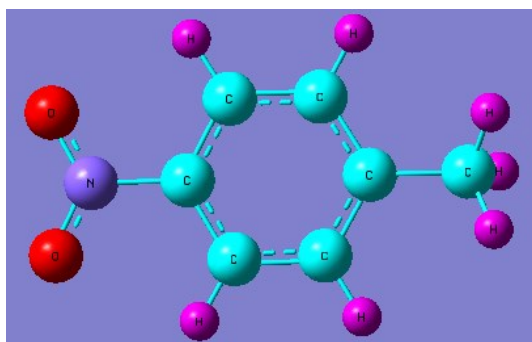


Supplementary material

Section S1

Geometries, vibrational frequencies and rotational constants are provided in the following.

p-Nitrotoluene R1



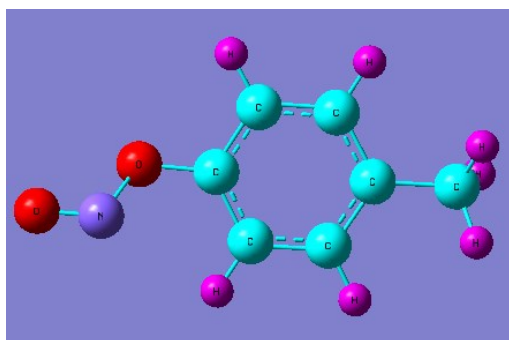
C	0.04197500	-1.21480600	-0.00425100
C	-1.34746100	-1.20362900	-0.01040500
C	0.71990900	-0.00000400	-0.00017800
C	-2.06475700	-0.00001800	-0.01053800
C	-1.34746600	1.20360900	-0.01047300
C	-3.57188800	0.00000600	0.01475900
C	0.04195900	1.21480000	-0.00431200
N	2.19585100	0.00000500	0.00339900
O	2.76613800	-1.08473500	0.00514100
O	2.76612300	1.08475200	0.00530200
H	0.60182200	-2.13990500	-0.00568400
H	-1.88411100	-2.14603600	-0.01749700
H	-1.88412600	2.14601300	-0.01761600
H	-3.97938400	-0.88585200	-0.47665400
H	-3.93930100	0.00111200	1.04680200
H	-3.97937300	0.88484500	-0.47851200
H	0.60180100	2.13990200	-0.00578200

<frequencies>

25.9707	51.3948	107.0520	220.1046	281.5483	358.3395
360.3327	417.46	472.0985	533.9901	624.0011	647.3227
686.6294	722.3745	799.4705	843.3063	848.4240	874.5502

979.6973	993.9970	1008.7428	1033.2053	1060.6696	1120.4362
1133.7669	1202.8215	1229.4702	1328.1064	1350.0604	1367.6724
1415.4664	1435.4483	1490.2606	1492.7221	1525.1363	1574.3200
1639.1429	1643.0798	3025.9795	3082.6374	3110.6049	3172.8384
3173.7342	3220.4508	3220.5591			
Rotational constants (GHZ):			3.90273	0.81263	0.67541

p-Nitrotoluene R2

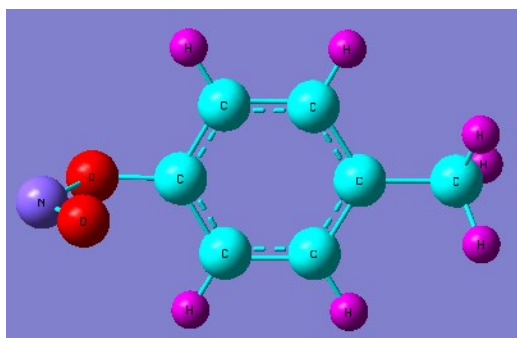


C	0.57770300	-0.24471300	-0.24963600
C	-0.23754000	-1.35848500	-0.06303800
C	0.03194300	1.03549300	-0.28108400
C	-1.60883400	-1.18198100	0.08793600
C	-2.18587100	0.09423200	0.06949600
C	-1.34179400	1.19411200	-0.11101300
H	0.20924800	-2.34505100	-0.03902800
H	0.67270600	1.89361000	-0.44297000
H	-2.24096700	-2.05234200	0.23117700
O	1.93394500	-0.45795300	-0.44141500
N	2.76833500	0.35879800	0.47338500
O	3.89291300	0.20675100	0.23732100
C	-3.67844500	0.27127900	0.20973700
H	-3.92869100	1.27092900	0.57133100
H	-4.18341000	0.13366100	-0.75264700
H	-4.10210300	-0.45626200	0.90648900
H	-1.76296300	2.19386400	-0.12967900

<frequencies>

45.0643	57.0948	100.0901	147.0975	206.4083	306.6876
341.5911	380.1722	422.0910	458.1001	528.0504	548.9391
653.9146	700.2536	717.2387	804.5075	833.5672	840.0087
916.6148	951.2347	971.3410	1007.0067	1033.9076	1061.1075
1131.0706	1187.8526	1227.9860	1230.2639	1325.4921	1330.7366
1416.2047	1437.2378	1489.5673	1496.2229	1532.3023	1620.3186
1644.1130	1794.7897	3022.1381	3075.7078	3102.7611	3163.1122
3164.9270	3194.3633	3195.2391			
Rotational constants (GHZ):			4.66900	0.66895	0.60140

p-Nitrotoluene R3



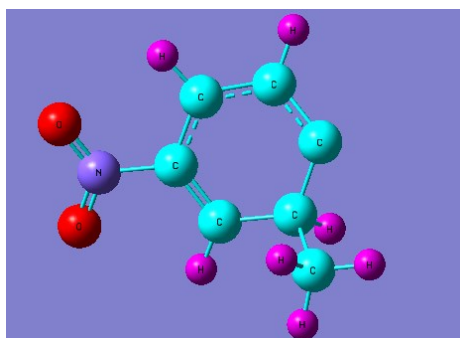
C	-0.71220600	0.00350700	-0.54026300
C	-0.03921500	1.21133800	-0.37180500
C	-0.04054800	-1.20651000	-0.37921000
C	1.31712800	1.20123800	-0.05894800
C	2.01783100	-0.00019000	0.09690100
C	1.31534100	-1.20011200	-0.06612900
H	-0.57714800	2.14356700	-0.49793000
H	-0.57970800	-2.13722400	-0.51120500
H	1.83887300	2.14442700	0.06591900
O	-2.05149900	0.00543800	-0.89593700
N	-3.04557200	-0.00144200	0.24465500
O	-2.57048900	-0.00766700	1.29972100
C	3.49553000	-0.00328900	0.40437500
H	3.77408900	-0.86680800	1.01282500
H	4.08717500	-0.04729400	-0.51659900
H	3.79261800	0.90013700	0.94144900
H	1.83584500	-2.14478000	0.05316200

