

# Hydrogen-abstractions from toluene and derivatives by phthalimide-*N*-oxyl radicals: a theoretical study

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## SUPPORTING INFORMATION

## Contents:

UB3LYP/6-31G(d,p) optimized geometries, vibration frequencies and rotational constants for the TSs of PINO<sup>•</sup> + ...reaction (see Table 1).

<i>p</i> -(CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CH <sub>3</sub> )	S.I.3
<i>p</i> -(H-C <sub>6</sub> H <sub>4</sub> -CH <sub>3</sub> )	S.I.4
<i>p</i> -(C(O)OH-C <sub>6</sub> H <sub>4</sub> -CH <sub>3</sub> )	S.I.6
<i>p</i> -(NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -CH <sub>3</sub> )	S.I.8
<i>p</i> -(CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CHO)	S.I.9
<i>p</i> -(H-C <sub>6</sub> H <sub>4</sub> -CHO)	S.I.11
<i>p</i> -(C(O)OH-C <sub>6</sub> H <sub>4</sub> -CHO)	S.I.12
<i>p</i> -(NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -CHO)	S.I.14
<i>p</i> -(CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> -CH <sub>2</sub> OH)	S.I.16
<i>p</i> -(CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CH <sub>2</sub> OH)	S.I.17
<i>p</i> -(H-C <sub>6</sub> H <sub>4</sub> -CH <sub>2</sub> OH)	S.I.19
<i>p</i> -(NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -CH <sub>2</sub> OH)	S.I.21

*p*-(CH<sub>3</sub>-C<sub>6</sub>H<sub>4</sub>-CH<sub>3</sub>)

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -898.480581356

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.579258	-2.156950	-0.002781
C	2.470999	-0.709666	-0.003062
C	2.397823	0.020755	1.207721
C	2.273510	1.402850	1.202059
C	2.388576	0.019535	-1.213523
C	2.204977	2.123438	-0.003278
C	2.264139	1.402126	-1.207987
H	2.963917	-2.614868	0.908972
H	2.957636	-2.615659	-0.916758
H	2.440163	-0.516056	2.151338
H	2.230562	1.939939	2.146353
H	2.423566	-0.517904	-2.157083
H	2.213673	1.938461	-2.152261
H	1.310338	-2.627353	0.001540
O	0.163504	-2.988136	0.004793
N	-0.590254	-1.891055	0.003475
C	-1.033169	-1.249167	1.187907
C	-1.036810	-1.254600	-1.182508
O	-0.746898	-1.574193	2.318310
O	-0.753815	-1.584715	-2.312270
C	-1.890995	-0.131607	-0.698407
C	-2.608407	0.809314	-1.422446
C	-1.888774	-0.128354	0.701262
C	-3.335399	1.765964	-0.700965
C	-2.603857	0.815969	1.423177
C	-3.333135	1.769256	0.699550
H	-2.602695	0.796321	-2.507547
H	-3.910861	2.516696	-1.234441
H	-2.594702	0.808024	2.508304
H	-3.906895	2.522484	1.231344
C	2.040602	3.622660	-0.001728
H	0.981025	3.902832	0.061929
H	2.547205	4.080686	0.853313
H	2.440488	4.070978	-0.915937

Rotational constants (GHz): 0.4218700 0.3216500 0.2527900

Vibrational harmonic frequencies (cm<sup>-1</sup>):

-1652.4665	14.6210	18.4279
27.7897	36.4717	54.7435
60.6097	98.5592	139.8416
149.7854	185.0599	238.4288
270.5570	293.4837	311.5879

335.2500	361.4803	386.8190
408.7630	414.0377	455.8436
463.5177	483.1956	517.9036
522.7712	523.6776	554.0995
603.9333	650.8902	677.0348
704.6461	716.5828	718.5458
723.9992	751.3125	784.8796
795.1294	827.5311	839.8835
849.8339	892.7330	910.3645
962.0911	969.2153	973.1650
989.6151	1006.9356	1015.4010
1025.7175	1029.6957	1047.0088
1059.5857	1083.9636	1094.9768
1132.1041	1150.0173	1170.3581
1184.4242	1192.6109	1205.6528
1232.9009	1241.5793	1280.0486
1311.8999	1342.7919	1351.6201
1388.8638	1401.3879	1424.9280
1459.7120	1480.8276	1499.1549
1501.9382	1502.3677	1506.2389
1514.5183	1547.7287	1591.9384
1644.5005	1655.8242	1661.7580
1820.7432	1860.4963	3036.0715
3097.3864	3107.6658	3128.3907
3179.4686	3179.9955	3192.0821
3193.6765	3198.7956	3200.9093
3205.3142	3217.6766	3220.8144

Zero-point correction (Hartree): 0.258456

*p*-(H-C<sub>6</sub>H<sub>4</sub>-CH<sub>3</sub>)

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -859.159834465

Electronic state : 2-A

Cartesian coordinates (Angs):

