

Supporting Information of

Intramolecular Proton Transfer (IPT) in Alkoxyamine: A Theoretical Investigation

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1. Calculations of energies of IPT and alkoxyamine homolysis reactions and NBO interactions

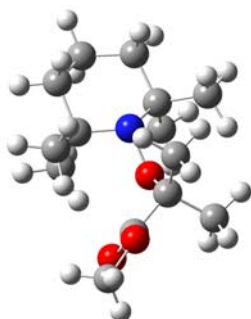
1.1. Optimization of structures by DFT

All calculations were performed using Gaussian package 09, revision A02.¹

The geometry of the species were optimized at the B3LYP/6-31+G(d,p) level of theory. Vibrational frequencies calculated at B3LYP/6-31+G(d,p) level to insure that the obtained geometries are minima (no imaginary frequency) or transition states (one imaginary frequency). The electronic energies were calculated at the BMK/6-311++G(3df,3pd) level of theory. The vibrational frequencies were scaled by a usual factor of 0.9642. The corresponding thermal corrections were included to obtain the enthalpy and Gibbs free energy values under the standard conditions ($p = 1$ atm and $T = 298.15$ K). Implicit solvent calculations have been carried out using the PCM² approach using standard UFF atom radii at the same level of theory described above. Energy values are given in hartree, and atomic cartesian coordinates are given in angströms

1.1.1 Reactants

1



ZPE = 0.385718

E (BMK) = -829.8799066

E (B3LYP) = -830.1864930

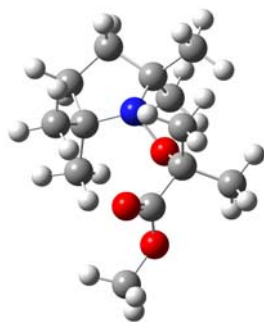
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ΔG_{corr} = 0.337961

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C	2.065240	0.983995	0.056422
C	3.310481	0.420112	-0.666633
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H	2.477382	-2.922844	-0.503163
H	3.836512	-1.192052	0.693710
H	4.443489	-1.403473	-0.939389
H	3.167046	0.536166	-1.749292
H	4.168729	1.044834	-0.391067
O	-0.203445	0.581137	0.552281
C	-1.436539	0.965920	-0.103811
C	-2.516514	-0.066584	0.308663
O	-2.526410	-0.671262	1.359435
O	-3.513826	-0.157642	-0.600792

C	-0.121378	-2.117843	-0.732349
H	-1.069511	-1.968623	-0.215963
H	-0.213881	-1.788852	-1.771251
H	0.074545	-3.195726	-0.735530
C	1.032870	-1.816615	1.460266
H	0.930930	-2.905822	1.523372
H	1.948049	-1.543862	1.987848
H	0.182714	-1.365840	1.976065
C	1.783834	2.373637	-0.545001
H	0.954886	2.871624	-0.038132
H	2.670367	3.006849	-0.431727
H	1.555597	2.296562	-1.611725
C	2.350252	1.172203	1.566963
H	2.799305	0.293753	2.032359
H	3.050398	2.004555	1.699099
H	1.430596	1.411645	2.104494
N	0.891101	0.090496	-0.264789
C	-4.617258	-1.012442	-0.239175
H	-5.078677	-0.665950	0.688639
H	-5.319453	-0.945302	-1.069728
H	-4.273929	-2.040955	-0.106032
C	-1.340594	1.154959	-1.617277
H	-0.595257	1.915591	-1.849518
H	-1.060883	0.235119	-2.129420
H	-2.309604	1.484277	-1.997345
C	-1.862774	2.277447	0.590708
H	-2.879807	2.558620	0.298500
H	-1.828773	2.150567	1.675832
H	-1.185440	3.086759	0.306659

2a



ZPE = 0.357112

E (BMK) = -790.5889966

E (B3LYP) = -790.8767524

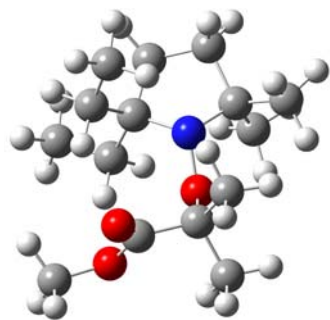
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ΔG_{corr} = 0.309424

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C	-3.251191	-0.368328	0.352126
C	-2.262988	0.655185	-0.233989
H	-2.893136	-2.489781	0.811098
H	-2.836669	-2.094502	-0.903088
H	-4.241030	-0.287939	-0.108093
H	-3.367415	-0.190252	1.427344
N	-0.976635	0.058895	0.243995
C	-2.456893	2.051263	0.367754
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H	-3.343866	1.215617	-2.032459
H	-1.581761	1.347405	-2.190391
H	-2.361789	-0.237863	-2.251255
C	-0.473610	-2.011821	1.499721

H	0.573987	-1.729177	1.633575
H	-0.534440	-3.106749	1.508063
C	-0.304937	-2.071644	-1.011125
H	0.773363	-1.914100	-0.946930
H	-0.643584	-1.653879	-1.962278
O	0.106862	0.594225	-0.524557
C	1.213182	1.179440	0.230246
C	1.681664	2.350651	-0.643740
H	0.916302	3.131893	-0.641625
H	2.613993	2.774874	-0.255996
H	1.850430	2.018898	-1.669843
C	0.848070	1.643833	1.635439
H	0.063771	2.400666	1.585597
H	0.506091	0.819645	2.258965
H	1.733543	2.084368	2.102509
C	2.332418	0.113223	0.315042
O	2.739955	-0.393954	1.341760
O	2.820069	-0.203338	-0.901601
C	3.857816	-1.201774	-0.926641
H	4.125602	-1.314370	-1.976862
H	4.718657	-0.871543	-0.340251
H	3.488941	-2.146290	-0.519151
H	-1.038387	-1.630298	2.356830
H	-0.491445	-3.151616	-1.024005

2b



ZPE = 0.412329

E (BMK) = -869.1770683

E (B3LYP) = -869.5044961

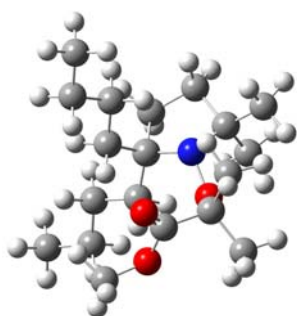
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ΔG_{corr} = 0.360886

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H	3.119823	-0.325934	1.530288
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H	3.211842	-2.879097	0.245537
H	1.940874	-2.479372	1.419153
C	2.389019	-1.158866	-1.757481
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C	-2.379573	-0.307474	0.300308
O	-2.851297	-0.176093	1.412120
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H	-4.598491	1.104285	-0.083929
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2c



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E (B3LYP) = -1026.773533

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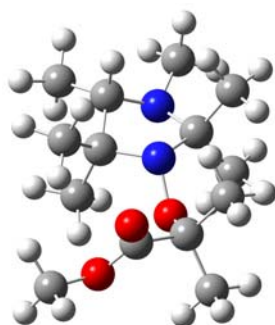
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H	1.773560	-2.654141	-0.568090
H	-0.113635	-3.962995	-1.293472
H	-1.167236	-3.271501	-0.050969
N	-0.622501	-0.741234	-0.766503
C	-2.233150	-2.078618	-2.137643
H	-2.525943	-1.299295	-2.847226
H	-2.355041	-3.044252	-2.641380
H	-2.912364	-2.047540	-1.281444
C	0.125075	-1.860038	-2.945595
H	-0.107744	-2.710898	-3.595388
H	-0.050885	-0.940368	-3.508673
H	1.188761	-1.910181	-2.701497

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H	-0.812476	-2.298652	2.251563
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H	-2.670405	-0.992807	5.272315
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C	4.339736	0.340647	-0.245476
H	3.027586	0.052035	1.436994
H	3.353241	-1.413704	0.527594
C	5.642941	0.172193	0.543956
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H	4.124333	1.410672	-0.372889
H	6.481652	0.667976	0.042918
H	5.556282	0.600419	1.549874
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O	-0.561694	0.473243	-1.535668
C	-1.533244	1.501695	-1.199510
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H	-2.124302	3.303170	-2.269250

H	-0.480158	2.739635	-2.645534
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H	-3.332766	0.500910	-1.840661
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H	-3.596835	1.809112	-0.670212
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C	0.649777	3.683883	0.921711
H	1.617081	4.054174	0.583156
H	-0.036374	4.511889	1.114831
H	0.761006	3.091364	1.833043

3a



ZPE = 0.399786

E (BMK) = -885.2141526

E (B3LYP) = -885.5341083

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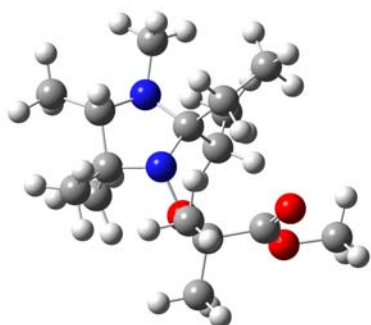
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C	0.515316	1.706507	-1.377869

H	-0.528771	1.561840	-1.658344
H	0.737872	2.777249	-1.428997
H	1.146361	1.185994	-2.102446
C	-0.034504	2.020807	1.065438
H	0.329076	3.054838	1.077685
H	-1.094390	2.054313	0.808023
H	0.061430	1.605033	2.072362
C	1.603225	-2.004171	-1.255827
H	0.861939	-2.796037	-1.123566
H	2.578332	-2.479181	-1.405569
C	1.941480	-1.930337	1.244094
H	1.103908	-2.605098	1.427306
H	2.050771	-1.288145	2.123264
O	-0.608589	-0.671109	-0.694738
C	-1.830237	-1.160707	-0.087667
C	-2.536846	-1.863610	-1.258594
H	-1.952841	-2.736757	-1.562147
H	-3.535263	-2.197455	-0.958398
H	-2.631623	-1.186138	-2.109468
C	-1.600115	-2.120607	1.075412
H	-1.022119	-2.980918	0.727740
H	-1.068788	-1.630470	1.890875
H	-2.560692	-2.475348	1.456407
C	-2.728002	0.009360	0.379776
O	-3.241587	0.096601	1.476681
O	-2.934237	0.912045	-0.602808
C	-3.830149	1.994665	-0.286191
H	-3.876017	2.606015	-1.187060
H	-4.819382	1.606763	-0.030821
H	-3.447641	2.576444	0.556056
H	1.353428	-1.433906	-2.151285

H	2.845200	-2.539994	1.141202
N	2.718141	-0.053939	-0.256409
C	4.097758	-0.431947	0.013636
H	4.330874	-0.534054	1.089192
H	4.330002	-1.380679	-0.477543
H	4.770387	0.320373	-0.407101
C	3.059262	2.402870	0.014772
H	4.065535	2.377297	0.443612
H	3.151200	2.482341	-1.072136
H	2.572621	3.307925	0.392308
H	2.339048	1.057389	1.517553

3b



ZPE = 0.454694

E (BMK) = -963.7956633

E (B3LYP) = -964.1555849

ΔH_{corr} = 0.481706

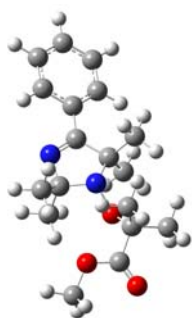
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H	2.683878	-0.732343	-1.512789
N	0.435344	-0.633359	-0.235201

C	1.732881	-1.654727	1.710384
H	0.800433	-2.040142	2.128985
H	2.526962	-2.374749	1.933141
H	1.978154	-0.713470	2.206554
C	1.515242	-2.848567	-0.490288
H	2.430806	-3.419007	-0.300877
H	0.680523	-3.429752	-0.086684
H	1.383580	-2.749685	-1.571498
O	-0.718713	-0.990658	0.534677
C	-1.923382	-1.344161	-0.209737
C	-1.670569	-1.900890	-1.606770
H	-1.073446	-2.811523	-1.541372
H	-2.629983	-2.141024	-2.072235
H	-1.151757	-1.183801	-2.241243
C	-2.609958	-2.382833	0.689726
H	-2.009695	-3.296775	0.709228
H	-2.709367	-2.000115	1.707322
H	-3.606604	-2.626716	0.306945
C	-2.832920	-0.094494	-0.306795
O	-3.262556	0.378152	-1.341088
O	-3.127226	0.408821	0.907831
C	-3.980893	1.568728	0.921573
H	-4.108153	1.821802	1.973738
H	-3.512097	2.393965	0.379973
H	-4.943815	1.339265	0.458851
N	2.292143	0.752731	-0.034130
C	3.059930	1.810620	-0.674499
H	2.981852	1.815320	-1.777076
H	2.751589	2.788405	-0.303456
H	4.115672	1.690585	-0.417204
C	0.227500	1.506349	-1.371938

C	0.095388	3.035138	-1.450346
H	-0.775639	1.093748	-1.504388
H	0.804742	1.137239	-2.228343
H	-0.385014	3.303489	-2.397719
H	-0.536081	3.430646	-0.648433
H	1.052558	3.560805	-1.412994
C	0.239761	1.455382	1.219961
C	1.000088	2.657219	1.798488
H	0.215869	0.672949	1.980510
H	-0.807508	1.728193	1.053262
H	0.534631	2.962077	2.742629
H	2.040330	2.394042	2.010298
H	0.995331	3.530149	1.139320
C	4.129660	-0.940967	0.060255
H	4.334453	-2.006503	-0.087585
H	4.881671	-0.390418	-0.512140
H	4.262204	-0.701858	1.119226

4a



ZPE = 0.400650

E (BMK) = -1036.385652

E (B3LYP) = -1036.765165

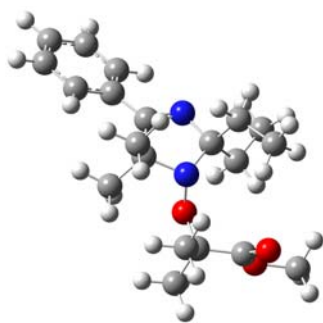
ΔH_{corr} = 0.426775

ΔG_{corr} = 0.34624

C	-0.168638	1.408855	-0.080356
C	1.803285	0.306711	-0.076021
C	0.772986	-0.832242	-0.124465
N	1.287386	1.481331	-0.060835
C	3.282612	0.150011	-0.029506
C	3.952028	-1.023430	-0.415527
C	4.055398	1.241349	0.413421
C	5.346234	-1.102714	-0.366342
H	3.397808	-1.881899	-0.773361
C	5.444530	1.160426	0.466592
H	3.542038	2.148645	0.711711
C	6.098226	-0.013687	0.076378
H	5.841474	-2.018212	-0.676858
H	6.019587	2.013320	0.815830
H	7.181715	-0.077845	0.118505
C	1.002537	-1.898283	0.961569
H	1.915333	-2.472394	0.784875
H	1.072305	-1.432534	1.948433
H	0.165746	-2.603037	0.971888
C	0.697610	-1.488450	-1.521818
H	0.615868	-0.745363	-2.318041
H	1.585884	-2.094339	-1.714160
H	-0.176702	-2.139868	-1.576961
C	-0.680294	1.884374	-1.451895
H	-1.771159	1.869867	-1.476252
H	-0.329136	2.906673	-1.618995
H	-0.304413	1.256856	-2.262758
C	-0.727806	2.304689	1.032721
H	-0.436152	3.344272	0.854548
H	-1.818697	2.242199	1.052083

H	-0.332638	1.992569	2.003439
N	-0.452618	-0.035997	0.234947
O	-1.608643	-0.499228	-0.458054
C	-2.687628	-1.046528	0.359947
C	-2.513788	-0.848102	1.868856
H	-3.404755	-1.235624	2.374609
H	-1.643481	-1.398557	2.228936
H	-2.389720	0.202689	2.127853
C	-2.828036	-2.529135	0.003571
H	-2.928939	-2.655572	-1.076986
H	-1.943028	-3.072629	0.344372
H	-3.712432	-2.962121	0.477164
C	-3.962905	-0.299123	-0.096340
O	-4.967784	-0.839592	-0.511095
O	-3.851931	1.036225	0.049446
C	-5.006519	1.808205	-0.337017
H	-4.732057	2.847995	-0.161178
H	-5.238370	1.642168	-1.391556
H	-5.871570	1.528605	0.269099

4b



ZPE = 0.456011

E (BMK) = -1114.97207

E (B3LYP) = -1115.392224

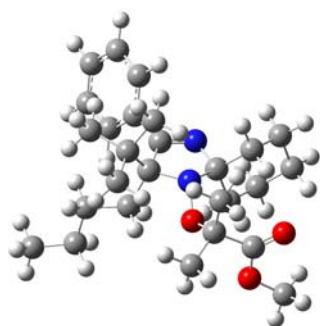
$\Delta H_{\text{corr}} = 0.484694$

$\Delta G_{\text{corr}} = 0.398446$

C	0.169821	1.145620	0.449632
C	-1.839851	0.149370	0.180609
C	-0.902524	-1.026737	0.517615
N	-1.251757	1.284402	0.135663
C	-3.295574	0.060503	-0.124943
C	-4.115892	-1.002372	0.289286
C	-3.888480	1.108030	-0.856970
C	-5.480795	-1.015710	-0.010477
H	-3.705889	-1.822928	0.864399
C	-5.247245	1.091732	-1.161595
H	-3.261228	1.932116	-1.177567
C	-6.052333	0.028319	-0.738763
H	-6.094693	-1.845200	0.328602
H	-5.679814	1.909086	-1.731654
H	-7.112205	0.014527	-0.976038
C	-1.031543	-2.158350	-0.515268
H	-0.871523	-1.799220	-1.532817
H	-0.313111	-2.955927	-0.315334
H	-2.033502	-2.588388	-0.454851
C	-1.132680	-1.581685	1.942402
H	-1.113618	-0.787781	2.692213
H	-2.090525	-2.101602	2.026830
H	-0.339405	-2.294245	2.184030
C	0.373451	1.747190	1.867290
H	-0.080811	2.743773	1.865912
H	-0.220046	1.150174	2.567072
C	0.989720	1.880888	-0.628975
H	2.053010	1.715910	-0.445009

H	0.770193	1.418938	-1.594637
N	0.458235	-0.349415	0.512614
O	1.195088	-0.780411	-0.647573
C	2.432894	-1.499675	-0.365469
C	2.653151	-2.335459	-1.633163
H	3.632788	-2.823474	-1.604663
H	1.881547	-3.107021	-1.700449
H	2.605315	-1.705344	-2.522859
C	2.373263	-2.380051	0.880256
H	2.190397	-1.789212	1.776299
H	1.586575	-3.130684	0.773037
H	3.328537	-2.898773	1.000148
C	3.585947	-0.478629	-0.202996
O	4.179615	-0.258853	0.833603
O	3.877303	0.145950	-1.362321
C	4.935097	1.121873	-1.306088
H	5.026410	1.508634	-2.320641
H	4.678601	1.923526	-0.609180
H	5.868277	0.653486	-0.984024
C	1.818660	1.824560	2.365401
H	2.309276	0.848537	2.342933
H	2.423851	2.514417	1.767934
H	1.836798	2.189215	3.398344
C	0.710170	3.387934	-0.705007
H	1.041422	3.918544	0.193508
H	1.247043	3.820757	-1.556265
H	-0.356609	3.585639	-0.839547