<frequencies>

17.9646	34.3493	84.8445	181.7167	213.0276	317.2825
331.5494	420.8895	430.0296	460.6044	463.2996	553.2387
653.6515	703.5482	713.9232	819.6357	837.1392	838.7530
914.2344	957.9089	974.2382	1007.1170	1033.1259	1060.1230
1128.9022	1176.5700	1210.8517	1228.6422	1320.7865	1329.1840
1415.5975	1434.4764	1489.9815	1494.2522	1529.3162	1616.5579
1641.9980	1791.3801	3022.4933	3077.1404	3103.7150	3162.8200
3163.6083	3190.2655	3191.3506			

Rotational constants (GHZ): 3.55507 0.77718 0.73496

p-Nitrotoluene R4



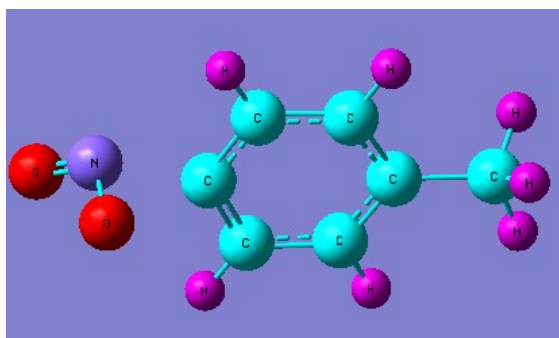
C	0.36205900	-0.84991400	-0.40211400
C	1.80323300	-0.47466100	-0.35056400
C	-0.54565700	0.09327400	-0.06127800
C	2.13206600	0.96764300	-0.19850300
C	1.08463000	1.89501600	-0.21621200
C	-0.19333000	1.46560100	0.11463300
N	-1.98108800	-0.27387900	0.03978000
O	-2.31607100	-1.37827600	-0.36246200
O	-2.73672400	0.55379600	0.53132000
H	0.04126000	-1.83175200	-0.73087200
H	2.24464700	-0.73657500	-1.33535700
H	1.29034300	2.96006500	-0.27350400
H	-0.95547800	2.14501900	0.47924600
C	2.58203800	-1.33524100	0.68413800
H	2.47006300	-2.40279200	0.47957000
H	3.63599100	-1.05784400	0.63962900
H	2.21291400	-1.13343400	1.69135900

<frequencies>

41.4128	75.8813	133.6834	212.3794	233.2231	263.8213
341.3577	392.7869	432.3215	508.1107	538.9003	600.7750
656.9749	729.5121	783.7856	821.4041	857.8074	884.4871
922.8228	947.3590	966.7782	982.9488	1056.4224	1069.0843
1098.2996	1156.1856	1182.9590	1219.7849	1313.7458	1338.6208
1372.6469	1396.5352	1408.1540	1483.2712	1492.8971	1500.1476
1580.0651	1636.9679	2908.1477	3036.1665	3109.9033	3124.9897
3144.6265	3190.2415	3191.9910			

Rotational constants (GHZ): 2.55914 0.99364 0.76570

p-Nitrotoluene TS1-2



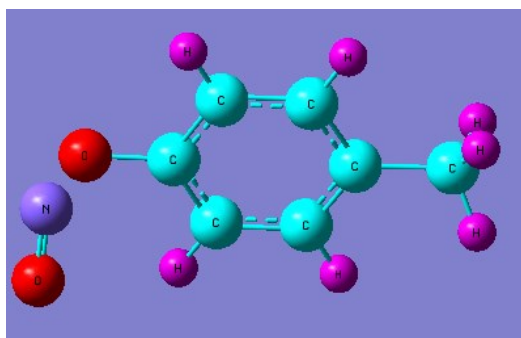
C	-0.68470600	0.15670900	0.09972400
C	-0.12836600	-1.10479600	0.20065600
C	0.05912900	1.32118100	-0.05110300
C	1.26495500	-1.19837000	0.11664100
C	2.06813000	-0.07032300	-0.04220100
C	1.43707100	1.18537700	-0.12072600
H	-0.74951400	-1.98163900	0.32275500
H	-0.42371500	2.28652200	-0.11560700
H	1.72124200	-2.17987700	0.18663400
O	-2.22762300	0.27990000	1.01874800
N	-2.35661700	0.19771500	-0.28270200
O	-3.20990500	-0.48518500	-0.77669100
C	3.56960700	-0.17877100	-0.13790500
H	3.92800100	0.13846800	-1.12248700
H	4.06196000	0.45479500	0.60577400
H	3.90418800	-1.20523100	0.02217800
H	2.03947100	2.07919000	-0.24730900

<frequencies>

-808.3269	13.4272	98.0077	105.8578	161.2497	245.8727
270.8580	361.0210	405.8739	420.4695	473.1679	549.2777
634.0514	682.2549	735.9512	786.5370	798.9055	806.6101
936.3769	968.2051	971.3096	1007.4511	1037.5204	1061.5246
1130.0890	1167.2822	1193.8881	1224.6962	1324.5034	1329.6562
1418.2060	1424.7651	1486.2172	1489.3387	1497.7204	1549.4831
1612.3261	1621.9725	3024.4361	3072.7343	3106.2949	3165.7510
3171.5006	3214.0294	3214.6928			

Rotational constants (GHZ): 3.99551 0.76527 0.69602

p-Nitrotoluene TS2-3



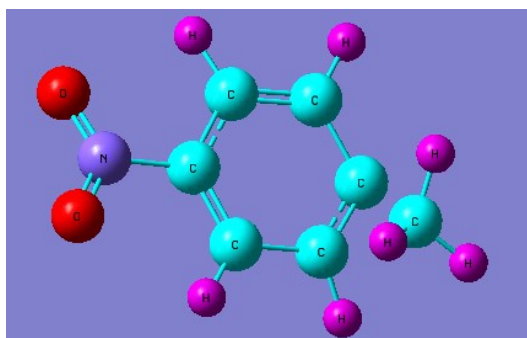
C	-0.65376500	0.21328900	-0.49733500
C	0.11044400	1.33223800	-0.14922000
C	-0.05644100	-1.04963000	-0.52833200
C	1.45950500	1.18194500	0.15381400
C	2.07796000	-0.07459500	0.11775000
C	1.29672800	-1.18309200	-0.22679200
H	-0.36248500	2.30720500	-0.13053300
H	-0.65493200	-1.90889300	-0.80677800
H	2.04424700	2.05667900	0.42067500
O	-1.98154200	0.35534200	-0.82079600
N	-2.88948500	0.33319000	0.52285100
O	-3.15463100	-0.73525100	0.81899700
C	3.55141900	-0.22130900	0.41105400
H	3.79190500	-1.23196800	0.74828000
H	4.15207300	-0.02220100	-0.48338700
H	3.87631900	0.48003500	1.18352100
H	1.75355200	-2.16698700	-0.26297400

