

Autoxidation Catalysis with Nitroxyl Radicals: More-Reactive Radicals or Just More Radicals?

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SUPPORTING INFORMATION

Analysis of the equilibrium reaction (1) @ 400 K

Conditions: 10 mol% NHPI, RH = cyclohexane and $[RH] = 5.585 \times 10^{21} \text{ cm}^{-3}$, $[ROOH] = 10^{19} \text{ cm}^{-3}$ (taken very small for the proof of concept, *i.e.* <0.2 % yield)

⇒ Estimation of the pseudo first order rate constants for $ROO^\bullet$ and $PINO^\bullet$ losses.

A. GASPHASE CONDITIONS

$ROO^\bullet + RH \Rightarrow k^{(1)} = 1.57 \times 10^{-11} \times \exp(-17.8 \text{ kcal/mol} / RT) \times [5.585 \times 10^{21}] \approx 16 \text{ s}^{-1}$
 $ROO^\bullet + NHPI \Rightarrow k^{(1)} = 1.3 \times 10^{-12} \times \exp(-0.7 \text{ kcal/mol} / RT) \times [5.585 \times 10^{20}] \approx 3 \times 10^8 \text{ s}^{-1}$

⇒ reaction of peroxy radicals with NHPI is much faster than with RH

$PINO^\bullet + RH \Rightarrow k^{(1)} = 1.57 \times 10^{-11} \times \exp(-16.2 \text{ kcal/mol} / RT) \times [5.585 \times 10^{21}] \approx 130 \text{ s}^{-1}$
 $PINO^\bullet + ROOH \Rightarrow k^{(1)} = 1.3 \times 10^{-12} \times \exp(-3.4 \text{ kcal/mol} / RT) \times [1 \times 10^{19}] \approx 2 \times 10^5 \text{ s}^{-1}$

⇒ reaction of $PINO^\bullet$ with $ROO-H$ is much faster than with RH

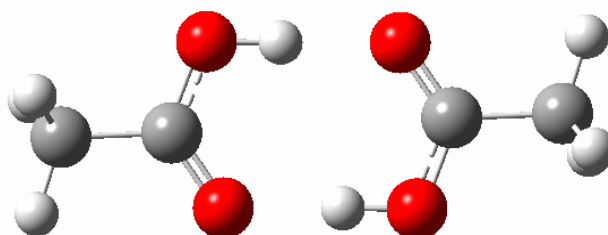
⇒ Equilibrium (1) is certainly established in the gas phase

B. IN ACETIC ACID (H-BONDING SOLVENT)

Conditions : $[RH] = 2 \times 10^{20} \text{ cm}^{-3}$; $[NHPI](\text{total}) = 2 \times 10^{19}$ (i.e. 10 mol%),
 $[ROOH](\text{total}) = 5 \times 10^{17} \text{ cm}^{-3}$

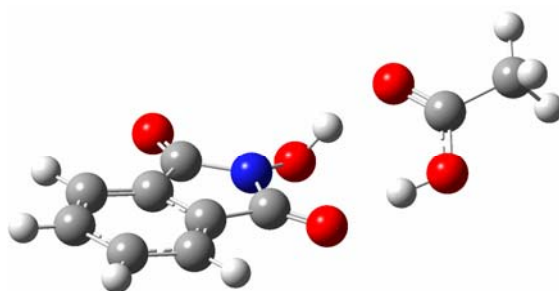
(i) Calculation of the free NHPI and ROOH concentrations

Acetic acid forms dimers, even in the gas phase:



In the liquid phase the dimers are far dominant, even at temperatures of 400 K.

Thus, before NHPI can form an H-bond with HOAc, one has to break up a $(\text{HOAc})_2$ dimer according to:



$$K_{eq}(400\text{K}) = 6.55 \times 10^{-22} \text{ cm}^3$$

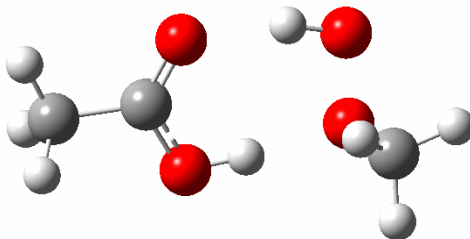
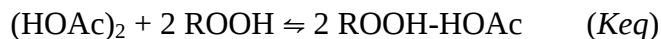
[Calculation is based on the B3LYP/6-311++G(df,pd)//B3LYP/6-31G(d,p) $\Delta_r E$ of -11.9 kcal/mol, and vibration/rotational data at B3LYP/6-31G(d,p) level ⇒ K_{eq} = ratio of partition functions]

based on $[(\text{HOAc})_2] \approx 5 \times 10^{21} \text{ cm}^{-3}$

⇒ $\text{NHPI}(\text{free})/\text{NHPI-HOAc} \approx 0.55$

⇒ $[\text{NHPI}]_{\text{free}} \approx 7 \times 10^{18} \text{ cm}^{-3}$

Analogous for ROOH:



$$K_{eq}(400\text{K}) = 9 \times 10^{-25} \text{ cm}^3 \text{ (again evaluated as the ratio of partition functions)}$$

$$\text{ROOH}(\text{free})/\text{ROOH-HOAc} \approx 15$$

$$\Rightarrow [\text{ROOH}]_{\text{free}} \approx 5 \times 10^{17} \text{ cm}^{-3}$$

(ii) Calculation of the pseudo first-order rate constants for $\text{ROO}^\bullet$ and $\text{PINO}^\bullet$ removal:

$$\begin{aligned} \text{ROO}^\bullet + \text{RH} &\Rightarrow k^{(1)} = 1.57 \times 10^{-11} \times \exp(-17.8 \text{ kcal/mol} / RT) \times [2 \times 10^{20}] \approx 0.6 \text{ s}^{-1} \\ \text{ROO}^\bullet + \text{NHPI}(\text{vrij}) &\Rightarrow k^{(1)} = 1.3 \times 10^{-12} \times \exp(-0.7 \text{ kcal/mol} / RT) \times [7 \times 10^{18}] \approx 3 \times 10^6 \text{ s}^{-1} \end{aligned}$$

$\Rightarrow$ reaction of peroxy radicals with NHPI is much faster than with RH, even though the concentration of free NHPI is very low.

$$\begin{aligned} \text{PINO}^\bullet + \text{RH} &\Rightarrow k^{(1)} = 1.57 \times 10^{-11} \times \exp(-16.2 \text{ kcal/mol} / RT) \times [2 \times 10^{20}] \approx 4 \text{ s}^{-1} \\ \text{PINO}^\bullet + \text{ROOH}(\text{free}) &\Rightarrow k^{(1)} = 1.3 \times 10^{-12} \times \exp(-3.4 \text{ kcal/mol} / RT) \times [5 \times 10^{17}] \approx 9000 \text{ s}^{-1} \end{aligned}$$

$\Rightarrow$ reaction of $\text{PINO}^\bullet$ with ROO-H is much faster than with RH

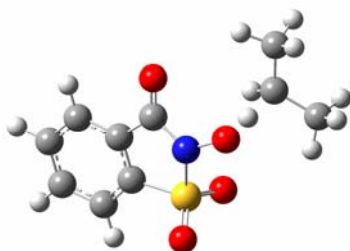
$\Rightarrow$ Equilibrium is still established.

Even if the substrate (RH) would become more reactive (*i.e.* feature weaker C-H bonds) this equilibrium condition remains fulfilled.

GEOMETRIES AND ENERGIES OF THE $>\text{NO}^\bullet + \text{R-H}$ REACTIONS CONSIDERED IN THE PAPER

I. TSs for $>\text{NO}^\bullet + \text{propane}$ (H^{sec}) (B3LYP/6-31G(d,p)-level optimisation)

Compound 1



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1141.94446826

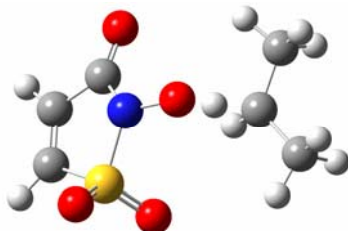
Electronic state : 2-A

Cartesian coordinates (Angs):

N	0.504651	-0.039485	1.017449
O	1.816265	-0.140641	1.282148
C	-0.102024	1.189757	0.713558
O	0.408456	2.278188	0.887910
C	-1.455740	0.909079	0.157541
C	-2.443836	1.860858	-0.081804
C	-1.699917	-0.434847	-0.135318
C	-2.913409	-0.879460	-0.641808
C	-3.899995	0.083087	-0.881230
C	-3.666654	1.436308	-0.606357
H	-2.247692	2.903380	0.145420
H	-3.088695	-1.929952	-0.847670
H	-4.858737	-0.226149	-1.285635
H	-4.449289	2.163147	-0.800274
C	3.997039	-0.771692	-1.084471
C	3.156289	0.449282	-0.813260
C	3.843246	1.730781	-0.413831
H	3.374392	-1.657888	-1.232582
H	4.593903	-0.625997	-1.998641
H	3.121939	2.483384	-0.084166
H	4.400198	2.146497	-1.268109
H	2.418994	0.115822	0.313135
H	2.325973	0.579921	-1.514380
S	-0.272770	-1.432094	0.258000
O	-0.591063	-2.449184	1.253688
O	0.501913	-1.788230	-0.933769

H	4.700938	-0.966184	-0.267913
H	4.565262	1.563940	0.392735
Rotational constants (GHz): 0.7926300 0.3442400 0.2819500			
Vibrational harmonic frequencies (cm-1):			
-1487.7499	35.5919	37.1316	
46.5753	79.8151	112.0028	
116.5988	139.7145	154.6983	
170.2623	195.4817	222.8783	
232.8257	270.8423	304.5092	
323.5869	372.1406	380.3141	
414.1648	424.7303	447.9675	
489.0510	530.0194	561.1285	
574.7942	595.7239	677.4606	
693.3421	746.8602	754.5683	
789.4897	833.4755	898.1207	
901.0622	922.4476	943.1923	
944.9586	972.9589	1011.9191	
1019.5453	1047.6767	1066.6689	
1074.6653	1134.6511	1139.7179	
1161.5082	1186.6963	1191.8765	
1197.5661	1227.5151	1290.5425	
1318.2032	1336.3948	1367.5839	
1377.0464	1412.7906	1421.1957	
1482.3539	1485.5317	1493.3513	
1494.4765	1498.6348	1501.9742	
1512.0560	1639.3575	1647.2049	
1810.8761	3001.2965	3006.4338	
3083.2715	3084.9839	3100.9988	
3135.1534	3138.2181	3199.8686	
3212.0949	3223.1293	3226.4373	
Zero-point correction (Hartree): 0.205655			

Compound 2



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -988.280782963

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-0.462927	0.397829	0.753888
O	0.681585	-0.012282	1.323066
C	-0.565979	1.637806	0.106522
O	0.219318	2.555441	0.222290
C	-1.794996	1.622593	-0.746919
C	-2.352550	0.422895	-0.918386
C	2.959926	-1.694279	-0.321464
C	2.507937	-0.261808	-0.447147
C	3.469765	0.837979	-0.073961
H	2.134130	-2.388781	-0.496344
H	3.742731	-1.910989	-1.065205
H	2.972325	1.811174	-0.046801
H	4.285917	0.895297	-0.810982
H	1.503363	-0.138865	0.492811
H	1.918919	-0.061289	-1.347818
S	-1.482716	-0.832333	0.004558
O	-2.369132	-1.442615	0.987809
O	-0.640209	-1.665272	-0.855351
H	3.388796	-1.896197	0.666003
H	3.928624	0.654281	0.903410
H	-2.145839	2.548189	-1.188571
H	-3.242143	0.146421	-1.471024

Rotational constants (GHz): 1.1660000 0.6328000 0.4836800

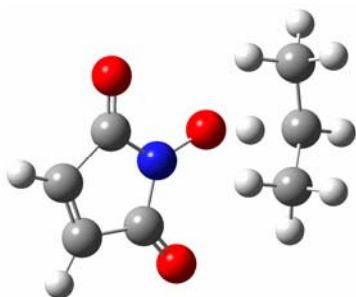
Vibrational harmonic frequencies (cm-1):

-1486.8036	33.8583	48.6468
58.0835	97.2707	119.0220
142.6016	168.5597	192.0853
221.4997	244.3075	278.6081
326.7698	347.8464	381.1343
391.1550	467.3590	493.5182
534.9597	572.2158	593.7227
664.7580	686.3364	792.7814
833.9519	840.2031	900.6920
922.2334	944.5085	961.4436

977.8996	1055.2184	1072.3007
1134.7820	1144.5266	1161.3957
1189.0348	1199.3665	1295.8483
1324.9727	1342.7305	1366.1775
1412.6284	1421.5629	1482.1466
1485.1039	1493.9971	1498.9024
1512.0808	1650.9917	1815.7314
3002.8004	3007.9907	3083.9459
3086.0840	3099.6339	3135.9482
3138.7462	3236.1669	3257.9690

Zero-point correction (Hartree): 0.157984

Compound 3



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -553.067286180

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-0.630099	0.039889	-0.575925
O	0.399863	-0.124569	-1.421679
C	-1.000183	1.276955	-0.016714
C	-1.507644	-0.994131	-0.196132
O	-0.399690	2.322306	-0.128091
O	-1.405574	-2.163816	-0.487589
C	-2.549649	-0.316123	0.648512
C	-2.258590	0.986157	0.751257
H	-3.375153	-0.866335	1.081355
H	-2.787315	1.762642	1.288936
C	2.004236	-1.152919	1.250023
C	2.498569	-0.541153	-0.037342
C	3.127675	0.828969	0.022670
H	1.422239	-2.061970	1.070368
H	1.388433	-0.449136	1.821476
H	3.010501	-1.248976	-0.696783
H	3.393158	1.194801	-0.973112