C	3.039815	-1.335624	-0.058557
C	2.653931	0.064423	-0.083410
C	2.540904	0.809299	1.115695
C	2.147238	2.141723	1.092446
C	2.330361	0.709794	-1.301711
C	1.845934	2.766199	-0.123968
C	1.936772	2.042658	-1.319057
H	3.577563	-1.676343	0.826599
H	3.419580	-1.752926	-0.991391

H	2.763478	0.322899	2.061233
H	2.073036	2.698562	2.021988
H	2.389288	0.146089	-2.228555
H	1.538784	3.807772	-0.139903
H	1.699560	2.522961	-2.263906
H	1.885491	-2.039665	0.070709
O	0.843556	-2.619258	0.168771
N	-0.124067	-1.706651	0.118457
C	-0.659010	-1.072746	1.269539
C	-0.732718	-1.284786	-1.091402
O	-0.276493	-1.232502	2.406571
O	-0.416741	-1.644020	-2.203344
C	-1.792985	-0.330673	-0.656326
C	-2.716756	0.371485	-1.416663
C	-1.748986	-0.205065	0.737214
C	-3.608973	1.212719	-0.738342
C	-2.627268	0.626688	1.416220
C	-3.564773	1.338500	0.655791
H	-2.741565	0.265838	-2.496414
H	-4.347373	1.776355	-1.300785
H	-2.583492	0.715651	2.496846
H	-4.269387	1.998032	1.153576

Rotational constants (GHz): 0.5266200 0.3264200 0.2900500

Vibrational harmonic frequencies (cm<sup>-1</sup>):

-1668.5689	8.5263	20.3838
28.5154	59.3142	61.0391
116.1340	139.6517	167.0532
210.7028	239.0964	311.2477
325.1244	341.9674	348.9902
405.7063	413.8899	463.6559
468.9124	490.4477	514.8954
523.6751	543.3474	563.3175
603.8225	628.2935	676.8795
694.2209	704.6768	716.5957
719.9163	772.5592	784.8125
795.6318	829.5302	844.0928
892.4216	910.5176	918.2263
972.5521	973.7300	996.3186
998.6823	1007.4340	1007.9750
1016.2811	1046.9548	1049.1795
1085.2945	1094.7873	1120.3251
1131.8671	1159.1113	1184.9251
1185.0432	1192.8348	1204.2014
1233.1259	1274.2320	1312.0706
1351.1565	1364.2020	1388.8426
1401.7851	1479.0973	1490.0921

1502.6792	1506.6063	1509.9742
1532.3794	1609.4267	1634.6785
1655.7172	1661.9338	1821.5793
1861.0395	3109.1073	3184.0340
3189.3115	3192.8138	3196.2130
3197.4748	3204.3115	3205.8689
3212.5660	3217.8025	3221.0570

Zero-point correction (Hartree): 0.231021

*p*-(C(O)OH-C<sub>6</sub>H<sub>4</sub>-CH<sub>3</sub>)

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1047.73364279

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.122755	-3.495825	-0.085515
C	-1.004639	-2.344723	-0.087451
C	-1.322631	-1.671946	-1.294328
C	-2.143032	-0.555753	-1.290501
C	-1.531205	-1.828872	1.122680
C	-2.669129	-0.066761	-0.082542
C	-2.354097	-0.712793	1.125469
H	-0.019356	-4.034883	-1.027119
H	-0.160971	-4.140089	0.792803
H	-0.908594	-2.039646	-2.228645
H	-2.394575	-0.040505	-2.211236
H	-1.280540	-2.319340	2.058681
H	1.138471	-2.989691	0.035677
O	2.220524	-2.504322	0.124717
N	2.072390	-1.183510	0.093311
C	2.076074	-0.428169	-1.109674
C	1.916618	-0.387062	1.259518
O	2.144916	-0.886864	-2.227275
O	1.838552	-0.804902	2.392129
C	1.871015	1.010483	0.743245
C	1.754246	2.205072	1.439019
C	1.964544	0.986178	-0.653882
C	1.733869	3.390441	0.692082
C	1.942330	2.155106	-1.400756
C	1.826060	3.365916	-0.705272
H	1.682750	2.211869	2.521761
H	1.644527	4.344437	1.202958
H	2.013069	2.123685	-2.483072

H	1.805929	4.300971	-1.256851
H	-2.757928	-0.332337	2.056648
C	-3.543426	1.131940	-0.137005
O	-3.834647	1.733608	-1.152719
O	-4.003594	1.511062	1.082107
H	-4.558566	2.292041	0.923024

Rotational constants (GHz): 0.3406100 0.2532100 0.1921100

Vibrational harmonic frequencies (cm<sup>-1</sup>):