<frequencies>

-205.7564	27.5930	45.3102	82.0167	171.2586	292.7002
308.3630	400.4410	415.7786	428.4510	473.6851	545.2874
646.9787	675.0042	719.8829	748.9331	838.5740	841.6587
851.2344	955.2041	975.8736	1005.0221	1031.2128	1060.0830
1125.6920	1177.2413	1221.1599	1227.3425	1308.6403	1327.5021
1414.9879	1433.0560	1489.5472	1493.6389	1526.8370	1605.1405
1638.3720	1879.0738	3020.6325	3074.4019	3101.6368	3158.1027
3159.6704	3189.6015	3191.5572			

Rotational constants (GHZ): 3.62642 0.73828 0.67572

p-Nitrotoluene TS1-4



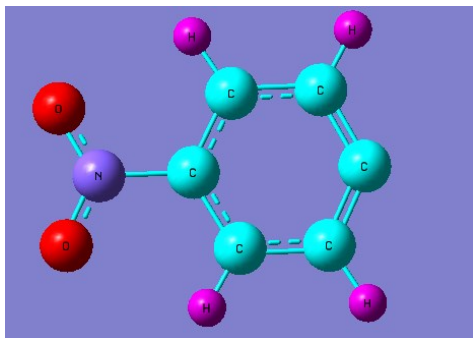
C	0.21074400	-1.00535300	-0.38606400
C	1.63071800	-0.73049500	-0.60835400
C	-0.58334900	0.05379500	-0.10653800
C	2.18429300	0.57325300	-0.52678300
C	1.27517800	1.58306700	-0.02055700
C	2.74124800	-0.78088900	0.81276000
C	-0.07421300	1.38333500	0.04620600
N	-2.04379300	-0.16708800	0.07081100
O	-2.75540000	0.82622700	0.12960000
O	-2.44275400	-1.32091900	0.14271500
H	2.15100000	-1.47944800	-1.20294400
H	1.66631900	2.57339000	0.19581100
H	-0.77584000	2.18416900	0.24298600
H	-0.19970300	-2.00602300	-0.43958500
H	2.19335900	-1.55632500	1.34898700
H	3.69970000	-1.12821700	0.45010900
H	2.84923800	0.07934100	1.46642400

<frequencies>

-535.2819	42.7331	112.5385	154.7912	214.9029	245.1717
341.8105	375.4765	421.4167	502.3992	532.2852	602.3222
621.7272	662.1416	727.8744	818.8454	846.8696	865.5585
900.6727	916.6752	941.1883	1010.6840	1023.2060	1047.9488
1091.8134	1141.2928	1205.8842	1288.2806	1318.7305	1342.8200
1373.6881	1396.2250	1444.9222	1453.2846	1465.6434	1535.8904
1592.0922	1660.5277	3063.0502	3102.2872	3143.3294	3154.0798
3200.7168	3202.9049	3222.6917			

Rotational constants (GHZ): 3.01641 0.94064 0.76979

p-Nitrotoluene R1 decomposition C6H4NO2



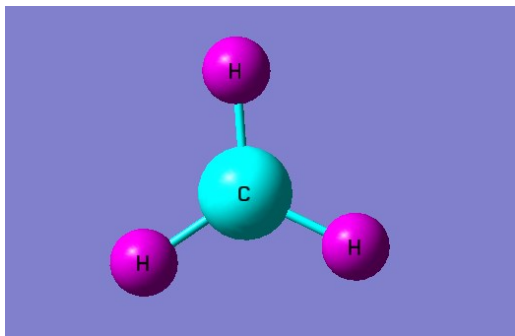
C	-0.48900000	-1.22401800	0.00000000
C	-1.88717700	-1.22739500	0.00000000
C	0.17738500	0.00000000	0.00000000
C	-2.50812100	0.00000000	0.00000000
C	-1.88717700	1.22739500	0.00000000
C	-0.48900000	1.22401800	0.00000000
N	1.65757900	0.00000000	0.00000000
O	2.22589200	-1.08453400	0.00000000
O	2.22589200	1.08453400	0.00000000
H	0.07970000	-2.14429900	0.00000000
H	-2.43909100	-2.15981800	0.00000000
H	-2.43909100	2.15981800	0.00000000
H	0.07970000	2.14430000	0.00000000

<frequencies>

48.4456	177.7912	258.4571	396.8734	404.9775	436.6264
527.2253	606.7823	646.5060	687.2757	714.5278	810.7394
816.6663	862.3135	966.2523	979.8757	995.7012	1041.5208
1103.4834	1109.7150	1171.6171	1298.1000	1331.4147	1370.1187
1406.0744	1467.7563	1571.2418	1582.1022	1644.4686	3183.0253
3183.7678	3215.8212	3215.8736			

Rotational constants (GHZ): 3.93565 1.34454 1.00217

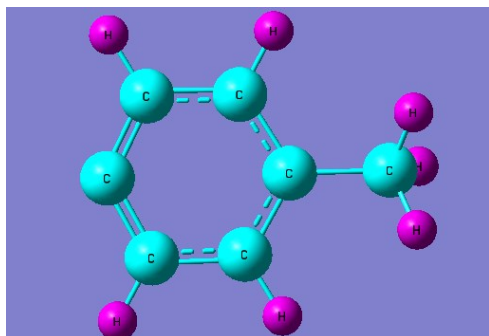
p-Nitrotoluene R1 decomposition CH3



C	0.00000200	-0.00000300	-0.00001400
H	1.00967800	-0.38513000	0.00002700
H	-0.17130100	1.06696700	0.00002700

H	-0.83838700	-0.68182100	0.00002700		
<frequencies>					
536.9517	1402.2722	1402.3867	3102.9360	3282.7699	3282.8919
Rotational constants (GHZ):		286.28026	286.26962	143.13747	

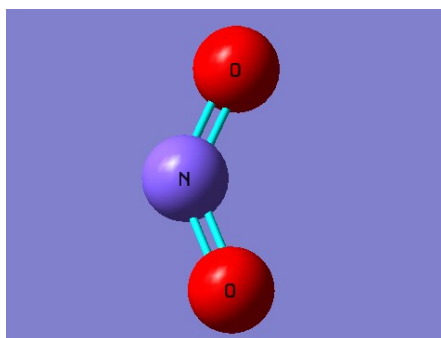
p-Nitrotoluene R1 decomposition C6H4CH3



C	-1.27209100	1.21979400	0.00284000		
C	0.12947700	1.20479700	-0.00854100		
C	-1.90313900	-0.00001200	0.00961100		
C	0.84238500	0.00001400	-0.01122600		
C	0.12949600	-1.20478800	-0.00854100		
C	2.35370500	0.00000800	0.00871200		
C	-1.27206400	-1.21981100	0.00283900		
H	-1.81752100	2.15690300	0.00212600		
H	0.66867800	2.14756400	-0.01785400		
H	0.66871500	-2.14754700	-0.01785300		
H	2.75880700	0.88417700	-0.48874500		
H	2.73335900	-0.00084500	1.03624200		
H	2.75882500	-0.88333600	-0.49020400		
H	-1.81747900	-2.15692900	0.00212600		