4c



ZPE = 0.628192

E (BMK) = -1388.825671

E (B3LYP) = -1389.373299

ΔH_{corr} = 0.664598

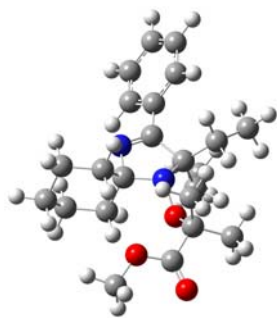
ΔG_{corr} = 0.56215

C	1.401310	-0.815903	0.104665
C	0.752265	0.542608	0.471847
N	0.582427	-1.759738	-0.159851
C	2.859197	-1.152674	-0.003955
C	3.419834	-2.069865	0.898718
C	3.653214	-0.679944	-1.057858
C	4.752889	-2.465851	0.780165
H	2.803162	-2.475927	1.694257
C	4.985482	-1.082448	-1.183418
H	3.225430	-0.021701	-1.805545
C	5.544239	-1.966955	-0.258196
H	5.169634	-3.170980	1.493719
H	5.581951	-0.711132	-2.011987
H	6.581033	-2.276020	-0.353842
N	-0.694966	0.041766	0.602031
O	-1.631487	0.992585	0.068233
C	-2.860473	1.241972	0.825304
C	-3.099146	2.753672	0.685515

H	-4.098628	3.018506	1.046928
H	-2.361761	3.303545	1.275461
H	-3.018103	3.056805	-0.359813
C	-2.840587	0.816045	2.290205
H	-2.679353	-0.253440	2.407916
H	-2.066124	1.352390	2.837204
H	-3.810227	1.060185	2.733040
C	-4.004284	0.488370	0.097195
O	-4.668799	-0.407585	0.579098
O	-4.197555	0.954872	-1.152031
C	-5.241504	0.315846	-1.912401
H	-5.252222	0.826833	-2.874640
H	-5.022883	-0.746814	-2.042192
H	-6.202775	0.424473	-1.404506
C	-0.793434	-1.299705	-0.088555
C	-1.610682	-2.284498	0.776581
C	-1.364066	-1.259070	-1.528306
C	-1.709385	-3.684283	0.147508
H	-2.619468	-1.879410	0.906914
H	-1.148084	-2.338152	1.768378
C	-1.457476	-2.662138	-2.152555
H	-2.356850	-0.804569	-1.498566
H	-0.742040	-0.606945	-2.149081
C	-2.279301	-3.618966	-1.276828
H	-2.339520	-4.320983	0.780698
H	-0.713111	-4.141299	0.120394
H	-1.904616	-2.580009	-3.151569
H	-0.447996	-3.068080	-2.286778
H	-2.298475	-4.619941	-1.725496
H	-3.322331	-3.272122	-1.234226
C	1.230206	1.102897	1.889206

C	2.758772	1.332842	2.007027
C	0.543730	2.454442	2.182603
C	0.855941	0.101809	3.006070
H	3.328090	0.405135	1.943420
H	3.156137	2.024446	1.265383
H	2.960573	1.767870	2.993052
H	-0.538142	2.391734	2.084912
H	0.772012	2.767457	3.207870
H	0.892833	3.246548	1.514449
H	1.192150	0.491828	3.973367
H	-0.218240	-0.073569	3.053041
H	1.346431	-0.866116	2.857218
C	0.853795	1.560687	-0.718802
C	2.090669	2.446107	-0.961387
H	-0.005704	2.226941	-0.625340
H	0.666520	0.986359	-1.633920
C	2.003050	3.149059	-2.326165
H	2.165051	3.216816	-0.186337
H	3.024447	1.879046	-0.916297
C	3.163786	4.118103	-2.578998
H	1.976496	2.393134	-3.123624
H	1.050589	3.692668	-2.394044
H	3.078185	4.596093	-3.560852
H	3.188728	4.912503	-1.823607
H	4.129464	3.599767	-2.544134

4d



ZPE = 0.519741

E (BMK) = -1231.655066

E (B3LYP) = -1232.124096

ΔH_{corr} = 0.55035

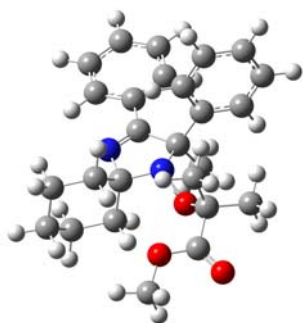
ΔG_{corr} = 0.460382

C	-1.706726	0.203397	-0.106496
C	-0.792403	-1.013902	0.134497
N	-1.086738	1.318140	-0.225293
C	-3.199513	0.225738	-0.170574
C	-3.893266	1.143047	0.636860
C	-3.933543	-0.556296	-1.075288
C	-5.281893	1.251347	0.567301
H	-3.329529	1.773401	1.316971
C	-5.323771	-0.439280	-1.154667
H	-3.423483	-1.235635	-1.747810
C	-6.004350	0.456737	-0.327838
H	-5.799053	1.960334	1.207567
H	-5.872052	-1.045213	-1.870428
H	-7.085552	0.542032	-0.386474
N	0.501657	-0.376155	-0.317788
O	1.611544	-0.875415	0.430672
C	2.652411	-1.587461	-0.305781
C	2.531307	-1.520488	-1.831724

H	3.397986	-2.026667	-2.270202
H	1.627294	-2.029031	-2.169102
H	2.503041	-0.493181	-2.192295
C	2.660797	-3.035796	0.193515
H	2.722075	-3.063549	1.283933
H	1.744465	-3.540377	-0.122059
H	3.519882	-3.579682	-0.206552
C	3.981449	-0.913857	0.113822
O	4.926099	-1.499486	0.602506
O	3.994896	0.406271	-0.156443
C	5.208446	1.104649	0.186155
H	5.030227	2.144889	-0.084894
H	5.410623	1.012467	1.255723
H	6.052733	0.697387	-0.375262
C	0.355490	1.118858	-0.163555
C	0.909882	1.709084	1.155854
C	1.011890	1.824679	-1.369532
C	0.779160	3.241469	1.209261
H	1.962272	1.421056	1.231803
H	0.389994	1.263583	2.009460
C	0.883375	3.354864	-1.312660
H	2.071575	1.546835	-1.377418
H	0.557752	1.430502	-2.285328
C	1.445593	3.914819	0.001502
H	1.225451	3.605510	2.143361
H	-0.282157	3.517468	1.234948
H	1.405343	3.796045	-2.171182
H	-0.173566	3.632323	-1.403809
H	1.302430	5.001626	0.046254
H	2.531183	3.738470	0.039659
C	-0.748902	-1.436430	1.640657

C	-2.077676	-1.480907	2.410370
H	-2.501652	-0.482016	2.544399
H	-2.839275	-2.095768	1.925795
H	-1.902094	-1.897134	3.408666
C	-1.038310	-2.234392	-0.798796
C	-2.054677	-3.308754	-0.382760
H	-0.068232	-2.731148	-0.891726
H	-1.268118	-1.858632	-1.802708
H	-1.762298	-3.801622	0.549162
H	-3.066833	-2.920581	-0.251336
H	-0.262606	-2.416391	1.691758
H	-0.074919	-0.755709	2.162969
H	-2.096282	-4.083198	-1.156904

4e



ZPE = 0.515813

E (BMK) = -1344.741829

E (B3LYP) = -1345.252444

ΔH_{corr} = 0.546931

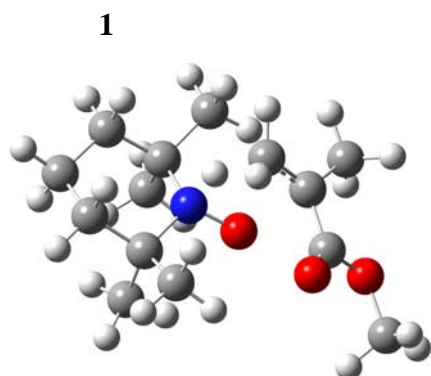
ΔG_{corr} = 0.454641

C	-0.765537	0.450809	-0.583016
N	-0.822051	-1.777572	0.230688
N	0.567939	0.075753	0.007810

O	1.647645	0.516659	-0.806316
C	2.514064	1.550477	-0.242771
C	2.317784	1.805795	1.254631
H	3.059053	2.543748	1.579794
H	1.321273	2.206291	1.444657
H	2.446638	0.896534	1.841153
C	2.303332	2.829321	-1.056535
H	2.427824	2.629431	-2.123716
H	1.295563	3.209963	-0.874994
H	3.029666	3.594507	-0.771691
C	3.951775	1.031198	-0.473789
O	4.819805	1.641228	-1.063982
O	4.155539	-0.175631	0.092276
C	5.481698	-0.720341	-0.054875
H	5.459363	-1.681621	0.457833
H	5.723059	-0.851794	-1.112269
H	6.219207	-0.055706	0.401490
C	0.587344	-1.421589	0.199276
C	1.295422	-2.212033	-0.929550
C	1.242494	-1.754525	1.556568
C	1.336493	-3.722583	-0.642727
H	2.312839	-1.820307	-1.018327
H	0.794014	-2.024014	-1.883991
C	1.294128	-3.263302	1.843396
H	2.260822	-1.349992	1.536008
H	0.694013	-1.227060	2.344904
C	1.995521	-4.025944	0.710360
H	1.879268	-4.226392	-1.452371
H	0.315394	-4.122992	-0.646231
H	1.809441	-3.435234	2.796786
H	0.272455	-3.644925	1.960017

H	1.976983	-5.104816	0.908622
H	3.054932	-3.731034	0.673237
C	-0.749627	0.570292	-2.121761
H	-1.747742	0.798383	-2.503509
H	-0.057055	1.348096	-2.446879
H	-0.425789	-0.369842	-2.570646
C	-1.263786	1.724460	0.120175
C	-1.520061	2.921503	-0.561523
C	-1.460246	1.702253	1.511054
C	-1.960227	4.061189	0.122754
H	-1.381930	2.981118	-1.635522
C	-1.904512	2.832221	2.196019
H	-1.257863	0.787693	2.060458
C	-2.156501	4.021552	1.503106
H	-2.148079	4.977659	-0.429732
H	-2.054899	2.785279	3.270955
H	-2.501720	4.903745	2.034323
C	-1.556963	-0.808190	-0.174229
C	-3.030056	-0.976526	-0.289054
C	-3.892753	0.060672	-0.680626
C	-3.587900	-2.238533	-0.003987
C	-5.269069	-0.156869	-0.786234
H	-3.502620	1.048834	-0.888377
C	-4.959423	-2.452772	-0.106908
H	-2.923548	-3.040975	0.296412
C	-5.808477	-1.411538	-0.500102
H	-5.917560	0.660487	-1.088132
H	-5.368859	-3.433686	0.117446
H	-6.878763	-1.578687	-0.580930

1.1.2 Transition states of IPT



ZPE = 0.381185

E (BMK) = -829.8188498

E (B3LYP) = -830.1404882

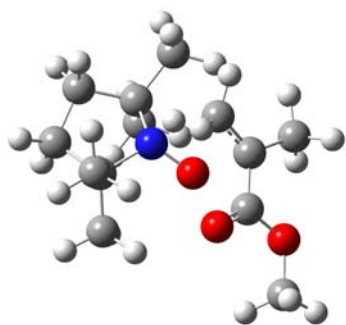
ΔH_{corr} = 0.403029

ΔG_{corr} = 0.334367

C	3.579646	-0.610758	-0.576341
C	2.432892	-1.566381	-0.905205
C	1.209072	-1.434893	0.024308
C	1.883749	1.094791	0.346133
C	3.069415	0.829633	-0.603631
H	2.106205	-1.388268	-1.938971
H	2.770873	-2.608777	-0.863186
H	4.014970	-0.848943	0.401331
H	4.387331	-0.732751	-1.307655
H	2.759744	1.077279	-1.628438
H	3.869515	1.533024	-0.342616
O	-0.314479	0.254522	0.804123
C	-1.746415	0.963201	-0.757081
C	-2.678283	-0.142677	-0.396462
O	-2.806483	-1.190512	-1.008992
O	-3.427830	0.158966	0.691231
C	0.059073	-2.267078	-0.556067
H	-0.816419	-2.249504	0.091404

H	-0.247041	-1.925558	-1.545209
H	0.400030	-3.303413	-0.649185
C	1.490769	-1.968826	1.443056
H	1.481689	-3.063224	1.414100
H	2.457074	-1.663724	1.845475
H	0.703327	-1.638642	2.124721
C	1.325109	2.494752	0.057890
H	0.509092	2.737684	0.738578
H	2.127842	3.223873	0.206733
H	0.975618	2.592963	-0.971608
C	2.306025	1.069683	1.828820
H	2.972560	0.244263	2.078622
H	2.837747	1.998478	2.060333
H	1.419765	1.013749	2.465231
N	0.773740	0.050845	0.069861
C	-4.354957	-0.853507	1.112038
H	-3.821812	-1.760744	1.407893
H	-4.883784	-0.427056	1.964653
H	-5.052675	-1.096613	0.306467
C	-0.884261	0.770123	-1.848575
H	0.229077	0.361452	-1.129127
H	-1.078219	-0.091627	-2.482995
H	-0.540882	1.657297	-2.378162
C	-2.052450	2.322602	-0.186913
H	-3.070781	2.620700	-0.468791
H	-2.006628	2.317855	0.904664
H	-1.366360	3.076514	-0.575999

2a



ZPE = 0.352373

E (BMK) = -790.5304551

E (B3LYP) = -790.8332748

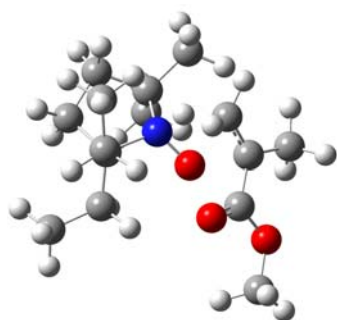
ΔH_{corr} = 0.373477

ΔG_{corr} = 0.305657

N	-0.902760	0.046830	-0.011386
C	-2.162857	0.882710	-0.289599
C	-1.301534	-1.458641	0.090741
C	-2.051806	2.269610	0.344234
C	-3.248329	0.013344	0.358539
C	-2.357324	1.023123	-1.807398
O	0.137630	0.328248	-0.781653
C	-0.667153	-2.246980	-1.055321
C	-0.831955	-2.018761	1.440481
C	-2.846349	-1.425453	0.009659
H	-1.200215	2.818723	-0.066071
H	-2.959338	2.841061	0.122918
H	-1.946387	2.214023	1.431170
H	-4.246851	0.276500	-0.003867
H	-3.243755	0.163098	1.445320
H	-2.473700	0.056288	-2.303228
H	-3.255587	1.618266	-2.004112
H	-1.494683	1.524272	-2.251113

C	1.541880	1.086055	0.675069
H	-0.931515	-1.825806	-2.028468
H	-1.029434	-3.280435	-1.011651
H	0.420933	-2.254649	-0.970524
H	-1.299825	-1.493628	2.280796
H	-1.116758	-3.074592	1.506515
H	0.253990	-1.949834	1.538677
H	-3.293853	-2.158273	0.687805
H	-3.179513	-1.677404	-1.002526
C	0.728933	0.966751	1.812608
C	1.808415	2.405795	0.003781
C	2.422432	-0.068931	0.345005
H	0.371383	1.887250	2.270361
H	0.949954	0.159064	2.505686
H	-0.378031	0.448247	1.137524
H	1.041710	3.135622	0.276318
H	2.779277	2.805420	0.325572
H	1.834508	2.304577	-1.082829
O	3.276264	0.210487	-0.667828
O	2.412645	-1.150927	0.913277
C	4.138894	-0.863625	-1.074656
H	4.748672	-1.206916	-0.235189
H	3.549839	-1.702074	-1.455032
H	4.766711	-0.449081	-1.863574

2b



ZPE = 0.407800

E (BMK) = -869.1171552

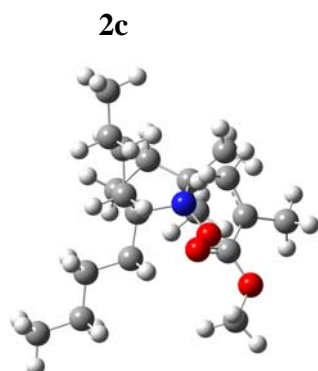
E (B3LYP) = -869.4596176

ΔH_{corr} = 0.431556

ΔG_{corr} = 0.358331

C	1.332215	0.994332	0.012047
C	2.840601	0.733504	-0.209690
C	3.056184	-0.766519	0.031611
C	1.796856	-1.436531	-0.532978
H	3.461028	1.352699	0.444314
H	3.116581	0.986308	-1.238583
H	3.960559	-1.145046	-0.455282
H	3.145929	-0.980388	1.101942
N	0.699271	-0.433495	-0.130839
C	1.530537	-2.812159	0.080064
H	0.584516	-3.225293	-0.280157
H	2.331173	-3.498889	-0.214297
H	1.505958	-2.774102	1.172759
C	1.845352	-1.553643	-2.064224
H	2.614188	-2.281281	-2.345644
H	0.879940	-1.888014	-2.448459
H	2.085622	-0.601802	-2.544624
C	1.017882	1.569534	1.413281

C	1.697547	0.923736	2.629729
H	-0.069149	1.562635	1.542683
H	1.311912	2.624977	1.393975
H	1.452898	-0.136824	2.738278
H	2.788608	1.015694	2.593674
C	0.727888	1.904925	-1.079590
C	1.376539	3.292266	-1.201368
H	-0.342214	2.015752	-0.885967
H	0.808727	1.386261	-2.040033
H	1.217464	3.909442	-0.311870
H	2.456151	3.234424	-1.380301
O	-0.408224	-0.513498	-0.858925
C	-1.846019	-1.141020	0.605754
C	-2.333223	-2.364345	-0.122152
H	-1.675670	-3.214479	0.076807
H	-3.340166	-2.633590	0.223380
H	-2.385691	-2.196861	-1.199565
C	-0.987134	-1.213328	1.712063
H	-0.753219	-2.202686	2.100886
H	0.166494	-0.818836	1.012100
H	-1.062602	-0.427159	2.458950
C	-2.562114	0.146869	0.384250
O	-2.379563	1.175961	1.017462
O	-3.478175	0.058915	-0.608485
C	-4.193248	1.267585	-0.910517
H	-4.893254	1.000772	-1.702467
H	-4.727306	1.629671	-0.028343
H	-3.503568	2.042880	-1.253837
H	0.935927	3.829532	-2.047957
H	1.362786	1.426404	3.543404