H	2.453890	1.558893	0.483106
H	1.357270	-0.342437	-0.795970
H	4.050306	0.803202	0.623259
H	2.854086	-1.427801	1.894064

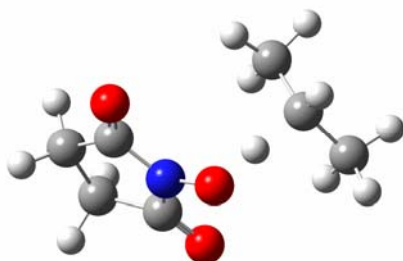
Rotational constants (GHz): 1.5058300 0.8121000 0.6422200

Vibrational harmonic frequencies (cm⁻¹):

-1564.1051	14.7703	46.8487
53.4484	115.2465	124.5839
134.9394	183.2867	200.7158
293.7730	307.6474	319.2276
358.0590	390.8676	516.0046
578.7275	591.3574	609.4508
678.9173	750.9393	762.2188
815.8744	827.5314	894.1466
929.3226	941.5112	969.6796
1043.0885	1061.7143	1068.6683
1131.6521	1168.0716	1174.1676
1192.4484	1203.9664	1334.9227
1365.7082	1403.8879	1412.6508
1428.2471	1486.4683	1490.9058
1496.0152	1506.2088	1509.3493
1652.3589	1819.7018	1864.5381
3002.8048	3007.5581	3077.0050
3090.4307	3098.5535	3124.5717
3133.9908	3247.3902	3267.4686

Zero-point correction (Hartree): 0.157817

Compound 4



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -554.309403348

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-0.595216	0.014737	-0.602993
O	0.450918	-0.194760	-1.415946
C	-0.888860	1.276896	-0.062210

C	-1.470169	-1.018269	-0.221205
O	-0.194452	2.260469	-0.181084
O	-1.327259	-2.185377	-0.499510
C	-2.578985	-0.363620	0.595239
C	-2.205112	1.129342	0.691885
H	-2.637758	-0.858476	1.568593
H	-3.533616	-0.537411	0.090393
H	-2.064714	1.476718	1.719106
H	-2.946173	1.788689	0.230478
C	2.009630	-1.036354	1.356873
C	2.519970	-0.583942	0.010253
C	3.217294	0.752552	-0.069079
H	1.385354	-1.931280	1.274209
H	1.434462	-0.248069	1.855670
H	2.996459	-1.380872	-0.569601
H	3.499244	0.998744	-1.096608
H	2.578658	1.556751	0.309326
H	1.407248	-0.408305	-0.753325
H	4.138295	0.741312	0.534159
H	2.852799	-1.283251	2.020337

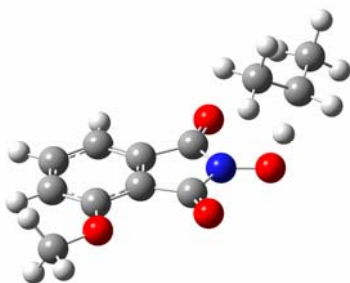
Rotational constants (GHz): 1.4832800 0.7865500 0.6312200

Vibrational harmonic frequencies (cm-1):

-1568.4816	22.6003	48.5716
58.7793	72.7352	102.1368
120.6081	162.4009	192.6020
217.2095	323.8571	335.9793
362.2626	393.4479	513.1406
558.9036	569.7531	577.2397
599.1497	660.5056	720.9529
810.3862	827.7544	891.9711
931.6181	943.6175	1008.1702
1018.5696	1045.7370	1071.7272
1117.8480	1130.9865	1163.2525
1193.2696	1202.8503	1215.8108
1245.2012	1284.0282	1319.1409
1363.8593	1384.9658	1411.9199
1426.7310	1468.6958	1480.7885
1488.9326	1491.8427	1492.9302
1499.6983	1512.1893	1825.0499
1877.7179	3004.9668	3009.9408
3077.3977	3083.9401	3089.9677
3093.4511	3097.9797	3121.1404
3124.5143	3135.5294	3136.5420

Zero-point correction (Hartree): 0.181651

Compound 5a



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -821.253749647

Electronic state : 2-A

Cartesian coordinates (Angs):

N	1.071842	0.009050	-0.907528
O	2.244118	-0.395954	-1.417950
C	0.804082	1.339547	-0.541512
C	-0.030455	-0.871453	-0.714120
O	1.594792	2.259613	-0.549210
O	0.001477	-2.065429	-0.902645
C	-1.123426	0.019987	-0.233121
C	-2.452766	-0.268531	0.101998
C	-0.632109	1.326614	-0.129083
C	-1.412693	2.386654	0.303659
C	-2.741249	2.098196	0.637211
C	-3.257341	0.803180	0.541421
H	-3.395493	2.894415	0.980248
H	-4.292102	0.630039	0.811273
C	2.883052	-1.342075	1.658114
C	3.799392	-0.961010	0.522086
C	4.613585	0.301915	0.658237
H	2.217354	-2.165822	1.383187
H	2.272750	-0.493085	1.986210
H	3.470017	-1.668957	2.530836
H	4.337346	-1.806754	0.082610
H	5.199459	0.502967	-0.243062
H	5.318327	0.218244	1.500439
H	3.973831	1.170324	0.846195
H	2.946013	-0.683829	-0.542391
H	-1.003929	3.388287	0.375489
O	-2.869733	-1.546314	-0.019345
C	-4.220219	-1.861361	0.299589
H	-4.922339	-1.314234	-0.341152
H	-4.323351	-2.931161	0.117212
H	-4.445115	-1.649070	1.351926

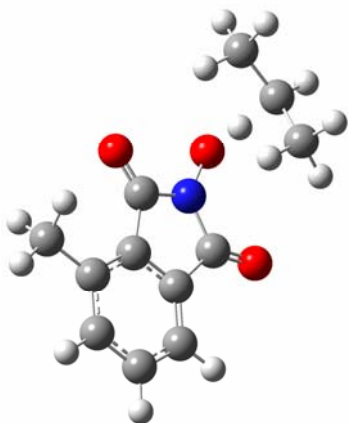
Rotational constants (GHz): 0.7929500 0.2952900 0.2450000

Vibrational harmonic frequencies (cm-1):

-1557.1188	22.7110	37.2907
42.4491	70.1407	93.9912
113.4199	116.3627	144.2258
162.5676	179.1949	189.6714
208.9247	225.3501	274.9966
298.5995	318.2327	328.7515
332.2778	371.4089	386.6700
462.1700	465.3023	528.1424
551.8529	568.3482	600.6004
652.6399	682.1229	721.8609
734.7834	769.8768	811.4185
817.4984	870.3542	894.6400
906.8098	907.2099	932.0630
942.8455	986.3061	1030.8641
1061.1629	1081.8050	1116.9941
1131.6006	1140.2116	1175.5161
1188.1677	1193.2980	1201.2713
1208.6847	1212.9843	1278.0368
1333.0275	1365.8913	1391.5655
1408.7519	1414.8372	1427.9567
1475.7509	1484.2547	1487.4834
1491.2722	1496.9498	1506.1991
1506.9210	1510.3800	1513.8236
1534.2446	1647.5529	1662.7042
1816.3816	1856.9867	3000.7915
3005.4947	3026.4059	3077.4007
3090.0567	3092.6213	3098.5281
3125.2561	3133.6003	3165.0091
3196.5816	3226.9220	3231.7036

Zero-point correction (Hartree): 0.238178

Compound 5b



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -746.054283894

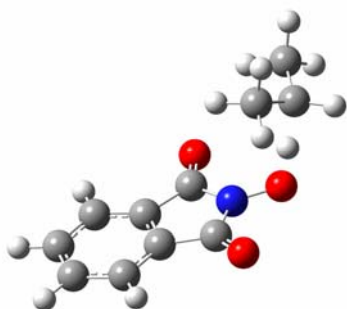
Electronic state : 2-A

Cartesian coordinates (Angs):

N	0.765953	-0.323452	-0.883565
O	2.000992	-0.308504	-1.406666
C	0.010867	0.849162	-0.646714
C	0.076476	-1.513098	-0.555798
O	0.415830	1.984276	-0.790889
O	0.528157	-2.635275	-0.616269
C	-1.271439	-1.045831	-0.118007
C	-2.359201	-1.794897	0.301201
C	-1.313535	0.353627	-0.172930
C	-2.452884	1.075239	0.191327
C	-3.553322	0.306009	0.614139
C	-3.512660	-1.090641	0.668986
H	-2.309334	-2.877973	0.339144
H	-4.464849	0.819625	0.908370
H	-4.391558	-1.633716	1.003813
C	2.969885	-0.664028	1.699353
C	3.664820	-0.053447	0.507740
C	3.936537	1.430486	0.525250
H	2.668517	-1.698054	1.506567
H	2.082574	-0.089098	1.987749
H	3.641862	-0.672330	2.571784
H	4.482929	-0.662652	0.111001
H	4.394393	1.767759	-0.408865
H	4.626783	1.686084	1.344413
H	3.016162	2.003797	0.676851
H	2.766444	-0.212427	-0.539455
C	-2.510014	2.579733	0.130675
H	-1.688868	3.029670	0.695654
H	-2.401131	2.934445	-0.899445

H	-3.458588	2.951160	0.526633
Rotational constants (GHz):	0.8467900	0.3623900	0.2950400
Vibrational harmonic frequencies (cm-1):			
-1562.6472	26.9269	39.2495	
46.0815	49.0723	94.8453	
101.6328	115.4132	144.5548	
180.7048	189.4943	206.8892	
213.0331	229.6886	313.2506	
326.0519	331.3883	360.0293	
384.7608	461.3216	464.9093	
497.8093	508.9384	535.4427	
586.0144	632.4346	679.1635	
722.1471	726.1664	780.2252	
810.5190	818.3079	868.0043	
895.3103	913.4718	931.8119	
933.2435	943.6430	996.0483	
1010.4328	1045.9676	1061.0170	
1064.7999	1110.9998	1131.0699	
1138.6632	1188.3301	1192.5351	
1199.6134	1209.2280	1263.0598	
1285.6513	1366.6390	1388.6966	
1401.3037	1415.3209	1427.3430	
1431.0610	1460.1055	1486.8891	
1490.4674	1491.6650	1495.4505	
1502.9535	1503.7079	1510.7440	
1522.5067	1644.9251	1665.3293	
1810.4138	1853.6921	3001.7971	
3006.6498	3057.8464	3077.6982	
3091.1073	3099.0913	3120.3346	
3125.3451	3134.3299	3140.7519	
3185.3620	3202.6601	3221.8795	
Zero-point correction (Hartree): 0.233042			

Compound 5c



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -706.732765066

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-0.558972	0.156922	-0.881749
O	-1.782445	0.277433	-1.417082
C	0.045127	-1.091065	-0.601768
C	0.269051	1.266924	-0.587126
O	-0.483519	-2.175433	-0.713595
O	-0.044521	2.431773	-0.689863
C	1.548690	0.655746	-0.121950
C	2.725891	1.267882	0.282205
C	1.416283	-0.737912	-0.130482
C	2.456700	-1.565686	0.264948
C	3.651288	-0.955345	0.671314
C	3.783692	0.438639	0.679843
H	2.816418	2.349275	0.286082
H	4.488369	-1.571765	0.985120
H	4.721421	0.882578	1.000373
C	-2.748822	0.891443	1.654856
C	-3.482676	0.289675	0.482089
C	-3.902612	-1.156663	0.572007
H	-2.344374	1.879796	1.416711
H	-1.927098	0.248546	1.990342
H	-3.430056	1.010778	2.511822
H	-4.230579	0.954531	0.038613
H	-4.375141	-1.497969	-0.353216
H	-4.629671	-1.295779	1.387328
H	-3.048072	-1.809886	0.776157
H	-2.562308	0.304179	-0.553894
H	2.342111	-2.644741	0.255505

Rotational constants (GHz): 1.0722600 0.3847100 0.3344000

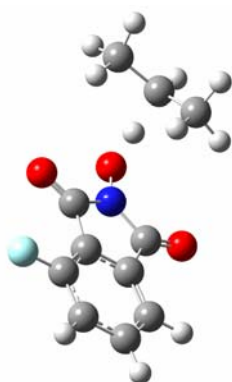
Vibrational harmonic frequencies (cm-1):

-1564.9262	25.8747	38.3510
45.2560	94.5574	115.4766
139.0255	145.8272	178.1754
200.4417	219.3292	239.6383

315.7574	328.0365	339.8080
383.1252	413.2715	464.0865
473.2739	524.1644	532.6620
603.9751	677.0171	704.2809
715.9176	719.3753	782.0194
795.5653	818.5154	891.7407
895.4606	911.3959	930.4523
943.0160	974.5679	1009.0064
1011.8123	1045.6846	1060.1275
1096.1817	1131.4223	1139.1738
1184.7698	1192.1474	1192.6790
1200.3918	1229.6746	1312.1524
1366.3519	1388.8666	1403.6013
1415.2822	1427.4903	1486.4027
1491.4433	1494.6277	1501.4263
1503.1715	1506.5062	1510.5318
1656.1193	1661.8917	1819.3707
1860.1359	3002.3103	3007.1161
3077.7320	3090.2270	3098.4166
3125.7227	3134.1790	3193.5259
3206.4717	3218.2515	3221.4984