<frequencies>					
19.5352	220.2356	344.6081	401.3508	460.1722	530.7982
616.3115	681.2869	777.0338	784.7859	805.6600	935.4785
958.6188	995.2650	1004.2889	1051.9833	1062.7095	1110.9918
1180.0954	1218.8603	1301.1410	1322.1862	1394.9667	1415.4595
1478.8696	1490.5480	1494.7111	1593.4716	1619.1420	3022.3199
3076.5448	3102.0919	3150.5979	3150.7867	3173.7515	3175.9822
Rotational constants (GHZ):		5.47150	2.66951	1.81440	

p-Nitrotoluene R1 decomposition NO2

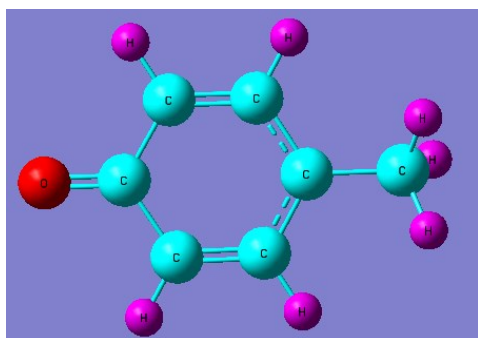


N	0.00000000	0.00000000	0.32194100
O	0.00000000	-1.09996700	-0.14084900
O	0.00000000	1.09996700	-0.14084900

<frequencies>

764.6896	1391.2897	1701.4273	
Rotational constants (GHZ):	242.27262	13.05707	12.38935

p-Nitrotoluene R2 decomposition C₆H₄CH₃O



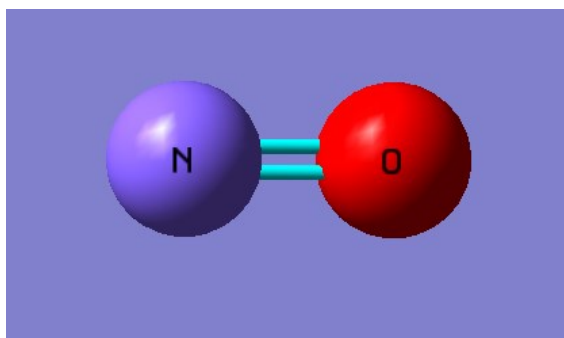
C	-1.54633700	-0.00010200	0.00397900
C	-0.78245600	-1.23431500	-0.00236800
C	-0.78291400	1.23428000	-0.00237100
C	0.59021800	-1.21718200	-0.01205300
C	1.31164900	0.00044900	-0.01403000
C	0.58996200	1.21762000	-0.01204000
H	-1.34245700	-2.16228800	-0.00236600
H	-1.34318200	2.16208900	-0.00234500
H	1.14228000	-2.15190400	-0.01962700
O	-2.79847100	-0.00032200	0.01169400
C	2.81361900	-0.00002500	0.01383000
H	3.22429000	0.89526400	-0.45794300
H	3.17879600	-0.01917000	1.04828900
H	3.22391700	-0.87827100	-0.48964000
H	1.14167600	2.15251800	-0.01961100

<frequencies>

23.9159	121.2677	285.7774	320.3302	378.9907	455.6243
462.0339	502.2968	624.5995	703.7678	750.2658	793.2933

814.9046	846.9268	967.8950	980.3258	990.8952	996.6784
1041.4886	1121.8405	1169.6601	1230.0396	1273.0425	1308.8958
1410.0075	1429.2508	1443.0144	1470.0210	1485.8558	1496.7112
1518.3668	1600.5565	3011.6212	3072.3687	3107.8268	3157.6323
3158.9905	3192.1900	3193.4566			
Rotational constants (GHZ):					
	5.37349		1.52752	1.19827	

p-Nitrotoluene R2 decomposition NO



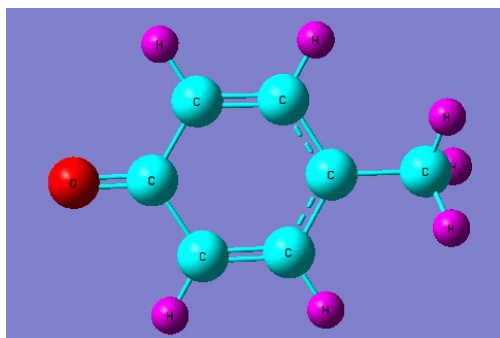
N	0.00000000	0.00000000	-0.61228500
O	0.00000000	0.00000000	0.53574900

<frequencies>

1979.6462

Rotational constants (GHZ):	51.35640	0	0
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p-Nitrotoluene R3 decomposition C₆H₄CH₃O



C	1.54637400	-0.00000200	0.00429400
C	0.78262000	1.23412400	-0.00271500
C	0.78260800	-1.23412500	-0.00271500
C	-0.59001200	1.21727800	-0.01184300
C	-1.31159000	0.00001000	-0.01447600
C	-0.59001800	-1.21726800	-0.01184200
H	1.34276900	2.16199900	-0.00292600
H	1.34275000	-2.16200400	-0.00292800
H	-1.14184500	2.15211400	-0.01936400
O	2.79826600	-0.00000800	0.01189200
C	-2.81352600	0.00000000	0.01395500

H	-3.22419200	-0.88669700	-0.47398300
H	-3.17829100	-0.00044100	1.04873500
H	-3.22420000	0.88708900	-0.47325400
H	-1.14185900	-2.15209900	-0.01936300

<frequencies>

24.4136	120.9287	285.4800	320.2555	378.7243	455.4626
462.0625	502.0867	624.6478	703.5731	750.3746	793.2426
815.1313	846.9135	967.9291	980.3618	991.0212	996.7280
1041.5006	1121.9662	1169.8624	1230.1848	1273.3159	1309.1978
1410.0346	1429.8744	1443.3228	1470.0819	1485.9042	1497.5905
1518.6208	1601.0631	3011.6132	3072.4066	3107.7848	3157.6665
3159.0016	3192.2210	3193.4899			