ZPE = 0.517140

E (BMK) = -1026.30152

E (B3LYP) = -1026.728477

ΔH_{corr} = 0.546693

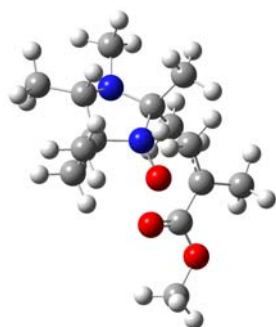
ΔG_{corr} = 0.458879

C	0.982206	0.580131	0.362873
C	1.627161	1.597648	1.333771
C	0.467544	2.277571	2.073153
C	-0.563724	1.161880	2.286880
H	2.262636	2.314809	0.806599
H	2.267912	1.075273	2.051475
H	0.777409	2.720707	3.024891
H	0.032801	3.076929	1.463901
N	-0.451083	0.371834	0.969617
C	-1.983055	1.697021	2.483967
H	-2.705894	0.879225	2.547109
H	-2.029106	2.258953	3.422837
H	-2.280725	2.370335	1.675206
C	-0.187814	0.249067	3.464226
H	-0.279078	0.812061	4.399377
H	-0.854199	-0.614712	3.501725
H	0.837116	-0.122670	3.389105

C	0.868073	1.112175	-1.085228
C	0.343089	2.539822	-1.308313
H	0.264398	0.399244	-1.657851
H	1.875741	1.066330	-1.515443
C	0.282478	2.904096	-2.799705
H	-0.659146	2.661004	-0.878371
H	0.988166	3.267919	-0.797869
C	-0.224655	4.328108	-3.053917
H	1.282352	2.788459	-3.240788
H	-0.363135	2.185002	-3.321087
H	-0.255947	4.555587	-4.124957
H	-1.237237	4.465690	-2.655735
H	0.423031	5.072386	-2.574762
C	1.711421	-0.781302	0.367695
C	3.198878	-0.740818	-0.021957
H	1.178664	-1.462245	-0.302621
H	1.620660	-1.213166	1.370366
C	3.873973	-2.111732	0.135762
H	3.316622	-0.413308	-1.062756
H	3.740333	-0.009226	0.594071
C	5.354310	-2.105533	-0.262118
H	3.776273	-2.445294	1.178035
H	3.334259	-2.850568	-0.472040
H	5.806425	-3.095478	-0.136824
H	5.481837	-1.812303	-1.311063
H	5.926984	-1.398701	0.350540
O	-0.877946	-0.883287	1.046886
C	-2.558409	-0.854566	-0.278887
C	-3.573335	-1.381237	0.699173
H	-3.965210	-0.569052	1.316745
H	-4.419280	-1.830290	0.162085

H	-3.145474	-2.148549	1.347028
C	-2.499267	0.496496	-0.651750
H	-3.284854	1.153264	-0.282788
H	-1.374209	0.802169	0.133686
H	-2.133287	0.725459	-1.649395
C	-1.836302	-1.829514	-1.144150
O	-1.104644	-1.539120	-2.078730
O	-2.090673	-3.112080	-0.793357
C	-1.405315	-4.117752	-1.556423
H	-1.749852	-5.071441	-1.156227
H	-1.652943	-4.031501	-2.617433
H	-0.323892	-4.018609	-1.432801

3a



ZPE = 0.394847

E (BMK) = -885.1534798

E (B3LYP) = -885.4889829

ΔH_{corr} = 0.418729

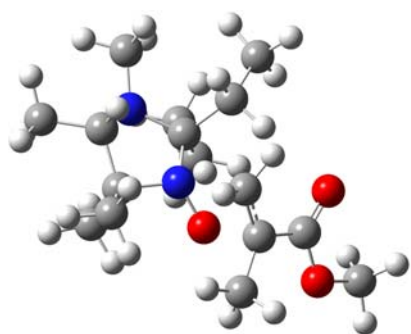
ΔG_{corr} = 0.345306

C	-1.576412	1.149982	-0.296371
C	-2.488557	-0.931473	0.421582
C	-1.032414	-1.269967	0.041333
N	-0.433725	0.145414	-0.005328
C	-0.898289	-1.919821	-1.340805
H	0.151474	-1.922354	-1.639522

H	-1.253375	-2.954008	-1.301939
H	-1.474905	-1.379195	-2.094725
C	-0.329105	-2.118832	1.101499
H	-0.741172	-3.133170	1.086918
H	0.743873	-2.183521	0.906497
H	-0.473342	-1.713197	2.107667
C	-1.345766	1.852191	-1.633486
H	-0.444360	2.467072	-1.603470
H	-2.203088	2.498568	-1.848921
C	-1.639358	2.177447	0.848483
H	-0.694101	2.719369	0.924108
H	-1.842304	1.704520	1.814146
O	0.654938	0.296329	-0.745634
C	2.083673	0.928689	0.749009
C	1.267636	0.779416	1.878891
H	1.430633	-0.097442	2.500431
H	0.972912	1.681601	2.411516
H	0.114575	0.424673	1.162610
H	-1.243199	1.123989	-2.438704
H	-2.424484	2.913663	0.653823
N	-2.756416	0.266056	-0.376985
C	-4.051867	0.893352	-0.158523
H	-4.243725	1.167527	0.894764
H	-4.137047	1.795948	-0.769353
H	-4.844266	0.212925	-0.480019
C	-3.496662	-2.054171	0.173933
H	-4.475890	-1.805267	0.593098
H	-3.618248	-2.246180	-0.895840
H	-3.163139	-2.976387	0.660081
H	-2.508067	-0.698492	1.506957
C	2.929170	-0.231778	0.347857

O	2.920345	-1.331207	0.879321
O	3.751308	0.069028	-0.684455
C	4.575272	-1.007053	-1.161032
H	5.174035	-0.579963	-1.965647
H	5.216287	-1.384668	-0.360394
H	3.953773	-1.823794	-1.536748
C	2.389193	2.277317	0.154531
H	3.355640	2.645030	0.524714
H	2.445191	2.232440	-0.934222
H	1.625483	3.005025	0.443098

3b



ZPE = 0.450761

E (BMK) = -963.7322668

E (B3LYP) = -964.1103869

ΔH_{corr} = 0.477146

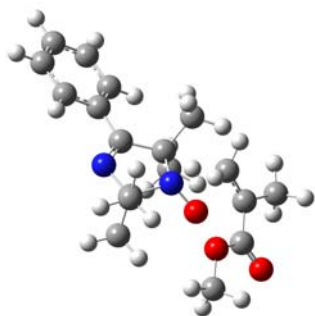
ΔG_{corr} = 0.398977

C	1.014775	0.857565	0.014225
C	2.538216	-0.964354	-0.422476
C	1.347942	-1.604937	0.306687
H	2.365259	-1.084619	-1.512711
N	0.293537	-0.530644	0.043350
C	1.564945	-1.767400	1.817963

H	0.602978	-1.953168	2.301243
H	2.223068	-2.620124	2.011095
H	2.016444	-0.877164	2.259680
C	0.928007	-2.943022	-0.301540
H	1.700754	-3.692039	-0.103626
H	0.000631	-3.295475	0.155732
H	0.789113	-2.879371	-1.383702
O	-0.800522	-0.606932	0.784215
C	-2.296178	-1.100228	-0.707536
C	-1.456527	-1.094861	-1.831401
H	-1.254660	-2.052422	-2.307450
H	-1.527664	-0.248385	-2.509520
H	-0.279571	-0.793734	-1.130423
C	-2.787039	-2.371632	-0.070023
H	-2.169220	-3.218713	-0.377130
H	-2.785570	-2.301308	1.019461
H	-3.817383	-2.577716	-0.388633
C	-2.991228	0.171473	-0.359391
O	-2.836644	1.241262	-0.929522
O	-3.855900	0.015850	0.669194
C	-4.540982	1.204316	1.096252
H	-5.197211	0.885929	1.906357
H	-3.824475	1.948697	1.452611
H	-5.120773	1.630754	0.273782
N	2.442242	0.446658	-0.031048
C	3.368959	1.318090	-0.741682
H	3.210425	1.339033	-1.834908
H	3.299329	2.337676	-0.363972
H	4.390996	0.978002	-0.557678
C	0.479619	1.593611	-1.241895
C	0.699939	3.108953	-1.377844

H	-0.602512	1.444476	-1.242842
H	0.867760	1.086278	-2.134657
H	0.220317	3.448517	-2.302101
H	0.230618	3.659426	-0.557459
H	1.750394	3.404401	-1.429019
C	0.676000	1.604978	1.329705
C	1.698603	2.643164	1.812442
H	0.551047	0.857916	2.115308
H	-0.307173	2.071432	1.210448
H	1.358814	3.066232	2.764139
H	2.675089	2.181170	1.985186
H	1.830925	3.476827	1.117286
C	3.898663	-1.586266	-0.098122
H	3.863837	-2.670799	-0.243657
H	4.680678	-1.201420	-0.758216
H	4.189520	-1.380544	0.935987

4a



ZPE = 0.395997

E (BMK) = -1036.324302

E (B3LYP) = -1036.719824

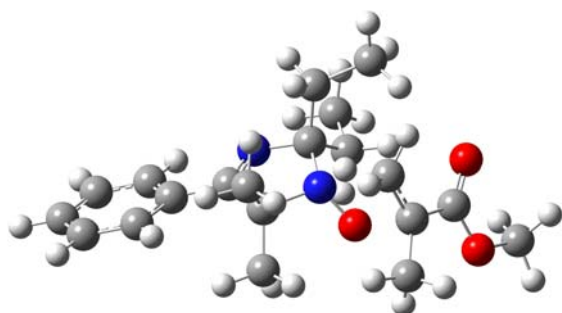
ΔH_{corr} = 0.421698

ΔG_{corr} = 0.342719

C	-0.184192	-1.434150	0.337148
C	1.779907	-0.311829	0.167314
C	0.787807	0.843429	0.329557
N	1.255773	-1.482704	0.179694
C	3.248359	-0.162826	-0.017690
C	3.958919	0.988642	0.360014
C	3.964853	-1.234658	-0.584153
C	5.342494	1.065618	0.182381
H	3.445568	1.827254	0.813562
C	5.343146	-1.154757	-0.766551
H	3.419141	-2.125532	-0.874610
C	6.039428	-0.002989	-0.383643
H	5.872926	1.962137	0.489699
H	5.876075	-1.990766	-1.210295
H	7.114331	0.059735	-0.526138
C	0.902619	1.906012	-0.771034
H	1.834117	2.466475	-0.668495
H	0.887249	1.458929	-1.768712
H	0.074080	2.614696	-0.690939
C	0.827407	1.490891	1.724543
H	0.925385	0.746177	2.517830
H	1.661530	2.191756	1.803939
H	-0.107405	2.032896	1.883338
C	-0.586986	-1.930552	1.729150
H	-1.666441	-1.838016	1.860988
H	-0.291904	-2.978749	1.827941
H	-0.093608	-1.355095	2.515118
C	-0.847771	-2.271627	-0.758490
H	-0.579784	-3.321631	-0.612833
H	-1.933664	-2.165827	-0.713708
H	-0.498825	-1.966818	-1.749260

N	-0.535903	0.060992	0.171159
O	-1.567305	0.509239	0.870056
C	-2.887096	1.172442	-0.713893
C	-2.118484	0.727301	-1.800041
H	-2.427633	-0.179223	-2.312700
H	-1.673614	1.487922	-2.439733
H	-1.035900	0.272570	-1.029949
C	-2.954403	2.622407	-0.320216
H	-3.027775	2.734491	0.762901
H	-2.079868	3.166062	-0.685960
H	-3.847273	3.086257	-0.759561
C	-3.970492	0.334890	-0.125309
O	-4.787671	0.747313	0.678351
O	-3.991534	-0.940917	-0.592794
C	-5.026297	-1.778150	-0.049438
H	-4.896728	-2.749350	-0.527878
H	-4.920081	-1.864046	1.034922
H	-6.012223	-1.365971	-0.278237

4b



ZPE = 0.451045

E (BMK) = -1114.909798

E (B3LYP) = -1115.345698

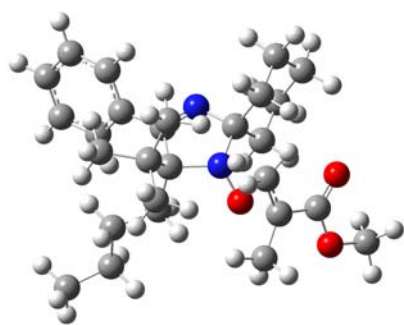
ΔH_{corr} = 0.479475

$\Delta G_{\text{corr}} = 0.39456$

C	0.045717	1.274189	0.347335
C	-1.880447	0.084439	0.097609
C	-0.873397	-1.037707	0.371551
N	-1.380122	1.263124	0.084737
C	-3.335104	-0.098136	-0.171035
C	-4.037176	-1.284058	0.103377
C	-4.051851	0.984331	-0.718846
C	-5.407106	-1.383788	-0.153881
H	-3.531324	-2.141512	0.528329
C	-5.415503	0.883184	-0.979778
H	-3.515855	1.901829	-0.933111
C	-6.102051	-0.302999	-0.697283
H	-5.927473	-2.309807	0.072734
H	-5.944696	1.730175	-1.406930
H	-7.165940	-0.382788	-0.900851
C	-0.880208	-2.129619	-0.703347
H	-0.798116	-1.703479	-1.704355
H	-0.038119	-2.808236	-0.560101
H	-1.805736	-2.705597	-0.640589
C	-1.036301	-1.640453	1.780782
H	-0.956681	-0.878277	2.559644
H	-2.009821	-2.122574	1.889900
H	-0.268428	-2.397774	1.959262
C	0.251376	1.869762	1.766317
H	-0.465295	2.692930	1.858278
H	-0.071123	1.117446	2.494993
C	0.778576	2.049366	-0.760118
H	1.852360	2.009774	-0.559547
H	0.620171	1.515642	-1.700830

N	0.454652	-0.237247	0.307608
O	1.257545	-0.589782	-0.686196
C	2.907633	-1.445430	0.406958
C	2.870374	-2.804839	-0.236261
H	3.848640	-3.294491	-0.140968
H	2.132335	-3.442114	0.259219
H	2.633416	-2.740941	-1.299757
C	2.427937	-1.219005	1.705591
H	1.236462	-0.612210	1.306856
H	2.119867	-2.089856	2.282060
H	2.890196	-0.424282	2.284957
C	3.774587	-0.395382	-0.197513
O	4.024425	0.688518	0.307048
O	4.284534	-0.778092	-1.390868
C	5.097179	0.195828	-2.066236
H	5.431786	-0.290625	-2.982554
H	4.508413	1.086896	-2.297981
H	5.950559	0.481580	-1.446197
C	1.654994	2.375424	2.124292
H	2.439759	1.650822	1.903913
H	1.905389	3.289987	1.578951
H	1.694040	2.613437	3.192945
C	0.309924	3.503644	-0.906582
H	0.483156	4.094119	-0.001456
H	0.860427	3.986235	-1.721182
H	-0.757040	3.554907	-1.139479

4c



ZPE = 0.623854

E (BMK) = -1388.762438

E (B3LYP) = -1389.325579

ΔH_{corr} = 0.659657

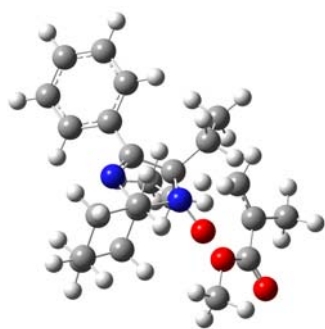
ΔG_{corr} = 0.559305

C	1.396436	-0.806999	0.026238
C	0.743929	0.523991	0.451670
N	0.608250	-1.783204	-0.206051
C	2.860347	-1.082484	-0.154981
C	3.482271	-2.047700	0.652661
C	3.598066	-0.503065	-1.196634
C	4.820623	-2.389435	0.455649
H	2.908166	-2.533337	1.435496
C	4.935561	-0.852631	-1.402076
H	3.122250	0.196060	-1.874847
C	5.555262	-1.787128	-0.569799
H	5.285990	-3.132617	1.096758
H	5.488084	-0.400578	-2.220827
H	6.596001	-2.054599	-0.727451
N	-0.795477	0.076573	0.322908
O	-1.558671	0.855145	-0.437411
C	-3.160058	1.366438	0.888745
C	-3.081729	2.863028	0.745046

H	-4.048150	3.314921	1.004820
H	-2.329037	3.280993	1.416931
H	-2.846602	3.155325	-0.280150
C	-2.702262	0.681809	2.024315
H	-1.510926	0.208198	1.426038
H	-2.381522	1.276822	2.876246
H	-3.201363	-0.249396	2.279922
C	-4.090932	0.629250	-0.016364
O	-4.397512	-0.547701	0.094488
O	-4.590338	1.420660	-0.992587
C	-5.478761	0.782757	-1.925243
H	-5.798583	1.570911	-2.606848
H	-4.955465	-0.006548	-2.470683
H	-6.336192	0.349871	-1.404038
C	-0.784599	-1.424022	-0.121499
C	-1.514924	-2.322183	0.896716
C	-1.423824	-1.585070	-1.516405
C	-1.528998	-3.795533	0.451247
H	-2.545086	-1.963664	0.979097
H	-1.042448	-2.230845	1.879854
C	-1.440995	-3.056781	-1.964990
H	-2.444078	-1.200813	-1.464970
H	-0.878484	-0.966568	-2.235791
C	-2.154267	-3.952639	-0.942012
H	-2.089200	-4.382926	1.189103
H	-0.504060	-4.185285	0.440035
H	-1.940336	-3.121866	-2.939718
H	-0.412613	-3.409519	-2.107580
H	-2.110268	-5.001588	-1.260404
H	-3.217232	-3.677658	-0.894797
C	1.105826	0.916362	1.952634

C	2.632209	1.079896	2.183216
C	0.440590	2.256910	2.335510
C	0.658246	-0.176318	2.953848
H	3.165635	0.130395	2.128134
H	3.108614	1.772823	1.492757
H	2.778595	1.476108	3.194644
H	-0.624636	2.268624	2.116819
H	0.563701	2.429638	3.410653
H	0.897948	3.102221	1.815658
H	1.032506	0.082320	3.950192
H	-0.424379	-0.275615	3.030758
H	1.073429	-1.155067	2.694666
C	0.927070	1.658007	-0.601993
C	2.177466	2.557104	-0.661362
H	0.053775	2.306190	-0.500323
H	0.796953	1.188541	-1.584303
C	2.161942	3.414174	-1.938075
H	2.209778	3.231032	0.201322
H	3.107749	1.982854	-0.636497
C	3.335786	4.396914	-2.017079
H	2.176091	2.755086	-2.817511
H	1.214887	3.968040	-1.992424
H	3.302871	4.983238	-2.941635
H	3.321006	5.100893	-1.176573
H	4.297699	3.871078	-1.990338