Zero-point correction (Hartree): 0.205612

Compound 5d



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -805.959240478
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	0.762062	-0.321298	-0.879757
O	1.997391	-0.340883	-1.399837
C	0.041404	0.878638	-0.653073
C	0.044011	-1.490540	-0.550971

O	0.478284	1.996440	-0.803288
O	0.462307	-2.625505	-0.605260
C	-1.296371	-0.990830	-0.118527
C	-2.402634	-1.712756	0.297705
C	-1.293563	0.410476	-0.180528
C	-2.434586	1.106929	0.186251
C	-3.569087	0.406370	0.607867
C	-3.548184	-0.988942	0.661319
H	-2.374557	-2.796167	0.336737
H	-4.453844	0.967400	0.888933
H	-4.437711	-1.516471	0.991406
C	2.970830	-0.675707	1.711038
C	3.667612	-0.089104	0.508358
C	3.965235	1.390004	0.509452
H	2.653834	-1.707719	1.532876
H	2.094337	-0.084134	1.998873
H	3.648615	-0.683492	2.578840
H	4.473670	-0.715846	0.113955
H	4.417094	1.711231	-0.433129
H	4.670913	1.638606	1.317444
H	3.057916	1.981533	0.668749
H	2.767061	-0.244563	-0.529099
F	-2.469291	2.443451	0.142938

Rotational constants (GHz): 0.8501200 0.3554200 0.2902700

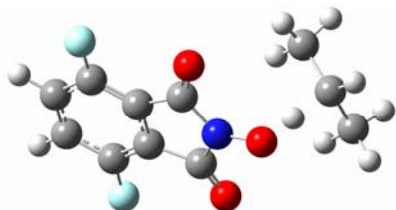
Vibrational harmonic frequencies (cm-1):

-1562.1038	26.1377	39.5674
48.0530	92.6736	100.6133
116.1240	144.4730	179.9018
187.1746	197.4893	211.9555
250.9823	315.3733	325.3789
331.6011	374.2431	394.8920
458.7966	465.4246	514.5639
542.6917	549.3004	585.7085
635.2715	671.0350	721.1609
731.1200	769.4245	813.0932
819.6589	878.7354	895.1709
926.5488	930.5408	937.2147
943.6147	992.6101	1049.5393
1063.7694	1087.4009	1131.0691
1139.6872	1181.4036	1192.2120
1198.4176	1206.5344	1270.2830
1309.1476	1366.6388	1387.9661
1410.2428	1414.9939	1427.3303
1477.2044	1486.3300	1491.5320
1493.9802	1502.0164	1510.7305
1525.3590	1660.3699	1666.0833

1821.2678	1861.2491	3003.0183
3007.9024	3077.7448	3092.1613
3098.6326	3125.1243	3135.4554
3204.0589	3223.4370	3228.5070

Zero-point correction (Hartree): 0.197397

Compound 5e



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -905.183804891

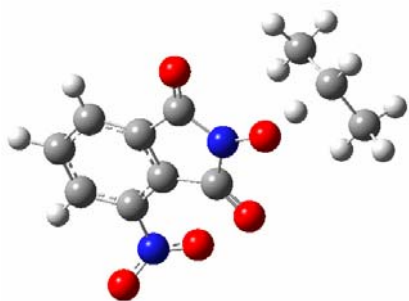
Electronic state : 2-A

Cartesian coordinates (Angs):

N	0.904704	-0.180299	-0.903424
O	2.134257	-0.311194	-1.419360
C	0.314709	1.075179	-0.632489
C	0.068285	-1.286627	-0.624925
O	0.861027	2.149339	-0.735788
O	0.379740	-2.450250	-0.725469
C	-1.214166	-0.663744	-0.179729
C	-2.413064	-1.238095	0.207458
C	-1.068246	0.733768	-0.184132
C	-2.122223	1.546070	0.198722
C	-3.336052	0.967143	0.587060
C	-3.480715	-0.418287	0.591443
H	-4.155194	1.613652	0.882230
H	-4.415518	-0.879751	0.890253
C	3.061502	-0.958502	1.661658
C	3.810221	-0.353221	0.499978
C	4.247257	1.086830	0.608067
H	2.649163	-1.940684	1.411948
H	2.244625	-0.309978	1.998286
H	3.736045	-1.092467	2.521609
H	4.554362	-1.022209	0.056184
H	4.724638	1.434177	-0.312332
H	4.975694	1.205360	1.425279
H	3.401334	1.748206	0.821344
H	2.904621	-0.349272	-0.540423
F	-2.002063	2.878221	0.203326

F -2.571042 -2.566129 0.220658
 Rotational constants (GHz): 0.6806800 0.3308600 0.2537500
 Vibrational harmonic frequencies (cm-1):
 -1563.1315 24.3679 35.3981
 43.0705 91.3693 92.8802
 114.8367 140.9190 151.7042
 178.3224 181.5914 199.0695
 218.6380 278.3587 317.6243
 328.6992 361.1746 389.3549
 393.0487 394.5154 450.4209
 469.8906 503.0165 552.7017
 560.8141 566.1188 623.8418
 672.5255 705.6775 740.4282
 768.5709 818.8722 845.3809
 851.1265 895.1280 924.6351
 929.2073 942.6701 946.6040
 959.7247 1063.2023 1107.5064
 1131.0831 1142.2446 1182.1726
 1192.2922 1201.1675 1233.6203
 1299.3899 1317.0997 1366.1521
 1386.4264 1414.8985 1416.3935
 1426.6537 1439.1629 1485.4183
 1491.1170 1493.0109 1500.8251
 1510.5826 1544.1829 1665.4272
 1674.5092 1823.5292 1863.1275
 3003.6766 3008.5234 3077.6157
 3090.8080 3098.4543 3126.1403
 3134.9573 3220.8622 3232.5393
 Zero-point correction (Hartree): 0.189150

Compound 5f



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -911.212200434
 Electronic state : 2-A

Cartesian coordinates (Angs):

N	-1.178246	0.488438	-0.831695
O	-2.384180	0.291374	-1.380098
C	-0.217778	-0.547830	-0.717161
C	-0.704599	1.757548	-0.453842
O	-0.408277	-1.698687	-1.022575
O	-1.335969	2.790086	-0.441832
C	0.718817	1.517716	-0.071339
C	1.658190	2.453500	0.335874
C	1.005225	0.149669	-0.176407
C	2.291385	-0.279884	0.136717
C	3.268835	0.646612	0.514214
C	2.951283	2.001309	0.621976
H	1.386950	3.501081	0.413926
H	4.268277	0.285880	0.726173
H	3.718369	2.703688	0.931387
C	-3.469121	0.204451	1.710811
C	-3.977404	-0.464844	0.457645
C	-3.916362	-1.970521	0.381202
H	-3.406639	1.290707	1.594910
H	-2.483085	-0.175917	2.000621
H	-4.148593	0.001151	2.552907
H	-4.901525	-0.027614	0.065900
H	-4.238678	-2.338955	-0.596518
H	-4.578499	-2.417299	1.139032
H	-2.903967	-2.342870	0.567710
H	-3.127799	-0.045552	-0.532733
N	2.675278	-1.703556	0.132212
O	3.825080	-1.963381	-0.221075
O	1.838988	-2.511246	0.514945

Rotational constants (GHz): 0.6322400 0.2985000 0.2283500

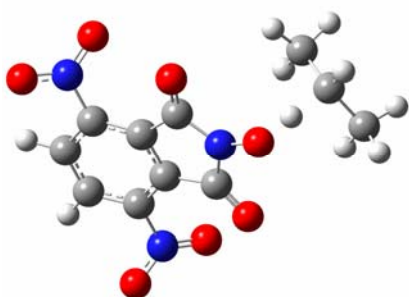
Vibrational harmonic frequencies (cm-1):

-1551.2815	1.9899	35.9700
36.8990	57.4150	74.7252
94.4132	115.5093	142.7068
166.6459	179.7656	187.2093
193.3726	217.8297	276.2423
321.1515	328.8456	341.5000
353.9422	376.5323	405.3609
464.5096	473.8682	518.6650
550.5123	594.1032	612.3847
672.2269	709.4854	717.5672
755.8710	769.7775	779.6752
819.1540	838.4287	877.9175
894.7369	910.0507	925.9381
941.1267	956.1086	1006.3200

1038.5666	1067.2572	1090.6591
1130.4869	1148.1297	1171.0890
1183.8124	1191.2645	1199.5023
1222.0628	1271.6437	1364.9727
1386.2481	1401.2197	1411.9664
1412.1464	1426.3056	1475.4967
1483.4984	1489.6123	1490.3667
1499.5272	1503.7203	1509.4983
1638.5375	1651.0524	1672.5936
1826.0683	1866.6188	3005.1154
3010.0549	3078.1800	3091.7240
3097.6452	3125.0406	3136.3926
3210.6262	3225.8023	3240.7589

Zero-point correction (Hartree): 0.207636

Compound 5g



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1115.68710083

Electronic state : 2-A

Cartesian coordinates (Angs):

N	1.348217	-0.274396	-0.881644
O	2.543276	-0.465596	-1.452067
C	0.815579	1.011693	-0.662017
C	0.440793	-1.331700	-0.665861
O	1.394909	2.052560	-0.848385
O	0.665280	-2.500077	-0.858565
C	-0.815149	-0.640362	-0.199693
C	-2.073398	-1.137696	0.120965
C	-0.593371	0.745458	-0.197081
C	-1.633785	1.609400	0.126468
C	-2.912609	1.109352	0.382693
C	-3.132500	-0.264598	0.379828
H	-3.718539	1.803391	0.589118
H	-4.114991	-0.673258	0.583685
C	3.548048	-1.263683	1.565296
C	4.283531	-0.654445	0.396942
C	4.805353	0.753953	0.541760

H	3.077037	-2.214824	1.299802
H	2.780617	-0.587364	1.958436
H	4.248933	-1.462687	2.390526
H	4.974150	-1.344351	-0.098898
H	5.251382	1.118426	-0.387541
H	5.582917	0.791181	1.320165
H	4.013380	1.450131	0.836452
H	3.357046	-0.567420	-0.592781
N	-1.441298	3.067977	0.243139
O	-2.336983	3.774685	-0.213840
O	-0.434768	3.450858	0.822539
N	-2.346294	-2.583980	0.230554
O	-3.416869	-2.973253	-0.230910
O	-1.511254	-3.264759	0.808840

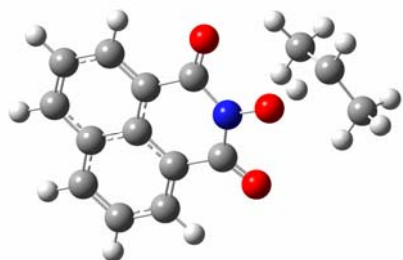
Rotational constants (GHz): 0.3509500 0.2667400 0.1673100

Vibrational harmonic frequencies (cm-1):

-1539.9433	17.5020	32.0357
39.0297	47.0188	63.5819
70.6923	73.2185	93.5022
111.9216	142.4003	162.6411
170.4674	183.0323	191.8803
218.8827	221.8944	280.4262
304.2961	325.8493	329.8618
346.4105	374.6441	391.8753
395.6724	460.0962	478.4292
527.8547	532.3968	604.7224
605.2469	619.9839	688.0327
712.9143	731.2473	748.3679
766.0524	782.5009	796.7801
820.6061	855.6004	876.6769
893.6161	895.8513	924.8228
928.6526	941.7101	985.9718
1070.4584	1077.2791	1129.2419
1159.0749	1169.3356	1182.5802
1190.2634	1199.2488	1217.7986
1243.6320	1364.8307	1379.5379
1392.9861	1408.6136	1413.9876
1414.3631	1425.0621	1438.1964
1478.5693	1486.6710	1490.6591
1498.3165	1500.9615	1510.0425
1637.0758	1643.1869	1667.8305
1676.2699	1831.9608	1871.9224
3007.4017	3012.4665	3079.3446
3091.0512	3098.3052	3127.0695
3136.3303	3236.6090	3246.5743

Zero-point correction (Hartree): 0.209528

Compound 6



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -860.387617132

Electronic state : 2-A

Cartesian coordinates (Angs):

N	1.104629	-0.195631	-0.858959
O	2.356900	-0.320667	-1.340889
C	0.645412	1.121583	-0.615477
C	0.403072	-1.399324	-0.597591
O	1.396890	2.075223	-0.716032
O	0.959695	-2.478360	-0.686513
C	-0.786369	1.231312	-0.240974
C	-1.578936	0.067090	-0.060365
C	-1.022580	-1.228941	-0.222425
C	-2.954009	0.201849	0.303388
C	-1.341177	2.486991	-0.064717
C	-2.699707	2.623921	0.289219
C	-3.489401	1.506661	0.469288
C	-3.727451	-0.974827	0.488017
C	-3.164823	-2.224393	0.325867
C	-1.805612	-2.353558	-0.028270
H	-0.707813	3.356183	-0.207002
H	-3.121295	3.615599	0.420301
H	-4.535661	1.612141	0.743836
H	-4.774320	-0.875606	0.762551
H	-3.767071	-3.115816	0.470824
H	-1.349157	-3.329245	-0.157307
C	3.190105	-0.736223	1.814525
C	4.002710	-0.365848	0.597592
C	4.617301	1.012041	0.551061
H	2.674740	-1.691548	1.678465
H	2.448586	0.034554	2.053448
H	3.843504	-0.834356	2.695439
H	4.659484	-1.168371	0.247256
H	5.139094	1.188013	-0.393875
H	5.350819	1.133399	1.363379
H	3.856044	1.789513	0.666456
H	3.111551	-0.364612	-0.438413