Rotational constants (GHZ): 5.37464 1.52767 1.19842

p-Nitrotoluene R3 decomposition NO



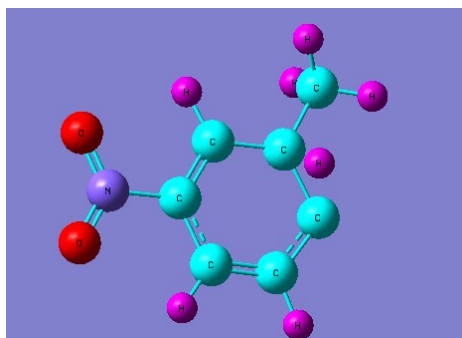
N	0.00000000	0.00000000	-0.61228500
O	0.00000000	0.00000000	0.53574900

<frequencies>

1979.6462

Rotational constants (GHZ): 51.35640 0 0

TS4-5



C	0.40326200	-0.81619300	-0.02288000
C	1.78066300	-0.33866300	-0.07683200
C	0.95959600	1.93918900	0.04191200
C	2.12546900	1.08429100	0.03591700

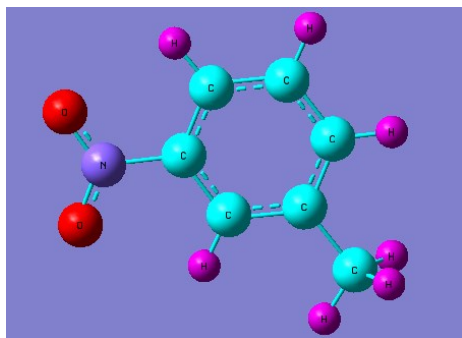
C	-0.59705100	0.10288300	-0.01808100
N	-2.01079800	-0.36509400	0.00397900
C	-0.33919700	1.49776100	0.00658800
C	2.88059100	-1.37563200	0.08817800
O	-2.88226700	0.49209800	0.02526400
O	-2.21004800	-1.57089700	-0.00281300
H	1.94080300	0.19734900	-1.12981900
H	1.12918600	3.00934700	0.12149300
H	-1.18103400	2.17937100	0.01227400
H	0.17144600	-1.87381000	0.01595200
H	2.70639000	-2.26453300	-0.52371500
H	3.84351700	-0.93494100	-0.16732100
H	2.92380200	-1.68855000	1.13486200

<frequencies>

-543.2132	35.0252	141.1818	159.2770	191.3884	208.1181
343.0858	364.6341	394.4869	497.1831	530.5769	543.6485
648.6609	669.8161	718.5381	807.0996	845.9124	876.1656
907.5770	936.8029	959.4612	982.8527	1030.0681	1080.7125
1107.4843	1127.9595	1197.1478	1235.2056	1238.9224	1360.3478
1374.8148	1413.8952	1446.1541	1486.0738	1496.0186	1533.7972
1596.0365	1652.1495	2343.7960	3036.6685	3095.1646	3135.2205
3147.2365	3196.8575	3200.5136			

Rotational constants (GHZ): 2.62521 0.97513 0.71732

m-Nitrotoluene R5



C	1.99816900	0.98463200	-0.00001000
C	1.74426200	-0.39437300	-0.00001100
C	0.96042100	1.91326200	-0.00000100
C	-0.36512500	1.48797500	0.00000500
C	-0.60894400	0.12040300	0.00000100
N	-2.01104400	-0.35590300	0.00000100
C	0.41646100	-0.82134500	-0.00000900
C	2.88129800	-1.38682300	0.00001400
O	-2.89867900	0.48794500	0.00001300
O	-2.20245700	-1.56584500	-0.00001000

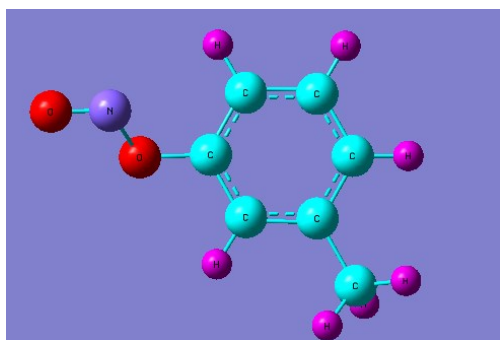
H	3.02555200	1.33448600	-0.00002000
H	1.18277900	2.97380600	-0.00000400
H	-1.19189800	2.18417200	0.00000900
H	0.16506000	-1.87353200	-0.00001800
H	3.51652900	-1.25625900	-0.88099600
H	3.51604800	-1.25675300	0.88144700
H	2.51306400	-2.41378500	-0.00036600

<frequencies>

37.7551	42.9383	161.9823	209.9515	216.0920	355.7978
397.0732	430.7027	500.0437	505.5295	556.3139	675.1294
686.2476	724.8140	809.8186	817.7286	910.4083	920.5009
950.1790	1000.5226	1009.0784	1021.0651	1066.4937	1108.6584
1113.4243	1190.4314	1234.5634	1316.5241	1350.0107	1369.8018
1416.5120	1455.5498	1487.5914	1500.6195	1513.5589	1584.0887
1621.9849	1658.2550	3029.7705	3080.1957	3112.1954	3164.1600
3187.5954	3211.8701	3225.5591			

Rotational constants (GHZ): 2.66695 0.97948 0.71957

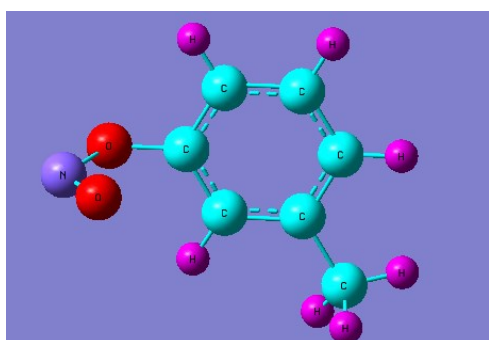
m-Nitrotoluene R6



C	0.43854300	-0.01883300	0.24666300
C	0.25438700	1.35990900	0.18235500
C	-0.63481600	-0.89895100	0.13000500
C	-1.03450900	1.84856000	-0.01917100
C	-2.11428200	0.97648000	-0.13317000
C	-1.93027900	-0.40949200	-0.05123500
H	1.09764300	2.02946500	0.29482700
H	-0.44364100	-1.96469200	0.18458500
H	-1.19645700	2.91885400	-0.07905000
H	-3.11194700	1.37492000	-0.28400100
O	1.69083800	-0.56952000	0.47122600
N	2.71826400	-0.03763300	-0.45672600
O	3.76106100	-0.46890800	-0.19259600
C	-3.10407700	-1.35486100	-0.13703300
H	-3.54360500	-1.52067000	0.85254900
H	-3.89019700	-0.95496200	-0.78146700