-1698.7192	14.2207	15.2126
31.7069	47.9035	51.6947
77.9304	87.0123	138.3658
139.6414	179.6927	192.4751
239.9270	246.0177	311.7227
327.6145	338.5530	349.4112
367.2268	410.5601	414.0018
462.5894	472.0148	497.8331
502.2076	517.7988	523.5964
546.1577	600.1945	605.4302
609.5493	645.1654	676.4002
705.2466	712.6539	716.6799
720.2017	737.4121	781.6268
784.5934	796.3375	845.0321
848.0453	865.5150	892.0085
911.5842	975.5982	983.1119
995.1390	1000.7407	1009.9573
1015.6131	1028.0253	1047.9163
1085.3778	1093.6120	1119.1049
1127.6458	1134.0655	1153.6870
1185.9343	1189.3735	1193.5841
1222.0883	1234.3584	1274.1810
1312.8270	1339.4089	1361.2543
1384.0227	1396.2986	1402.5573
1457.9199	1476.8068	1502.4535
1507.1285	1509.4283	1541.8617
1588.6283	1640.2748	1655.0887
1661.3060	1814.4366	1823.8921
1862.4248	3113.0365	3194.6940
3198.1332	3199.1496	3201.8394
3207.5087	3219.1958	3222.4547
3225.6217	3230.7974	3770.2356

Zero-point correction (Hartree): 0.246148

*p*-(NO<sub>2</sub>-C<sub>6</sub>H<sub>4</sub>-CH<sub>3</sub>)

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1063.65552154

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.243048	-3.492653	-0.046729
C	-1.079321	-2.309029	-0.040586
C	-1.426740	-1.657506	-1.251316
C	-2.194767	-0.503520	-1.248627
C	-1.523715	-1.738659	1.179217
C	-2.620713	0.018984	-0.024335
C	-2.292911	-0.585632	1.192367
H	-0.196978	-4.057604	-0.977244
H	-0.259004	-4.110270	0.850756
H	-1.075648	-2.068060	-2.193031
H	-2.470036	0.001476	-2.165944
H	-1.249557	-2.213105	2.116393
H	1.045015	-3.018112	0.006563
O	2.130420	-2.556514	0.044151
N	2.009230	-1.233452	0.035005
C	1.980915	-0.460890	-1.158520
C	1.913574	-0.449451	1.217954
O	1.992790	-0.907461	-2.282713
O	1.864700	-0.884742	2.345301
C	1.876376	0.954536	0.721518
C	1.804874	2.141331	1.436851
C	1.916517	0.947755	-0.678961
C	1.775460	3.336817	0.706664
C	1.885848	2.127368	-1.408921
C	1.815326	3.329975	-0.693439
H	1.772673	2.134989	2.521412
H	1.718624	4.284785	1.232872
H	1.915261	2.110256	-2.493455
H	1.788791	4.272707	-1.231329
H	-2.642646	-0.142897	2.116460
N	-3.427545	1.244539	-0.015512
O	-3.694642	1.760556	-1.101505
O	-3.786310	1.684619	1.077424

Rotational constants (GHz): 0.3422100 0.2629800 0.1979500

Vibrational harmonic frequencies (cm<sup>-1</sup>):

-1704.4752	10.8673	13.5088
27.0984	47.5702	50.4132
70.3674	88.1597	137.2330
139.1231	180.5186	226.7884
240.4295	250.6326	311.9422
331.4504	341.0078	361.7370



376.9064	413.4585	414.2771
461.1735	473.0902	504.5690
510.8526	523.2585	534.6777
546.4726	600.7077	641.0904
642.9418	675.7556	698.6572
705.4212	716.4626	719.5319
764.0293	783.7680	796.9622
817.9639	838.9206	863.3922
872.6590	891.2342	913.0185
977.8005	984.6316	988.8683
998.8779	1012.2335	1015.2424
1024.0029	1048.0586	1086.8083
1092.1265	1115.2801	1125.7944
1127.9581	1144.4922	1186.8976
1194.0008	1206.6909	1234.6259
1270.7589	1313.2629	1331.3869
1372.6869	1378.6770	1397.1308
1403.2230	1455.4445	1476.6973
1502.0003	1505.2212	1507.3440
1529.5237	1593.3372	1628.4269
1654.2936	1656.9089	1660.1129
1825.1737	1863.1146	3117.3681
3197.0925	3205.1193	3206.7288
3207.8586	3209.3680	3220.2725
3223.6403	3249.0294	3249.3344

Zero-point correction (Hartree): 0.233524

*p*-(CH<sub>3</sub>-C<sub>6</sub>H<sub>4</sub>-CHO)

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -972.493119112

Electronic state : 2-A

Cartesian coordinates (Angs):

H	0.557767	1.478040	0.635237
O	-0.256612	1.152624	1.479176
N	-1.312527	0.593279	0.877779
C	-2.458954	1.324866	0.470323
C	-1.422719	-0.794559	0.652721
C	-2.778885	-0.972315	0.059797
C	-3.391398	0.281711	-0.050224
C	-3.421301	-2.130325	-0.352750
C	-4.667346	0.419155	-0.575855
C	-4.711974	-2.000407	-0.883890
C	-5.324841	-0.746264	-0.993785
O	-2.597809	2.523319	0.547016