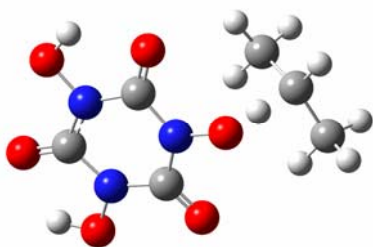
Rotational constants (GHz): 0.6430400 0.2800900 0.2186600

Vibrational harmonic frequencies (cm-1):

-1585.9110	21.3670	37.1553
43.2379	76.6387	84.8731
120.2742	146.0573	169.2042
181.5977	205.6585	233.9205
243.4657	290.2304	338.8434
365.1652	372.4147	378.9148
409.8084	425.8947	434.7567
441.3061	479.1941	516.4578
550.4454	554.9919	562.6262
621.6503	642.3293	709.8147
724.5520	737.1768	772.3793
799.8177	809.2679	812.3597
849.0658	892.5588	902.8948
928.9344	933.1679	943.3684
952.6981	966.9045	999.2232
1005.7394	1053.2895	1064.4613
1070.7616	1105.2515	1131.0234
1137.6157	1182.7864	1193.9940
1199.5059	1204.5635	1209.9320
1249.6334	1259.4668	1269.6352
1358.7133	1365.4782	1401.1559
1405.3627	1412.7050	1423.9126
1443.3190	1475.5256	1480.8823
1490.2576	1493.6287	1499.7755
1504.5253	1513.0480	1558.7879
1632.0087	1641.0826	1674.4163
1767.5665	1794.1421	3002.4976
3007.4165	3077.7886	3093.8284
3097.9024	3127.6221	3136.2720
3186.1610	3188.6312	3207.0887
3207.6529	3224.4388	3225.3050

Zero-point correction (Hartree): 0.253194

Compound 7



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -850.058603971

Electronic state : 2-A

Cartesian coordinates (Angs):

N	0.301284	-0.133790	-0.796440
O	1.482129	-0.311129	-1.417076
C	-0.075410	1.206512	-0.500382
C	-0.440760	-1.275053	-0.510066
O	0.653985	2.152249	-0.653951
O	-0.073005	-2.426063	-0.668203
C	2.655978	-0.947536	1.590339
C	3.326242	-0.443896	0.334917
C	3.914678	0.945620	0.353060
H	2.130789	-1.892046	1.418904
H	1.948605	-0.214622	1.994941
H	3.408069	-1.127568	2.373635
H	3.951739	-1.194312	-0.159585
H	4.312275	1.228268	-0.625413
H	4.743937	0.995089	1.075513
H	3.171279	1.692778	0.646762
H	2.341435	-0.377509	-0.589921
N	-1.380080	1.271129	-0.025725
N	-1.711338	-1.006986	-0.007920
C	-2.242970	0.226030	0.300027
O	-3.334391	0.441103	0.794885
O	-1.834794	2.536607	0.321070
H	-2.725347	2.325401	0.676536
O	-2.480866	-2.114711	0.317385
H	-1.882843	-2.842464	0.038961

Rotational constants (GHz): 0.8505500 0.4471400 0.3417400

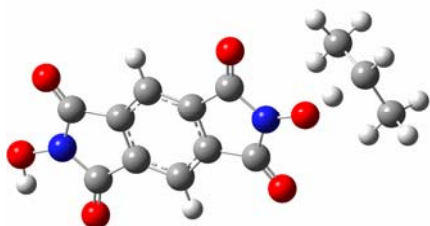
Vibrational harmonic frequencies (cm-1):

-1526.5315	18.8910	40.1745
45.3704	81.4808	86.7758
93.6949	121.5405	144.4020
167.3208	176.3015	189.8852
219.7733	312.2077	326.3613
334.9729	353.0281	363.0105
367.5797	380.2948	383.3593
398.5855	470.1880	470.6551
508.3400	577.9382	645.1406
691.1878	693.7306	701.6702
820.6971	829.3044	894.0350
927.5830	942.2747	1012.9914
1039.8536	1081.2875	1132.0313
1133.9029	1191.6221	1199.5380
1206.1071	1225.8226	1311.1049
1365.7485	1406.5527	1412.8617
1424.9774	1458.9524	1478.5878
1488.4870	1491.3166	1498.5072

1510.5072	1531.6839	1544.8195
1784.1878	1812.6888	1865.4980
3007.5078	3012.5109	3077.4221
3093.5238	3099.8984	3125.0779
3139.6978	3583.3108	3587.5767

Zero-point correction (Hartree): 0.175678

Compound 8



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1062.71743737

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-2.335688	0.170408	-0.906772
O	-3.629149	0.225872	-1.250135
C	-1.622731	-1.041320	-0.771628
C	-1.540200	1.321555	-0.706370
O	-2.087690	-2.156260	-0.841558
O	-1.925817	2.467630	-0.718319
C	-0.164672	0.784281	-0.465192
C	1.017220	1.484539	-0.226193
C	-0.214045	-0.615602	-0.504648
C	0.915335	-1.408883	-0.308395
C	2.093803	-0.709240	-0.074145
C	2.144250	0.694766	-0.033638
H	1.054164	2.568103	-0.194306
C	-4.209815	0.777611	1.937795
C	-5.043443	0.119748	0.865881
C	-5.356067	-1.349414	1.008572
H	-3.899894	1.786590	1.649766
H	-3.316180	0.189017	2.174676
H	-4.789289	0.864368	2.869889
H	-5.884399	0.730964	0.522849
H	-5.906154	-1.731558	0.144346
H	-5.977822	-1.521839	1.900708
H	-4.444982	-1.945893	1.122306
H	-4.280460	0.190318	-0.271753

H	0.874340	-2.492301	-0.338470
C	3.556714	1.131053	0.240867
C	3.472677	-1.222366	0.172235
O	3.923960	-2.352379	0.232919
O	4.011621	2.244667	0.353504
N	4.249274	-0.082729	0.341186
O	5.599298	-0.168891	0.595081
H	5.743635	-1.137007	0.596308

Rotational constants (GHz): 0.7059000 0.1475400 0.1332900

Vibrational harmonic frequencies (cm-1):

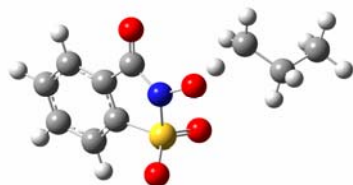
-1558.3136	23.8029	29.7761
39.2119	66.4345	74.4636
105.7497	108.7652	112.3165
145.7165	149.4778	174.4497
185.4447	202.0113	205.3699
247.8262	256.2194	258.9214
261.2365	298.4317	315.5736
335.4394	351.6548	377.0724
412.2423	423.1844	503.0433
513.4643	554.3805	567.8184
591.2483	609.1558	645.0540
666.0430	688.0207	725.3762
744.3108	757.5232	761.8343
780.9280	822.1548	846.7702
895.1921	927.7901	940.6534
942.6087	946.1193	998.7150
1023.5565	1065.2070	1071.8598
1130.8072	1136.9710	1148.0812
1158.7176	1174.5717	1191.4989
1199.9489	1237.7065	1282.5415
1366.7861	1388.7737	1409.5922
1413.8273	1426.2311	1431.3367
1484.7562	1487.2068	1490.0182
1490.7416	1494.5553	1500.0583
1509.7945	1519.8478	1648.1061
1661.3092	1803.2271	1822.1814
1859.1416	1867.1359	3005.5641
3010.4761	3077.6041	3091.1715
3098.6507	3126.2321	3135.7254
3230.6619	3231.3985	3643.9653

Zero-point correction (Hartree): 0.223571

II. TSs for $\text{>NO}^\bullet + \text{propane (H}^{\text{prim}}/\text{H}^{\text{sec}})$, *t*-butane, propene and 1-butene (B3LYP/6-31G(d,p)-level optimisation)

A. Compound 1

H^{prim}



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1141.93753097

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-0.267350	0.293284	-1.175467
O	-1.535817	0.434947	-1.600436
C	0.485744	1.382408	-0.705940
O	0.181653	2.547991	-0.850423
C	1.696253	0.841636	-0.025167
C	2.784131	1.595970	0.407057
C	1.685839	-0.540875	0.173927
C	2.739520	-1.215902	0.774885
C	3.827351	-0.450666	1.208650
C	3.847909	0.937960	1.028324
H	2.785626	2.669604	0.251178
H	2.719194	-2.292391	0.906814
H	4.665905	-0.942884	1.691245
H	4.704715	1.508479	1.372980
C	-4.026683	-0.140518	0.472401
C	-3.071246	1.017044	0.374695
H	-3.463694	-1.063589	0.644973
H	-2.193719	0.708844	-0.720047
H	-2.347743	1.121963	1.185423
S	0.180417	-1.257265	-0.464026
O	0.455845	-2.239839	-1.505927
O	-0.780154	-1.565241	0.598970
H	-3.472718	1.970563	0.026153
H	-4.566521	-0.261295	-0.474460
C	-5.050170	0.057857	1.612734
H	-5.649157	0.961005	1.456919
H	-5.732192	-0.797352	1.662790
H	-4.549021	0.147960	2.581841

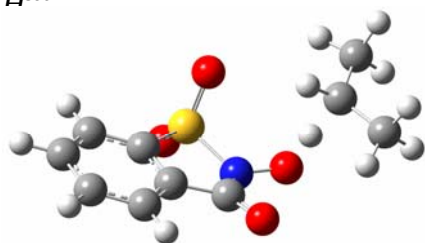
Rotational constants (GHz): 0.7990400 0.2978300 0.2678900

Vibrational harmonic frequencies (cm-1):

-1352.7500	25.6497	37.9475
43.5138	68.0007	90.6639
112.0176	112.3633	149.8197
161.1737	222.5432	245.9672
263.0660	298.5537	322.3241
332.0710	370.3178	405.8804
421.5566	439.4349	489.0498
513.5692	532.4477	562.8514
596.8166	619.6800	678.5988
693.9926	747.1645	755.3381
762.5053	790.5612	898.4185
900.6775	914.1341	939.4362
942.5404	973.5654	1012.2609
1017.3485	1028.2065	1047.4270
1070.1685	1098.9077	1139.9832
1161.5084	1164.7332	1191.4968
1216.1114	1227.5976	1291.8355
1319.5169	1322.9580	1337.1151
1354.8079	1377.0844	1412.1778
1470.8185	1492.8627	1493.9709
1502.1198	1504.7052	1508.0048
1521.7033	1639.6153	1647.4073
1819.0992	3044.4721	3051.2234
3095.8482	3098.6592	3119.6557
3124.8668	3186.1554	3199.9642
3212.2198	3223.3027	3226.7152

Zero-point correction (Hartree): 0.205967

L^{sec}



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1141.94446826

Electronic state : 2-A

Cartesian coordinates (Angs):

N	0.504651	-0.039485	1.017449
O	1.816265	-0.140641	1.282148
C	-0.102024	1.189757	0.713558
O	0.408456	2.278188	0.887910
C	-1.455740	0.909079	0.157541

C	-2.443836	1.860858	-0.081804
C	-1.699917	-0.434847	-0.135318
C	-2.913409	-0.879460	-0.641808
C	-3.899995	0.083087	-0.881230
C	-3.666654	1.436308	-0.606357
H	-2.247692	2.903380	0.145420
H	-3.088695	-1.929952	-0.847670
H	-4.858737	-0.226149	-1.285635
H	-4.449289	2.163147	-0.800274
C	3.997039	-0.771692	-1.084471
C	3.156289	0.449282	-0.813260
C	3.843246	1.730781	-0.413831
H	3.374392	-1.657888	-1.232582
H	4.593903	-0.625997	-1.998641
H	3.121939	2.483384	-0.084166
H	4.400198	2.146497	-1.268109
H	2.418994	0.115822	0.313135
H	2.325973	0.579921	-1.514380
S	-0.272770	-1.432094	0.258000
O	-0.591063	-2.449184	1.253688
O	0.501913	-1.788230	-0.933769
H	4.700938	-0.966184	-0.267913
H	4.565262	1.563940	0.392735

Rotational constants (GHz): 0.7926300 0.3442400 0.2819500

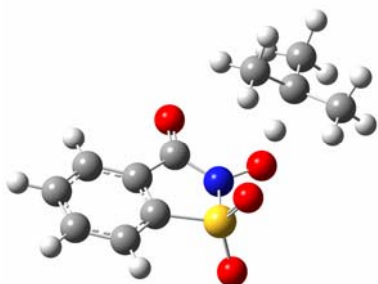
Vibrational harmonic frequencies (cm⁻¹):

-1487.7499	35.5919	37.1316
46.5753	79.8151	112.0028
116.5988	139.7145	154.6983
170.2623	195.4817	222.8783
232.8257	270.8423	304.5092
323.5869	372.1406	380.3141
414.1648	424.7303	447.9675
489.0510	530.0194	561.1285
574.7942	595.7239	677.4606
693.3421	746.8602	754.5683
789.4897	833.4755	898.1207
901.0622	922.4476	943.1923
944.9586	972.9589	1011.9191
1019.5453	1047.6767	1066.6689
1074.6653	1134.6511	1139.7179
1161.5082	1186.6963	1191.8765
1197.5661	1227.5151	1290.5425
1318.2032	1336.3948	1367.5839
1377.0464	1412.7906	1421.1957
1482.3539	1485.5317	1493.3513
1494.4765	1498.6348	1501.9742

1512.0560	1639.3575	1647.2049
1810.8761	3001.2965	3006.4338
3083.2715	3084.9839	3100.9988
3135.1534	3138.2181	3199.8686
3212.0949	3223.1293	3226.4373

