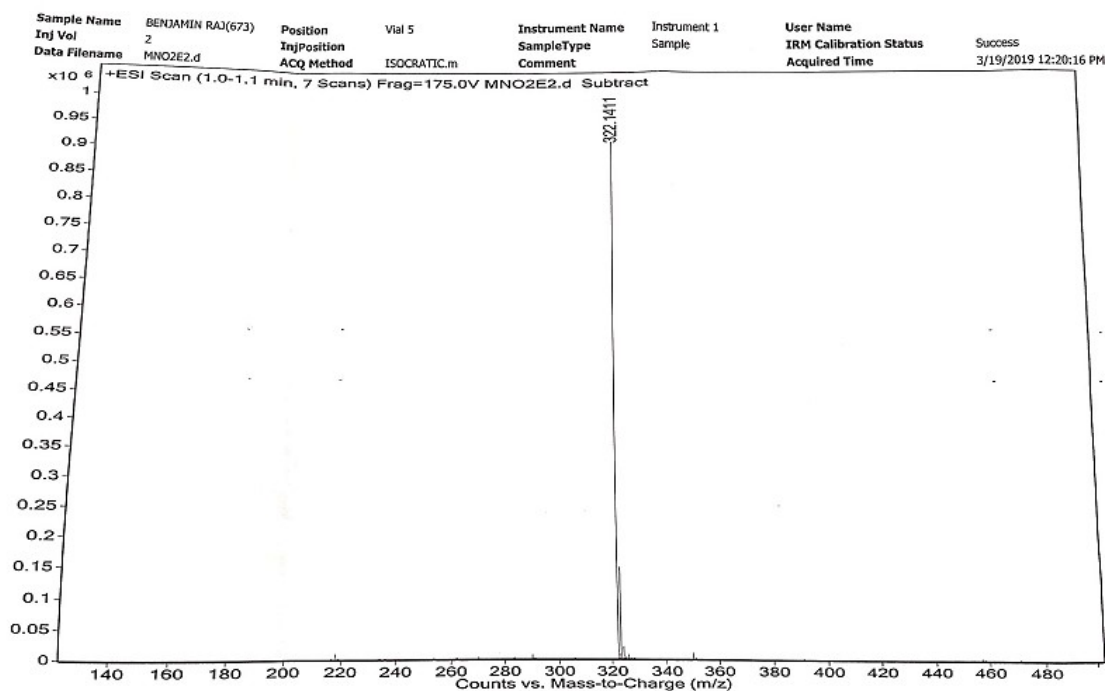


Supplementary Information

Synthesis of 2-amino alcohols from imidazole derivatives: Experimental and *in silico* study

Subham Behera, Priyamvada Kumari, Simon Watre Sangma, Sabyasachi Bhunia & Arun Kumar Padhy*
Department of Chemistry, Central University of Jharkhand, Cheri Manatu, Ranchi 835 222, India
E-mail: arun.padhy@uj.ac.in

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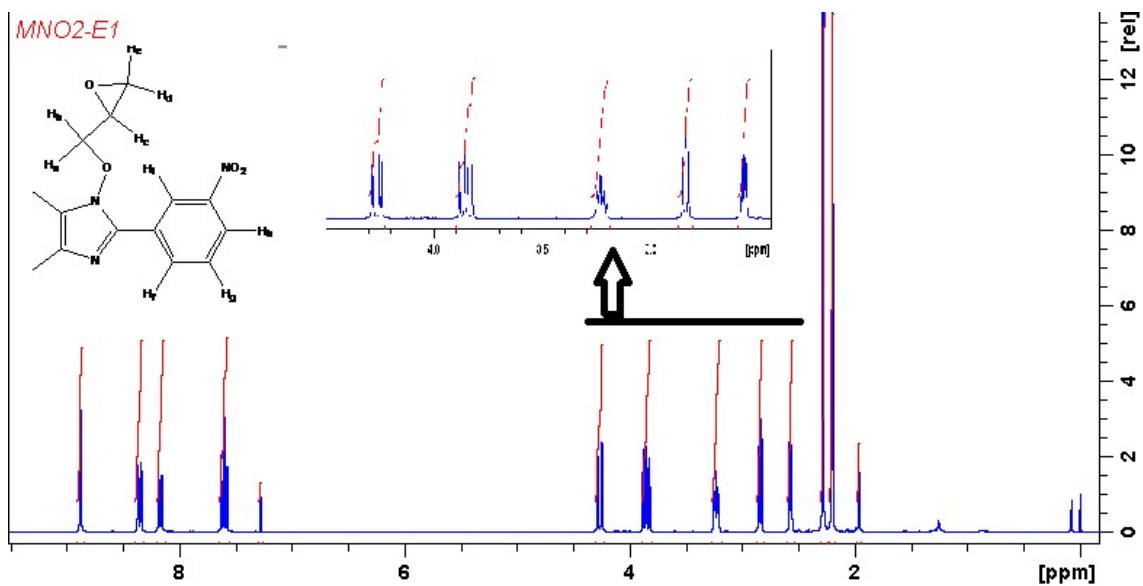