O	-0.566061	-1.620704	0.895265
H	-2.936240	-3.096926	-0.263455
H	-5.131783	1.396560	-0.656701
H	-5.246418	-2.885410	-1.216006
H	-6.325455	-0.677186	-1.409903
C	2.664203	0.816704	-0.199816
C	2.567549	-0.352754	0.567435
C	3.633654	-1.249674	0.584037
C	3.830980	1.080190	-0.944271
C	4.804346	-0.998777	-0.143543
C	4.884393	0.180128	-0.909677
C	1.545805	1.773679	-0.235743
O	1.448836	2.765430	-0.907071
H	1.658651	-0.565962	1.121744
H	3.553995	-2.160425	1.170736
H	3.887645	1.988410	-1.535861
H	5.785337	0.383665	-1.483027
C	5.966996	-1.958899	-0.102803
H	6.348819	-2.163972	-1.108455
H	6.798468	-1.540028	0.477087
H	5.687034	-2.909828	0.357319

Rotational constants (GHz): 0.6443700 0.1457400 0.1281700

Vibrational harmonic frequencies (cm<sup>-1</sup>):

-1518.3695	13.1011	27.1857
31.7807	38.0792	65.0131
72.8539	97.4213	106.8814
140.7208	162.1899	209.9894
233.5770	241.4644	253.4764
324.1291	338.5203	344.3803
371.3256	412.3580	418.1767
420.4055	465.1851	476.4445
486.2604	524.0947	551.7486
601.4016	626.1223	652.6163
676.5275	702.3480	716.4065
718.5186	722.4217	778.5082
784.5734	794.6612	837.4978
864.5228	867.3162	893.3016
910.5206	973.6204	984.9330
999.9540	1008.3625	1013.1532
1014.2963	1037.5516	1046.6382
1064.1029	1096.3985	1138.1601
1148.0304	1182.2769	1185.2066
1192.4607	1218.1733	1229.5685
1232.6640	1239.2293	1312.3198
1346.0129	1357.9558	1380.6126
1403.0111	1425.2692	1448.4760

1453.7934	1497.3722	1502.4712
1503.4918	1506.1760	1542.2258
1615.5608	1655.2246	1656.3129
1661.7370	1811.7968	1842.8993
1861.7494	3044.1063	3102.1037
3135.8172	3182.9079	3193.4092
3194.1860	3206.3834	3214.1976
3214.8330	3218.0833	3221.4082

Zero-point correction (Hartree): 0.240781

*p*-(H-C<sub>6</sub>H<sub>4</sub>-CHO)

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -933.171888473

Electronic state : 2-A

Cartesian coordinates (Angs):

H	1.027253	1.243661	0.633982
O	0.196121	0.985499	1.478736
N	-0.912911	0.537752	0.879956
C	-1.991536	1.379310	0.500153
C	-1.149970	-0.829337	0.626129
C	-2.522348	-0.870489	0.045678
C	-3.019520	0.436125	-0.030639
C	-3.271484	-1.956083	-0.383780
C	-4.282691	0.700192	-0.538299
C	-4.550000	-1.697972	-0.897102
C	-5.047358	-0.391288	-0.973147
O	-2.019466	2.583427	0.602772
O	-0.367814	-1.733332	0.840498
H	-2.875564	-2.964431	-0.320239
H	-4.657199	1.717188	-0.593143
H	-5.165845	-2.523325	-1.241546
H	-6.041541	-0.222523	-1.375950
C	3.075835	0.417133	-0.215913
C	2.880287	-0.745592	0.544388
C	3.873514	-1.724395	0.558741
C	4.259208	0.602898	-0.955726
C	5.050595	-1.538841	-0.169092
C	5.244390	-0.376155	-0.926155
C	2.032150	1.461095	-0.245173
O	2.011979	2.456107	-0.916752
H	1.954482	-0.885602	1.093823
H	3.727243	-2.630781	1.137745
H	4.383301	1.511535	-1.536045

H	5.822936	-2.302632	-0.150425
H	6.162317	-0.240566	-1.490296

Rotational constants (GHz): 0.7290700 0.1713500 0.1513700

Vibrational harmonic frequencies (cm<sup>-1</sup>):

-1529.4470	16.9316	28.3790
38.9172	63.1424	79.9652
102.4932	140.4624	143.8780
165.0521	234.7309	236.6504
242.0283	324.9573	332.7083
350.8785	412.3439	417.7695
437.5225	451.6620	465.0846
486.9289	524.1024	551.7486
601.7240	625.6470	676.1507
681.0553	701.2545	702.7993
716.4494	719.7933	777.1324
780.0856	794.8988	851.9294
869.6506	893.1046	910.9524
963.8802	974.2075	995.5626
1008.7449	1014.1564	1014.6086
1019.7204	1046.6573	1051.8891
1096.2515	1114.6900	1138.0008
1177.9548	1185.1901	1190.8278
1192.4919	1214.6689	1226.5710
1230.3313	1312.4415	1350.2676
1371.0872	1382.3575	1403.1445
1452.7023	1490.2657	1502.4152
1506.5283	1526.8090	1631.0431
1646.0132	1656.2289	1661.6662
1812.2908	1847.0918	1863.0921
3188.9306	3193.6984	3201.6065
3206.6836	3209.7000	3217.8173
3218.5194	3219.7820	3221.7721