4d



ZPE = 0.515376

E (BMK) = -1231.593679

E (B3LYP) = -1232.078758

ΔH_{corr} = 0.545565

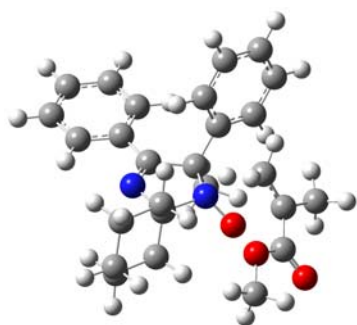
ΔG_{corr} = 0.456898

C	-1.678072	0.210637	-0.059604
C	-0.819000	-0.987247	0.369780
N	-1.046232	1.319824	-0.174203
C	-3.152958	0.220892	-0.295103
C	-3.927608	1.203101	0.345332
C	-3.784078	-0.646118	-1.200030
C	-5.299727	1.293862	0.114347
H	-3.439977	1.895351	1.023927
C	-5.156572	-0.546172	-1.442224
H	-3.205022	-1.380402	-1.747076
C	-5.920887	0.416101	-0.779162
H	-5.882801	2.053244	0.627360
H	-5.624946	-1.217851	-2.155891
H	-6.988853	0.487571	-0.963327
N	0.579611	-0.369646	0.101772
O	1.564328	-0.820158	0.861897
C	2.832274	-1.805777	-0.612342
C	2.098062	-1.439209	-1.751172

H	2.481669	-0.636556	-2.374556
H	1.592765	-2.235971	-2.294938
H	1.056029	-0.796202	-1.064956
C	2.787658	-3.194878	-0.035598
H	2.806382	-3.170839	1.055593
H	1.900231	-3.734867	-0.374498
H	3.669455	-3.759916	-0.364912
C	3.981270	-0.995294	-0.119554
O	4.741280	-1.359245	0.760345
O	4.138308	0.188102	-0.769035
C	5.241431	0.993589	-0.321319
H	5.221227	1.888193	-0.944383
H	5.122923	1.254073	0.733517
H	6.184607	0.456976	-0.450657
C	0.377187	1.165379	0.045903
C	0.818285	1.828651	1.365426
C	1.145184	1.767198	-1.145699
C	0.731696	3.362728	1.308983
H	1.845930	1.505272	1.559826
H	0.205306	1.451064	2.188998
C	1.042404	3.300094	-1.193276
H	2.193563	1.466343	-1.057200
H	0.753139	1.336080	-2.073654
C	1.514854	3.936138	0.120674
H	1.109977	3.774171	2.252712
H	-0.319717	3.666308	1.228424
H	1.637158	3.672316	-2.036449
H	0.001667	3.588499	-1.384076
H	1.398504	5.026035	0.079903
H	2.587925	3.738461	0.260114
C	-0.926509	-1.286087	1.896696

C	-2.330456	-1.309956	2.518435
H	-2.793708	-0.319610	2.516529
H	-3.017941	-1.993103	2.015394
H	-2.251008	-1.630600	3.562854
C	-0.930148	-2.277940	-0.479235
C	-1.986221	-3.327130	-0.098188
H	0.044254	-2.764895	-0.390193
H	-1.036827	-2.004806	-1.535731
H	-1.800240	-3.741517	0.896510
H	-3.008279	-2.943771	-0.117054
H	-0.419773	-2.240072	2.072714
H	-0.325741	-0.546006	2.426707
H	-1.931269	-4.159196	-0.808588

4e



ZPE = 0.510832

E (BMK) = -1344.67949

E (B3LYP) = -1345.206307

ΔH_{corr} = 0.541643

ΔG_{corr} = 0.450721

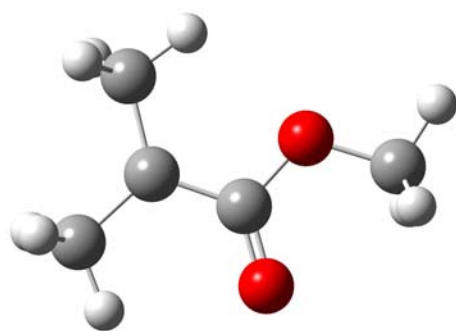
C	-0.821465	0.479029	-0.694606
N	-0.858768	-1.740417	0.163873
N	0.633669	0.039333	-0.342411
O	1.556883	0.351948	-1.235198

C	2.754249	1.774482	-0.109628
C	2.066461	1.673427	1.107978
H	1.475612	2.531967	1.421230
H	1.095253	0.780820	0.650316
H	2.524738	1.109042	1.915581
C	2.568009	2.941001	-1.039014
H	2.660336	2.633427	-2.082255
H	1.593651	3.406684	-0.876429
H	3.343573	3.695108	-0.849264
C	3.964748	0.953440	-0.390825
O	4.715923	1.144222	-1.330889
O	4.183791	-0.028560	0.524213
C	5.349108	-0.836653	0.291077
H	5.371730	-1.559135	1.107506
H	5.276721	-1.345643	-0.673505
H	6.251619	-0.220277	0.299793
C	0.554390	-1.456047	0.073091
C	1.208552	-2.348824	-0.999809
C	1.233033	-1.664241	1.439667
C	1.234292	-3.827328	-0.579315
H	2.224508	-1.977522	-1.161831
H	0.673920	-2.226635	-1.947106
C	1.257842	-3.143986	1.856119
H	2.256401	-1.282596	1.363894
H	0.712180	-1.064580	2.195326
C	1.919217	-4.018794	0.781471
H	1.752410	-4.407951	-1.352188
H	0.208064	-4.211449	-0.527263
H	1.791752	-3.239360	2.809538
H	0.231806	-3.490824	2.029021
H	1.885725	-5.074236	1.078182

H	2.982139	-3.749506	0.695329
C	-0.932357	0.645204	-2.217312
H	-1.920459	1.018978	-2.493969
H	-0.161579	1.327532	-2.577970
H	-0.775444	-0.314595	-2.713823
C	-1.187150	1.734780	0.098700
C	-1.238852	3.001458	-0.499525
C	-1.461686	1.640239	1.473550
C	-1.553523	4.138642	0.251718
H	-1.033683	3.114299	-1.558130
C	-1.774862	2.771645	2.225946
H	-1.434923	0.670608	1.962887
C	-1.822061	4.029536	1.616909
H	-1.585898	5.109231	-0.235072
H	-1.986336	2.670145	3.286501
H	-2.068169	4.912075	2.199985
C	-1.589236	-0.764334	-0.229390
C	-3.069449	-0.902914	-0.276783
C	-3.926725	0.164757	-0.591405
C	-3.638939	-2.162066	-0.004811
C	-5.310733	-0.020340	-0.632861
H	-3.524693	1.150848	-0.788098
C	-5.018475	-2.344391	-0.045094
H	-2.978680	-2.988160	0.234371
C	-5.862257	-1.273009	-0.360213
H	-5.955536	0.819407	-0.874903
H	-5.438008	-3.323851	0.166011
H	-6.938591	-1.415436	-0.392733

1.1.3 Alkoxyamine homolysis products

Alkyl radical



ZPE = 0.127619

E (BMK) = -346.2772435

E (B3LYP) = -346.3963887

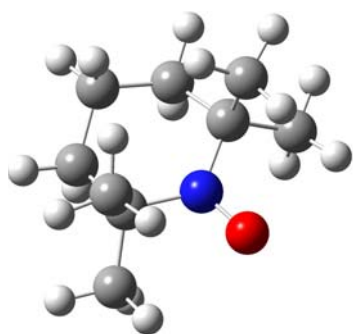
ΔH_{corr} = 0.137887

ΔG_{corr} = 0.092176

$\langle S^2 \rangle$ = 0.756318

C	-0.285309	-0.352600	-0.002803
O	-0.618882	-1.535396	-0.002069
O	-1.202808	0.658830	0.000272
C	1.091638	0.119228	-0.006950
C	-2.577888	0.245525	0.002618
H	-3.158699	1.168100	0.009428
H	-2.803651	-0.345060	-0.889277
H	-2.797799	-0.354749	0.889417
C	2.188221	-0.894050	0.004401
H	1.792238	-1.909848	0.036608
H	2.822822	-0.789338	-0.887920
H	2.850110	-0.740911	0.869206
C	1.446699	1.571021	-0.002334
H	2.174390	1.791874	-0.795617
H	0.576141	2.213804	-0.131607
H	1.937796	1.843910	0.944541

1•



ZPE = 0.252233

E (BMK) = -483.552544

E (B3LYP) = -483.7592844

ΔH_{corr} = 0.265634

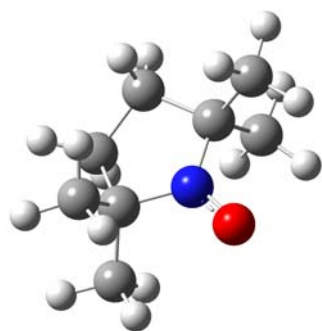
ΔG_{corr} = 0.215159

$\langle S^2 \rangle$ = 0.754343

C	0.000004	2.129534	0.004971
C	1.247192	1.396481	-0.492608
C	1.332838	-0.071993	-0.025815
C	-1.332838	-0.071988	-0.025815
C	-1.247186	1.396485	-0.492611
H	1.249493	1.417492	-1.590679
H	2.160922	1.908024	-0.167543
H	0.000002	2.201910	1.099475
H	0.000006	3.159561	-0.370443
H	-1.249483	1.417495	-1.590682
H	-2.160915	1.908032	-0.167549
C	2.350976	-0.827601	-0.896232
H	2.458827	-1.861365	-0.563962
H	2.034995	-0.835080	-1.944100
H	3.323790	-0.328774	-0.830849
C	1.759550	-0.170830	1.455641
H	2.792541	0.176285	1.566169

H	1.129979	0.435212	2.112316
H	1.705153	-1.211013	1.787595
C	-2.350977	-0.827597	-0.896231
H	-2.458823	-1.861363	-0.563964
H	-3.323792	-0.328774	-0.830842
H	-2.035000	-0.835071	-1.944100
C	-1.759549	-0.170823	1.455641
H	-1.129977	0.435219	2.112315
H	-2.792539	0.176293	1.566169
H	-1.705153	-1.211006	1.787597
N	-0.000002	-0.747866	-0.204823
O	-0.000008	-2.027252	-0.069350

2a•



ZPE = 0.223550

E (BMK) = -444.2604275

E (B3LYP) = -444.4476503

$\Delta H_{\text{corr}} = 0.236313$

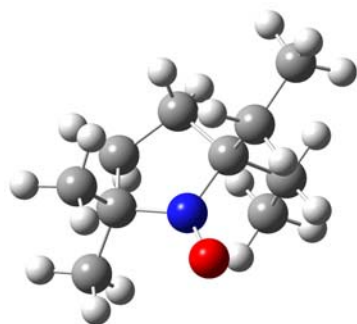
$\Delta G_{\text{corr}} = 0.186572$

$\langle S^2 \rangle = 0.754579$

C	1.261371	0.126165	0.012433
C	0.716792	1.545054	0.284604
C	-0.716847	1.545127	-0.284096

C	-1.261345	0.126146	-0.012396
H	1.345585	2.316274	-0.170222
H	0.697149	1.732408	1.364197
H	-1.345687	2.316175	0.170962
H	-0.697214	1.732804	-1.363639
N	0.000000	-0.670699	-0.000352
C	-2.193343	-0.391423	-1.113650
H	-2.470226	-1.431300	-0.920901
H	-3.104643	0.215114	-1.148592
H	-1.706511	-0.343484	-2.092764
C	-1.941815	0.007954	1.365407
H	-2.898063	0.542317	1.363361
H	-2.129938	-1.044298	1.597735
H	-1.315622	0.427211	2.159556
C	1.942206	0.008628	-1.365245
H	2.130564	-1.043481	-1.598027
H	2.898350	0.543165	-1.362686
C	2.193009	-0.392037	1.113688
H	2.469717	-1.431879	0.920494
H	1.705942	-0.344480	2.092704
O	-0.000015	-1.948473	-0.000505
H	1.316118	0.428154	-2.159326
H	3.104430	0.214291	1.149175

2b•



ZPE = 0.279041

E (BMK) = -522.8497971

E (B3LYP) = -523.0768964

ΔH_{corr} = 0.294377

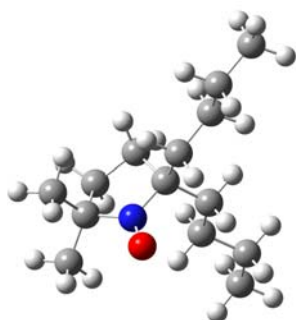
ΔG_{corr} = 0.238998

$\langle S^2 \rangle = 0.754552$

C	0.856520	0.010872	0.013318
C	0.427874	-0.184019	1.489862
C	-1.086678	0.116830	1.554832
C	-1.646614	-0.272664	0.173318
H	0.997569	0.457216	2.168610
H	0.618528	-1.218313	1.795869
H	-1.581319	-0.432030	2.361998
H	-1.257161	1.183944	1.728984
N	-0.460577	-0.016953	-0.693444
C	-2.818987	0.600419	-0.283936
H	-3.102123	0.350615	-1.309870
H	-3.682770	0.438190	0.369398
H	-2.554827	1.661882	-0.250631
C	-2.029105	-1.764816	0.090137
H	-2.933292	-1.955990	0.678257
H	-2.224091	-2.041841	-0.950077
H	-1.230910	-2.408342	0.473521
C	1.556516	1.361825	-0.273834
C	0.785781	2.624328	0.127098
H	1.764518	1.395777	-1.349838
H	2.525389	1.354580	0.238035
H	-0.176438	2.684758	-0.390373
H	0.598635	2.670267	1.205880

C	1.714396	-1.165012	-0.519536
C	3.090604	-1.331749	0.137697
H	1.827235	-1.032098	-1.600827
H	1.137317	-2.087666	-0.381880
H	3.757428	-0.491000	-0.076432
H	3.017091	-1.432513	1.226785
O	-0.539779	-0.029382	-1.969442
H	3.578171	-2.236286	-0.241152
H	1.361479	3.516507	-0.140355

2c•



ZPE = 0.388323

E (BMK) = -680.0343008

E (B3LYP) = -680.3460545

ΔH_{corr} = 0.409429

ΔG_{corr} = 0.339277

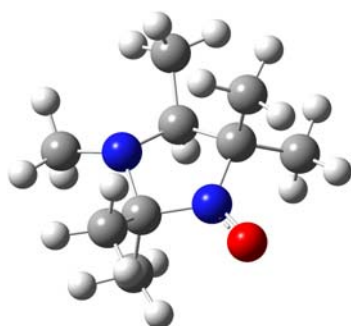
$\langle S^2 \rangle$ = 0.754562

C	0.254561	-0.075778	0.027519
C	0.098765	-0.523959	1.503331
C	-1.165004	-1.411629	1.564532
C	-1.259966	-2.090405	0.184581
H	0.029529	0.328664	2.184876
H	0.977947	-1.102892	1.805963

H	-1.113307	-2.145836	2.374365
H	-2.056487	-0.798551	1.732000
N	-0.621739	-1.058299	-0.681765
C	-2.697544	-2.339287	-0.281582
H	-2.704694	-2.721253	-1.305890
H	-3.180397	-3.073637	0.371724
H	-3.283205	-1.415255	-0.256540
C	-0.442133	-3.396253	0.111944
H	-0.930591	-4.180790	0.700072
H	-0.368769	-3.732808	-0.926362
H	0.571724	-3.259812	0.501446
C	-0.251364	1.358394	-0.263937
C	-1.701979	1.674441	0.123011
H	-0.125075	1.532764	-1.339964
H	0.413311	2.061877	0.251831
C	-2.104572	3.112864	-0.232281
H	-2.378478	0.977583	-0.387525
H	-1.849068	1.524585	1.201731
C	-3.550719	3.446640	0.152033
H	-1.422623	3.815140	0.267415
H	-1.967209	3.268549	-1.310821
H	-3.807703	4.477365	-0.115161
H	-4.259038	2.784065	-0.359307
H	-3.710869	3.333300	1.231089
C	1.700680	-0.254571	-0.500653
C	2.767787	0.643559	0.142044
H	1.682039	-0.094714	-1.584825
H	1.982927	-1.305095	-0.349893
C	4.187552	0.302340	-0.334854
H	2.565611	1.697291	-0.087800
H	2.729636	0.554494	1.237333

C	5.262789	1.209396	0.274225
H	4.410097	-0.745327	-0.089789
H	4.226012	0.373179	-1.430414
H	6.262497	0.939525	-0.082950
H	5.089050	2.260171	0.013266
H	5.269717	1.137242	1.368529
O	-0.661691	-1.127032	-1.957692

3a•



ZPE = 0.266031

E (BMK) = -538.8845626

E (B3LYP) = -539.1041992

ΔH_{corr} = 0.281584

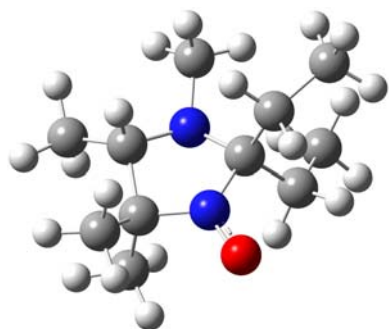
ΔG_{corr} = 0.226205

$\langle S^2 \rangle$ = 0.754516

C	-1.235723	-0.328553	0.034397
C	0.670549	1.051100	-0.368650
C	1.255361	-0.347142	-0.039477
N	0.003559	-1.142779	-0.032797
C	1.915787	-0.444569	1.348511
H	2.080994	-1.498487	1.589914
H	2.883325	0.067174	1.358043
H	1.277988	-0.005442	2.120128

C	2.201618	-0.870365	-1.124968
H	3.108833	-0.258163	-1.162952
H	2.488200	-1.902477	-0.907336
H	1.724477	-0.848338	-2.109543
C	-2.096467	-0.771177	1.222013
H	-2.387267	-1.817832	1.101101
H	-3.003943	-0.162215	1.282219
C	-2.004101	-0.505099	-1.293766
H	-2.186208	-1.570658	-1.457672
H	-1.429851	-0.121931	-2.142819
O	-0.014807	-2.418396	0.014514
H	-1.537075	-0.660599	2.153870
H	-2.969351	0.009473	-1.263133
N	-0.659223	1.013152	0.262538
C	-1.528067	2.137769	-0.053002
H	-1.682079	2.288601	-1.136870
H	-2.505334	1.993769	0.415491
H	-1.104819	3.056548	0.360634
C	1.515769	2.236170	0.096299
H	1.114578	3.180017	-0.283836
H	1.553486	2.293285	1.187698
H	2.537897	2.144404	-0.285830
H	0.575892	1.118626	-1.471556