Fig:1- 1H NMR spectra of 6f

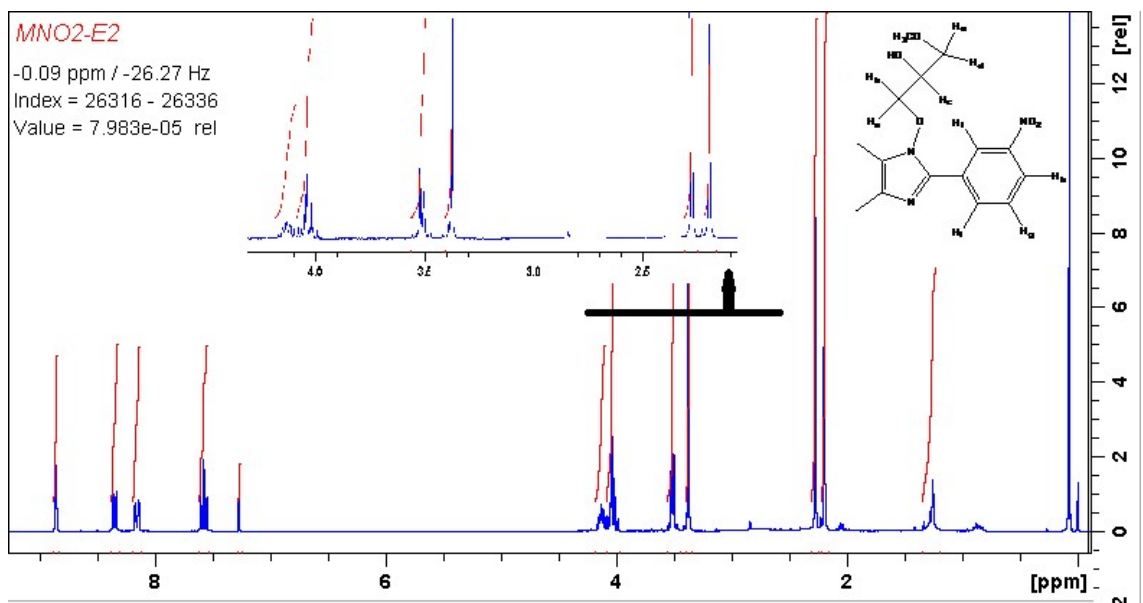


Fig:2- 1H NMR spectra of 7f

Fig:3- ^1H NMR spectra of 8f

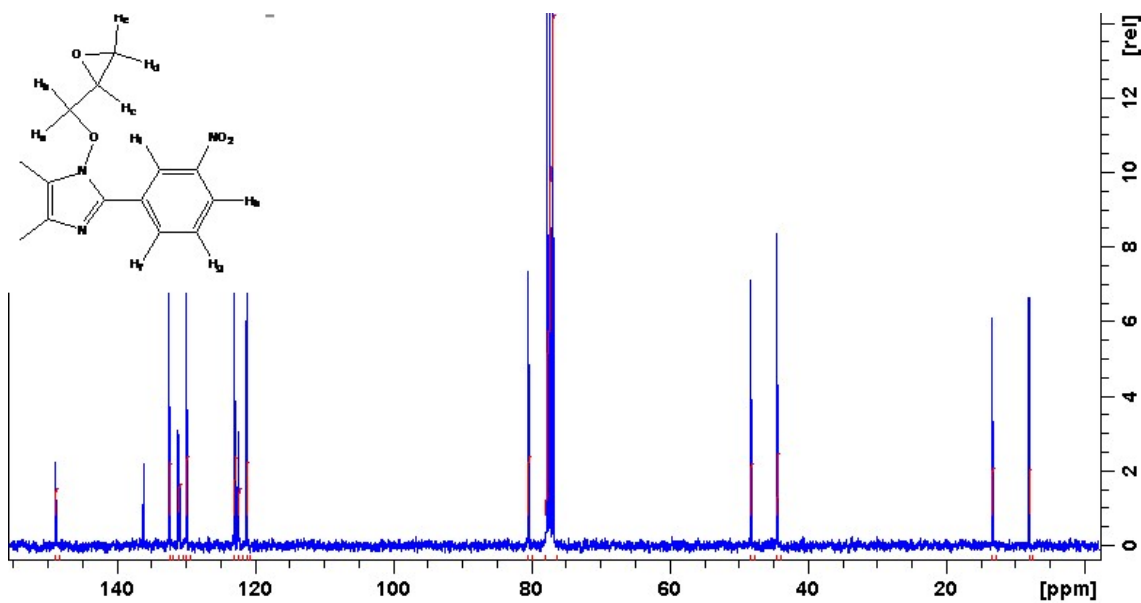
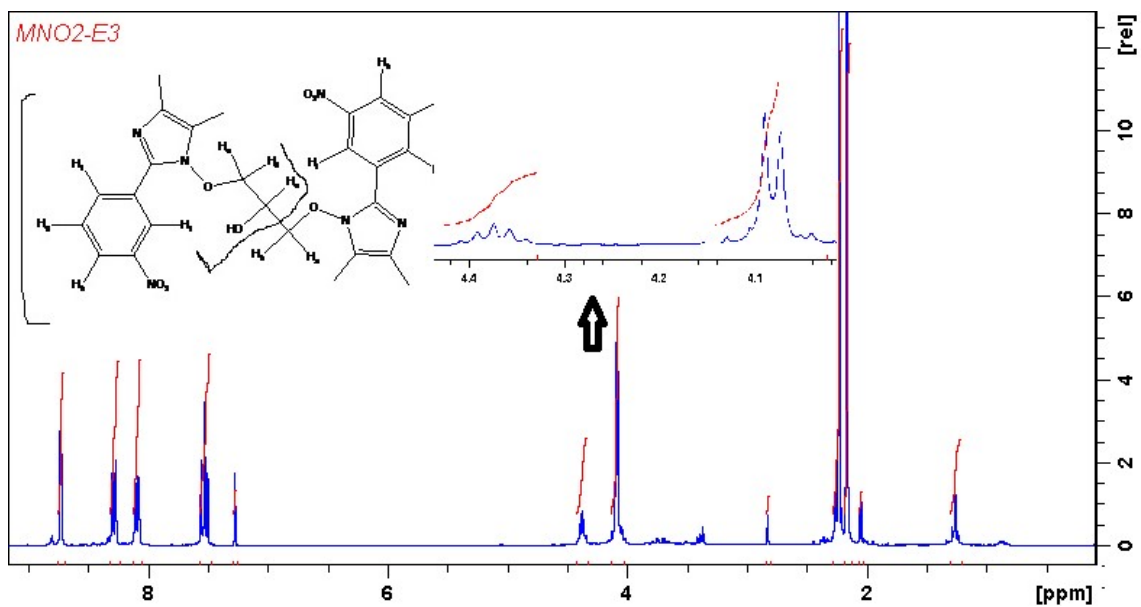


