.96071
O	−2.88173	−0.85796	0.83326
O	1.01048	1.44417	−2.10953
C	−1.74460	−2.36134	−1.12272
H	−1.56164	−2.61903	−2.17744
C	−0.37214	3.08206	−0.40726
H	−0.00454	3.47035	−1.36299
H	−1.32095	3.57602	−0.16192
C	0.66195	3.33467	0.68813
H	1.58042	2.79412	0.42330
H	0.29908	2.90561	1.63182
C	0.94678	4.82300	0.85873
H	1.69333	4.99565	1.64227
H	1.32778	5.25610	−0.07553
H	0.03371	5.36728	1.13457
C	−0.92421	−3.28505	−0.22099
H	−1.13547	−3.02006	0.82229
H	0.14695	−3.11121	−0.39019
C	−1.25817	−4.75164	−0.47421
H	−0.66838	−5.41032	0.17378
H	−2.32122	−4.94869	−0.28096
H	−1.04867	−5.02695	−1.51682
H	−2.80987	−2.50515	−0.91551
K	−4.61752	0.98076	0.60718
K	3.28882	0.15087	−1.89419

O	2.73919	−0.90309	0.19167
C	2.46586	−1.08504	1.52795
C	1.03844	−0.60517	1.86379
H	0.29872	−1.20579	1.31833
H	0.80991	−0.67883	2.93747
H	0.92065	0.44090	1.54822
C	3.45783	−0.28172	2.39476
H	4.48393	−0.60270	2.16715
H	3.36881	0.78687	2.15093
H	3.27959	−0.41046	3.47329
C	2.57691	−2.57382	1.91467
H	1.86957	−3.15840	1.31024
H	3.59246	−2.93397	1.69992
H	2.35820	−2.74989	2.97879

43 → 44 transition state geometry

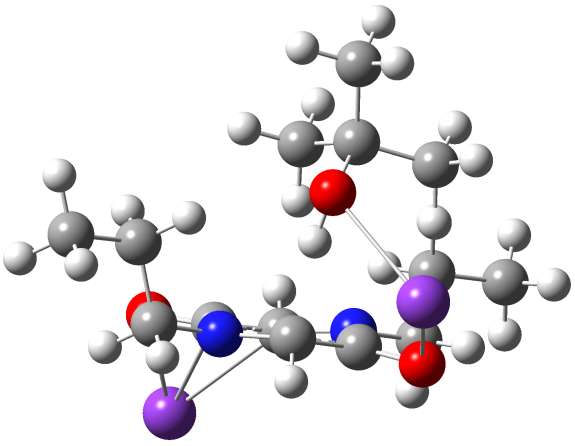


47
−2083.9292247

C	0.30972	−0.58472	−1.21878
C	0.06673	0.86139	−1.25498
C	−1.97221	0.53829	0.09423
C	−1.79832	−0.87588	0.04913
H	0.55777	−0.90143	−2.24581
H	1.51871	−0.70252	−0.36003
H	−2.20955	0.89719	1.09949
N	−0.97148	1.36839	−0.56088
N	−0.81824	−1.39819	−0.74558
O	−2.58802	−1.66484	0.67608
O	0.87054	1.61588	−1.88221
C	−0.64066	−2.83291	−0.81239
H	−0.16564	−3.06316	−1.77937
C	−1.19271	2.79934	−0.51518
H	−0.60426	3.26237	−1.31309
H	−2.26238	2.97558	−0.70954
C	−0.81044	3.41776	0.83013
H	0.25960	3.24052	1.00225

H	−1.35331	2.90693	1.63671
C	−1.11212	4.91291	0.86394
H	−0.82945	5.35666	1.82574
H	−0.56183	5.43903	0.07244
H	−2.18328	5.09803	0.70736
C	0.20983	−3.40650	0.32210
H	−0.31563	−3.20804	1.26517
H	1.16600	−2.86876	0.35626
C	0.43813	−4.90488	0.14817
H	1.03557	−5.31719	0.97021
H	−0.51700	−5.44730	0.11998
H	0.96898	−5.11341	−0.79113
H	−1.63038	−3.30328	−0.79789
K	−4.71238	−0.40864	0.05807
K	3.19658	0.51228	−1.95360
O	2.53616	−0.74884	0.22977
C	2.46658	−0.04784	1.45320
C	1.06591	−0.16577	2.06804
H	0.79109	−1.22178	2.17622
H	1.03640	0.30930	3.05776
H	0.31756	0.31952	1.43023
C	2.78448	1.43611	1.21437
H	3.81346	1.54650	0.84009
H	2.08446	1.84863	0.47324
H	2.69925	2.02539	2.13748
C	3.49950	−0.65225	2.40543
H	3.25930	−1.70721	2.58867
H	4.50034	−0.59891	1.95680
H	3.51623	−0.12123	3.36740

43 → 44 product complex geometry



47
−2083.9307727

C	−0.23548	0.67477	−1.31970
C	−0.06867	−0.75108	−1.33083
C	1.91336	−0.52263	0.10319

C	1.78669	0.89850	0.08424
H	−0.43422	1.05149	−2.33245
H	−1.73785	0.72791	−0.19437
H	2.19953	−0.87893	1.09530
N	0.83230	−1.31614	−0.47308
N	0.81034	1.46890	−0.67761
O	2.60747	1.64908	0.72114
O	−0.80969	−1.48926	−2.06095
C	0.62477	2.90248	−0.65278
H	0.16037	3.19739	−1.60684
C	1.02747	−2.74772	−0.47065
H	0.21763	−3.19214	−1.05676
H	1.98837	−2.98175	−0.97002
C	1.04133	−3.35608	0.93175
H	0.12891	−3.04455	1.45929
H	1.89305	−2.96613	1.50422
C	1.12407	−4.87881	0.86980
H	1.16396	−5.32017	1.87292
H	0.25228	−5.29600	0.34830
H	2.02343	−5.19697	0.32483
C	−0.24121	3.38519	0.51178
H	0.27285	3.11255	1.44284
H	−1.19686	2.84517	0.49294
C	−0.47465	4.89161	0.45554
H	−1.08083	5.23542	1.30241
H	0.47916	5.43638	0.47990
H	−0.99729	5.17291	−0.46933
H	1.60978	3.37907	−0.59087
K	4.66964	0.36832	−0.06240
K	−3.07517	−0.33322	−2.12690
O	−2.62468	0.69521	0.30742
C	−2.48561	−0.14014	1.45957
C	−1.15537	0.15012	2.15353
H	−1.10600	1.20642	2.44306
H	−1.05418	−0.46752	3.05542
H	−0.31373	−0.07042	1.48471
C	−2.54992	−1.60942	1.03214
H	−3.52754	−1.82633	0.57732
H	−1.75566	−1.83124	0.30628
H	−2.42821	−2.27511	1.89664
C	−3.65505	0.19640	2.37760
H	−3.60523	1.24987	2.67881
H	−4.60679	0.02770	1.85711
H	−3.63345	−0.43082	3.27807