H	-2.80463600	-2.32892400	-0.52988600		
<frequencies>					
47.0748	56.6293	121.7522	155.7906	210.9213	284.2575
291.0259	379.4407	453.6924	484.6015	526.8555	576.9019
600.9513	696.1577	715.2633	786.5908	843.0711	885.4986
913.2015	962.3408	978.9416	1016.0079	1022.0061	1060.2335
1112.9397	1163.6399	1189.5137	1265.2367	1313.0749	1341.6945
1415.8226	1455.3195	1490.9946	1498.7876	1516.0312	1619.5077
1644.4933	1795.9525	3023.9238	3079.0273	3105.3972	3163.0415
3180.0326	3182.4309	3200.4812			
Rotational constants (GHZ):	3.26425	0.75632	0.63044		

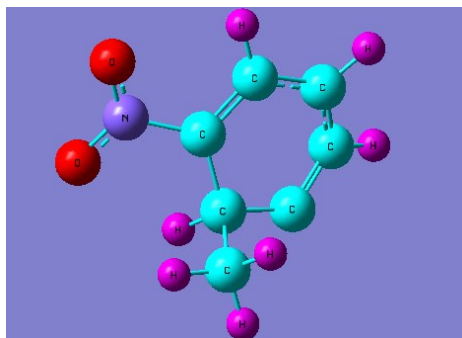
m-Nitrotoluene R7



C	-0.58101500	0.19515300	-0.50736500		
C	-0.31231700	1.52492000	-0.19038400		
C	0.40721300	-0.78213200	-0.41681000		
C	0.97658000	1.86873300	0.20649100		
C	1.97175200	0.89636700	0.29274700		
C	1.70214800	-0.44191600	-0.01493700		
H	-1.09723600	2.26651400	-0.27554400		
H	0.15860600	-1.80471600	-0.67929200		
H	1.20831200	2.90064800	0.44475900		
H	2.97296500	1.18119200	0.59848800		
O	-1.84538600	-0.15852200	-0.95405000		
N	-2.83608300	-0.57715600	0.10755600		
O	-2.42442400	-0.55792900	1.18889500		
C	2.77199700	-1.50027300	0.10550800		
H	2.65897200	-2.27097700	-0.66052700		
H	3.77045100	-1.06882400	0.00870700		
H	2.72084700	-1.99725200	1.08025200		
<frequencies>					
29.7653	30.9663	107.2656	208.7242	210.9174	255.3608
325.1331	407.2701	460.6094	478.6534	512.9994	530.4998
598.7954	697.0165	725.3653	791.8521	864.9581	891.1918
921.2884	952.1776	981.2096	1016.1960	1020.2432	1061.1685

1108.7834	1149.6094	1186.8683	1252.0999	1308.9899	1339.6517
1416.2455	1451.3454	1490.5814	1497.9971	1513.9273	1619.3505
1641.3992	1790.8183	3024.5051	3079.2566	3105.4483	3162.9065
3175.2785	3179.4440	3196.4052			
Rotational constants (GHZ):		2.49838	0.93501	0.77960	

m-Nitrotoluene R8

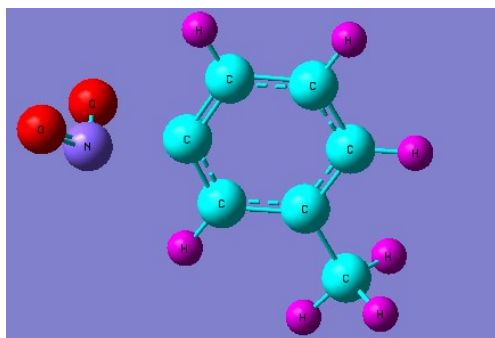


C	-2.46320600	-0.44035600	-0.55344400
C	-1.88455200	0.78617100	-0.47090400
C	-1.80386600	-1.41889700	0.23300900
C	-0.40550400	-1.36009300	0.40563500
C	0.27592600	-0.22618200	0.06293400
N	1.71075300	-0.28227200	-0.16449500
C	-0.45510900	1.04842800	-0.20476200
O	2.34549700	-1.20182700	0.34887700
O	2.21087300	0.62403800	-0.83252600
H	-3.44884700	-0.61104900	-0.97295700
H	-2.36665800	-2.22129700	0.70157900
H	0.13598000	-2.23699000	0.73855900
H	-0.03983000	1.47246000	-1.13664000
C	-0.26695800	2.12035500	0.89614500
H	-0.83380800	3.01210900	0.62278600
H	-0.64139700	1.74815200	1.85154200
H	0.78794700	2.37828000	1.00410000

<frequencies>

70.1785	95.9620	150.4903	210.8261	224.8258	295.8619
357.9594	386.3497	476.6043	515.3550	533.0843	564.5063
663.0581	747.7183	755.3617	814.6955	845.5232	873.7106
890.0054	948.3534	982.6382	1041.3520	1051.3532	1081.1615
1089.7574	1159.6531	1208.0670	1220.5076	1294.0729	1336.1041
1349.8757	1371.4239	1403.6526	1488.3487	1495.1849	1520.2052
1551.8285	1595.2884	2965.7342	3040.8356	3118.0091	3123.0000
3153.7802	3166.1138	3203.3972			
Rotational constants (GHZ):		2.24355	1.18167	0.88391	

m-Nitrotoluene TS5-6



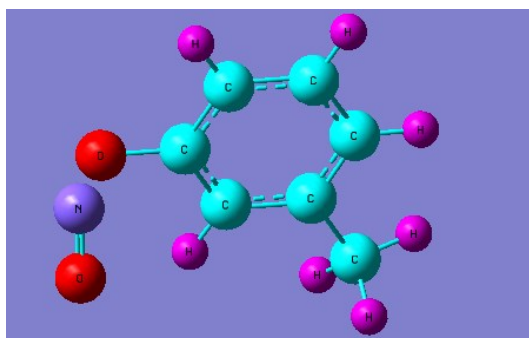
C	0.54660000	0.01563600	0.11739800
C	0.40126500	1.38918200	0.10126900
C	-0.50150200	-0.89381400	0.05482200
C	-0.90738400	1.87290800	-0.01116000
C	-1.98698800	1.00379500	-0.08099500
C	-1.79575700	-0.39054500	-0.04746000
H	1.25573600	2.04884900	0.15902200
H	-0.30858900	-1.95796500	0.07848500
H	-1.06806000	2.94477500	-0.03150700
H	-2.99254900	1.40076500	-0.16368800
O	2.00460800	-0.49222000	1.05176300
N	2.13725200	-0.55611900	-0.24762100
O	3.16326600	-0.24210600	-0.78062600
C	-2.97676400	-1.32628500	-0.13440800
H	-3.70080400	-1.11422300	0.65747600
H	-3.49620000	-1.21077400	-1.09044200
H	-2.67010900	-2.36924600	-0.04189000