Zero-point correction (Hartree): 0.213467

*p*-(C(O)OH-C<sub>6</sub>H<sub>4</sub>-CHO)

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1121.74297168

Electronic state : 2-A

Cartesian coordinates (Angs):

H	-0.182836	1.647950	0.684028
O	-0.953106	1.227256	1.508018
N	-1.950649	0.586396	0.889011
C	-3.166402	1.213309	0.505305

C	-1.919979	-0.797058	0.615191
C	-3.253398	-1.090253	0.018037
C	-3.989745	0.098952	-0.049346
C	-3.776682	-2.292396	-0.434957
C	-5.274307	0.124904	-0.571394
C	-5.075034	-2.274924	-0.962683
C	-5.811530	-1.085880	-1.030002
O	-3.422172	2.388753	0.621166
O	-0.980145	-1.536608	0.826552
H	-3.196428	-3.207627	-0.378814
H	-5.835141	1.052605	-0.619238
H	-5.518283	-3.197227	-1.325900
H	-6.814910	-1.103848	-1.444693
C	2.000647	1.225732	-0.163874
C	2.016972	0.033494	0.573444
C	3.172415	-0.745759	0.585738
C	3.134881	1.643636	-0.885867
C	4.304458	-0.329528	-0.126112
C	4.282978	0.866904	-0.861918
C	0.777096	2.060371	-0.188112
O	0.583732	3.041352	-0.850658
H	1.128821	-0.288757	1.108017
H	3.198452	-1.673969	1.144002
H	3.094193	2.570239	-1.448875
H	5.175500	1.160508	-1.403697
C	5.567734	-1.124440	-0.140921
O	6.571988	-0.806175	-0.744520
O	5.488526	-2.256612	0.595766
H	6.353967	-2.690764	0.516318

Rotational constants (GHz): 0.5482200 0.1078300 0.0958400

Vibrational harmonic frequencies (cm<sup>-1</sup>):

-1558.9316	10.8607	24.3672
33.5575	48.6427	63.3375
74.4120	81.4631	102.2081
140.9090	159.3167	167.3115
213.4320	237.1188	242.4302
252.5504	320.4385	336.6179
346.6741	357.6985	412.5925
418.7786	448.6265	464.9099
475.8172	494.4245	524.3069
535.9545	551.4788	601.5875
611.1481	639.8277	666.2438
676.4053	703.1291	712.5927
716.4550	719.5688	764.6160
780.5658	782.2046	795.4923
862.4947	873.6681	888.3853

893.8085	911.2197	974.9026
1004.9105	1009.4894	1009.7044
1014.3098	1036.6873	1046.9070
1096.1484	1122.0955	1137.3519
1138.6433	1174.6328	1185.7038
1192.7417	1200.1877	1217.2960
1222.7624	1230.7314	1312.7399
1339.7340	1364.7474	1383.5462
1393.9293	1403.4889	1448.9127
1457.6640	1502.4629	1506.8306
1536.6806	1615.7611	1655.7913
1657.8912	1661.7441	1812.7760
1824.6179	1850.7238	1865.0627
3194.5700	3207.3714	3213.6412
3214.9729	3218.9787	3222.2937
3228.6280	3237.4285	3767.7291

Zero-point correction (Hartree): 0.228399

*p*-(NO<sub>2</sub>-C<sub>6</sub>H<sub>4</sub>-CHO)

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1137.66309363

Electronic state : 2-A

Cartesian coordinates (Angs):

H	-0.163551	1.654553	0.666816
O	-0.931575	1.248109	1.485002
N	-1.932635	0.606861	0.872114
C	-3.149865	1.234442	0.489871
C	-1.906472	-0.778717	0.608538
C	-3.243856	-1.073662	0.023180
C	-3.978256	0.116867	-0.049491
C	-3.772357	-2.278552	-0.416518
C	-5.266047	0.141089	-0.563693
C	-5.074020	-2.262550	-0.935907
C	-5.808473	-1.072491	-1.008501
O	-3.399564	2.411646	0.596688
O	-0.964320	-1.516236	0.817929
H	-3.193905	-3.194637	-0.356428
H	-5.825509	1.069352	-0.615894
H	-5.521544	-3.186902	-1.288339
H	-6.814526	-1.091912	-1.416471
C	2.030266	1.192892	-0.165243
C	2.014486	-0.003841	0.565209
C	3.155172	-0.804376	0.591403
C	3.180318	1.598772	-0.867486
C	4.283551	-0.380910	-0.105135