3b•



ZPE = 0.321716

E (BMK) = -617.4670535

E (B3LYP) = -617.7263735

ΔH_{corr} = 0.339733

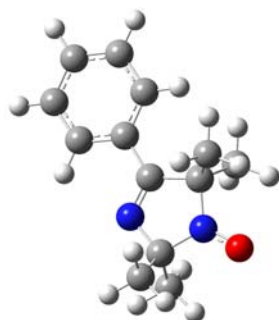
ΔG_{corr} = 0.279099

$\langle S^2 \rangle = 0.754433$

C	-0.770095	-0.312613	-0.014233
C	1.189846	1.017523	-0.452274
C	1.729967	-0.364798	-0.024885
H	1.154767	1.025952	-1.560393
N	0.470910	-1.141135	-0.093948
C	2.284126	-0.410746	1.412451
H	2.414667	-1.454962	1.710452
H	3.256669	0.088167	1.468627
H	1.603065	0.073058	2.117327
C	2.748980	-0.945387	-1.010653
H	3.669150	-0.351916	-0.998406
H	2.995329	-1.973104	-0.731624
H	2.351792	-0.953645	-2.030276
O	0.438242	-2.410822	0.037344
N	-0.178908	1.043933	0.100826
C	-0.977015	2.155064	-0.404258
H	-1.061627	2.170260	-1.506091
H	-1.981705	2.126612	0.016674
H	-0.521749	3.097765	-0.090364
C	-1.555625	-0.626544	-1.324905
C	-3.049494	-0.282970	-1.406400
H	-1.448526	-1.707608	-1.466721
H	-1.022185	-0.155685	-2.160235

H	-3.435965	-0.592527	-2.383657
H	-3.629615	-0.816558	-0.647604
H	-3.254501	0.785416	-1.300134
C	-1.528847	-0.724647	1.278395
C	-2.500793	0.293785	1.887374
H	-0.767584	-0.953252	2.030571
H	-2.044437	-1.669729	1.075169
H	-2.940302	-0.128088	2.797957
H	-1.979389	1.212884	2.170423
H	-3.327067	0.556233	1.221131
C	2.036415	2.209500	-0.004628
H	3.078177	2.067024	-0.310954
H	1.692078	3.138981	-0.466224
H	2.004221	2.332716	1.081539

4a•



ZPE = 0.267259

E (BMK) = -690.0562399

E (B3LYP) = -690.3350745

ΔH_{corr} = 0.284591

ΔG_{corr} = 0.222976

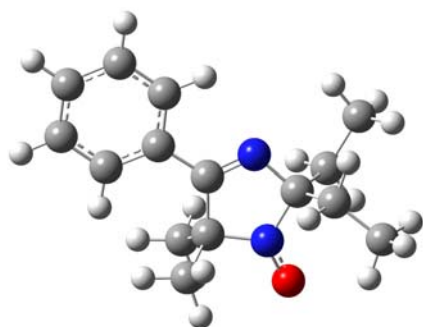
$\langle S^2 \rangle = 0.754538$

C	2.045287	-1.015589	0.000025
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C	-0.054513	-0.148220	-0.000001
C	0.807965	1.122957	-0.000061
N	0.611239	-1.249474	0.000045
C	-1.539726	-0.176866	-0.000007
C	-2.326547	0.986584	0.000081
C	-2.193106	-1.425305	-0.000079
C	-3.721637	0.907761	0.000098
H	-1.862429	1.964309	0.000147
C	-3.582538	-1.502955	-0.000071
H	-1.587863	-2.324813	-0.000142
C	-4.355076	-0.335393	0.000025
H	-4.309951	1.820656	0.000176
H	-4.066477	-2.475420	-0.000135
H	-5.439495	-0.396612	0.000040
C	0.682589	1.982975	1.273874
H	0.693246	1.360357	2.173173
H	1.538854	2.662924	1.313265
H	-0.233827	2.577197	1.275937
C	0.682374	1.983066	-1.273897
H	0.692688	1.360524	-2.173254
H	-0.233948	2.577435	-1.275664
H	1.538726	2.662896	-1.313473
C	2.691461	-1.592338	-1.268001
H	3.748135	-1.313140	-1.299075
H	2.604689	-2.682211	-1.265684
H	2.197122	-1.204463	-2.162963
C	2.691432	-1.591952	1.268246
H	2.604688	-2.681830	1.266264
H	3.748105	-1.312736	1.299249
H	2.197077	-1.203832	2.163095
N	2.141915	0.467805	-0.000205

O	3.241349	1.114012	-0.000154
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4b•



ZPE = 0.322576

E (BMK) = -768.6457422

E (B3LYP) = -768.9651918

ΔH_{corr} = 0.342502

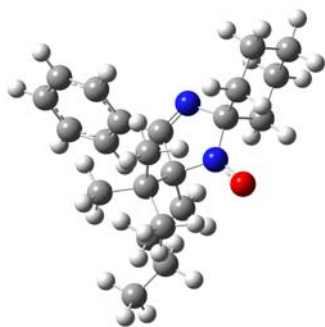
ΔG_{corr} = 0.27519

$\langle S^2 \rangle$ = 0.754555

C	1.733480	-0.446285	-0.029017
C	-0.485692	0.056382	-0.010092
C	0.147832	1.444531	0.150706
N	0.357422	-0.911813	-0.089990
C	-1.944618	-0.219584	-0.064580
C	-2.917694	0.787873	0.041743
C	-2.377200	-1.550285	-0.230083
C	-4.279098	0.477996	-0.014276
H	-2.626836	1.822386	0.170526
C	-3.733236	-1.858285	-0.285485
H	-1.628286	-2.329753	-0.313760
C	-4.692639	-0.844398	-0.177818
H	-5.013472	1.273645	0.070469
H	-4.045184	-2.890829	-0.413647

H	-5.750898	-1.084987	-0.221669
C	-0.126308	2.106461	1.516386
H	-0.004466	1.389391	2.333338
H	0.595562	2.916096	1.656602
H	-1.134727	2.522382	1.569421
C	-0.119531	2.421773	-1.011263
H	-0.003300	1.926124	-1.979383
H	-1.122572	2.851227	-0.961774
H	0.609002	3.235903	-0.948482
C	2.438639	-0.814903	-1.358574
H	2.333412	-1.897652	-1.487721
H	1.860804	-0.353160	-2.167881
C	2.443001	-0.997347	1.229233
H	3.398382	-0.471689	1.324498
H	1.838939	-0.705575	2.096328
N	1.577135	1.030756	0.098809
O	2.532661	1.838551	0.355124
C	3.910676	-0.402824	-1.471949
H	4.036824	0.671992	-1.320599
H	4.537824	-0.919500	-0.738011
H	4.289987	-0.659811	-2.466761
C	2.652230	-2.515013	1.238967
H	3.336458	-2.841585	0.449340
H	3.085385	-2.825855	2.195529
H	1.704932	-3.046303	1.107513

4c•



ZPE = 0.495039

E (BMK) = -1042.506447

E (B3LYP) = -1042.954460

ΔH_{corr} = 0.522291

ΔG_{corr} = 0.439179

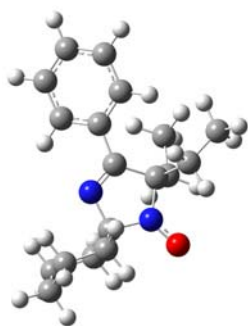
$\langle S^2 \rangle = 0.75452$

C	0.109959	0.653011	-0.001827
C	-0.236811	-0.785256	0.461025
N	1.336564	0.853223	-0.320843
C	-0.818376	1.821124	-0.098792
C	-0.534679	2.974444	0.650439
C	-1.903720	1.845403	-0.985756
C	-1.341929	4.107845	0.547754
H	0.324866	2.976307	1.313000
C	-2.704473	2.984537	-1.098688
H	-2.107723	0.988274	-1.616757
C	-2.434291	4.115039	-0.324061
H	-1.112779	4.987130	1.142923
H	-3.534782	2.989290	-1.799013
H	-3.061713	4.997556	-0.407843
N	1.161243	-1.337175	0.363662
O	1.440101	-2.580314	0.455175
C	2.125546	-0.358196	-0.209271

C	3.336290	-0.162397	0.727557
C	2.593142	-0.835436	-1.605066
C	4.416216	0.740632	0.111704
H	3.745388	-1.159342	0.933249
H	2.988521	0.251173	1.679100
C	3.674159	0.071492	-2.210031
H	2.975229	-1.855111	-1.478131
H	1.722811	-0.894390	-2.268095
C	4.871413	0.228759	-1.261866
H	5.268412	0.800637	0.799629
H	4.018856	1.757922	0.007117
H	3.998533	-0.347986	-3.170262
H	3.244234	1.058320	-2.422053
H	5.610532	0.913603	-1.694966
H	5.373042	-0.742779	-1.142520
C	-0.732314	-0.883768	1.975193
C	-2.033978	-0.089949	2.237601
C	-0.965049	-2.360169	2.373550
C	0.349852	-0.310662	2.918252
H	-2.336933	-0.262159	3.276710
H	-1.898122	0.985887	2.111658
H	-2.864192	-0.401065	1.603641
H	-0.073433	-2.967125	2.206329
H	-1.220932	-2.403748	3.438311
H	-1.792610	-2.813901	1.822050
H	-0.023799	-0.323751	3.947637
H	1.266954	-0.904051	2.889342
H	0.600748	0.727116	2.674370
C	-1.066373	-1.604152	-0.588362
C	-2.604794	-1.602572	-0.626095
H	-0.734227	-2.640258	-0.459644

H	-0.698071	-1.299729	-1.576969
C	-3.123842	-2.325316	-1.880112
H	-3.008132	-2.110334	0.256461
H	-3.014776	-0.588352	-0.606696
C	-4.652762	-2.424736	-1.927341
H	-2.762614	-1.802342	-2.776852
H	-2.689781	-3.333606	-1.922695
H	-4.990352	-2.939005	-2.833479
H	-5.040441	-2.980635	-1.065561
H	-5.117273	-1.431427	-1.915956

4d•



ZPE = 0.386550

E (BMK) = -885.3277549

E (B3LYP) = -885.6969521

ΔH_{corr} = 0.408239

ΔG_{corr} = 0.336544

$\langle S^2 \rangle = 0.754543$

C	0.423786	-0.145279	-0.099281
C	0.270393	1.382681	0.042878
N	-0.681854	-0.801519	-0.138641
C	1.701264	-0.908356	-0.135082
C	1.743494	-2.169028	0.488569

C	2.850470	-0.450262	-0.797071
C	2.905362	-2.938315	0.464614
H	0.853070	-2.531241	0.990697
C	4.010848	-1.227267	-0.831688
H	2.841230	0.502723	-1.309162
C	4.045857	-2.469918	-0.195900
H	2.921557	-3.903961	0.961811
H	4.886500	-0.859485	-1.358748
H	4.951655	-3.068923	-0.216019
N	-1.220805	1.428495	-0.058733
O	-1.891494	2.509591	0.034942
C	-1.834699	0.078110	-0.082342
C	-2.666829	-0.167446	1.197682
C	-2.716144	-0.077650	-1.341092
C	-3.429527	-1.500139	1.159012
H	-3.367576	0.671642	1.285323
H	-2.001368	-0.128363	2.067415
C	-3.477691	-1.410662	-1.368120
H	-3.418992	0.764362	-1.341638
H	-2.081541	0.025854	-2.228358
C	-4.310468	-1.611737	-0.093764
H	-4.039915	-1.591387	2.065784
H	-2.711756	-2.329939	1.173272
H	-4.122617	-1.438964	-2.254837
H	-2.760578	-2.234833	-1.469371
H	-4.811044	-2.587276	-0.118244
H	-5.103458	-0.850882	-0.050706
C	0.639396	1.904344	1.468155
C	2.041837	1.612404	2.018409
H	2.211659	0.540820	2.151655
H	2.842361	1.997483	1.384120

H	2.144137	2.086609	3.000804
C	0.813233	2.264230	-1.131682
C	2.102606	3.078121	-0.952353
H	0.010163	2.983843	-1.323027
H	0.885787	1.641367	-2.031220
H	2.028519	3.771587	-0.109656
H	2.998856	2.470238	-0.805493
H	0.446044	2.982813	1.464287
H	-0.093745	1.475700	2.160075
H	2.262488	3.681673	-1.852348

4e•



ZPE = 0.382419

E (BMK) = -998.4103601

E (B3LYP) = -998.8208559

ΔH_{corr} = 0.404596

ΔG_{corr} = 0.331439

$\langle S^2 \rangle$ = 0.754557

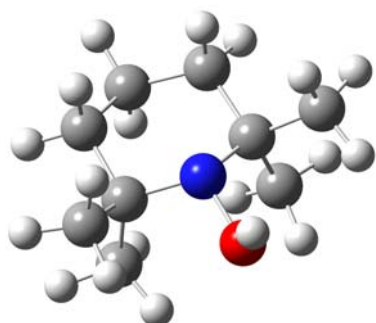
C	-0.365738	-0.610119	0.906798
N	1.162446	0.873839	-0.162459
N	0.991010	-1.221302	0.784035
O	1.311910	-2.324140	1.334049
C	1.966407	-0.297110	0.140758
C	3.099742	0.055012	1.131070

C	2.541830	-0.939816	-1.139580
C	4.206073	0.899512	0.481330
H	3.507649	-0.894874	1.496620
H	2.667277	0.577356	1.992031
C	3.649387	-0.090052	-1.779517
H	2.934580	-1.922634	-0.851191
H	1.724301	-1.113460	-1.847322
C	4.769485	0.222886	-0.776889
H	5.004201	1.071185	1.213786
H	3.800980	1.883843	0.214987
H	4.052482	-0.619978	-2.651015
H	3.217853	0.848931	-2.148671
H	5.527602	0.863723	-1.243170
H	5.276620	-0.710810	-0.493120
C	-0.690871	-0.435698	2.404407
H	-1.716907	-0.095239	2.558963
H	-0.544060	-1.387845	2.920340
H	-0.013027	0.296813	2.850675
C	-1.379351	-1.476572	0.144686
C	-2.194949	-2.402934	0.807637
C	-1.459375	-1.400500	-1.255023
C	-3.074758	-3.221867	0.093051
H	-2.146549	-2.501987	1.885850
C	-2.337992	-2.214258	-1.970306
H	-0.834960	-0.693956	-1.794003
C	-3.152410	-3.129511	-1.297241
H	-3.695271	-3.935217	0.627916
H	-2.386933	-2.131388	-3.052267
H	-3.837526	-3.764406	-1.851440
C	-0.054293	0.733745	0.228323
C	-1.038364	1.832835	0.072483

C	-0.582961	3.106344	-0.318776
C	-2.411779	1.652364	0.308082
C	-1.474887	4.164823	-0.468620
H	0.477489	3.245297	-0.497808
C	-3.304771	2.715719	0.156771
H	-2.795028	0.678446	0.589184
C	-2.841155	3.974134	-0.230667
H	-1.105822	5.141551	-0.768070
H	-4.363539	2.555869	0.338235
H	-3.536500	4.800517	-0.346589

1.1.4 IPT products

1H



ZPE = 0.263655

E (BMK) = -484.1669433

E (B3LYP) = -484.3720325

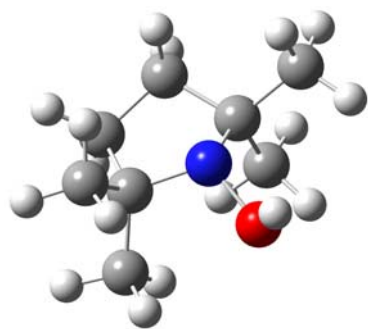
ΔH_{corr} = 0.277205

ΔG_{corr} = 0.22762

C	0.000459	2.170491	0.018284
C	1.251844	1.433425	-0.465927
C	1.296360	-0.050376	-0.033301
C	-1.296348	-0.049969	-0.033320
C	-1.251350	1.433919	-0.465654

H	1.284289	1.475144	-1.562622
H	2.162038	1.924295	-0.100518
H	0.000617	2.253315	1.111956
H	0.000643	3.197895	-0.365448
H	-1.284119	1.475888	-1.562330
H	-2.161274	1.925026	-0.099880
C	2.403015	-0.760422	-0.838306
H	2.528139	-1.796031	-0.509977
H	2.160927	-0.756330	-1.906129
H	3.359141	-0.244614	-0.697740
C	1.631030	-0.187418	1.471090
H	2.685492	0.061507	1.633657
H	1.037815	0.475718	2.103280
H	1.469614	-1.216156	1.802568
C	-2.402957	-0.759705	-0.838618
H	-2.528061	-1.795476	-0.510753
H	-3.359054	-0.243928	-0.697815
H	-2.160833	-0.755120	-1.906431
C	-1.631276	-0.187327	1.471028
H	-1.038778	0.476340	2.103339
H	-2.685976	0.060745	1.633380
H	-1.469155	-1.215945	1.802543
N	-0.000115	-0.665171	-0.450958
O	-0.000580	-2.044684	0.000127
H	-0.000675	-2.544316	-0.827044

2aH



ZPE = 0.235139

E (BMK) = -444.8699443

E (B3LYP) = -445.0553477

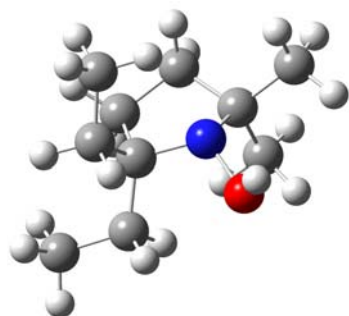
ΔH_{corr} = 0.247909

ΔG_{corr} = 0.199633

C	1.230650	0.137241	-0.015381
C	0.718861	1.565561	0.337160
C	-0.746028	1.618074	-0.141919
C	-1.235265	0.162008	-0.027750
H	1.332980	2.341674	-0.129829
H	0.772770	1.724109	1.419304
H	-1.361662	2.303396	0.449233
H	-0.798864	1.939064	-1.188150
N	-0.015771	-0.532237	-0.522512
C	-2.402619	-0.149275	-0.972060
H	-2.685323	-1.205586	-0.903863
H	-3.282428	0.449401	-0.710814
H	-2.125601	0.068974	-2.008221
C	-1.633653	-0.196157	1.420099
H	-2.587902	0.280984	1.668982
H	-1.751673	-1.277676	1.526643
H	-0.894168	0.139855	2.151705
C	2.245829	0.161819	-1.170724