<frequencies>

-798.5295	33.5193	93.0568	124.2027	179.3626	221.0276
228.9247	376.0761	407.2299	431.9579	505.1466	518.9292
624.4845	670.9735	738.0025	760.6979	806.5399	847.8982
877.0720	971.7904	987.5852	1019.3233	1040.7408	1058.6684
1104.8527	1176.5935	1188.3397	1211.0367	1305.7903	1337.2469
1414.9379	1440.6916	1485.1977	1492.9798	1500.5305	1558.0705
1584.7242	1638.4903	3029.8274	3080.9240	3111.7804	3170.0761
3186.5298	3206.4185	3218.3067			

Rotational constants (GHZ): 2.86223 0.88047 0.73318

m-Nitrotoluene TS6-7



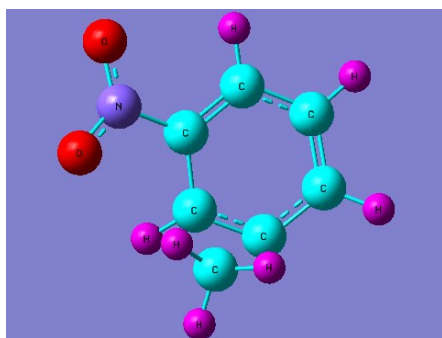
C	0.53293700	0.36341800	0.45816600
C	0.11162700	1.64310500	0.08130700
C	-0.35748300	-0.71274800	0.42518300
C	-1.20770400	1.82920000	-0.31781500
C	-2.09773000	0.75497500	-0.34443700
C	-1.68548100	-0.52953900	0.02633600
H	0.81365000	2.46701900	0.12499000
H	-0.00223400	-1.68795600	0.73947600
H	-1.54922000	2.81820100	-0.60276200
H	-3.12594600	0.91830500	-0.64977700
O	1.82419100	0.16272000	0.88515100
N	2.80996600	-0.06667600	-0.37883300
O	2.79112000	-1.15359600	-0.72231400
C	-2.64033500	-1.69856700	-0.02038300
H	-2.46496700	-2.38905400	0.80810700
H	-3.67929500	-1.36592800	0.02850600
H	-2.51923000	-2.26590800	-0.94955400

<frequencies>

-208.9841	26.0035	35.8512	98.7264	210.4664	240.6286
281.2773	378.8498	432.7418	459.0325	523.3436	546.5121
598.3462	673.5493	706.4242	743.5091	800.5459	888.9812
916.6035	937.9269	982.8557	1013.8470	1019.1702	1060.4398
1105.7070	1154.7281	1184.8702	1256.0676	1301.4224	1337.0223
1413.4902	1445.1684	1489.5811	1496.7214	1510.5990	1613.2819
1632.9177	1878.4881	3023.2443	3077.3545	3104.1180	3160.8450
3176.6697	3178.9079	3195.6122			

Rotational constants (GHZ): 2.40314 0.91377 0.72500

m-Nitrotoluene TS5-8



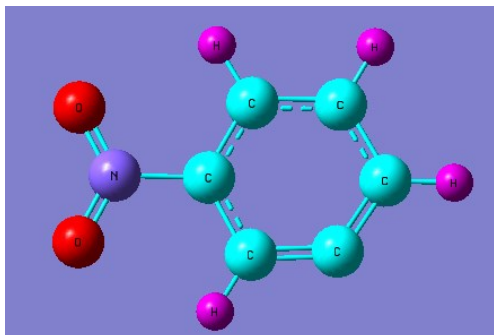
C	2.37868700	-0.53520100	-0.07233900
C	1.86635900	0.62563900	0.56391300
C	1.57659100	-1.65918000	-0.14923200
C	0.16379200	-1.50971400	-0.10101400
C	-0.38463100	-0.29334400	0.19107700
N	-1.80049600	-0.05704000	0.00628600
C	0.47230800	0.80668000	0.62751600
O	-2.14820400	1.12705600	-0.05970400
O	-2.56677900	-1.01369200	-0.06193500
H	0.04749900	1.48508500	1.36397300
H	3.42219800	-0.58226600	-0.36918100
H	1.99345400	-2.64335800	-0.33605000
H	-0.48672700	-2.33696700	-0.35699500
C	0.98897400	2.02700000	-0.55934500
H	1.25976800	2.93491400	-0.03583000
H	1.71406900	1.75644500	-1.32304200
H	0.00060100	2.10723100	-1.01722100

<frequencies>

-469.6695	81.1223	117.1425	185.1219	206.7646	229.5874
354.7668	372.7449	402.8319	502.8372	518.0442	586.2005
648.1941	667.0163	745.5193	785.9523	834.5710	849.3435
921.6126	946.2146	981.6538	994.1126	1020.0841	1079.0841
1107.2923	1164.4841	1191.0956	1288.5429	1323.6486	1336.8901
1375.6363	1411.6711	1431.3344	1456.6954	1465.2603	1514.8890
1547.9908	1623.6128	3047.9009	3116.0474	3141.0826	3148.5729
3170.1766	3205.1374	3217.4125			

Rotational constants (GHZ): 2.37180 1.20581 0.84850

m-Nitrotoluene R5 decomposition C6H4NO2



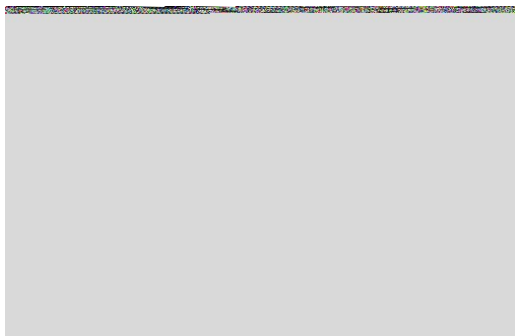
C	2.57160600	-0.14997100	0.00001900
C	1.77494300	-1.27086900	-0.00003900
C	1.91700600	1.09066500	0.00006800
C	0.52560500	1.15222500	0.00005700
C	-0.20654100	-0.03213700	-0.00000400
N	-1.68844300	0.03833200	-0.00001500
C	0.40407800	-1.29082700	-0.00005400
O	-2.20347900	1.14850600	0.00003300
O	-2.30426900	-1.01906100	-0.00007300
H	3.65394700	-0.20947000	0.00002800
H	2.49690600	2.00664400	0.00011500
H	0.00255700	2.09815700	0.00009400
H	-0.19251000	-2.19372500	-0.00010100

<frequencies>

49.0112	166.0416	256.6759	391.1360	410.3454	449.0599
525.0182	617.1765	630.2301	683.8762	715.4298	784.8768
864.6204	878.9463	928.9348	989.7847	997.6112	1047.3131
1085.5487	1103.2300	1173.8722	1274.1537	1334.4753	1367.5256
1434.4615	1463.5082	1560.0793	1604.9346	1634.8234	3173.1628
3187.5522	3206.0732	3225.5390			