Zero-point correction (Hartree): 0.205655

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E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1181.26555791

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-0.316438	0.125613	-1.045121
O	-1.606987	0.273815	-1.366554
C	0.271183	-1.125808	-0.817704
O	-0.251963	-2.195042	-1.063262
C	1.892683	0.426357	0.121875
C	3.108645	0.821346	0.662194
C	1.623070	-0.897703	-0.233036
C	2.588122	-1.879957	-0.025946
C	3.813591	-1.505885	0.530306
C	4.072138	-0.171948	0.868600
S	0.493415	1.472757	-0.243099
O	-0.269151	1.817892	0.960110
O	0.837503	2.510514	-1.208611
H	3.303505	1.857435	0.917613
H	4.578383	-2.257494	0.699478
H	5.032320	0.098263	1.296822
C	-2.381500	-0.951228	1.647398
C	-3.207440	-0.361785	0.521687
C	-4.053915	-1.358316	-0.245040
C	-3.863730	0.968540	0.829383
H	-1.678564	-0.220025	2.057173
H	-1.829837	-1.837821	1.320281
H	-3.046737	-1.263967	2.467940

H	-4.538753	-0.895624	-1.110237
H	-4.848470	-1.757059	0.404771
H	-3.452428	-2.202403	-0.594937
H	-4.651323	0.833618	1.587442
H	-3.140298	1.687538	1.223964
H	-4.335792	1.400110	-0.058765
H	-2.296285	-0.018316	-0.436049
H	2.372428	-2.906762	-0.301817

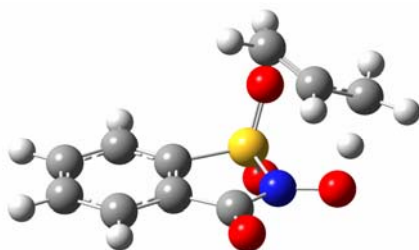
Rotational constants (GHz): 0.7385100 0.3039500 0.2583800

Vibrational harmonic frequencies (cm-1):

-1513.2141	31.1559	37.6030
55.5709	83.5435	107.8479
113.0014	118.5377	152.3571
165.9312	186.0416	213.1164
222.4652	245.9583	270.0959
283.6067	322.2412	344.8341
372.0027	377.5046	380.6924
415.4951	426.8355	449.9052
488.5282	531.1349	553.5324
562.9598	597.4107	675.9132
693.1412	747.0296	753.1103
788.2722	797.6864	897.7176
933.5968	935.2853	944.9537
972.2095	977.0297	1007.6313
1011.3884	1015.1607	1024.5173
1048.1764	1070.3996	1110.0357
1139.6249	1161.4571	1190.7005
1196.1522	1227.9683	1267.5912
1280.2931	1293.4978	1322.3201
1334.1156	1377.1566	1403.6926
1408.3351	1431.5263	1474.0969
1484.8340	1493.3297	1494.4716
1499.2135	1501.1826	1502.2765
1503.7635	1527.7265	1639.3988
1647.1580	1806.8456	3000.1239
3002.9580	3010.0841	3090.1690
3090.4389	3093.9518	3131.4067
3134.3465	3136.6185	3199.6491
3211.8670	3222.7847	3226.2282

Zero-point correction (Hartree): 0.233905

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E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1140.71170028

Electronic state : 2-A

Cartesian coordinates (Angs):

N	0.781739	0.322299	-1.038635
O	2.031037	0.532272	-1.434879
C	0.112872	-0.905567	-1.151882
O	0.548061	-1.887542	-1.716279
C	-1.207509	-0.765014	-0.473343
C	-2.203757	-1.737477	-0.452758
C	-1.413560	0.453496	0.178856
C	-2.592065	0.750149	0.849799
C	-3.586254	-0.234136	0.868744
C	-3.393595	-1.462632	0.225455
H	-2.037908	-2.680986	-0.961984
H	-2.737110	1.706364	1.341112
H	-4.519001	-0.038887	1.388548
H	-4.181329	-2.209088	0.252293
C	3.588133	-0.319676	0.410477
H	2.777102	0.089966	-0.577130
H	3.639723	0.583843	1.018194
S	0.001522	1.524887	-0.012243
O	-0.329928	2.714412	-0.789393
O	0.774644	1.656348	1.224393
C	2.937768	-1.462592	1.003891
H	3.076170	-2.422442	0.508055
C	2.128974	-1.405095	2.093510
H	1.932196	-0.464570	2.599616
H	1.652250	-2.296200	2.489559
H	4.484823	-0.514927	-0.179156

Rotational constants (GHz): 0.7019400 0.4081300 0.3488400

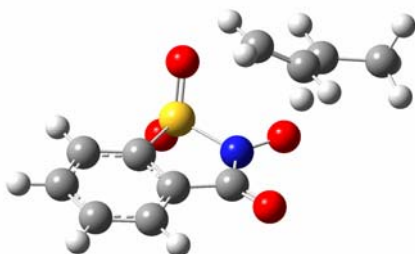
Vibrational harmonic frequencies (cm-1):

-1705.9510	32.0418	51.4202
57.9503	66.3957	83.1338
110.0935	151.8425	157.1448
210.8581	224.6449	265.9044
304.7562	326.8917	371.7892

395.1720	418.2393	423.3146
439.6795	484.8529	516.9345
529.1413	562.1961	587.2408
599.3133	633.2537	672.4552
692.7939	746.3572	751.5855
786.6105	897.1664	916.6493
947.1697	956.8707	971.7277
990.2166	1009.2889	1011.6184
1026.5319	1048.4036	1068.2177
1076.5826	1139.5427	1162.0137
1191.2668	1198.0059	1221.8905
1232.3688	1299.3940	1320.9726
1331.0127	1338.1171	1376.7773
1440.8928	1474.2490	1493.5036
1501.8129	1509.3472	1608.8300
1639.3667	1647.4216	1815.4074
3108.4052	3160.8806	3167.9811
3199.8465	3200.0445	3211.9120
3222.3648	3226.2610	3259.9982

Zero-point correction (Hartree): 0.182878

1-butene



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1180.03085332

Electronic state : 2-A

Cartesian coordinates (Angs):

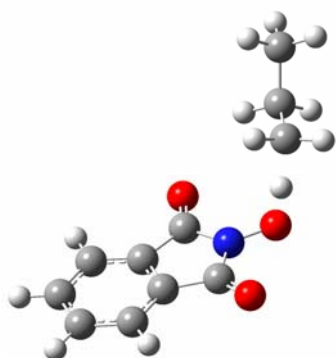
N	0.485295	0.375440	-1.006166
O	1.741127	0.634896	-1.344963
C	-0.114975	-0.888008	-1.113781
O	0.389020	-1.856205	-1.644288
C	-1.461677	-0.805692	-0.479062
C	-2.408030	-1.827055	-0.474515
C	-1.748284	0.408482	0.150405
C	-2.960360	0.653481	0.781209
C	-3.903813	-0.379668	0.784632
C	-3.630063	-1.604693	0.164515
H	-2.179625	-2.767248	-0.965333

H	-3.168115	1.607241	1.254449
H	-4.860453	-0.225676	1.274009
H	-4.379518	-2.389925	0.178787
C	4.613836	-0.323986	-0.220415
C	3.309716	-0.129843	0.530932
H	4.869113	0.562257	-0.808349
H	5.441014	-0.507340	0.478441
H	2.479189	0.225577	-0.430767
H	3.264819	0.772641	1.146740
S	-0.383446	1.547191	-0.014353
O	-0.753745	2.710792	-0.813297
O	0.348267	1.730251	1.240846
H	4.556564	-1.179536	-0.901012
C	2.667630	-1.288137	1.129386
H	2.858329	-2.250154	0.652959
C	1.823166	-1.239874	2.186237
H	1.577243	-0.299432	2.670520
H	1.359282	-2.139442	2.578729
Rotational constants (GHz): 0.6960800 0.3203900 0.2819000			
Vibrational harmonic frequencies (cm-1):			
-1625.8128	26.9287	33.4819	
56.4692	70.3528	85.2385	
109.8938	139.8546	152.3832	
170.3182	180.3398	218.1834	
226.8349	268.8128	286.1455	
306.4905	327.0105	372.7276	
397.1822	423.4187	449.6657	
474.8677	485.7639	527.6705	
534.4713	562.5618	596.6754	
635.1234	671.6499	691.9928	
746.0731	751.0844	786.4108	
839.1561	886.1050	897.3283	
922.3289	946.9309	971.6501	
997.4774	1009.7467	1011.3749	
1027.9203	1048.7780	1071.9410	
1085.9054	1112.5595	1139.4163	
1161.9708	1191.2888	1211.5291	
1229.7297	1239.4260	1299.1948	
1320.1262	1330.2222	1336.3106	
1346.0523	1376.5890	1422.5304	
1454.6319	1483.9689	1493.3311	
1500.9541	1501.8978	1506.6203	
1623.1440	1639.2143	1647.2506	
1814.0227	3030.3786	3097.6669	
3111.0920	3131.6097	3152.5165	
3165.2221	3199.4406	3211.6892	

3222.4259 3226.2441 3257.5232
 Zero-point correction (Hartree): 0.211119

B. Compound 5c

H^{prim}



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -706.726846485

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-0.277849	0.661552	-0.690441
O	-1.456148	1.119947	-1.144769
C	0.098691	-0.698484	-0.755895
C	0.719243	1.503481	-0.139991
O	-0.604885	-1.611794	-1.130406
O	0.614817	2.692543	0.056517
C	1.864768	0.583561	0.125229
C	3.119412	0.861711	0.647003
C	1.498121	-0.717413	-0.239289
C	2.373730	-1.783420	-0.094349
C	3.644913	-1.510510	0.429216
C	4.011610	-0.209272	0.794172
H	3.392052	1.873929	0.927512
H	4.357943	-2.319819	0.554618
H	5.003417	-0.028951	1.197833
C	-3.222727	0.685908	0.646798
C	-3.953512	-0.507323	0.089578
H	-3.771608	1.628173	0.699812
H	-4.439038	-0.234362	-0.854651
H	-3.235814	-1.301217	-0.144908
H	-2.231642	0.985986	-0.327689
H	2.078050	-2.787748	-0.379796
H	-2.590957	0.509776	1.521093

C	-5.018021	-1.043797	1.070467
H	-5.532347	-1.908439	0.638057
H	-4.562837	-1.359392	2.015026
H	-5.769921	-0.281020	1.297813

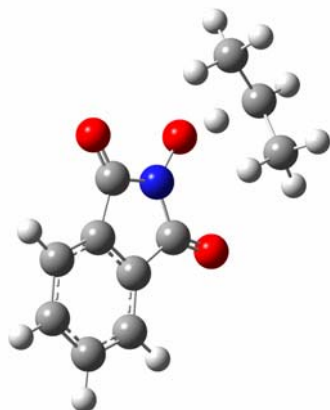
Rotational constants (GHz): 1.1135100 0.3206200 0.2768000

Vibrational harmonic frequencies (cm-1):

-1469.9525	25.5439	36.8993
56.5134	77.2424	100.4133
117.6878	140.1115	166.9649
237.6908	240.0437	246.2892
310.3988	335.7814	342.4297
412.2827	458.4642	464.8176
524.1057	540.1109	604.1751
627.3653	677.1425	705.6764
715.8827	719.3327	761.1534
783.0069	795.9817	889.7904
895.1849	910.9290	915.6061
923.9764	974.6243	1009.1480
1010.1203	1028.5788	1045.0711
1096.2229	1099.0893	1140.2093
1171.7217	1185.2138	1192.1923
1214.9433	1229.2428	1312.1855
1323.4117	1350.4769	1399.2230
1407.1664	1414.8591	1477.6750
1491.9360	1502.4285	1504.9555
1506.4238	1508.2750	1522.7380
1656.0640	1661.9945	1820.0386
1862.1077	3043.7409	3053.2088
3089.4047	3092.7942	3118.6699
3122.2069	3177.7223	3193.7014
3206.6178	3218.2895	3221.5584

Zero-point correction (Hartree): 0.205981

L^{sec}



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -706.732765066

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-0.558972	0.156922	-0.881749
O	-1.782445	0.277433	-1.417082
C	0.045127	-1.091065	-0.601768
C	0.269051	1.266924	-0.587126
O	-0.483519	-2.175433	-0.713595
O	-0.044521	2.431773	-0.689863
C	1.548690	0.655746	-0.121950
C	2.725891	1.267882	0.282205
C	1.416283	-0.737912	-0.130482
C	2.456700	-1.565686	0.264948
C	3.651288	-0.955345	0.671314
C	3.783692	0.438639	0.679843
H	2.816418	2.349275	0.286082
H	4.488369	-1.571765	0.985120
H	4.721421	0.882578	1.000373
C	-2.748822	0.891443	1.654856
C	-3.482676	0.289675	0.482089
C	-3.902612	-1.156663	0.572007
H	-2.344374	1.879796	1.416711
H	-1.927098	0.248546	1.990342
H	-3.430056	1.010778	2.511822
H	-4.230579	0.954531	0.038613
H	-4.375141	-1.497969	-0.353216
H	-4.629671	-1.295779	1.387328
H	-3.048072	-1.809886	0.776157
H	-2.562308	0.304179	-0.553894
H	2.342111	-2.644741	0.255505