Fig:4- ^{13}C NMR spectra of 6f

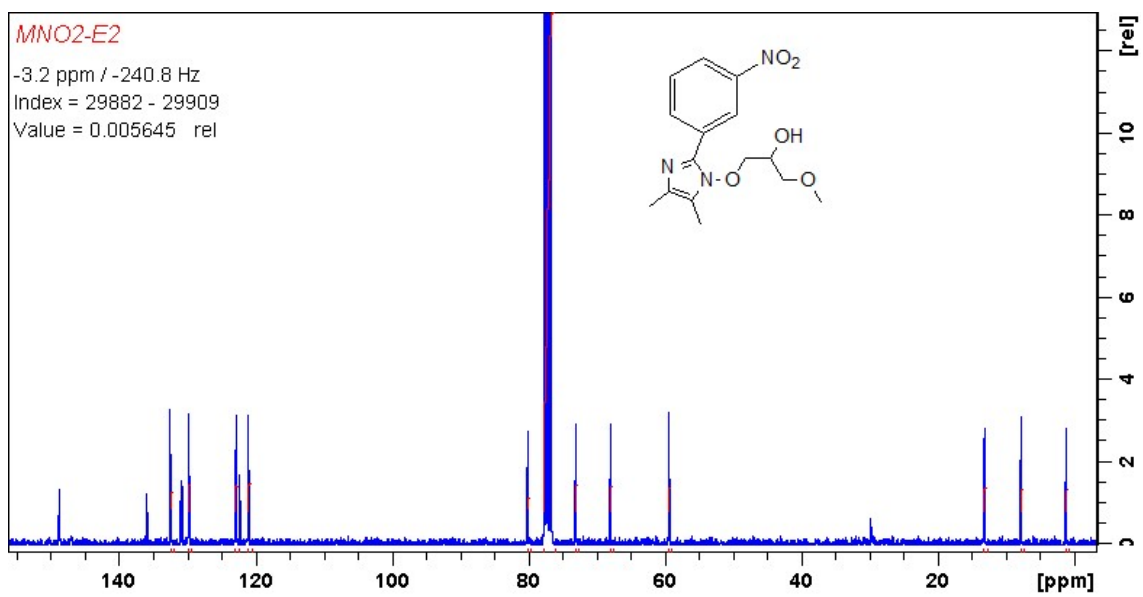
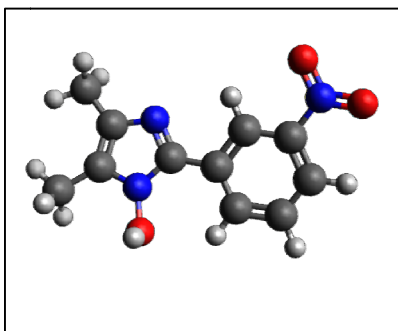


Fig-5: ^{13}C NMR spectra of 8f

Fig:6- HRMS of 8f

Supporting Information

Energies (in Hartree), Optimized Structures and Imaginary Frequencies of Transition States

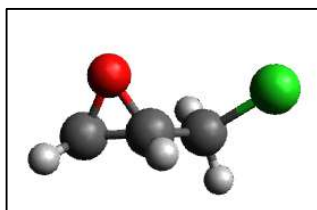


4,5-dimethyl-2-(3-nitrophenyl)-1H-imidazol-1-ol

E= -815.522200813264 E_h

Atom	X	Y	Z
C	-3.68733	2.92971	0.01382
C	-4.34114	1.71809	0.04162
N	-2.32888	2.73108	-0.03756
N	-3.32510	0.78850	0.00609
C	-2.11624	1.42395	-0.04486
C	-4.26647	4.30615	0.03010
H	-5.35638	4.28001	0.01887
H	-3.93221	4.88055	-0.83802
H	-3.95212	4.85334	0.92348
C	-5.77300	1.32472	0.10481
H	-6.01215	0.81631	1.04341
H	-6.03615	0.64783	-0.71153
H	-6.40379	2.20891	0.03267
O	-3.54485	-0.57109	0.00007
H	-3.56986	-0.84910	0.93116
C	-0.79722	0.79253	-0.09266
C	-0.58331	-0.52779	-0.51606
C	0.31079	1.56369	0.27543
C	1.57659	1.00588	0.21502
C	0.69959	-1.06333	-0.56242
C	1.80043	-0.30373	-0.19686
H	-1.42036	-1.13707	-0.82068
H	0.84073	-2.08309	-0.89500
H	2.80159	-0.70585	-0.22930
H	0.17765	2.58235	0.60299
N	2.72630	1.83080	0.60886
O	2.52015	2.97804	0.98416

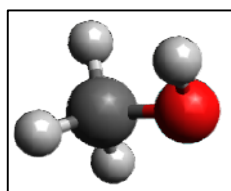
O 3.84405 1.33457 0.54461



Epichlorohydrin

E= -652.653742794466 E_h

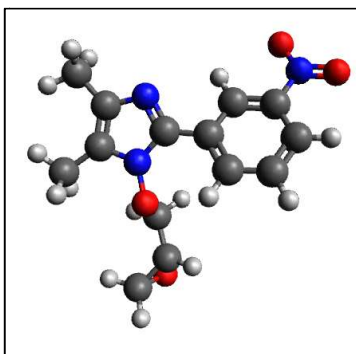
Atom	X	Y	Z
C	-3.50887	-0.27273	0.06403
C	-2.06803	-0.34886	0.32980
O	-2.57381	0.45713	-0.73196
C	-1.28437	-1.56328	-0.05582
H	-1.66607	0.21641	1.16743
Cl	0.43847	-1.15144	-0.41951
H	-1.69505	-2.02380	-0.95143
H	-1.26085	-2.28708	0.75779
H	-4.14038	0.32647	0.71344
H	-4.00649	-1.09441	-0.44390