C	4.320636	0.808215	-0.836511
C	0.818263	2.050257	-0.203364
O	0.656915	3.032375	-0.871069
H	1.113726	-0.316950	1.084156
H	3.181532	-1.739463	1.136120
H	3.162347	2.529265	-1.424803
H	5.227057	1.085169	-1.359882
N	5.496504	-1.226856	-0.073852
O	5.444796	-2.267867	0.576196
O	6.477149	-0.832166	-0.701149

Rotational constants (GHz): 0.5545500 0.1084300 0.0962600

Vibrational harmonic frequencies (cm<sup>-1</sup>):

-1583.1794	11.0560	24.1192
34.6233	45.6567	63.5999
72.4791	80.9235	103.4808
141.0725	159.2495	179.7076
220.4314	237.8628	243.2514
278.2825	321.2550	337.3015
353.9233	359.5492	412.4497
422.6803	457.8044	464.7003
482.1036	519.9579	524.2415
540.1110	556.5383	601.4715
636.1614	676.1785	695.2158
703.5179	712.1269	716.6094
720.9088	762.7227	780.2709
796.0880	832.4152	863.3850
880.8224	891.1953	896.0166
911.8042	975.9568	999.1734
1010.9695	1012.1329	1015.2509
1032.8118	1046.9984	1095.8913
1122.6218	1130.9332	1136.5100
1169.0894	1186.2022	1193.0359
1208.1804	1211.5939	1230.8008
1313.1248	1330.9330	1374.3385
1384.8066	1401.5150	1404.3296
1445.6700	1460.2928	1502.3083
1506.9841	1523.4439	1619.5918
1644.8743	1655.4296	1661.3014
1675.0560	1812.6814	1853.9119
1867.6764	3195.6857	3208.2900
3213.8499	3219.6532	3221.2494
3222.9543	3250.0669	3253.0329

Zero-point correction (Hartree): 0.215803

*p*-(CH<sub>3</sub>O-C<sub>6</sub>H<sub>4</sub>-CH<sub>2</sub>OH)

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1048.90371509

Electronic state : 2-A

Cartesian coordinates (Angs):

C	1.279567	-2.819563	0.071316
C	1.839376	-1.457314	-0.091004
C	2.395319	-0.794145	1.017465
C	2.912420	0.493529	0.911267
C	1.805975	-0.776123	-1.324649
C	2.875386	1.153491	-0.327069
C	2.318911	0.505419	-1.443589
H	1.896093	-3.485045	0.685044
H	2.419292	-1.295037	1.982220
H	3.336340	0.971283	1.786311
H	1.392914	-1.277041	-2.193305
H	2.312421	1.029945	-2.393539
H	0.229972	-2.652648	0.795961
O	-1.003417	-2.540173	1.171700
N	-1.438689	-1.359380	0.740325
C	-1.705041	-0.253378	1.598116
C	-1.702710	-1.081694	-0.607838
O	-1.507290	-0.221937	2.789517
O	-1.454276	-1.822512	-1.548575
C	-2.271428	0.292354	-0.620565
C	-2.734348	1.054552	-1.682527
C	-2.270408	0.787023	0.689595
C	-3.211164	2.341542	-1.395448
C	-2.734737	2.060019	0.980739
C	-3.211034	2.836072	-0.086070
H	-2.726990	0.662209	-2.694128
H	-3.585786	2.965906	-2.200929
H	-2.726833	2.434492	1.999194
H	-3.584761	3.837529	0.104995
O	0.825188	-3.488646	-1.046349
H	0.020586	-3.035862	-1.371630
O	3.350583	2.408572	-0.548901
C	3.935241	3.114030	0.537064
H	4.812978	2.588446	0.933374
H	4.245565	4.079512	0.135353
H	3.214767	3.274652	1.348855

Rotational constants (GHz): 0.3293900 0.2396900 0.1831700

Vibrational harmonic frequencies (cm<sup>-1</sup>):

-1385.6558	11.9580	27.3194
36.3391	54.5750	80.0456
84.1593	126.0045	144.2819



165.7241	170.4214	186.1699
201.7823	239.1703	249.6765
258.0435	303.9216	317.5306
349.4323	383.0967	407.0362
416.0146	420.9884	464.5882
469.4618	480.2828	524.8036
531.1370	569.0254	593.6576
614.7241	625.2349	649.6724
675.7505	701.6265	717.1202
718.6440	724.7129	760.9887
777.8993	794.0041	822.3959
842.1055	854.5621	895.5567
910.6605	947.6591	966.0233
973.2551	1008.4427	1010.3086
1021.8686	1035.5043	1053.5669
1072.5340	1096.9065	1136.9165
1138.5676	1161.0204	1176.3546
1185.8610	1192.8274	1193.9857
1210.7771	1230.4584	1231.6172
1269.6341	1305.7751	1313.2885
1323.3888	1344.7472	1377.1493
1401.3670	1409.5731	1449.9065
1462.7959	1473.1117	1487.9420
1502.4130	1504.2817	1506.6069
1516.7241	1551.0612	1610.7216
1652.6132	1657.2438	1661.0628
1776.4601	1856.4640	3022.6973
3086.6765	3087.9537	3155.4605
3183.3162	3194.5596	3207.4597
3208.2879	3219.1007	3222.4490
3223.3807	3228.8773	3579.2516