Rotational constants (GHz): 1.0722600 0.3847100 0.3344000

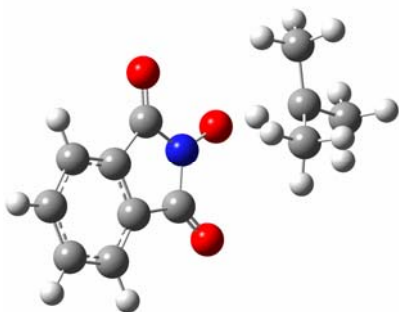
Vibrational harmonic frequencies (cm-1):

-1564.9262	25.8747	38.3510
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45.2560	94.5574	115.4766
139.0255	145.8272	178.1754
200.4417	219.3292	239.6383
315.7574	328.0365	339.8080
383.1252	413.2715	464.0865
473.2739	524.1644	532.6620
603.9751	677.0171	704.2809
715.9176	719.3753	782.0194
795.5653	818.5154	891.7407
895.4606	911.3959	930.4523
943.0160	974.5679	1009.0064
1011.8123	1045.6846	1060.1275
1096.1817	1131.4223	1139.1738
1184.7698	1192.1474	1192.6790
1200.3918	1229.6746	1312.1524
1366.3519	1388.8666	1403.6013
1415.2822	1427.4903	1486.4027
1491.4433	1494.6277	1501.4263
1503.1715	1506.5062	1510.5318
1656.1193	1661.8917	1819.3707
1860.1359	3002.3103	3007.1161
3077.7320	3090.2270	3098.4166
3125.7227	3134.1790	3193.5259
3206.4717	3218.2515	3221.4984

Zero-point correction (Hartree): 0.205612

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E(UB+HF-LYP/6-31G(d,p)) (Hartree): -746.053895121

Electronic state : 2-A

Cartesian coordinates (Angs):

N	0.246583	-0.029301	-0.877000
O	1.483979	-0.047853	-1.387100

C	-0.459994	1.164516	-0.598757
C	-0.485688	-1.203082	-0.577627
O	-0.020544	2.288555	-0.704976
O	-0.071877	-2.337775	-0.666922
C	-1.816112	-0.700570	-0.125165
C	-2.940376	-1.408042	0.273913
C	-1.800944	0.699364	-0.137595
C	-2.909604	1.437981	0.248636
C	-4.051334	0.730758	0.650179
C	-4.066466	-0.669313	0.662675
H	-2.939723	-2.493199	0.281226
H	-4.938928	1.275709	0.957393
H	-4.965512	-1.189411	0.979517
C	2.406279	-0.467072	1.715355
C	3.184949	0.012661	0.506568
C	3.587181	1.473719	0.529141
H	1.984067	-1.463896	1.553026
H	1.594973	0.220436	1.976454
H	3.070154	-0.529599	2.591881
H	4.062053	1.773368	-0.409975
H	4.309697	1.658093	1.339573
H	2.724037	2.125117	0.695916
H	2.264830	-0.021495	-0.492051
C	4.236831	-0.952738	-0.001669
H	5.064463	-1.028731	0.720835
H	3.825742	-1.957330	-0.140215
H	4.662935	-0.619312	-0.953040
H	-2.885661	2.522830	0.236526

Rotational constants (GHz): 1.0343200 0.3136200 0.2770500

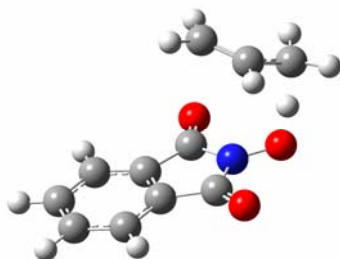
Vibrational harmonic frequencies (cm⁻¹):

-1561.7946	21.1354	24.6012
36.4243	93.3654	106.2468
125.2589	139.1702	173.6429
184.3853	208.8555	221.6726
233.1361	239.4377	317.9232
338.3788	353.4297	370.7082
390.1631	413.9714	464.1223
486.3168	523.7684	568.1221
604.3744	676.9635	704.1903
715.9182	719.5444	782.9904
795.4566	797.8582	891.7482
911.1853	932.6018	935.7168
973.1431	974.3159	1001.8577
1008.6742	1012.5461	1013.8235
1046.4840	1093.7402	1097.0446
1138.9876	1184.8813	1192.1503

1197.1598	1229.5748	1266.3553
1278.0861	1312.2770	1389.3017
1403.2112	1404.9019	1409.5419
1434.5722	1475.7517	1489.1834
1492.7359	1495.6307	1502.3314
1502.6073	1503.9451	1506.1856
1521.5671	1655.9933	1661.7655
1817.6338	1858.7543	3001.8029
3002.8173	3010.0626	3082.1984
3088.9410	3093.4369	3122.6437
3128.2719	3131.4283	3193.3740
3206.3799	3218.2763	3221.4886

Zero-point correction (Hartree): 0.233628

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E(UB+HF-LYP/6-31G(d,p)) (Hartree): -705.500812292

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-0.777163	0.054083	-1.034726
O	-1.986484	0.076994	-1.580922
C	-0.053723	-1.144129	-0.790240
C	-0.071044	1.224470	-0.650235
O	-0.462376	-2.266035	-0.984679
O	-0.496477	2.355917	-0.709353
C	1.248066	0.718749	-0.173589
C	2.346742	1.423544	0.296337
C	1.258316	-0.678832	-0.255760
C	2.367472	-1.417578	0.129861
C	3.482226	-0.713185	0.604428
C	3.472065	0.684893	0.686213
H	2.327325	2.506977	0.354821
H	4.369009	-1.258259	0.913730
H	4.351203	1.203042	1.057412
C	-3.612735	-0.040284	0.384686
H	-3.927500	-1.083538	0.335403
H	-2.791660	0.038813	-0.669072

H	2.363861	-2.500613	0.061800
C	-2.796463	0.335610	1.514445
H	-2.674314	1.402199	1.699964
C	-2.128539	-0.539694	2.308661
H	-1.505807	-0.200001	3.129930
H	-2.202627	-1.612958	2.153734
H	-4.380945	0.669372	0.076149

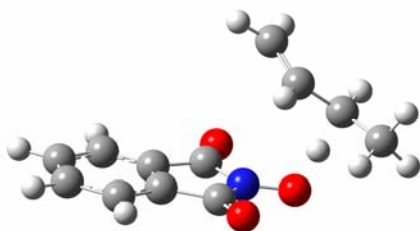
Rotational constants (GHz): 0.9719500 0.4326700 0.4026800

Vibrational harmonic frequencies (cm-1):

-1716.0823	23.9372	32.5764
37.7645	74.5324	119.8504
138.3177	159.5016	194.0621
239.3442	302.7849	322.0316
339.7672	413.6355	417.1235
462.6045	475.1093	523.2095
538.5316	549.9985	598.4965
638.4159	676.2103	705.1100
716.6002	720.3064	784.1276
796.1259	891.8753	908.5172
911.5154	951.1837	975.0337
997.3615	1008.2534	1009.3197
1017.2912	1047.8275	1077.9359
1093.5781	1128.6231	1179.0517
1185.5105	1193.1248	1220.3931
1234.5697	1312.2736	1316.8661
1388.0381	1401.7079	1443.3437
1478.7570	1502.8151	1506.4753
1513.0899	1613.6731	1655.5077
1661.4090	1823.2044	1862.6846
3106.7670	3157.5695	3163.1873
3193.7160	3196.1186	3206.6141
3218.3177	3221.5699	3253.7374

Zero-point correction (Hartree): 0.182774

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E(UB+HF-LYP/6-31G(d,p)) (Hartree): -744.820051627

Electronic state : 2-A

Cartesian coordinates (Angs):

N	0.433238	0.137582	-1.034698
O	1.639060	0.262353	-1.571331
C	-0.441301	1.235198	-0.805050
C	-0.107610	-1.105011	-0.619408
O	-0.188266	2.397099	-1.024095
O	0.473685	-2.168254	-0.641413
C	-1.483211	-0.773469	-0.150461
C	-2.477305	-1.609417	0.337028
C	-1.680030	0.608540	-0.259554
C	-2.877808	1.199562	0.114923
C	-3.888320	0.361812	0.606316
C	-3.691430	-1.020383	0.715406
H	-2.313074	-2.679087	0.417367
H	-4.839745	0.789604	0.907911
H	-4.493256	-1.643987	1.099250
C	4.176974	-0.923395	-0.038584
C	3.296931	0.243622	0.372081
H	4.646065	-0.741176	-1.009455
H	3.588977	-1.843188	-0.114972
H	4.978487	-1.088886	0.693571
H	3.772420	1.227181	0.305775
H	2.453055	0.314142	-0.626344
H	-3.018852	2.271942	0.026993
C	2.427818	0.082947	1.527527
H	2.120886	-0.936651	1.763421
C	1.943753	1.098030	2.280018
H	1.277151	0.917103	3.117200
H	2.208622	2.132123	2.075434

Rotational constants (GHz): 0.9248500 0.3480300 0.3228100

Vibrational harmonic frequencies (cm-1):

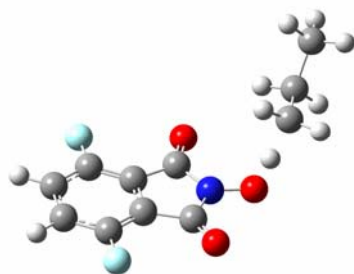
-1632.8790	23.1577	32.1155
37.3679	77.1524	109.1965
139.1333	156.3658	169.8551
184.4977	212.9081	240.1620
286.0798	316.7679	325.5526

342.2398	414.3093	463.2706
474.7526	484.1575	523.4874
551.0559	601.0425	650.1578
675.8585	705.0803	716.9324
720.4958	781.2284	795.7716
837.2825	885.2036	893.0343
911.1278	916.3626	974.4876
999.6264	1008.7961	1017.9305
1019.7660	1049.6590	1085.2631
1094.1077	1123.1907	1129.6999
1185.4728	1193.0132	1207.1245
1220.4980	1234.4472	1312.3429
1315.8109	1337.2717	1389.3681
1402.1502	1427.5337	1454.4245
1486.3288	1502.5996	1506.4103
1506.4916	1507.5122	1627.0789
1655.5159	1661.2059	1818.4801
1861.0462	3031.7543	3096.3429
3104.8256	3134.8276	3149.8741
3159.6014	3193.6815	3206.5201
3217.9808	3221.3303	3250.6152

Zero-point correction (Hartree): 0.211266

C. Compound 5e

Γ^{prim}



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -905.177841850

Electronic state : 2-A

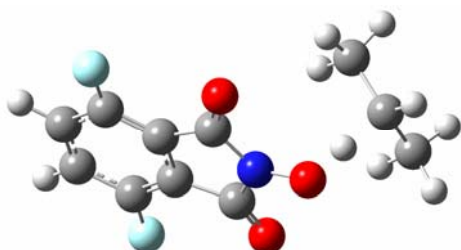
Cartesian coordinates (Angs):

N	0.635433	-0.643570	-0.777652
O	1.817519	-1.068597	-1.250969
C	0.290142	0.722615	-0.695753
C	-0.385657	-1.529340	-0.358594
O	1.023884	1.652821	-0.942780
O	-0.298588	-2.732624	-0.301811
C	-1.524728	-0.623750	-0.019853

C	-2.803141	-0.907358	0.429973
C	-1.124498	0.708421	-0.218833
C	-2.005204	1.746582	0.034041
C	-3.298805	1.461389	0.486161
C	-3.695720	0.140811	0.683319
H	-3.980515	2.282630	0.678321
H	-4.694837	-0.094040	1.033625
C	3.547298	-0.867051	0.612920
C	4.341169	0.333859	0.170660
H	4.055007	-1.833536	0.601992
H	4.840975	0.115853	-0.780354
H	3.663143	1.174034	-0.015564
H	2.577283	-1.040722	-0.401604
H	2.902701	-0.733409	1.485458
C	5.399399	0.745081	1.217054
H	5.959650	1.618320	0.867032
H	4.931637	1.004944	2.172345
H	6.113577	-0.064215	1.401140
F	-1.641931	3.020919	-0.147674
F	-3.202592	-2.168167	0.627572
Rotational constants (GHz): 0.7119400 0.2740300 0.2165600			
Vibrational harmonic frequencies (cm-1):			
-1487.9578	20.5756	29.4214	
54.2748	72.1936	92.0505	
99.6325	113.1993	146.0799	
168.9151	181.2979	231.5065	
245.2461	279.8419	311.2268	
337.6921	364.7975	389.6325	
394.5808	447.5673	470.0756	
498.3076	552.6724	563.8331	
566.3275	623.8408	627.7092	
672.8051	705.6744	741.5934	
760.1704	769.7222	845.8544	
850.8171	894.2903	913.5634	
922.0529	925.4820	945.2403	
960.0166	1029.6322	1097.4955	
1106.4434	1143.8151	1168.9854	
1183.5755	1214.7170	1233.6729	
1299.6085	1317.1987	1323.4270	
1348.9411	1398.8963	1411.7972	
1416.9102	1438.9614	1476.8485	
1489.4236	1504.4283	1507.6425	
1522.2109	1544.3424	1665.7396	
1674.4896	1824.2539	1865.1359	
3043.7793	3053.2957	3089.0395	
3092.9813	3119.1563	3122.3182	

3177.3945 3221.0599 3232.7152
 Zero-point correction (Hartree): 0.189430

H^{sec}



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -905.183804891

Electronic state : 2-A

Cartesian coordinates (Angs):