Methanol

E= -115.719267419946 E_h

Atom	X	Y	Z
C	-3.76977	1.35097	-0.00832
O	-2.57265	0.59595	0.02563
H	-4.55244	0.77258	-0.50532
H	-3.59640	2.28661	-0.54559
H	-4.07881	1.57335	1.01572
H	-2.32332	0.41399	-0.89643

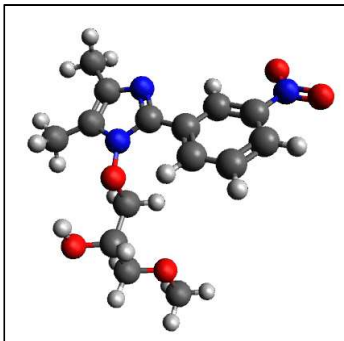


4,5-dimethyl-2-(3-nitrophenyl)-1-(oxiran-2-ylmethoxy)-1H-imidazole

E=-1007.399669468525 E_n

Atom	X	Y	Z
C	-4.61257	0.82969	0.43020
C	-4.22251	2.14385	0.30523
N	-2.85102	2.23161	0.29493
C	-2.37194	1.00426	0.41421
N	-3.42346	0.13193	0.49397
O	-3.35139	-1.23630	0.61511
C	-3.31219	-1.89014	-0.68266
C	-3.15851	-3.35996	-0.41000
H	-2.46268	-1.50567	-1.25175
H	-4.23635	-1.69382	-1.22876
C	-4.32476	-4.23513	-0.29077
O	-3.54094	-4.20767	-1.50016
H	-2.23672	-3.65483	0.08296
H	-5.32036	-3.81427	-0.38454
H	-4.24407	-5.15135	0.28354
C	-5.07573	3.36537	0.20726
H	-6.13557	3.11163	0.22339
H	-4.87357	3.90944	-0.71947
H	-4.87757	4.04912	1.03720
C	-5.93899	0.16349	0.51888
H	-6.14817	-0.45678	-0.35663
H	-6.72344	0.91559	0.58818
H	-6.00246	-0.47831	1.40065
C	-0.94983	0.66319	0.46593
C	-0.03719	1.56229	-0.09526
C	-0.45775	-0.49588	1.08395
C	1.31746	1.28197	-0.03040
C	0.90798	-0.75461	1.12948
C	1.81705	0.13174	0.57136
H	-1.14245	-1.19205	1.54491
H	1.26587	-1.65373	1.61337

H	2.87973	-0.05582	0.60143
H	-0.38700	2.46288	-0.57432
N	2.26106	2.23623	-0.62733
O	1.81334	3.24553	-1.15703
O	3.45729	1.98122	-0.56906

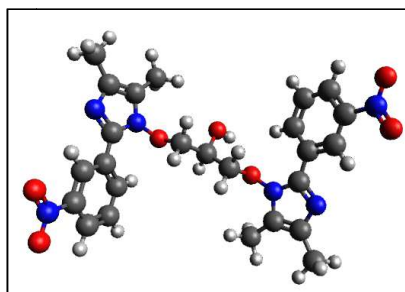


1-((4,5-dimethyl-2-(3-nitrophenyl)-1H-imidazol-1-yl)-oxy)-3-methoxypropan-2-ol

E=-1123.164376358429 E_n

Atom	X	Y	Z
H	-1.68188	-1.84213	-0.10357
H	-3.40156	-1.88862	-0.59479
C	-2.70470	-2.00493	0.23669
N	-3.18912	0.22362	0.74130
C	1.10127	-0.07367	1.85156
C	-0.26773	0.03894	1.64075
H	-0.94329	-0.58835	2.20183
H	1.47395	-0.79272	2.56851
C	-2.85661	-3.36613	0.87840
C	-2.20569	1.13375	0.46621
C	1.99387	0.73040	1.15956
C	-0.77868	0.96347	0.71839
C	-4.41494	0.72895	0.36329
H	3.05911	0.65478	1.31276
O	-3.02844	-1.03281	1.26770
C	1.47372	1.64984	0.25579
C	0.11608	1.78060	0.02182
O	3.60043	2.37591	-0.29138
H	-5.67996	-0.96095	-0.01969
N	2.39972	2.51264	-0.48846
O	1.93233	3.32920	-1.27180
H	-0.24897	2.50167	-0.69171
C	-5.67631	-0.03062	0.55300
C	-4.12187	1.97721	-0.13910
N	-2.76684	2.20632	-0.07151
H	-6.52119	0.57256	0.22631

H	-5.82601	-0.29192	1.60326
C	-5.05759	3.00512	-0.67853
H	-4.79119	3.27325	-1.70382
H	-5.02238	3.91933	-0.08064
H	-6.08433	2.64073	-0.67948
O	-4.22004	-3.64668	1.18673
H	-4.54225	-2.96163	1.78608
C	-2.39083	-4.46810	-0.05946
H	-2.24709	-3.39807	1.78911
O	-0.99919	-4.32547	-0.26633
H	-2.93180	-4.40569	-1.01323
H	-2.61859	-5.43881	0.39720
C	-0.47903	-5.30576	-1.15106
H	0.58950	-5.12053	-1.24719
H	-0.95077	-5.23418	-2.13774
H	-0.63880	-6.31555	-0.75585