H	2.487826	-0.857944	-1.490818
H	3.178413	0.649630	-0.863256
C	1.864938	-0.557017	1.203391
H	2.227122	-1.555540	0.946822
H	1.159484	-0.660612	2.031468
O	-0.040063	-1.930463	-0.188276
H	1.836874	0.699485	-2.032003
H	2.715457	0.039810	1.551879
H	-0.048690	-2.363183	-1.052188

2bH



ZPE = 0.290212

E (BMK) = -523.4581697

E (B3LYP) = -523.6839291

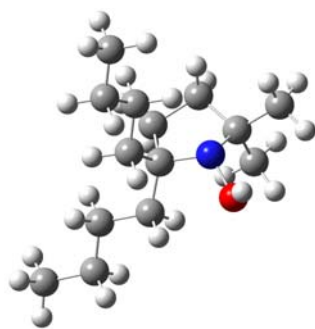
$\Delta H_{\text{corr}} = 0.305749$

$\Delta G_{\text{corr}} = 0.251065$

C	-0.825428	0.035547	0.005132
C	-0.428621	0.023656	-1.501673
C	1.068078	0.388496	-1.552997
C	1.632622	-0.137437	-0.220151
H	-1.040703	0.706842	-2.097687
H	-0.582234	-0.977959	-1.915092
H	1.580789	-0.051634	-2.414265

H	1.200939	1.474417	-1.603102
N	0.506323	0.236316	0.675113
C	2.894184	0.612120	0.227148
H	3.235660	0.250441	1.203386
H	3.709841	0.459737	-0.488624
H	2.694903	1.685620	0.305425
C	1.930149	-1.651699	-0.281666
H	2.833671	-1.826825	-0.876058
H	2.097254	-2.048458	0.723272
H	1.116360	-2.219083	-0.740999
C	-1.731664	1.234039	0.387755
C	-1.188478	2.626916	0.051635
H	-1.918528	1.173781	1.469079
H	-2.706346	1.105361	-0.097684
H	-0.217989	2.794802	0.526784
H	-1.064534	2.769868	-1.028077
C	-1.515412	-1.289310	0.427569
C	-2.834904	-1.605069	-0.293334
H	-1.692386	-1.259708	1.507180
H	-0.815985	-2.115168	0.262697
H	-3.624484	-0.887553	-0.049540
H	-2.721324	-1.616766	-1.383325
O	0.591456	-0.446735	1.937015
H	-3.195544	-2.595315	0.005919
H	-1.880670	3.400286	0.402342
H	0.712244	0.273439	2.569951

2cH



ZPE = 0.399405

E (BMK) = -680.6424571

E (B3LYP) = -680.9528324

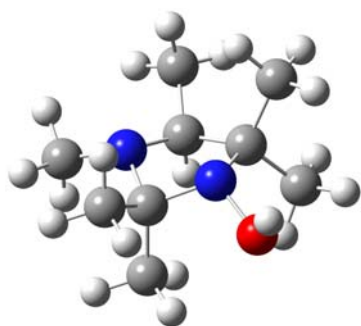
ΔH_{corr} = 0.420748

ΔG_{corr} = 0.351132

C	0.150090	0.007247	0.002150
C	0.054908	0.395587	-1.504225
C	-1.014588	1.501835	-1.593252
C	-0.923939	2.225307	-0.236886
H	-0.182615	-0.461959	-2.140285
H	1.019566	0.782833	-1.847080
H	-0.846400	2.185201	-2.431709
H	-2.013039	1.067118	-1.710278
N	-0.729571	1.045679	0.646742
C	-2.232240	2.926601	0.150361
H	-2.149019	3.382522	1.143097
H	-2.471190	3.722665	-0.563716
H	-3.060483	2.211122	0.165402
C	0.233271	3.247655	-0.209039
H	-0.037411	4.128260	-0.802093
H	0.430891	3.571424	0.816244
H	1.160237	2.841731	-0.622688
C	-0.457745	-1.386017	0.310888
C	-1.915271	-1.610063	-0.111199

H	-0.373106	-1.551908	1.395048
H	0.167219	-2.152880	-0.163884
C	-2.440720	-2.998212	0.281353
H	-2.545234	-0.836325	0.343046
H	-2.014690	-1.491961	-1.199509
C	-3.896193	-3.235605	-0.138399
H	-1.802034	-3.772128	-0.167383
H	-2.349847	-3.124192	1.369476
H	-4.242478	-4.231343	0.159892
H	-4.565970	-2.498609	0.320642
H	-4.013096	-3.155272	-1.225862
C	1.612822	0.062666	0.517172
C	2.599600	-0.906951	-0.154452
H	1.609100	-0.122173	1.596450
H	1.986423	1.085026	0.391277
C	4.047630	-0.681707	0.305984
H	2.321689	-1.945716	0.064909
H	2.556632	-0.803288	-1.247814
C	5.043726	-1.658988	-0.328731
H	4.346371	0.349209	0.070516
H	4.096363	-0.768969	1.400199
H	6.065921	-1.469043	0.016577
H	4.795550	-2.697244	-0.077687
H	5.041037	-1.573944	-1.422135
O	-0.252706	1.438098	1.944726
H	-0.969847	1.169171	2.533989

3aH



ZPE = 0.277741

E (BMK) = -539.4928136

E (B3LYP) = -539.7109416

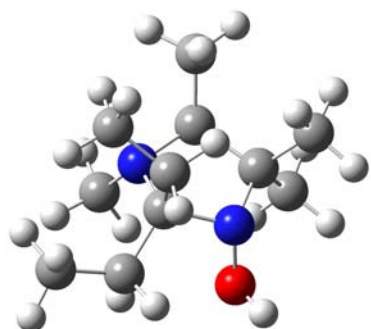
ΔH_{corr} = 0.29326

ΔG_{corr} = 0.239126

C	1.207226	-0.303351	-0.106906
C	-0.651088	1.080795	0.351079
C	-1.236986	-0.323459	-0.010680
N	-0.016981	-1.057658	-0.489740
C	-2.230208	-0.311206	-1.185077
H	-2.472493	-1.343554	-1.459636
H	-3.166407	0.194606	-0.924821
H	-1.792906	0.174821	-2.060877
C	-1.907081	-0.955824	1.219832
H	-2.714840	-0.299655	1.564157
H	-2.337590	-1.931151	0.980792
H	-1.202987	-1.093489	2.044209
C	2.296987	-0.596906	-1.143628
H	2.544750	-1.663240	-1.125728
H	3.217446	-0.043106	-0.931371
C	1.724997	-0.634723	1.312725
H	1.926886	-1.704386	1.397511
H	1.005146	-0.365566	2.090190

O	0.035638	-2.399424	0.019149
H	1.937373	-0.329107	-2.139967
H	2.656204	-0.094921	1.511472
N	0.685303	1.068351	-0.259308
C	1.564518	2.143140	0.175223
H	1.676758	2.205150	1.273771
H	2.556906	2.015009	-0.264242
H	1.176993	3.102355	-0.178386
C	-1.485857	2.286797	-0.081387
H	-1.053692	3.216535	0.300702
H	-1.547969	2.360632	-1.170509
H	-2.500446	2.214685	0.324410
H	-0.564155	1.129187	1.454914
H	-0.003391	-2.935836	-0.783543

3bH



ZPE = 0.333638

E (BMK) = -618.0628572

E (B3LYP) = -618.3218965

ΔH_{corr} = 0.351631

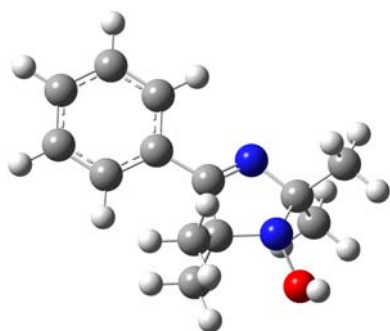
ΔG_{corr} = 0.292141

C	0.752814	-0.191123	-0.287307
C	-1.072660	0.690789	0.948367

C	-1.680449	-0.157691	-0.244946
H	-1.560978	0.350228	1.867959
N	-0.487034	-0.820503	-0.901077
C	-2.423601	0.658486	-1.321223
H	-2.757211	-0.017524	-2.114541
H	-3.307911	1.148023	-0.899124
H	-1.802483	1.426950	-1.783912
C	-2.680594	-1.179112	0.327051
H	-3.514877	-0.627570	0.775008
H	-3.083798	-1.830307	-0.453367
H	-2.230956	-1.810900	1.094488
O	-0.512435	-2.242341	-0.601007
N	0.356016	0.312244	1.046076
C	0.622741	-0.549284	2.203118
H	0.112775	-1.526986	2.173909
H	1.694366	-0.725892	2.311505
H	0.296405	-0.022050	3.104797
C	1.901873	-1.223491	-0.277633
C	3.316338	-0.721857	0.050750
H	1.920470	-1.666111	-1.279576
H	1.639779	-2.040913	0.394530
H	3.983378	-1.582917	0.169205
H	3.730578	-0.101860	-0.748531
H	3.356811	-0.140827	0.976998
C	1.094948	1.003742	-1.239290
C	1.940458	2.150159	-0.668016
H	0.161432	1.427887	-1.613239
H	1.581024	0.576230	-2.124874
H	2.003080	2.959785	-1.404763
H	1.494167	2.550404	0.244618
H	2.961351	1.850958	-0.425006

C	-1.288599	2.209836	0.894689
H	-2.356365	2.453124	0.934669
H	-0.806678	2.670641	1.762463
H	-0.871112	2.672055	-0.002253
H	-0.526249	-2.638609	-1.481267

4aH



ZPE = 0.279005

E (BMK) = -690.6669742

E (B3LYP) = -690.9443409

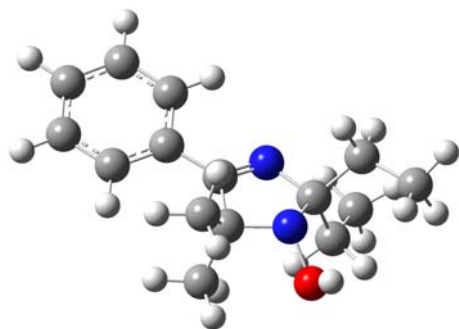
ΔH_{corr} = 0.296274

ΔG_{corr} = 0.236548

C	2.004152	-1.020299	0.053838
C	-0.083085	-0.159916	-0.002321
C	0.812310	1.079961	-0.168218
N	0.565882	-1.261978	0.121208
C	-1.569520	-0.166672	0.017433
C	-2.342223	0.987533	0.228427
C	-2.238971	-1.391237	-0.173508
C	-3.737706	0.920929	0.252704
H	-1.865849	1.946309	0.389661
C	-3.629659	-1.456305	-0.153658
H	-1.645062	-2.283686	-0.336239

C	-4.387241	-0.299078	0.059993
H	-4.314115	1.825585	0.423458
H	-4.125516	-2.410505	-0.307614
H	-5.472197	-0.349346	0.074259
C	0.886436	1.926710	1.123588
H	1.056637	1.311902	2.010099
H	1.708977	2.641292	1.042428
H	-0.039862	2.486118	1.274654
C	0.453008	1.968220	-1.372286
H	0.342537	1.363901	-2.276626
H	-0.468469	2.534076	-1.214352
H	1.263166	2.687119	-1.538116
C	2.647633	-1.991902	-0.943899
H	3.713457	-1.764411	-1.052848
H	2.545223	-3.023522	-0.594117
H	2.167711	-1.899302	-1.921645
C	2.622632	-1.205497	1.451408
H	2.433566	-2.228946	1.787073
H	3.700870	-1.033352	1.418214
H	2.186043	-0.520557	2.180883
N	2.084476	0.367351	-0.497312
O	3.237975	1.070486	-0.017517
H	3.729981	1.261157	-0.827322

4bH



ZPE = 0.334030

E (BMK) = -769.2556038

E (B3LYP) = -769.5734972

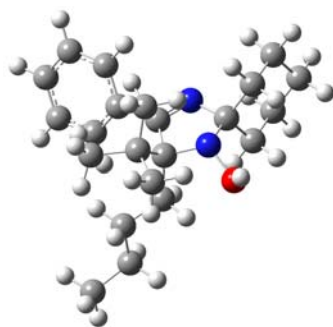
ΔH_{corr} = 0.354117

ΔG_{corr} = 0.287756

C	1.709442	-0.466792	-0.063493
C	-0.494219	0.048332	-0.034509
C	0.181518	1.427974	-0.005307
N	0.328048	-0.937697	-0.044201
C	-1.959422	-0.208434	-0.053834
C	-2.920013	0.767824	0.259371
C	-2.410123	-1.498073	-0.398470
C	-4.284043	0.465544	0.235378
H	-2.617047	1.769565	0.536084
C	-3.769432	-1.797883	-0.426134
H	-1.671710	-2.253310	-0.643451
C	-4.715123	-0.816362	-0.108367
H	-5.007443	1.235803	0.486831
H	-4.093748	-2.798139	-0.698936
H	-5.775826	-1.049277	-0.130978
C	0.083522	2.088916	1.389021
H	0.407868	1.412890	2.183336
H	0.718473	2.977133	1.419999
H	-0.943701	2.392938	1.602509
C	-0.304097	2.398832	-1.096747
H	-0.297888	1.911867	-2.075660
H	-1.309474	2.780953	-0.902103
H	0.377587	3.255558	-1.137848
C	2.420536	-1.162260	-1.248158

H	2.354887	-2.244582	-1.094896
H	1.831710	-0.937633	-2.144369
C	2.380495	-0.759299	1.301572
H	3.368108	-0.290659	1.308135
H	1.799388	-0.251961	2.077995
N	1.568320	0.998392	-0.367704
O	2.553146	1.800292	0.301505
C	3.879063	-0.755323	-1.481780
H	3.968936	0.314680	-1.696339
H	4.517162	-0.980387	-0.620691
H	4.286582	-1.295344	-2.343122
C	2.495185	-2.248326	1.651900
H	3.182120	-2.776826	0.982893
H	2.880667	-2.363678	2.670756
H	1.522443	-2.745953	1.598240
H	3.041432	2.201148	-0.429740

4cH



ZPE = 0.506477

E (BMK) = -1043.113224

E (B3LYP) = -1043.560121

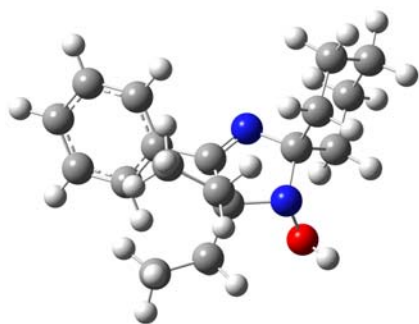
ΔH_{corr} = 0.533902

ΔG_{corr} = 0.451218

C	0.121878	0.688737	0.043035
C	-0.220572	-0.729412	0.567322
N	1.351822	0.874676	-0.262706
C	-0.815289	1.838561	-0.147067
C	-0.538514	3.053052	0.501208
C	-1.907785	1.780685	-1.025121
C	-1.355095	4.168225	0.307411
H	0.325760	3.117068	1.154199
C	-2.717357	2.900180	-1.229882
H	-2.114779	0.869336	-1.573315
C	-2.451240	4.094862	-0.556191
H	-1.129562	5.096212	0.825134
H	-3.552757	2.838737	-1.921543
H	-3.085606	4.962803	-0.710810
N	1.205983	-1.207963	0.729641
O	1.406096	-2.595304	0.439108
C	2.122107	-0.346395	-0.074348
C	3.395115	-0.060853	0.750739
C	2.512248	-0.923302	-1.458603
C	4.418465	0.810620	0.007046
H	3.845186	-1.031611	1.001021
H	3.098752	0.408942	1.694613
C	3.522826	-0.032802	-2.200591
H	2.941719	-1.917299	-1.296861
H	1.610252	-1.060331	-2.063812
C	4.783288	0.213583	-1.359449
H	5.316500	0.928240	0.626441
H	3.996238	1.812797	-0.136637
H	3.787555	-0.508511	-3.153235
H	3.053941	0.928588	-2.443250
H	5.471982	0.879890	-1.893478

H	5.316286	-0.737936	-1.213062
C	-0.872333	-0.721854	2.025600
C	-2.299305	-0.124751	2.091533
C	-0.925272	-2.163124	2.580851
C	0.000753	0.119640	2.986022
H	-2.587098	-0.035262	3.145456
H	-2.351988	0.874473	1.655323
H	-3.050753	-0.748306	1.608973
H	0.077283	-2.560596	2.764154
H	-1.453592	-2.165657	3.541126
H	-1.447986	-2.853627	1.912785
H	-0.394375	0.035204	4.004580
H	1.036754	-0.224151	2.987855
H	-0.011204	1.181722	2.720822
C	-0.944296	-1.588944	-0.533110
C	-2.474027	-1.730676	-0.635940
H	-0.537964	-2.598808	-0.435580
H	-0.575958	-1.227085	-1.501084
C	-2.870445	-2.466813	-1.926453
H	-2.859554	-2.302303	0.215920
H	-2.985383	-0.763531	-0.610626
C	-4.380842	-2.701146	-2.045665
H	-2.519786	-1.892082	-2.795251
H	-2.345057	-3.430629	-1.969981
H	-4.632150	-3.219491	-2.977296
H	-4.754532	-3.310979	-1.214558
H	-4.931981	-1.753163	-2.033267
H	1.664597	-2.965657	1.293749

4dH



ZPE = 0.398374

E (BMK) = -885.9321831

E (B3LYP) = -886.2999453

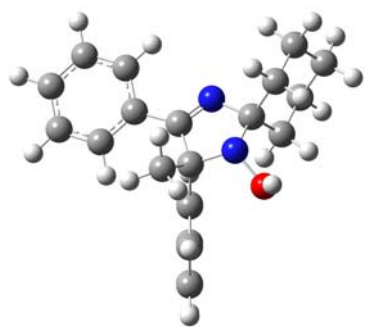
ΔH_{corr} = 0.41992

ΔG_{corr} = 0.350693

C	0.403755	-0.064679	-0.100317
C	0.185870	1.450792	0.149687
N	-0.683242	-0.731992	-0.197148
C	1.698256	-0.804529	-0.184792
C	1.900408	-1.926824	0.635999
C	2.686006	-0.478685	-1.127238
C	3.070245	-2.680485	0.542774
H	1.127147	-2.204837	1.344796
C	3.852313	-1.241225	-1.230371
H	2.534634	0.351916	-1.807164
C	4.053924	-2.338043	-0.389836
H	3.210441	-3.539371	1.193013
H	4.599592	-0.979515	-1.974135
H	4.963836	-2.926163	-0.466992
N	-1.292360	1.580555	-0.168786
O	-1.451064	2.108584	-1.509706
C	-1.840723	0.164337	-0.138430
C	-2.614717	-0.054032	1.189043