N	0.904704	-0.180299	-0.903424
O	2.134257	-0.311194	-1.419360
C	0.314709	1.075179	-0.632489
C	0.068285	-1.286627	-0.624925
O	0.861027	2.149339	-0.735788
O	0.379740	-2.450250	-0.725469
C	-1.214166	-0.663744	-0.179729
C	-2.413064	-1.238095	0.207458
C	-1.068246	0.733768	-0.184132
C	-2.122223	1.546070	0.198722
C	-3.336052	0.967143	0.587060
C	-3.480715	-0.418287	0.591443
H	-4.155194	1.613652	0.882230
H	-4.415518	-0.879751	0.890253
C	3.061502	-0.958502	1.661658
C	3.810221	-0.353221	0.499978
C	4.247257	1.086830	0.608067
H	2.649163	-1.940684	1.411948
H	2.244625	-0.309978	1.998286
H	3.736045	-1.092467	2.521609
H	4.554362	-1.022209	0.056184
H	4.724638	1.434177	-0.312332
H	4.975694	1.205360	1.425279
H	3.401334	1.748206	0.821344
H	2.904621	-0.349272	-0.540423
F	-2.002063	2.878221	0.203326
F	-2.571042	-2.566129	0.220658

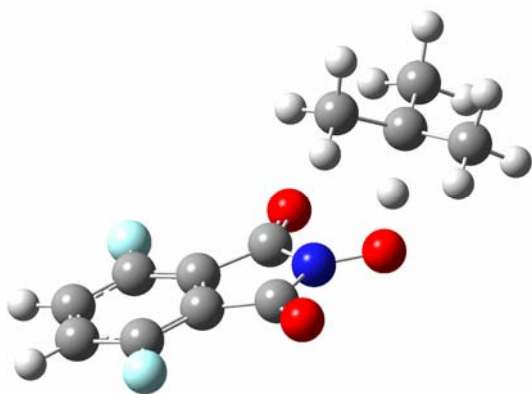
Rotational constants (GHz): 0.6806800 0.3308600 0.2537500

Vibrational harmonic frequencies (cm-1):

-1563.1315	24.3679	35.3981
43.0705	91.3693	92.8802
114.8367	140.9190	151.7042
178.3224	181.5914	199.0695
218.6380	278.3587	317.6243
328.6992	361.1746	389.3549
393.0487	394.5154	450.4209
469.8906	503.0165	552.7017
560.8141	566.1188	623.8418
672.5255	705.6775	740.4282
768.5709	818.8722	845.3809
851.1265	895.1280	924.6351
929.2073	942.6701	946.6040
959.7247	1063.2023	1107.5064
1131.0831	1142.2446	1182.1726
1192.2922	1201.1675	1233.6203
1299.3899	1317.0997	1366.1521
1386.4264	1414.8985	1416.3935
1426.6537	1439.1629	1485.4183
1491.1170	1493.0109	1500.8251
1510.5826	1544.1829	1665.4272
1674.5092	1823.5292	1863.1275
3003.6766	3008.5234	3077.6157
3090.8080	3098.4543	3126.1403
3134.9573	3220.8622	3232.5393

Zero-point correction (Hartree): 0.189150

Tertiair



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -944.504987558

Electronic state : 2-A

Cartesian coordinates (Angs):

N	0.612529	-0.024569	-0.897971
O	1.855548	-0.040195	-1.391176
C	-0.091898	1.170589	-0.625893
C	-0.116910	-1.203080	-0.616583
O	0.355167	2.290400	-0.721831
O	0.305511	-2.332464	-0.706644
C	-1.455425	-0.702855	-0.181736
C	-2.597428	-1.386267	0.200068
C	-1.440618	0.702308	-0.187249
C	-2.567938	1.412715	0.188994
C	-3.724296	0.723261	0.572397
C	-3.738950	-0.669564	0.577977
H	-4.601584	1.290719	0.863050
H	-4.627910	-1.216104	0.873211
C	2.745959	-0.459558	1.725939
C	3.537981	0.004633	0.519483
C	3.960673	1.460136	0.539916
H	2.314779	-1.453172	1.567610
H	1.941127	0.238850	1.978092
H	3.403892	-0.523526	2.606649
H	4.441639	1.751366	-0.398669
H	4.684218	1.634700	1.351424
H	3.106904	2.124195	0.704739
H	2.629772	-0.020538	-0.481180
C	4.579972	-0.977097	0.021604
H	5.401008	-1.061115	0.750519
H	4.156273	-1.976480	-0.116157
H	5.017213	-0.652752	-0.927767
F	-2.572906	2.750325	0.192481
F	-2.630602	-2.723372	0.214406

Rotational constants (GHz): 0.6640300 0.2692000 0.2143100

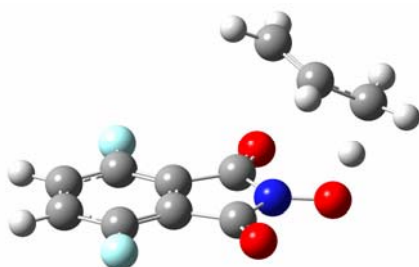
Vibrational harmonic frequencies (cm-1):

-1543.6684	19.9661	23.1365
35.4993	89.0100	91.0202
106.4339	123.7041	147.0438
173.5274	181.0872	184.7944
210.1736	222.5426	227.7012
280.7237	319.9577	354.1171
368.1432	370.5814	389.1127
393.6249	394.1776	451.1629
470.1500	537.6011	552.3717
565.5342	574.3544	623.8960
672.4629	705.6330	740.3620
769.1770	797.1483	844.8094
850.9659	924.2043	931.7652

935.0791	947.7196	959.0946
972.9388	1001.9460	1012.6019
1097.4159	1108.5532	1142.3005
1182.6321	1196.6025	1233.3080
1266.0700	1277.9432	1299.1036
1316.7845	1387.3426	1404.6718
1409.1258	1416.0801	1433.4002
1439.1999	1475.4128	1486.3428
1492.4492	1494.4646	1502.2362
1503.2954	1521.6552	1543.6513
1665.2630	1674.1732	1821.7479
1861.7364	3003.5476	3004.4894
3011.7364	3082.3781	3090.0692
3094.4034	3122.7604	3129.1721
3132.2506	3220.1613	3231.8666

Zero-point correction (Hartree): 0.217161

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E(UB+HF-LYP/6-31G(d,p)) (Hartree): -903.951825333

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-1.107651	0.044093	-1.046929
O	-2.325803	0.062789	-1.571185
C	-0.398504	-1.156315	-0.780724
C	-0.390284	1.221275	-0.711781
O	-0.828702	-2.274516	-0.934315
O	-0.812473	2.350057	-0.798824
C	0.933574	0.716167	-0.243592
C	2.058981	1.397076	0.189562
C	0.928641	-0.688448	-0.283711
C	2.049136	-1.400714	0.109910
C	3.187973	-0.713911	0.546108
C	3.192887	0.678625	0.585689
H	4.059762	-1.282822	0.850168
H	4.068625	1.223244	0.921238
C	-3.909558	-0.012531	0.430949

H	-4.235053	-1.053092	0.395805
H	-3.116644	0.049188	-0.637928
C	-3.064523	0.362074	1.540414
H	-2.933172	1.428318	1.721574
C	-2.383900	-0.516007	2.320828
H	-1.743300	-0.178547	3.129250
H	-2.466873	-1.589054	2.168840
F	2.063068	-2.737842	0.080780
F	2.082315	2.733559	0.236405
H	-4.678948	0.702282	0.137576

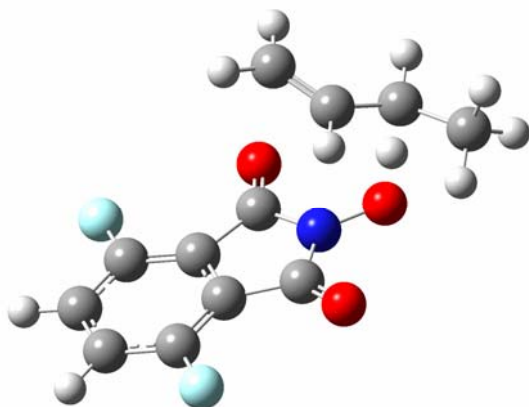
Rotational constants (GHz): 0.6378100 0.3767700 0.2977600

Vibrational harmonic frequencies (cm-1):

-1699.9785	22.7204	32.1216
38.3194	74.4984	90.1546
117.4452	145.6918	160.4671
179.4770	192.7694	276.1429
303.2319	323.1713	371.4836
389.1537	394.5603	416.5375
450.0872	468.6093	517.9204
542.4904	551.8114	562.5831
566.8845	620.3950	639.8072
671.9696	705.7500	740.9392
770.6291	845.4528	851.5170
911.7352	924.1509	950.8063
951.6481	959.4956	998.7686
1008.5994	1075.7895	1114.1160
1129.6855	1182.5103	1186.4961
1220.8179	1233.2232	1299.6855
1316.7636	1317.4466	1386.1187
1414.9449	1438.6687	1443.3987
1477.1532	1512.5601	1543.9756
1613.1830	1664.6665	1673.9077
1826.9064	1865.2870	3106.9031
3157.5590	3163.3429	3196.3378
3220.4032	3232.0683	3253.7915

Zero-point correction (Hartree): 0.166324

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E(UB+HF-LYP/6-31G(d,p)) (Hartree): -943.271118061

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-0.773757	-0.224821	-1.045443
O	-1.984445	-0.393000	-1.556614
C	0.107892	-1.302384	-0.763498
C	-0.248254	1.047239	-0.710491
O	-0.143512	-2.474019	-0.910963
O	-0.845892	2.096202	-0.789537
C	1.137368	0.756278	-0.240151
C	2.145110	1.604622	0.186916
C	1.347769	-0.632792	-0.271032
C	2.564484	-1.162021	0.125079
C	3.584884	-0.305671	0.554746
C	3.376327	1.071355	0.585298
H	4.533755	-0.732209	0.861035
H	4.158580	1.746046	0.915377
C	-4.557388	0.780684	-0.051633
C	-3.615148	-0.316529	0.410727
H	-5.025373	0.522968	-1.005703
H	-4.018994	1.724401	-0.182813
H	-5.359482	0.943670	0.680347
H	-4.044185	-1.323431	0.412115
H	-2.787353	-0.410171	-0.592556
C	-2.738699	-0.046337	1.540505
H	-2.478950	0.998895	1.712095
C	-2.195837	-0.991866	2.341956
H	-1.529344	-0.730694	3.157796
H	-2.412409	-2.047630	2.201145
F	2.783523	-2.481307	0.104824
F	1.963122	2.929415	0.224692

Rotational constants (GHz): 0.6212400 0.2998800 0.2452500

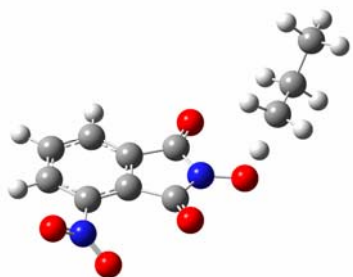
Vibrational harmonic frequencies (cm-1):

-1601.0543	19.0167	32.0594
34.2517	77.2908	91.6637
108.4110	145.6871	157.1446
168.4952	182.3511	185.4358
211.8975	277.3731	285.1106
315.7550	327.1191	375.0873
389.1142	394.8815	451.1879
468.9833	474.6550	528.8837
552.1152	564.3293	568.7861
621.1875	651.4447	671.5154
705.8936	740.9908	767.1837
835.8868	845.2391	852.2170
884.5269	919.8761	925.0559
952.7259	959.2863	998.3048
1017.2411	1083.7749	1112.1022
1123.2529	1130.7363	1186.3576
1211.0866	1221.4877	1233.5760
1299.5641	1315.3664	1316.9849
1336.8691	1387.8110	1415.4854
1426.2842	1438.5313	1452.7804
1485.3627	1505.2044	1507.4555
1543.9111	1627.2066	1664.6021
1674.0359	1822.8094	1863.7166
3032.6824	3096.6046	3105.4208
3135.1308	3150.0509	3160.0994
3220.8361	3232.5403	3251.1840

Zero-point correction (Hartree): 0.194798

C. Compound 5f

H^{prim}



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -911.206130953

Electronic state : 2-A

Cartesian coordinates (Angs):

N	0.911091	-0.313804	-0.908238
O	2.019625	-0.946809	-1.320580
C	0.821200	1.080705	-0.778805
C	-0.250529	-1.011596	-0.486639
O	1.707623	1.883150	-0.976260
O	-0.329772	-2.207419	-0.367585
C	-1.239683	0.087578	-0.187397
C	-2.560296	0.092459	0.250955
C	-0.579412	1.317050	-0.319160
C	-1.188432	2.531376	-0.038240
C	-2.511514	2.510201	0.416657
C	-3.189797	1.300053	0.569549
H	-3.020916	3.438326	0.654523
H	-4.211436	1.270834	0.929037
C	3.636828	-1.119476	0.645370
C	4.657230	-0.060749	0.320760
H	3.965758	-2.159608	0.602299
H	5.164024	-0.311690	-0.618247
H	4.154744	0.899511	0.160098
H	2.719008	-1.076304	-0.426938
H	-0.640510	3.459360	-0.163605
H	2.972547	-0.917589	1.489552
C	5.709572	0.086947	1.441174
H	6.437648	0.860974	1.177365
H	5.241878	0.371805	2.389290
H	6.253508	-0.849433	1.601976
N	-3.362581	-1.140225	0.360521
O	-4.196229	-1.175971	1.265520
O	-3.164601	-2.014859	-0.471929