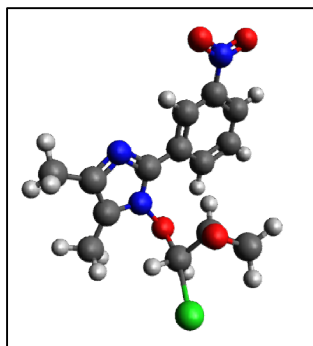


1,3-bis((4,5-dimethyl-2-(3-nitrophenyl)-1H-imidazol-1-yl)-oxy)propan-2-ol

$E = -1822.967633027439 E_h$

Atom	X	Y	Z
N	-3.59557	5.18926	-1.22986
C	-2.77635	4.63622	-2.18524
C	-3.14879	4.80478	-0.04314
N	-2.04811	4.01342	-0.23488
C	-1.78950	3.88709	-1.58433
C	-3.00661	4.87226	-3.63944
H	-2.86678	5.92680	-3.89250
H	-4.02667	4.59977	-3.92037
H	-2.31724	4.28668	-4.24725
C	-0.65971	3.07540	-2.10445
H	-0.64194	2.08406	-1.64462
H	0.30761	3.54700	-1.90719
H	-0.76041	2.95476	-3.18245
O	-1.29363	3.39202	0.72736

C	-3.74439	5.17952	1.23566
C	-3.44527	4.54377	2.45058
C	-4.67887	6.22186	1.23780
C	-5.26438	6.60414	2.43123
C	-4.04678	4.95269	3.63551
C	-4.96368	5.99360	3.64494
H	-2.74541	3.72289	2.47263
H	-3.79992	4.44717	4.56039
H	-5.43892	6.32162	4.55650
H	-4.93247	6.72500	0.31755
N	-6.23735	7.70512	2.41138
O	-6.59217	8.15312	1.32199
O	-6.65140	8.12493	3.48735
C	-0.19036	4.22618	1.16049
C	0.67732	3.33780	2.03255
H	-0.57913	5.08114	1.71752
H	0.36284	4.56958	0.28643
C	1.95951	4.05220	2.39101
O	0.01959	2.96726	3.24121
H	0.93207	2.44285	1.45464
H	-0.64560	2.29788	3.03841
O	2.88683	3.03385	2.84575
H	1.79857	4.78115	3.18739
H	2.37973	4.54746	1.51565
N	4.14742	3.54887	3.01096
C	5.08252	3.74056	2.03060
C	4.64534	3.97419	4.22447
N	6.16263	4.27358	2.58065
C	5.91482	4.41821	3.92743
C	3.85654	3.88511	5.47889
H	2.95785	4.50665	5.43555
H	4.46209	4.22281	6.31879
H	3.53822	2.85785	5.67350
C	6.94453	4.97812	4.84919
H	6.62542	4.88501	5.90438
H	7.12274	6.04987	4.63242
H	7.90607	4.44120	4.72391
C	4.91413	3.43486	0.61261
C	5.71081	4.11924	-0.30918
C	4.00251	2.48144	0.13669
C	5.56802	3.84777	-1.65906
C	3.87451	2.23546	-1.22533
C	4.65485	2.91902	-2.14520
H	3.39630	1.92377	0.83372
H	3.16270	1.49775	-1.57052
H	4.56715	2.73954	-3.20563
H	6.42253	4.85578	0.02788
N	6.40828	4.58146	-2.61390
O	7.23264	5.37274	-2.17452
O	6.24600	4.36752	-3.80861



TS1

E= -1467.619803228270 E_h

Atom	X	Y	Z
C	-4.73328	0.52141	0.38218
C	-3.76341	1.17664	-0.83003
O	-2.70794	-0.02297	-0.94809
H	-4.00437	0.92972	-2.01364
H	-3.07668	2.07937	-0.44358
Cl	-4.86594	3.13018	-1.09780
N	-1.80823	-0.04213	0.19906
C	-0.88331	0.96061	0.42668
C	-0.31437	0.63966	1.68826
N	-0.89134	-0.50874	2.18389
C	-1.81291	-0.92189	1.26514
C	0.75812	1.39467	2.44004
H	1.53651	1.79777	1.75799
H	1.25509	0.72652	3.17675
H	0.33271	2.26690	3.00178
C	-0.61581	2.04611	-0.56612
H	-0.75266	1.66243	-1.60196
H	0.42433	2.42262	-0.44873
H	-1.30272	2.92444	-0.45582
C	-2.62731	-2.14030	1.37579
C	-2.62970	-2.81042	2.63010
C	-3.36852	-3.99404	2.77597
C	-4.12935	-4.55786	1.72202
C	-3.39250	-2.70003	0.29996
C	-4.13154	-3.88838	0.48099
H	-2.05122	-2.39995	3.47644
H	-4.68391	-5.49465	1.88333
H	-3.38809	-2.19216	-0.67846
H	-4.70408	-4.31069	-0.36781
N	-3.33789	-4.68247	4.09586
O	-2.66904	-4.17206	5.01301
O	-3.98347	-5.73420	4.21710
O	-5.12074	1.37943	1.48025
C	-6.18319	0.81062	0.60677

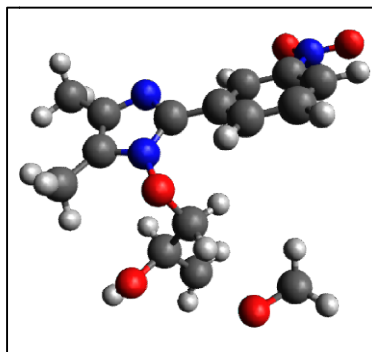
H	-4.35764	-0.48897	0.68300
H	-6.83775	0.02411	1.07324
H	-6.63471	1.60552	-0.03232