C	-2.779085	-0.142865	-1.325533
C	-3.263052	-1.444077	1.290644
H	-3.385372	0.725307	1.243694
H	-1.945626	0.099365	2.040093
C	-3.408555	-1.541462	-1.223428
H	-3.570821	0.616224	-1.344254
H	-2.223135	-0.045291	-2.260027
C	-4.174251	-1.733106	0.091591
H	-3.828608	-1.507851	2.228746
H	-2.475568	-2.206239	1.340141
H	-4.077179	-1.691623	-2.080223
H	-2.617498	-2.296964	-1.299187
H	-4.576059	-2.751937	0.155440
H	-5.038761	-1.052445	0.116120
C	0.310904	1.812512	1.670187
C	1.435334	1.164450	2.490181
H	1.287899	0.085869	2.594379
H	2.428217	1.318936	2.062197
H	1.438696	1.591881	3.499146
C	1.023280	2.433432	-0.711320
C	2.441707	2.779188	-0.230146
H	0.454704	3.367865	-0.751029
H	1.054769	2.073205	-1.743058
H	2.431284	3.311226	0.725568
H	3.087974	1.905938	-0.120525
H	0.389431	2.905218	1.725531
H	-0.640375	1.572201	2.146551
H	2.909695	3.445787	-0.963011
H	-1.991317	2.894491	-1.358791

4eH



ZPE = 0.394048

E (BMK) = -999.019902

E (B3LYP) = -999.4283465

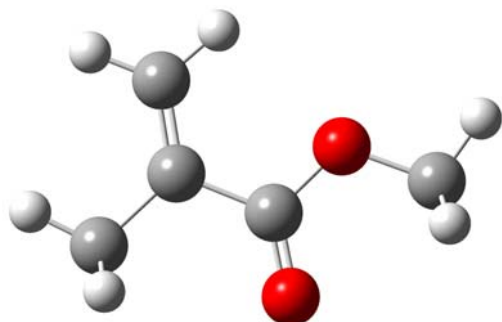
ΔH_{corr} = 0.416281

ΔG_{corr} = 0.344768

C	0.308604	0.567340	1.050728
N	-0.906066	-1.155321	-0.045834
N	-1.162634	0.696686	1.312930
O	-1.600589	2.057380	1.308205
C	-1.902722	-0.157950	0.331930
C	-3.074332	-0.841100	1.069026
C	-2.430771	0.586007	-0.916662
C	-3.919650	-1.742459	0.156791
H	-3.703187	-0.043785	1.489011
H	-2.666480	-1.407914	1.913005
C	-3.257214	-0.330630	-1.833938
H	-3.051529	1.417145	-0.565026
H	-1.594679	1.029146	-1.463789
C	-4.424330	-0.982951	-1.078847
H	-4.763032	-2.151722	0.726853
H	-3.309749	-2.595175	-0.166409
H	-3.632698	0.254888	-2.682392
H	-2.610157	-1.113466	-2.248853

H	-4.975092	-1.660983	-1.742527
H	-5.135332	-0.203901	-0.765161
C	1.002817	0.477268	2.426403
H	2.091958	0.452342	2.345432
H	0.724696	1.338518	3.040683
H	0.665742	-0.422177	2.947870
C	0.902085	1.687464	0.171568
C	1.296227	2.907201	0.743519
C	1.051905	1.537969	-1.215853
C	1.817693	3.939044	-0.039386
H	1.190321	3.065206	1.810665
C	1.577641	2.565338	-2.003648
H	0.767842	0.606810	-1.695635
C	1.962254	3.773143	-1.418822
H	2.108917	4.874015	0.431191
H	1.688436	2.415753	-3.073965
H	2.371212	4.573581	-2.028649
C	0.265895	-0.791746	0.331018
C	1.445072	-1.662233	0.094477
C	1.238914	-3.027600	-0.178884
C	2.762459	-1.174251	0.122471
C	2.317358	-3.877114	-0.414576
H	0.221878	-3.403684	-0.200002
C	3.842406	-2.026848	-0.117488
H	2.950464	-0.122678	0.304680
C	3.625272	-3.380115	-0.384092
H	2.139390	-4.928998	-0.619324
H	4.853052	-1.629344	-0.099374
H	4.466424	-4.042760	-0.566679
H	-1.958279	2.175921	2.198670

Methyl methacrylate



ZPE = 0.118790

E (BMK) = -345.7000471

E (B3LYP) = -345.8129611

ΔH_{corr} = 0.12802

ΔG_{corr} = 0.085949

C	0.240362	-0.300486	0.000007
O	0.482633	-1.494781	0.000013
O	1.209472	0.643775	0.000016
C	2.561493	0.151565	-0.000021
H	3.192519	1.040057	-0.000739
H	2.747788	-0.453741	0.890515
H	2.747344	-0.454917	-0.889838
C	-1.147235	0.258695	-0.000003
C	-1.362677	1.582585	0.000003
H	-0.543549	2.292133	0.000011
H	-2.373401	1.980756	0.000003
C	-2.247355	-0.769976	-0.000010
H	-2.173731	-1.421909	-0.876830
H	-2.173736	-1.421915	0.876806
H	-3.227604	-0.286720	-0.000012

1.1.5 Electronic energy values for O-H bond scan in figure 3

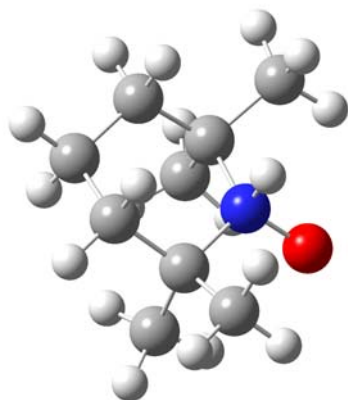
O...H (Å)	E(a.u.)
2.526	-790.820538
2.476	-790.820491
2.426	-790.820317
2.376	-790.820009
2.326	-790.819563
2.276	-790.818975
2.226	-790.818234
2.176	-790.817327
2.126	-790.816246
2.076	-790.814975
2.026	-790.813495
1.976	-790.811787
1.926	-790.809846
1.876	-790.807638
1.826	-790.805114
1.776	-790.802240
1.726	-790.798965
1.676	-790.795238
1.626	-790.790992
1.576	-790.786168
1.526	-790.780716
1.476	-790.774594
1.426	-790.767764
1.376	-790.760207
1.326	-790.751927
1.276	-790.742972
1.226	-790.733464
1.176	-790.723678
1.126	-790.785919
1.076	-790.792237
1.026	-790.796714

1.1.6 Thermodynamic data at 400K

alkox	IPT								exp %	C-ON				exp E _a
	ΔH^\ddagger	ΔG^\ddagger	ΔH_{rxn}	ΔG_{rxn}	$\Delta_{4a}^{IPT} H^\ddagger$	$\Delta_{4a}^{IPT} G^\ddagger$	$\Delta_{4a}^{IPT} H_{rxn}$	$\Delta_{4a}^{IPT} G_{rxn}$		ΔH_{rxn}	ΔG_{rxn}	$\Delta_{4a}^{CO} H_{rxn}$	$\Delta_{4a}^{CO} G_{rxn}$	
1	146,8	152,2	25,9	-49,4	-0,5	-1,1	-15,8	-17,0	0	119,1	27,8	-5,9	-3,6	115,5
2a	139,9	145,1	42,3	-31,6	-7,5	-8,2	0,6	0,8	-	122,6	30,7	-2,4	-0,7	-
2b	143,8	152,8	41,6	-32,0	-3,5	-0,5	-0,1	0,4	-	119,5	30,6	-5,6	-0,8	-
2c	144,2	150,7	41,9	-35,5	-3,1	-2,6	0,2	-3,1	1	119,3	27,2	-5,8	-4,2	118,5
3a	145,4	147,7	43,2	-34,4	-2,0	-5,6	1,5	-2,0	21,5	125,3	30,4	0,2	-1,0	125,5
3b	146,3	155,5	40,8	-32,1	-1,0	2,3	-0,9	0,3	0	123,4	33,6	-1,6	2,2	118,6
4a	147,3	153,3	41,7	-32,4	0,0	0,0	0,0	0,0	31	125,0	31,4	0,0	0,0	121,6
4b	149,5	154,5	35,7	-41,7	2,1	1,2	-6,0	-9,3	-	116,9	23,3	-8,1	-8,1	-
4c	152,6	160,5	24,7	-52,9	5,3	7,2	-17,0	-20,5	0	97,8	5,8	-27,2	-25,6	115,5
4d	148,1	153,3	37,3	-37,0	0,8	0,0	-4,4	-4,6	0	119,7	23,8	-5,4	-7,6	122,7
4e	149,4	154,7	43,3	-30,9	2,1	1,4	1,6	1,5	10,5	130,1	37,2	5,0	5,8	130,3

1.1.8 1,2 proton shift reaction data for 1

Reactant



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.531758
C	1.407882	0.000000	2.158011
C	2.227275	1.295149	-0.031399
C	0.769481	1.216263	-0.524297
H	-0.548453	0.886041	1.884745
H	-0.542489	-0.869105	1.923018
H	0.437291	-0.928168	-0.385405
H	-1.031702	0.028352	-0.369342
H	0.238156	2.129386	-0.217097
H	0.783807	1.227262	-1.620834
O	3.515970	1.191266	2.020526
C	1.325787	0.350316	3.650580
H	2.323517	0.356277	4.092363
H	0.872916	1.338060	3.804954
H	0.700166	-0.385674	4.165624
C	2.142442	-1.333257	1.993731
H	1.741732	-2.050198	2.717219
H	2.028773	-1.769209	0.999633
H	3.204399	-1.179033	2.198705
C	2.806305	2.690458	-0.305394
H	3.836626	2.747922	0.049302
H	2.775712	2.895035	-1.380365
H	2.222620	3.471406	0.198583
C	3.137394	0.239398	-0.664822
H	2.675260	-0.747350	-0.727805
H	3.388492	0.552759	-1.683038
H	4.056847	0.168360	-0.079066
N	2.250940	1.154349	1.525255
H	1.740218	2.000089	1.834422

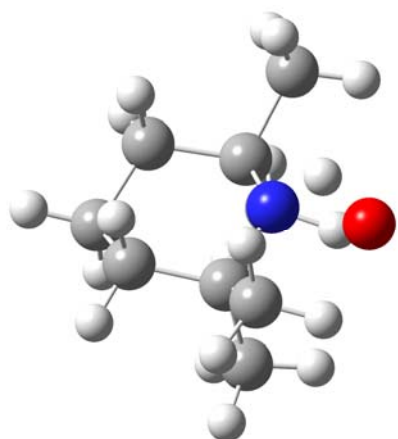
ZPE = 0.264752

E (BMK) = -484.1448504

ΔH_{corr} = 0.278031

ΔG_{corr} = 0.228809

TS



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.531371
C	1.416078	0.000000	2.150780
C	2.243493	1.264068	-0.002090
C	0.788702	1.204925	-0.520772
H	-0.536866	0.890693	1.885116
H	-0.539771	-0.870013	1.923684
H	0.423927	-0.934657	-0.385860
H	-1.030895	0.043855	-0.370455
H	0.270946	2.124813	-0.216749
H	0.820922	1.208760	-1.616733
O	3.622792	1.147141	2.065901
C	1.317125	0.353159	3.645186
H	2.300522	0.316595	4.118178
H	0.898094	1.356589	3.782257
H	0.656134	-0.360945	4.146724
C	2.115260	-1.365041	2.008720
H	1.678399	-2.069024	2.724020
H	2.008561	-1.798241	1.012505
H	3.178706	-1.253115	2.233459
C	2.826995	2.659835	-0.283378
H	3.870399	2.714945	0.033482
H	2.771096	2.870148	-1.356242
H	2.258065	3.434256	0.243722
C	3.143905	0.206451	-0.667732

H	2.676247	-0.778199	-0.724753
H	3.374799	0.522625	-1.689893
H	4.078751	0.121914	-0.108388
N	2.208421	1.094816	1.491591
H	2.639733	1.927755	2.146422

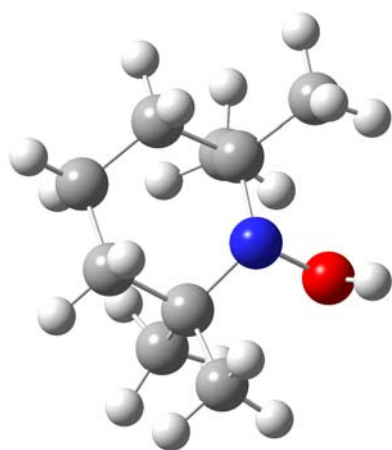
ZPE = 0.259843

E (BMK) = -484.0964823

ΔH_{corr} = 0.27312

ΔG_{corr} = 0.223933

Product



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.530938
C	1.419013	0.000000	2.145026
C	2.254829	1.236869	0.025317
C	0.807052	1.194306	-0.515825
H	-0.529840	0.894432	1.884186
H	-0.542932	-0.868578	1.923026
H	0.412834	-0.940048	-0.385746
H	-1.029814	0.056680	-0.372989
H	0.298434	2.120143	-0.216397
H	0.850846	1.193989	-1.611734
O	3.521485	1.107609	2.034845
C	1.301258	0.331920	3.645921
H	2.273096	0.265313	4.142941
H	0.903908	1.342900	3.783406
H	0.623518	-0.376275	4.134916
C	2.090245	-1.387484	2.009231
H	1.614146	-2.091481	2.700627
H	2.004746	-1.807434	1.005425

H	3.150158	-1.322021	2.267128
C	2.850666	2.624787	-0.283524
H	3.902991	2.677290	0.009368
H	2.789423	2.828911	-1.358034
H	2.297405	3.405044	0.249364
C	3.141743	0.168562	-0.657475
H	2.674029	-0.817007	-0.691939
H	3.345638	0.470844	-1.690607
H	4.097155	0.079383	-0.134554
N	2.167332	1.128746	1.513226
H	3.574526	1.931760	2.536655

ZPE = 0.263659

E (BMK) = -484.166946

ΔH_{corr} = 0.277208

ΔG_{corr} = 0.227624

1. 2 Geometrical data

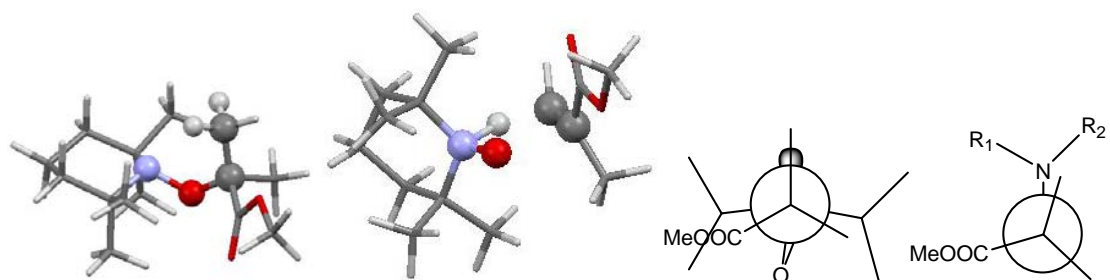
Table 1SI. Selected calculated geometrical parameters (distance d , valence angle α , and torsion angle θ) by DFT at B3LYP/6-31G+(d,p) level for reactants.

	1	2a	2b	2c	3a	3b	4a	4b	4c	4d	4e
distance d (Å)											
N1—O2	1.451	1.432	1.439	1.439	1.437	1.433	1.425	1.4404	1.437	1.429	1.422
O2—C3	1.449	1.462	1.454	1.454	1.449	1.460	1.460	1.4591	1.465	1.460	1.462
C3—C7	1.528	1.524	1.526	1.526	1.525	1.525	1.532	1.5266	1.526	1.532	1.532
C7—H	1.090	1.089	1.090	1.090	1.090	1.089	1.091	1.0888	1.088	1.091	1.091
N1•••H	2.703	2.615	2.621	2.615	2.624	2.617	2.693	2.5827	2.699	2.725	2.678
N1•••C3	2.493	2.460	2.461	2.459	2.446	2.464	2.456	2.4487	2.485	2.468	2.454
valence angle α (°)											
<N1HC7>	84.6	87.5	92.5	93.4	91.9	88.9	81.6	90.72	85.9	81.3	82.6
<N1O2C3>	118.5	116.4	116.5	116.4	115.9	116.8	116.7	115.20	117.9	117.4	116.7
torsion angle θ (°)											
<N1O2C3C7>	-15.1	-23.3	-40.1	-42.2	-43.8	-26.7	9.0	34.71	18.4	9.2	12.3
<O2C3C7H>	62.1	61.7	60.1	59.0	62.4	60.8	56.1	59.70	60.9	56.0	56.3

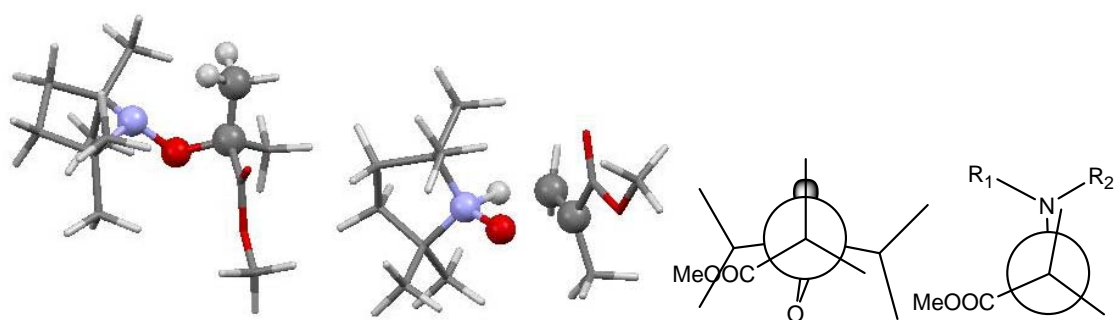
Table 2SI. Selected calculated geometrical parameters (distance d , valence angle α , and torsion angle) by DFT at B3LYP/6-31+G(d,p) level for transition states of IPT.