Zero-point correction (Hartree): 0.269805

*p*-(CH<sub>3</sub>-C<sub>6</sub>H<sub>4</sub>-CH<sub>2</sub>OH)

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -973.699215321

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.281175	-2.029229	-0.026851
C	2.356638	-0.546196	-0.029497
C	2.568552	0.142495	1.180877
C	2.630722	1.529976	1.205832
C	2.195853	0.204437	-1.205697
C	2.481163	2.284717	0.029959
C	2.261546	1.595018	-1.170803

H	3.063614	-2.514895	0.565753
H	2.675981	-0.419971	2.105274
H	2.795459	2.041159	2.151116
H	2.041355	-0.312518	-2.146643
H	2.146949	2.157450	-2.094317
H	1.208993	-2.293456	0.637506
O	-0.001125	-2.622968	0.932614
N	-0.785352	-1.607761	0.581288
C	-1.438848	-0.753188	1.517117
C	-1.075817	-1.283906	-0.751580
O	-1.309512	-0.794430	2.717090
O	-0.559451	-1.792834	-1.736038
C	-2.069847	-0.180712	-0.677558
C	-2.721476	0.499277	-1.695519
C	-2.283424	0.138402	0.669346
C	-3.611687	1.517573	-1.326226
C	-3.157207	1.147697	1.042233
C	-3.825539	1.836806	0.019798
H	-2.546300	0.245058	-2.735717
H	-4.143983	2.068602	-2.095655
H	-3.312659	1.389067	2.088672
H	-4.519659	2.631969	0.274664
O	2.114844	-2.688804	-1.224596
H	1.228049	-2.468994	-1.577015
C	2.583198	3.790200	0.058894
H	2.133037	4.205123	0.966305
H	3.631259	4.115379	0.041355
H	2.087313	4.242430	-0.804831

Rotational constants (GHz): 0.3864500 0.2639300 0.2139700

Vibrational harmonic frequencies (cm<sup>-1</sup>):

-1436.1242	14.6920	28.4104
39.3050	46.0736	61.5258
83.0272	108.4778	142.1747
161.9916	172.2367	200.4575
202.4706	250.3650	279.5754
315.8492	339.1917	349.4984
379.3749	409.2010	412.9440
414.5493	464.7899	474.8400
510.3700	524.7959	561.0542
586.6007	620.9340	631.7661
651.9759	675.9155	701.9242
715.1891	717.3081	722.9682
764.9459	778.4594	794.3209
819.8591	851.1390	852.5153
895.1387	910.7505	963.0682
972.1846	973.7339	1008.8752

1010.7392	1011.7325	1030.6820
1037.2430	1053.4371	1062.9971
1096.7179	1137.3077	1143.0171
1164.3921	1186.1402	1193.2457
1201.8916	1230.6965	1232.0183
1240.4397	1267.3243	1313.3967
1324.7226	1344.7099	1369.5509
1401.0814	1409.2072	1426.4812
1447.6338	1457.2410	1468.9722
1499.9709	1502.4410	1505.0927
1506.5625	1547.1146	1610.3826
1654.4160	1656.8581	1661.0967
1778.4628	1858.4955	3038.4340
3091.6615	3097.8639	3127.3712
3175.3871	3179.7171	3191.7612
3194.6958	3207.5802	3217.9436
3219.3332	3222.5114	3573.4054

Zero-point correction (Hartree): 0.264583

*p*-(H-C<sub>6</sub>H<sub>4</sub>-CH<sub>2</sub>OH)

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -934.378817866

Electronic state : 2-A

Cartesian coordinates (Angs):

C	2.761482	-1.238442	-0.046933
C	2.509661	0.226534	-0.020168
C	2.563695	0.913353	1.208448
C	2.320575	2.281997	1.264836
C	2.195989	0.944630	-1.186968
C	2.013960	2.989040	0.097060
C	1.954748	2.315895	-1.125973
H	3.631582	-1.552186	0.539103
H	2.792244	0.363920	2.118448
H	2.368128	2.799918	2.218296
H	2.167248	0.422632	-2.137304
H	1.825703	4.057775	0.141241
H	1.727288	2.862946	-2.036576
H	1.769925	-1.740116	0.609697
O	0.660469	-2.320317	0.896606
N	-0.321981	-1.489990	0.558592
C	-1.144876	-0.811203	1.505377
C	-0.675704	-1.216552	-0.770488
O	-1.009662	-0.842911	2.704799
O	-0.059665	-1.585424	-1.760014