VIBRATIONAL FREQUENCIES

0:	0.00 cm ⁻¹
1:	0.00 cm ⁻¹
2:	0.00 cm ⁻¹
3:	0.00 cm ⁻¹
4:	0.00 cm ⁻¹
5:	0.00 cm ⁻¹
6:	-144.64 cm ⁻¹ ***imaginary mode***
7:	17.47 cm ⁻¹
8:	50.88 cm ⁻¹
9:	99.34 cm ⁻¹
10:	105.01 cm ⁻¹
11:	113.64 cm ⁻¹
12:	135.93 cm ⁻¹
13:	141.49 cm ⁻¹
14:	149.29 cm ⁻¹
15:	185.08 cm ⁻¹
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17:	224.03 cm ⁻¹
18:	243.46 cm ⁻¹
19:	256.86 cm ⁻¹
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22:	310.93 cm ⁻¹
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26:	383.16 cm ⁻¹
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33:	485.60 cm ⁻¹
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36:	566.92 cm ⁻¹
37:	612.72 cm ⁻¹
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92: 1503.02 cm^{**}-1

93: 1512.49 cm⁻¹
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 95: 1574.40 cm⁻¹
 96: 1956.76 cm⁻¹
 97: 2214.03 cm⁻¹
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 102: 2874.22 cm⁻¹
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 104: 2901.71 cm⁻¹
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 106: 2924.40 cm⁻¹
 107: 2966.36 cm⁻¹
 108: 3007.10 cm⁻¹
 109: 3017.58 cm⁻¹
 110: 3039.60 cm⁻¹



TS2

E=-1123.059638973081 E_h

Atom	X	Y	Z
C	-5.93557	1.92476	0.03003
C	-6.25531	1.02199	1.01958
N	-5.12838	0.23059	1.12800
C	-4.17424	0.66193	0.24544
N	-4.66315	1.68609	-0.43558
C	-2.83331	0.10740	0.08509
C	-2.18627	0.27933	-1.14078
C	-0.90285	-0.21381	-1.30111
C	-0.22520	-0.88280	-0.28875
C	-0.87105	-1.04555	0.92749
C	-2.15643	-0.55438	1.11896
H	-2.68302	0.78569	-1.95269
H	0.77323	-1.25720	-0.45303
H	-0.36572	-1.55281	1.73814
H	-2.63322	-0.67647	2.08011
N	-0.23695	-0.02746	-2.59637
O	-0.83496	0.57998	-3.47492

O	0.88858	-0.48788	-2.73865
O	-5.02456	-0.82204	2.01029
C	-5.08572	-2.10409	1.35157
C	-6.47037	-2.44245	0.81316
C	-7.44516	0.85804	1.89202
H	-7.18253	0.99580	2.94395
H	-7.89340	-0.13132	1.79665
H	-8.19343	1.60234	1.62670
C	-6.76124	3.04376	-0.50818
H	-6.84517	2.97369	-1.59514
H	-6.31065	4.01213	-0.27531
H	-7.76656	3.02966	-0.08892
H	-4.35244	-2.14357	0.54841
H	-4.81901	-2.82139	2.12249
C	-6.42107	-3.59703	-0.09240
O	-7.35703	-2.58741	1.90133
H	-6.78453	-1.60726	0.15183
H	-8.26355	-2.64813	1.57275
O	-5.08275	-5.19379	1.13201
H	-5.74411	-3.57089	-0.93573
H	-7.26010	-4.27705	-0.13583
C	-3.92527	-5.35219	0.37582
H	-3.29701	-6.11388	0.86829
H	-3.31726	-4.43703	0.30205
H	-4.11318	-5.71253	-0.64746

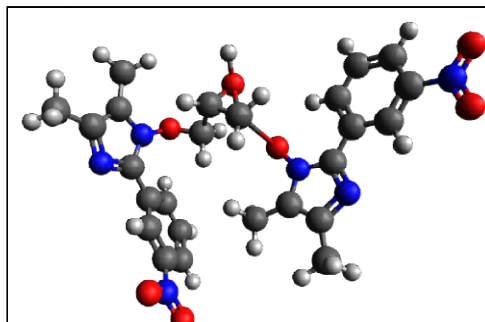
VIBRATIONAL FREQUENCIES

0:	0.00 cm ^{**} -1
1:	0.00 cm ^{**} -1
2:	0.00 cm ^{**} -1
3:	0.00 cm ^{**} -1
4:	0.00 cm ^{**} -1
5:	0.00 cm ^{**} -1
6:	-258.46 cm ^{**} -1 ***imaginary mode***
7:	2.87 cm ^{**} -1
8:	23.39 cm ^{**} -1
9:	32.52 cm ^{**} -1
10:	40.18 cm ^{**} -1
11:	51.78 cm ^{**} -1
12:	61.84 cm ^{**} -1
13:	70.09 cm ^{**} -1
14:	80.56 cm ^{**} -1
15:	91.35 cm ^{**} -1
16:	95.78 cm ^{**} -1
17:	122.89 cm ^{**} -1
18:	133.05 cm ^{**} -1
19:	142.72 cm ^{**} -1
20:	155.34 cm ^{**} -1

21: 178.31 cm**⁻¹
22: 192.50 cm**⁻¹
23: 205.04 cm**⁻¹
24: 228.45 cm**⁻¹
25: 240.87 cm**⁻¹
26: 251.33 cm**⁻¹
27: 255.73 cm**⁻¹
28: 292.86 cm**⁻¹
29: 304.35 cm**⁻¹
30: 312.52 cm**⁻¹
31: 345.12 cm**⁻¹
32: 372.33 cm**⁻¹
33: 377.28 cm**⁻¹
34: 415.16 cm**⁻¹
35: 435.17 cm**⁻¹
36: 456.96 cm**⁻¹
37: 486.02 cm**⁻¹
38: 531.36 cm**⁻¹
39: 540.89 cm**⁻¹
40: 570.50 cm**⁻¹
41: 598.49 cm**⁻¹
42: 617.72 cm**⁻¹
43: 630.48 cm**⁻¹
44: 662.06 cm**⁻¹
45: 673.68 cm**⁻¹
46: 692.90 cm**⁻¹
47: 712.61 cm**⁻¹
48: 721.10 cm**⁻¹
49: 745.97 cm**⁻¹
50: 771.87 cm**⁻¹
51: 810.98 cm**⁻¹
52: 828.51 cm**⁻¹
53: 851.30 cm**⁻¹
54: 893.94 cm**⁻¹
55: 915.36 cm**⁻¹
56: 930.44 cm**⁻¹
57: 941.98 cm**⁻¹
58: 963.21 cm**⁻¹
59: 985.59 cm**⁻¹
60: 995.70 cm**⁻¹
61: 1014.07 cm**⁻¹
62: 1020.83 cm**⁻¹
63: 1021.63 cm**⁻¹
64: 1037.37 cm**⁻¹
65: 1055.10 cm**⁻¹
66: 1055.55 cm**⁻¹
67: 1071.66 cm**⁻¹
68: 1094.04 cm**⁻¹
69: 1095.43 cm**⁻¹
70: 1115.62 cm**⁻¹