	1	2a	2b	2c	3a	3b	4a	4b	4c	4d	4e
distance d (Å)											
N1—O2	1.328	1.325	1.328	1.328	1.325	1.324	1.324	1.325	1.329	1.323	1.322
O2—C3	2.234	2.161	2.146	2.141	2.162	2.170	2.166	2.156	2.141	2.180	2.174
C3—C7	1.404	1.403	1.402	1.403	1.402	1.403	1.403	1.403	1.403	1.403	1.402
C7—H	1.387	1.396	1.406	1.406	1.403	1.403	1.402	1.395	1.415	1.404	1.396
N1•••H	1.353	1.325	1.319	1.318	1.320	1.332	1.318	1.323	1.321	1.330	1.322
N1•••C3	2.805	2.744	2.743	2.740	2.742	2.756	2.747	2.736	2.752	2.765	2.749
valence angle α (°)											
<N1HC7>	148.2	147.7	147.7	147.6	147.8	147.5	147.6	147.5	147.4	147.3	147.9
<N1O2C3>	100.8	101.1	101.7	101.7	101.0	101.4	101.1	100.9	102.4	101.4	100.9
torsion angle θ (°)											
<N1O2C3C7>	4.7	-0.7	-0.7	-0.8	5.4	-1.4	4.9	-1.7	1.4	4.4	3.5
<O2C3C7H>	-3.3	-1.0	-0.1	0.0	-4.0	0.9	-3.8	0.2	1.5	-3.9	-2.6

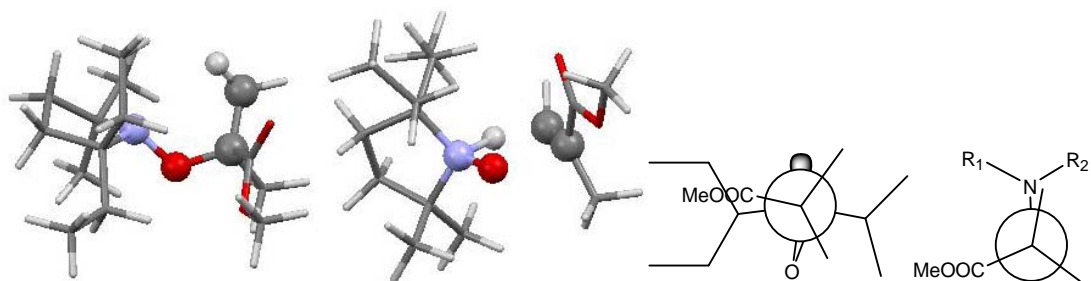
1.3 Figure 1SI



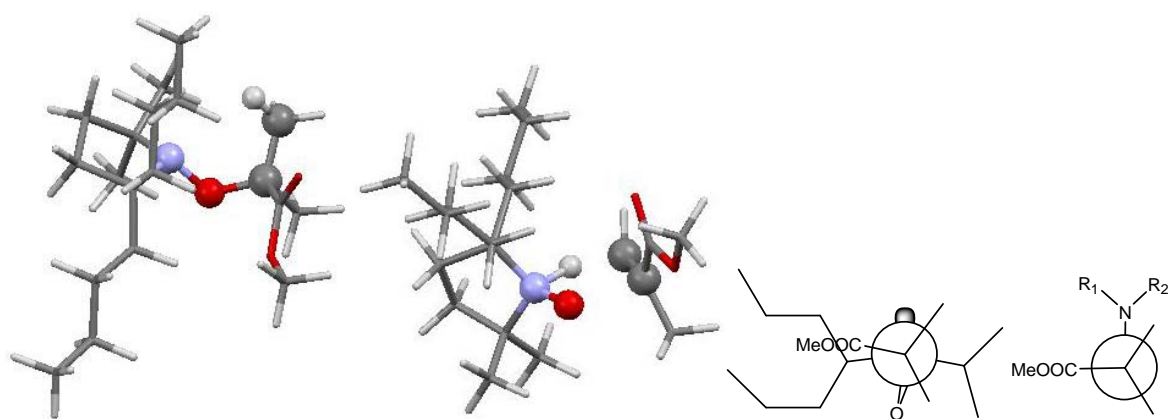
1a



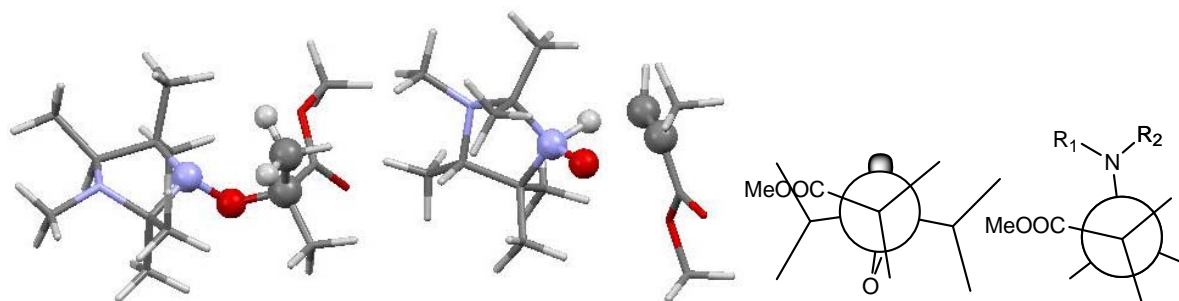
2a



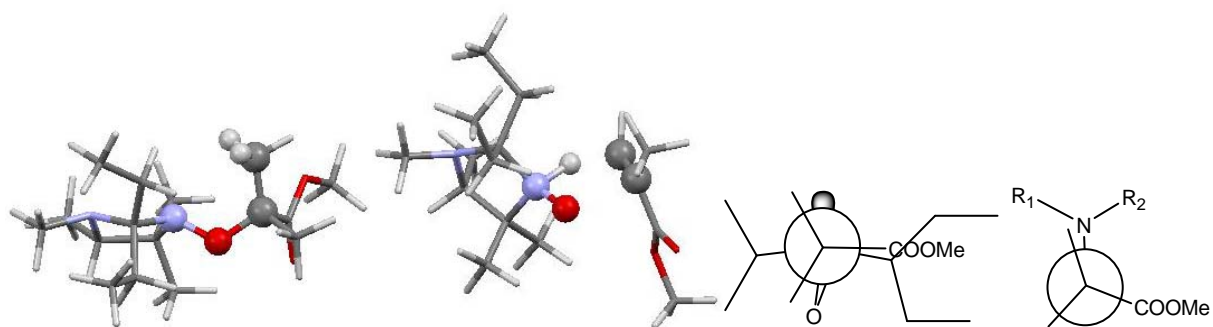
2b



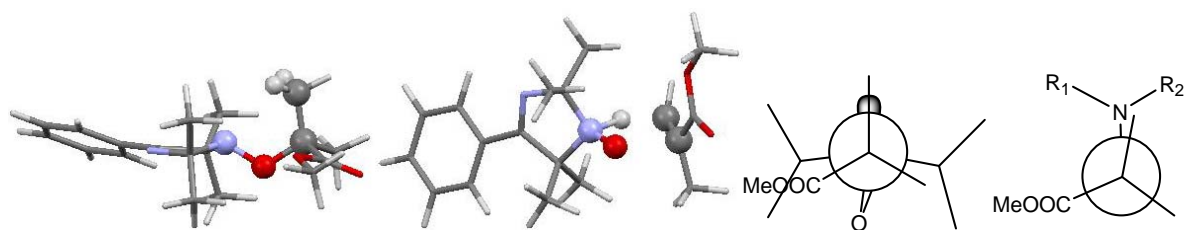
2c



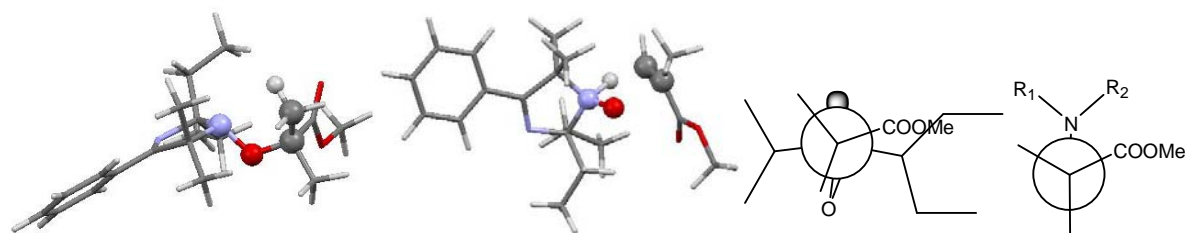
3a



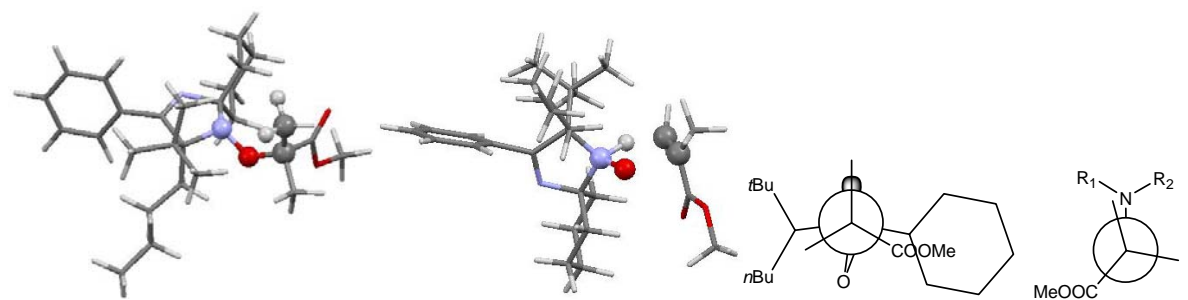
3b



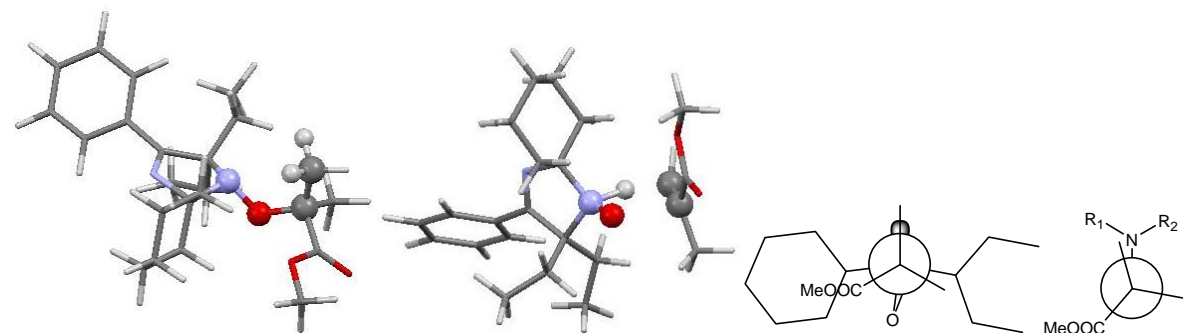
4a



4b



4c



4d

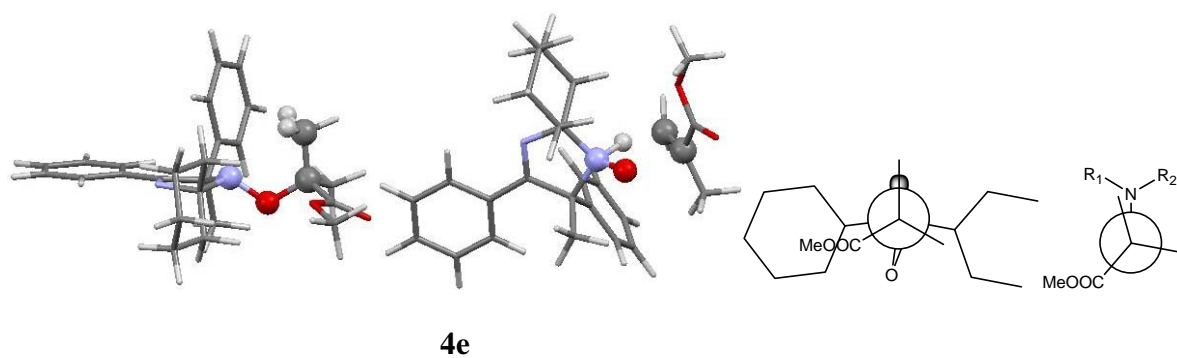


Figure 1SI. Optimized structure with the B3LYP/6-31+G(d,p) method of starting materials (left column) and of their corresponding TS for IPT (middle column). In the right column are displayed the Newman projections along the C3...N1 axis (left) and the C3—O2 bond (right) in starting materials.

1.4 Figure 2SI

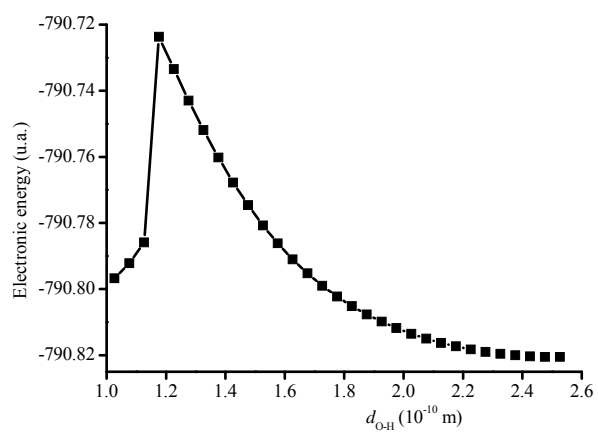


Figure 2SI. Scan of the O-H bond formation from **2a** to the products at the RB3LYP/6-31G(d) level of theory.

1.5 Figure 3SI

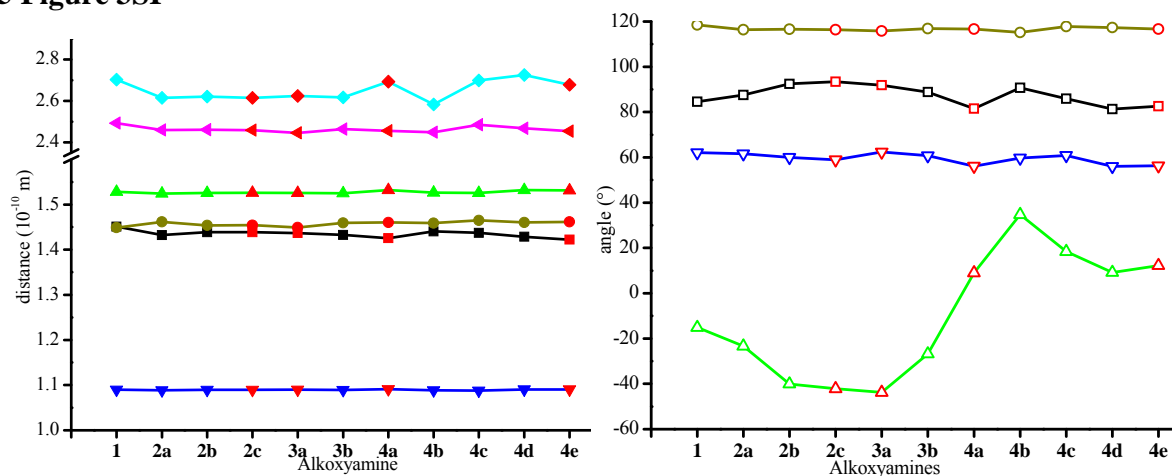
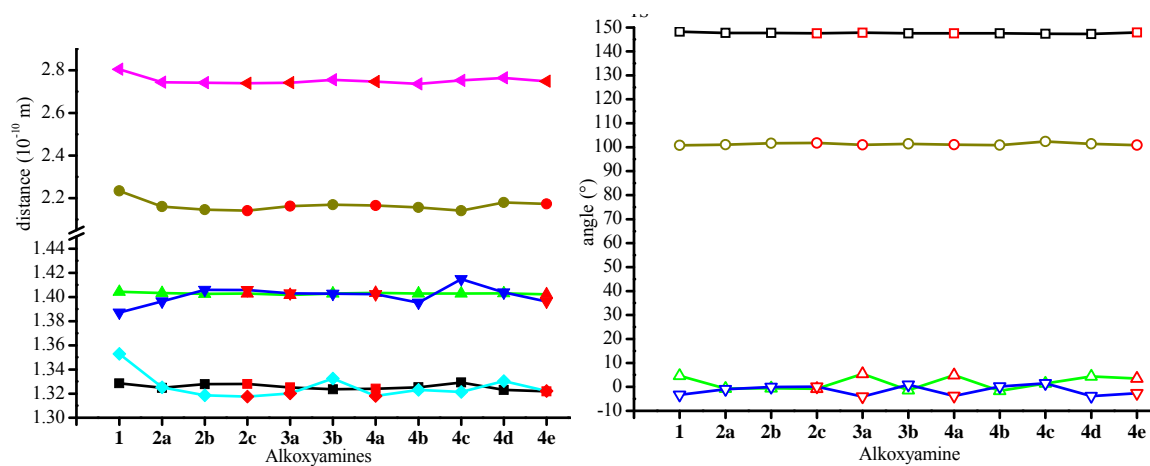


Figure 3SIa. (a) Lengths l_{C3-O2} (●), l_{N1-O2} (■), l_{C3-C7} (▲) and l_{C7-H} (▼), and distances $d_{N1...C3}$ (◄) and $d_{N1...H}$ (◆), and (b) $\langle C3O2N1 \rangle$ (○) and $\langle N1HC7 \rangle$ (◻) valence angles and $\langle N1O2C3C7 \rangle$ (△) and $\langle O2C3C7H \rangle$ (▽) torsion angles reported in starting materials for families 1-4. Red-highlighted symbols are molecules exhibiting IPT

1.6 Figure 4SI



Figures 4SI. (a) Lengths l_{C3-O2} (●), l_{N1-O2} (■), l_{C3-C7} (▲) and l_{C7-H} (▼), and distances $d_{N1...C3}$ (◄) and $d_{N1...H}$ (◆), and (b) $\langle C3O2N1 \rangle$ (○) and $\langle N1HC7 \rangle$ (□) valence angles and $\langle N1O2C3C7 \rangle$ (△) and $\langle O2C3C7H \rangle$ (▽) torsion angles reported at TS for families 1-4. Red-highlighted symbols are molecules exhibiting IPT

1.7 Table 3SI

Table 1SI. Correcting factors $\kappa(T)$ for the tunneling effect at 298.15 K and frequency frequencies ν^\ddagger (in cm^{-1}) at TS

alkoxyamines	$\kappa(T)$	ν^\ddagger
1	11.1	<i>i</i> 1194
2a	8.7	<i>i</i> 1167
2b	9.9	<i>i</i> 1183
2c	9.6	<i>i</i> 1179
3a	8.9	<i>i</i> 1170
3b	12.5	<i>i</i> 1208
4a	8.6	<i>i</i> 1166
4b	8.8	<i>i</i> 1162
4c	22.3	<i>i</i> 1254
4d	10.7	<i>i</i> 1192
4e	8.4	<i>i</i> 1162

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- ¹ Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A. Jr., Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A., Burant, J. C.; Iyengar, S. S.,

Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

² Tomasi, J.; Mennucci, B. ; Cammi, R. *Chem. Rev.* **2005**, *105*, 2999-3093.