C	-1.884253	-0.355527	-0.683189
C	-2.666605	0.184072	-1.693157
C	-2.161214	-0.109810	0.667708
C	-3.754427	0.982154	-1.311881
C	-3.231075	0.683147	1.052405
C	-4.031535	1.228165	0.038024
H	-2.441017	-0.010782	-2.736462
H	-4.392449	1.417714	-2.074868
H	-3.434667	0.870266	2.101686
H	-4.879744	1.852418	0.302329
O	2.742224	-1.895858	-1.255783
H	1.830172	-1.863215	-1.611203
Rotational constants (GHz):	0.4857400	0.2749400	0.2502400
Vibrational harmonic frequencies (cm-1):			
-1465.4028	14.8565	27.6082	
38.2196	69.9281	86.8308	
129.9814	148.5687	172.2197	
184.3458	214.0084	223.2600	
251.7921	315.2479	348.4238	
360.2178	411.0128	413.2915	
425.4074	464.7971	473.2363	
495.7088	524.7169	569.8690	
609.3536	626.4443	629.2864	
651.5364	675.9706	700.6058	
701.8982	717.4132	721.6177	
758.6584	778.6411	794.4491	
828.2287	853.0613	895.0090	
911.0398	916.5333	974.1699	
974.2271	998.1099	1007.9582	
1009.4664	1014.8466	1034.6210	
1051.2692	1053.3155	1096.6119	
1106.9619	1137.0004	1164.7377	
1186.0914	1186.3945	1193.3346	
1199.1757	1225.2626	1232.2048	
1260.2760	1313.6528	1322.1541	
1362.7382	1369.6387	1400.3213	
1408.4698	1454.8840	1459.4738	
1492.7215	1501.9344	1506.5556	
1529.3769	1625.5547	1645.0273	
1656.5259	1660.6694	1778.7929	
1859.3303	3093.5279	3179.6359	
3186.5766	3194.9497	3197.3256	
3207.7670	3209.0508	3218.4402	
3219.3615	3222.5709	3574.3993	
Zero-point correction (Hartree):	0.237136		

*p*-(NO<sub>2</sub>-C<sub>6</sub>H<sub>4</sub>-CH<sub>2</sub>OH)

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -1138.87465113

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.674821	3.098412	-0.038710
C	-1.450385	1.831441	-0.049493
C	-1.975470	1.332294	1.160301
C	-2.682286	0.138366	1.189692
C	-1.649057	1.099980	-1.235006
C	-2.860400	-0.563882	-0.004311
C	-2.355890	-0.096782	-1.217720
H	-1.135521	3.897446	0.550673
H	-1.817515	1.885031	2.082329
H	-3.092922	-0.260528	2.108639
H	-1.261541	1.488588	-2.169745
H	-2.529123	-0.669760	-2.120111
H	0.389595	2.802807	0.645816
O	1.588547	2.506537	0.945185
N	1.796486	1.241786	0.595069
C	1.960908	0.175350	1.533414
C	1.910578	0.820641	-0.739141
O	1.851796	0.275325	2.730776
O	1.694281	1.516884	-1.720722
C	2.264066	-0.619504	-0.663297
C	2.519301	-1.526641	-1.681276
C	2.288750	-1.005012	0.684108
C	2.811733	-2.846861	-1.311759
C	2.571018	-2.310203	1.056511
C	2.836395	-3.232263	0.033938
H	2.493984	-1.219052	-2.721430
H	3.020156	-3.584209	-2.080830
H	2.582344	-2.599670	2.102131
H	3.062002	-4.263326	0.288229
O	-0.192553	3.593141	-1.225069
H	0.484461	2.973708	-1.570950
N	-3.600548	-1.832466	0.018671
O	-4.043626	-2.215451	1.101522
O	-3.730211	-2.437473	-1.045997

Rotational constants (GHz): 0.3034400 0.2198200 0.1668000

Vibrational harmonic frequencies (cm<sup>-1</sup>):

-1602.1916	12.4498	27.5804
36.8871	54.3327	70.4165
84.1421	96.9333	140.0929
159.6160	170.5607	180.1575

200.8113	251.3369	261.7606
274.0824	311.7648	342.0200
352.1379	379.6844	413.2699
419.7102	463.3039	472.9373
495.5649	504.7890	524.4613
539.2350	570.7440	614.3587
638.0656	654.6724	675.5260
689.9770	697.9175	704.3373
717.5324	721.9161	757.6381
778.7003	795.9788	818.5481
850.4491	861.0864	875.6219
894.0552	912.8111	977.3905
988.5619	990.5309	1009.3563
1012.8810	1025.6801	1033.1519
1052.2979	1095.4713	1127.4211
1131.3743	1132.9697	1168.9502
1187.6635	1194.3501	1202.3189
1226.4015	1233.6481	1262.6190
1314.6096	1317.5446	1345.3850
1383.3962	1389.9932	1402.0033
1408.3924	1446.9785	1457.8134
1468.9315	1501.9262	1506.7745
1526.4835	1608.2292	1640.7682
1655.3820	1659.2897	1664.5800
1778.9725	1862.5967	3100.9106
3195.3752	3198.0181	3210.1958
3220.9307	3224.2519	3224.6161
3247.5361	3249.1544	3549.8311

Zero-point correction (Hartree): 0.239854