71: 1119.50 cm^{**}-1
72: 1155.10 cm^{**}-1
73: 1164.56 cm^{**}-1
74: 1171.07 cm^{**}-1
75: 1172.47 cm^{**}-1
76: 1192.16 cm^{**}-1
77: 1214.75 cm^{**}-1
78: 1242.82 cm^{**}-1
79: 1297.25 cm^{**}-1
80: 1300.00 cm^{**}-1
81: 1305.94 cm^{**}-1
82: 1317.30 cm^{**}-1
83: 1346.17 cm^{**}-1
84: 1361.61 cm^{**}-1
85: 1382.04 cm^{**}-1
86: 1392.01 cm^{**}-1
87: 1403.67 cm^{**}-1
88: 1410.98 cm^{**}-1
89: 1417.66 cm^{**}-1
90: 1431.40 cm^{**}-1
91: 1439.70 cm^{**}-1
92: 1444.24 cm^{**}-1
93: 1456.86 cm^{**}-1
94: 1461.75 cm^{**}-1
95: 1465.90 cm^{**}-1
96: 1469.07 cm^{**}-1
97: 1471.92 cm^{**}-1
98: 1474.05 cm^{**}-1
99: 1483.15 cm^{**}-1
100: 1490.33 cm^{**}-1
101: 1491.00 cm^{**}-1
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103: 1561.10 cm^{**}-1
104: 1610.58 cm^{**}-1
105: 1620.85 cm^{**}-1
106: 1652.72 cm^{**}-1
107: 2871.16 cm^{**}-1
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109: 2943.56 cm^{**}-1
110: 2950.76 cm^{**}-1
111: 3027.79 cm^{**}-1
112: 3037.60 cm^{**}-1
113: 3074.43 cm^{**}-1
114: 3093.58 cm^{**}-1
115: 3094.35 cm^{**}-1
116: 3116.09 cm^{**}-1
117: 3131.87 cm^{**}-1
118: 3162.77 cm^{**}-1
119: 3166.25 cm^{**}-1
120: 3197.00 cm^{**}-1

121: 3220.85 cm⁻¹
 122: 3234.40 cm⁻¹
 123: 3241.09 cm⁻¹
 124: 3276.93 cm⁻¹
 125: 3778.64 cm⁻¹



TS3

E=-1822.894513925493 E_n

Atom	X	Y	Z
C	-6.33538	1.48600	-0.07982
C	-6.44794	0.71015	1.05184
N	-5.19500	0.14616	1.19630
C	-4.37530	0.57522	0.18734
N	-5.06368	1.38465	-0.59992
C	-2.97499	0.19784	0.01230
C	-2.46025	0.11004	-1.28195
C	-1.13264	-0.24495	-1.45404
C	-0.28604	-0.51596	-0.38672
C	-0.80197	-0.41650	0.89662
C	-2.12958	-0.06258	1.09878
H	-3.09165	0.29980	-2.13535
H	0.74040	-0.79829	-0.56161
H	-0.16399	-0.61586	1.74678
H	-2.51304	0.01494	2.10600
N	-0.60913	-0.36256	-2.82011
O	-1.35244	-0.08545	-3.75230
O	0.54823	-0.73499	-2.96516
O	-4.88418	-0.75445	2.19176
C	-4.70773	-2.08857	1.67538
C	-6.00498	-2.71462	1.16121
C	-7.54797	0.47700	2.02166
H	-7.29070	0.86565	3.01040
H	-7.77366	-0.58406	2.13736
H	-8.44834	0.98400	1.68022
C	-7.36338	2.36189	-0.71170
H	-7.48667	2.11315	-1.76821
H	-7.07217	3.41396	-0.65352
H	-8.32996	2.25252	-0.22125
H	-3.95806	-2.08543	0.89058
H	-4.34243	-2.66022	2.52405

C	-5.73120	-3.83791	0.26371
O	-6.83113	-3.02251	2.26306
H	-6.48683	-1.96298	0.50123
H	-7.72604	-3.21216	1.95131
O	-3.82291	-4.96472	1.22736
H	-5.14935	-3.65971	-0.63034
H	-6.32423	-4.73986	0.32092
N	-3.25776	-5.64042	0.24601
C	-3.56132	-6.92334	-0.16684
N	-2.78436	-7.24838	-1.19104
C	-1.98177	-6.16180	-1.45489
C	-2.26355	-5.14046	-0.57586
C	-0.97796	-6.19099	-2.55606
H	-0.26204	-7.00440	-2.41237
H	-0.42264	-5.25522	-2.60993
H	-1.46389	-6.35233	-3.52220
C	-1.73026	-3.76663	-0.40874
H	-0.88049	-3.61150	-1.07083
H	-1.40469	-3.58575	0.61731
H	-2.48236	-3.01068	-0.64794
C	-4.59155	-7.78137	0.40011
C	-5.31614	-7.47143	1.56272
C	-6.29354	-8.33530	2.04485
C	-6.57736	-9.52596	1.39491
C	-5.85003	-9.82446	0.24709
C	-4.87503	-8.98495	-0.25838
H	-5.10688	-6.55148	2.08451
H	-6.83833	-8.07452	2.94250
H	-7.33252	-10.20511	1.75863
H	-4.33755	-9.24973	-1.15445
N	-6.13086	-11.07892	-0.46132
O	-5.48091	-11.34038	-1.46573
O	-7.00486	-11.81150	-0.01430