Rotational constants (GHz): 0.7472600 0.2274600 0.1946800

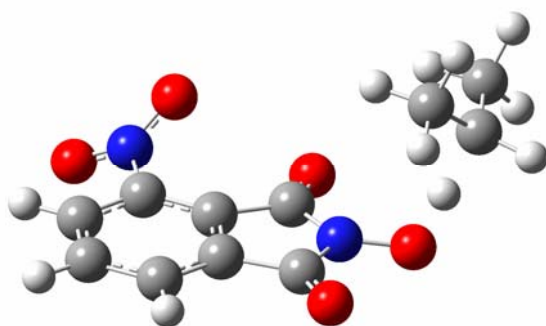
Vibrational harmonic frequencies (cm-1):

-1475.4195	21.9969	31.7997
49.2262	57.0516	74.2332
76.8930	95.3252	115.5704
168.6946	171.0443	187.9199
241.6717	245.9000	276.6332
315.8505	332.4127	343.3388
355.3413	399.3370	462.1912
464.5541	519.6418	550.9002
597.5545	613.2413	627.3021
669.8462	710.7882	718.8899
755.9877	760.9361	770.5200
780.2030	838.8370	877.0610
894.3281	908.6440	914.9054
922.1066	957.1715	1006.8828
1028.3985	1037.7259	1090.1230

1097.6937	1148.9591	1170.3009
1170.8743	1184.0623	1214.3677
1221.7553	1271.6890	1322.2590
1348.8081	1398.8215	1401.4634
1411.2255	1413.3562	1475.2135
1476.5740	1486.2206	1503.8338
1504.2867	1507.9355	1521.7710
1638.6394	1651.1213	1673.5915
1824.7706	1869.1833	3044.9307
3053.8759	3089.6873	3093.0526
3120.3518	3123.8679	3178.1005
3210.6950	3225.9375	3241.4208

Zero-point correction (Hartree): 0.208064

L^{sec}



E(UB+HF-LYP/6-31G(d,p)) (Hartree): -911.212200434

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-1.178246	0.488438	-0.831695
O	-2.384180	0.291374	-1.380098
C	-0.217778	-0.547830	-0.717161
C	-0.704599	1.757548	-0.453842
O	-0.408277	-1.698687	-1.022575
O	-1.335969	2.790086	-0.441832
C	0.718817	1.517716	-0.071339
C	1.658190	2.453500	0.335874
C	1.005225	0.149669	-0.176407
C	2.291385	-0.279884	0.136717
C	3.268835	0.646612	0.514214
C	2.951283	2.001309	0.621976
H	1.386950	3.501081	0.413926
H	4.268277	0.285880	0.726173
H	3.718369	2.703688	0.931387
C	-3.469121	0.204451	1.710811
C	-3.977404	-0.464844	0.457645

C	-3.916362	-1.970521	0.381202
H	-3.406639	1.290707	1.594910
H	-2.483085	-0.175917	2.000621
H	-4.148593	0.001151	2.552907
H	-4.901525	-0.027614	0.065900
H	-4.238678	-2.338955	-0.596518
H	-4.578499	-2.417299	1.139032
H	-2.903967	-2.342870	0.567710
H	-3.127799	-0.045552	-0.532733
N	2.675278	-1.703556	0.132212
O	3.825080	-1.963381	-0.221075
O	1.838988	-2.511246	0.514945

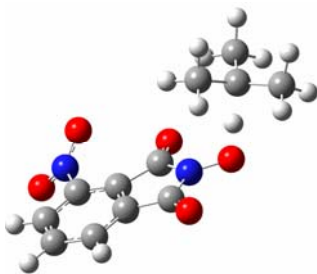
Rotational constants (GHz): 0.6322400 0.2985000 0.2283500

Vibrational harmonic frequencies (cm-1):

-1551.2815	1.9899	35.9700
36.8990	57.4150	74.7252
94.4132	115.5093	142.7068
166.6459	179.7656	187.2093
193.3726	217.8297	276.2423
321.1515	328.8456	341.5000
353.9422	376.5323	405.3609
464.5096	473.8682	518.6650
550.5123	594.1032	612.3847
672.2269	709.4854	717.5672
755.8710	769.7775	779.6752
819.1540	838.4287	877.9175
894.7369	910.0507	925.9381
941.1267	956.1086	1006.3200
1038.5666	1067.2572	1090.6591
1130.4869	1148.1297	1171.0890
1183.8124	1191.2645	1199.5023
1222.0628	1271.6437	1364.9727
1386.2481	1401.2197	1411.9664
1412.1464	1426.3056	1475.4967
1483.4984	1489.6123	1490.3667
1499.5272	1503.7203	1509.4983
1638.5375	1651.0524	1672.5936
1826.0683	1866.6188	3005.1154
3010.0549	3078.1800	3091.7240
3097.6452	3125.0406	3136.3926
3210.6262	3225.8023	3240.7589

Zero-point correction (Hartree): 0.207636

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E(UB+HF-LYP/6-31G(d,p)) (Hartree): -950.533402144

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-0.869756	0.455185	-0.825978
O	-2.076311	0.236224	-1.358289
C	0.106756	-0.566151	-0.709058
C	-0.415934	1.730890	-0.446203
O	-0.067572	-1.721110	-1.008921
O	-1.065288	2.752489	-0.428667
C	1.012908	1.515067	-0.070216
C	1.939068	2.466435	0.330923
C	1.320952	0.151618	-0.175016
C	2.615575	-0.256413	0.131717
C	3.579923	0.686375	0.502950
C	3.240933	2.035763	0.610789
H	1.651234	3.509573	0.409079
H	4.586195	0.342193	0.710034
H	3.998058	2.750967	0.915336
C	-3.120435	0.109004	1.733483
C	-3.689385	-0.502927	0.468327
C	-3.612346	-2.014750	0.384689
H	-3.033914	1.197195	1.652272
H	-2.137473	-0.305553	1.980031
H	-3.783171	-0.106234	2.585919
H	-3.942061	-2.379999	-0.592355
H	-4.265052	-2.468746	1.146390
H	-2.595466	-2.379182	0.557650
H	-2.826065	-0.110771	-0.483485
N	3.022700	-1.673561	0.126931
O	4.174441	-1.915143	-0.233170
O	2.202256	-2.494301	0.516096
C	-4.988578	0.113537	-0.012621
H	-5.805755	-0.140239	0.680158
H	-4.923557	1.204748	-0.061253
H	-5.270419	-0.261268	-1.001414

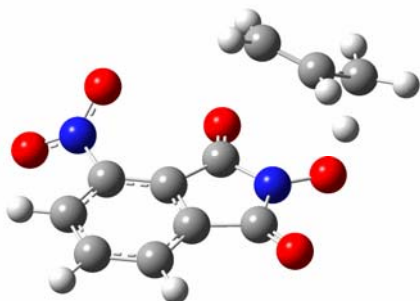
Rotational constants (GHz): 0.6328300 0.2404200 0.1928900

Vibrational harmonic frequencies (cm-1):

-1530.6895	20.3493	30.1804
35.0602	57.4367	73.7665
94.5366	106.9059	124.0886
162.7516	177.1134	181.6171
187.4398	209.8722	220.7941
233.0030	276.6200	322.1593
337.7088	352.3959	356.7538
369.0972	390.6958	404.8489
464.6038	483.0498	537.5835
567.8975	594.2390	612.6266
672.1977	709.5839	717.6508
756.3371	769.5756	779.6090
796.3847	837.8374	878.1628
910.5967	929.0662	935.8413
955.7823	972.7383	1001.2502
1006.0001	1011.9300	1040.2186
1091.2772	1099.0761	1147.6965
1171.2263	1183.7375	1194.9522
1222.0270	1265.3202	1271.8212
1276.4324	1386.6769	1401.2320
1405.7497	1409.0827	1412.1601
1434.1102	1474.7948	1475.4474
1481.2111	1490.5892	1493.1175
1501.8717	1502.8710	1503.5996
1520.3525	1638.4275	1650.9929
1672.3709	1824.4663	1865.5771
3005.5566	3006.1909	3013.6112
3083.8636	3090.4924	3096.6984
3122.9532	3129.1434	3134.6181
3210.4663	3225.6986	3240.6868

Zero-point correction (Hartree): 0.235777

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E(UB+HF-LYP/6-31G(d,p)) (Hartree): -909.980337560

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-1.409597	0.382709	-0.956578
O	-2.576178	0.095545	-1.517478
C	-0.337651	-0.550690	-0.901898
C	-1.089330	1.650660	-0.428563
O	-0.387946	-1.675918	-1.329674
O	-1.833051	2.600044	-0.334142
C	0.344146	1.531483	-0.030504
C	1.166708	2.520130	0.489919
C	0.782798	0.219160	-0.252687
C	2.100301	-0.098205	0.063300
C	2.961798	0.887358	0.555345
C	2.495177	2.184521	0.774197
H	0.780424	3.520358	0.655597
H	3.989354	0.617277	0.767949
H	3.173437	2.933040	1.170689
C	-3.897618	-1.078053	0.327810
H	-3.797569	-2.108487	-0.015985
H	-3.265007	-0.437330	-0.645277
N	2.633458	-1.467901	-0.051680
O	3.811564	-1.575610	-0.389583
O	1.878922	-2.388355	0.235659
C	-3.183629	-0.730765	1.534505
H	-3.479478	0.190046	2.036304
C	-2.141590	-1.438864	2.042079
H	-1.791060	-2.350877	1.566200
H	-1.626522	-1.121936	2.943256
H	-4.903741	-0.671825	0.219788

Rotational constants (GHz): 0.6248000 0.3344000 0.2651700

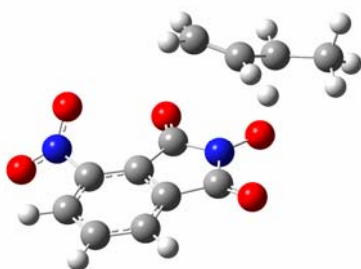
Vibrational harmonic frequencies (cm-1):

-1678.2009	19.4790	32.9059
35.5677	57.6122	75.0013
84.9627	121.6229	155.1406
171.3195	186.6770	199.9021
276.1008	302.5878	329.8076
338.0445	353.6691	402.2091
415.5953	462.8662	476.2565
526.9399	539.5897	562.2305
593.4468	607.7605	638.5275
672.0059	710.2774	718.6542
756.3848	770.9567	780.0236
838.4695	878.5479	911.6523
919.9446	949.5562	956.0024
998.2852	1006.5539	1008.1995
1042.6622	1075.7335	1094.7741

1136.7143	1172.8396	1184.1411
1193.2444	1220.9707	1225.0646
1272.4074	1316.0776	1387.3929
1400.4022	1411.9886	1442.3033
1474.6465	1477.2749	1503.3662
1512.7910	1610.8205	1638.6347
1650.3155	1672.1954	1828.1825
1868.2144	3107.2481	3157.4011
3163.4919	3196.4674	3210.2234
3225.6666	3239.8211	3255.8926

Zero-point correction (Hartree): 0.185012

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E(UB+HF-LYP/6-31G(d,p)) (Hartree): -949.299431925

Electronic state : 2-A

Cartesian coordinates (Angs):

N	-1.055393	0.333774	-1.001496
O	-2.212095	0.026151	-1.568392
C	0.023235	-0.590196	-0.907553
C	-0.759862	1.608825	-0.479411
O	-0.007174	-1.722170	-1.317981
O	-1.519749	2.548006	-0.402729
C	0.666907	1.512118	-0.053771
C	1.468283	2.517361	0.467719
C	1.124805	0.202266	-0.251926
C	2.441324	-0.093827	0.088116
C	3.282101	0.908641	0.582370
C	2.795855	2.202086	0.778249
H	1.066970	3.514682	0.614043
H	4.309460	0.654298	0.814353
H	3.458125	2.963822	1.176626
C	-5.013341	-0.194119	0.117156
C	-3.683938	-0.901251	0.309961
H	-5.401513	-0.350738	-0.893036
H	-4.913919	0.883941	0.278643
H	-5.763473	-0.572921	0.823927

H	-3.687982	-1.962137	0.041134
H	-2.948275	-0.433768	-0.656423
N	2.996379	-1.456605	-0.004952
O	4.181347	-1.549268	-0.323573
O	2.251682	-2.385797	0.278965
C	-2.897845	-0.597756	1.496182
H	-3.058120	0.381947	1.948153
C	-1.958854	-1.414057	2.029546
H	-1.746568	-2.390858	1.603009
H	-1.385712	-1.124373	2.904555

Rotational constants (GHz): 0.6300100 0.2601500 0.2175400

Vibrational harmonic frequencies (cm-1):

-1567.1548	18.6104	20.9468
30.9113	56.5864	72.0639
79.3170	103.4683	150.9681
161.6445	175.6171	185.3064
186.4604	214.3206	275.7653
284.3855	308.7491	332.3072
339.1388	353.7154	403.5121
462.7623	476.0794	482.9487
531.9297	553.8588	593.2726
609.7017	641.9469	671.7004
709.5272	718.6221	755.9668
768.0877	780.0290	828.5366
838.9012	878.8965	883.9213
911.6237	924.2654	955.5064
997.4334	1006.0347	1012.4142
1045.8836	1084.9359	1093.6245
1118.6841	1137.0066	1172.4819
1184.0356	1213.6954	1223.1272
1227.9949	1272.5240	1315.8459
1338.8792	1389.5943	1400.4646
1411.8190	1425.9798	1450.5799
1476.0446	1484.5366	1502.8153
1503.2622	1508.0402	1625.0062
1638.1666	1650.4300	1672.0907
1826.0084	1867.9241	3032.8229
3096.7538	3104.6461	3133.4728
3147.2159	3161.1223	3210.0804
3225.4172	3239.8635	3252.5969

Zero-point correction (Hartree): 0.213267