VIBRATIONAL FREQUENCIES

0:	0.00 cm ^{**} -1
1:	0.00 cm ^{**} -1
2:	0.00 cm ^{**} -1
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4:	0.00 cm ^{**} -1
5:	0.00 cm ^{**} -1
6:	-196.06 cm ^{**} -1 ***imaginary mode***
7:	9.23 cm ^{**} -1
8:	13.89 cm ^{**} -1
9:	17.21 cm ^{**} -1
10:	21.27 cm ^{**} -1
11:	28.58 cm ^{**} -1
12:	32.01 cm ^{**} -1

13: 46.23 cm**⁻¹
14: 49.32 cm**⁻¹
15: 52.69 cm**⁻¹
16: 63.58 cm**⁻¹
17: 70.59 cm**⁻¹
18: 71.31 cm**⁻¹
19: 80.77 cm**⁻¹
20: 82.50 cm**⁻¹
21: 84.30 cm**⁻¹
22: 92.40 cm**⁻¹
23: 101.10 cm**⁻¹
24: 114.49 cm**⁻¹
25: 121.86 cm**⁻¹
26: 135.10 cm**⁻¹
27: 157.19 cm**⁻¹
28: 161.40 cm**⁻¹
29: 168.93 cm**⁻¹
30: 179.13 cm**⁻¹
31: 182.77 cm**⁻¹
32: 203.41 cm**⁻¹
33: 213.69 cm**⁻¹
34: 225.41 cm**⁻¹
35: 242.32 cm**⁻¹
36: 251.71 cm**⁻¹
37: 252.56 cm**⁻¹
38: 257.29 cm**⁻¹
39: 285.40 cm**⁻¹
40: 294.09 cm**⁻¹
41: 301.22 cm**⁻¹
42: 307.70 cm**⁻¹
43: 309.55 cm**⁻¹
44: 341.07 cm**⁻¹
45: 342.64 cm**⁻¹
46: 363.31 cm**⁻¹
47: 375.70 cm**⁻¹
48: 378.22 cm**⁻¹
49: 393.27 cm**⁻¹
50: 415.42 cm**⁻¹
51: 417.56 cm**⁻¹
52: 435.38 cm**⁻¹
53: 439.09 cm**⁻¹
54: 455.65 cm**⁻¹
55: 475.72 cm**⁻¹
56: 528.31 cm**⁻¹
57: 538.89 cm**⁻¹
58: 540.26 cm**⁻¹
59: 543.58 cm**⁻¹
60: 559.29 cm**⁻¹
61: 587.19 cm**⁻¹
62: 596.81 cm**⁻¹

63: 617.25 cm**⁻¹
64: 622.55 cm**⁻¹
65: 637.27 cm**⁻¹
66: 661.41 cm**⁻¹
67: 662.55 cm**⁻¹
68: 672.59 cm**⁻¹
69: 679.59 cm**⁻¹
70: 689.49 cm**⁻¹
71: 693.05 cm**⁻¹
72: 711.77 cm**⁻¹
73: 715.57 cm**⁻¹
74: 720.96 cm**⁻¹
75: 722.93 cm**⁻¹
76: 746.58 cm**⁻¹
77: 769.81 cm**⁻¹
78: 772.07 cm**⁻¹
79: 773.22 cm**⁻¹
80: 810.41 cm**⁻¹
81: 826.55 cm**⁻¹
82: 826.70 cm**⁻¹
83: 829.39 cm**⁻¹
84: 852.40 cm**⁻¹
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90: 941.78 cm**⁻¹
91: 961.80 cm**⁻¹
92: 963.18 cm**⁻¹
93: 984.34 cm**⁻¹
94: 987.01 cm**⁻¹
95: 998.64 cm**⁻¹
96: 1007.70 cm**⁻¹
97: 1015.52 cm**⁻¹
98: 1016.16 cm**⁻¹
99: 1019.04 cm**⁻¹
100: 1020.43 cm**⁻¹
101: 1022.63 cm**⁻¹
102: 1045.10 cm**⁻¹
103: 1051.37 cm**⁻¹
104: 1055.26 cm**⁻¹
105: 1067.36 cm**⁻¹
106: 1071.53 cm**⁻¹
107: 1091.62 cm**⁻¹
108: 1094.83 cm**⁻¹
109: 1097.31 cm**⁻¹
110: 1109.68 cm**⁻¹
111: 1116.87 cm**⁻¹
112: 1120.81 cm**⁻¹

113: 1133.20 cm^{**}-1
114: 1159.12 cm^{**}-1
115: 1166.77 cm^{**}-1
116: 1172.86 cm^{**}-1
117: 1183.95 cm^{**}-1
118: 1192.78 cm^{**}-1
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121: 1249.14 cm^{**}-1
122: 1283.95 cm^{**}-1
123: 1299.10 cm^{**}-1
124: 1300.66 cm^{**}-1
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135: 1392.75 cm^{**}-1
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141: 1430.72 cm^{**}-1
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143: 1461.86 cm^{**}-1
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155: 1491.82 cm^{**}-1
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157: 1535.71 cm^{**}-1
158: 1552.37 cm^{**}-1
159: 1563.55 cm^{**}-1
160: 1605.28 cm^{**}-1
161: 1612.30 cm^{**}-1
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190: 3281.95 cm^{**}-1
191: 3773.24 cm^{**}-1