Rotational constants (GHZ): 4.18095 1.29874 0.99092

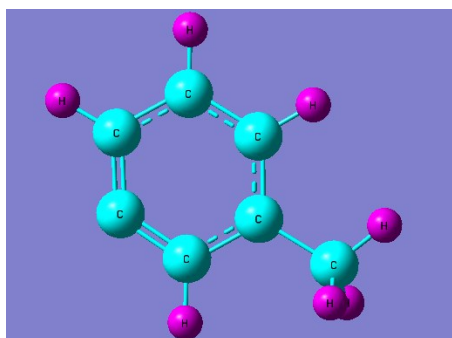
m-Nitrotoluene R5 decomposition CH3



C	0.00000200	-0.00000300	-0.00001400
H	1.00967800	-0.38513000	0.00002700
H	-0.17130100	1.06696700	0.00002700

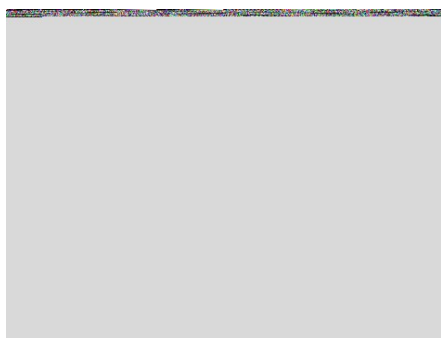
H	-0.83838700	-0.68182100	0.00002700		
<frequencies>					
536.9517	1402.2722	1402.3867	3102.9360	3282.7699	3282.8919
Rotational constants (GHZ):					
	286.28026	286.26962	143.13747		

m-Nitrotoluene R5 decomposition C6H4CH3



C	-0.07167500	-1.15651700	0.00003400		
C	-0.88096200	-0.01540200	0.00004600		
C	1.32156100	-1.06762300	-0.00000700		
C	1.95222500	0.18309700	-0.00003300		
C	1.11725700	1.27588800	-0.00001200		
C	-0.25393300	1.24744000	0.00003700		
C	-2.38770400	-0.11689600	-0.00003400		
H	-0.53950600	-2.13533000	0.00006800		
H	1.92155100	-1.97198800	-0.00000200		
H	3.03265100	0.27014900	-0.00005400		
H	-0.84798400	2.15625200	0.00006100		
H	-2.71419100	-1.15863000	0.00128000		
H	-2.81671800	0.37100200	0.88046600		
H	-2.81641500	0.36862500	-0.88200600		
<frequencies>					
28.8804	208.3576	348.7641	415.9061	483.7187	517.9809
628.1125	669.1076	755.1008	788.1364	854.4798	888.5633
972.3601	996.7502	999.7232	1056.7676	1060.2924	1097.4968
1177.3986	1207.9551	1298.6658	1307.3640	1413.5489	1434.4807
1484.3296	1486.5443	1494.0941	1558.5191	1634.3113	3025.3336
3074.9694	3103.5216	3154.1167	3154.7073	3170.7434	3181.2346
Rotational constants (GHZ):					
	5.95457	2.53924	1.79998		

m-Nitrotoluene R5 decomposition NO2

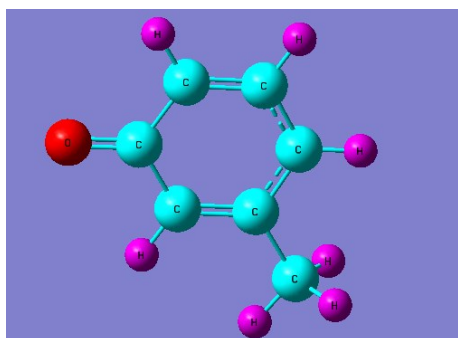


N	0.00000000	0.00000000	0.32194100
O	0.00000000	-1.09996700	-0.14084900
O	0.00000000	1.09996700	-0.14084900

<frequencies>

764.6896	1391.2897	1701.4273	
Rotational constants (GHZ):	242.27262	13.05707	12.38935

m-Nitrotoluene R6 decomposition C6H4CH3O



C	1.28610800	-0.49538900	-0.00000200
C	1.43833700	0.94768400	-0.00000300
C	-0.06712100	-1.02130600	0.00000300
C	0.32947200	1.76207400	-0.00000100
C	-0.96136300	1.20602200	0.00000400
C	-1.16936900	-0.19644100	0.00000500
H	2.44732300	1.34247200	-0.00000500
H	-0.16717500	-2.10125200	0.00001300
H	0.44235400	2.84071300	0.00000000
H	-1.82278300	1.86627500	0.00001100
O	2.28128900	-1.25645300	0.00000100
C	-2.57552600	-0.74435200	-0.00000300
H	-3.12900600	-0.40530100	0.88098400
H	-3.12880600	-0.40578200	-0.88130300
H	-2.57545000	-1.83525700	0.00029000

<frequencies>

82.3599	184.7708	199.4096	300.4970	409.2357	478.2305
498.7701	537.4350	539.3865	660.0439	728.0152	790.2096

852.4080	909.4014	913.2642	976.5079	977.8427	1026.6184
1061.6228	1097.0922	1165.8723	1186.7156	1276.4016	1333.2247
1357.6022	1415.0843	1437.1390	1480.7423	1485.8495	1492.5203
1554.7963	1592.8807	3027.0367	3076.8750	3112.4699	3160.7900
3176.3126	3181.2155	3198.6500			
Rotational constants (GHZ):		3.71702	1.84496	1.24246	

m-Nitrotoluene R6 decomposition NO



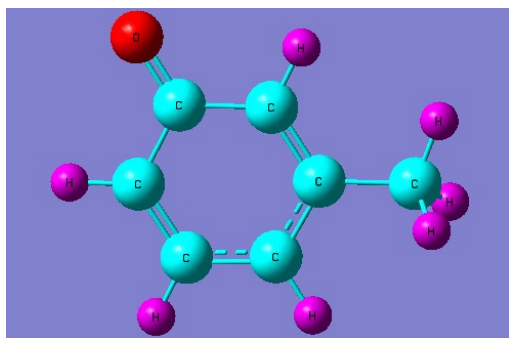
N	0.00000000	0.00000000	-0.61228500
O	0.00000000	0.00000000	0.53574900

<frequencies>

1979.6462

Rotational constants (GHZ):	51.35640	0	0
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m-Nitrotoluene R7 decomposition C6H4CH3O



C	1.28687800	-0.49411900	0.00000700
C	1.44143400	0.94997100	0.00001200
C	-0.06616500	-1.02368700	0.00000000
C	0.32877900	1.76658100	-0.00000900
C	-0.96463900	1.20834300	0.00000500
C	-1.17258100	-0.19703300	-0.00000700
H	2.45208300	1.34531300	0.00001000
H	-0.16559400	-2.10540600	-0.00001900
H	0.44144800	2.84713200	-0.00002100
H	-1.82808200	1.86909100	-0.00001000
O	2.28815800	-1.25922600	-0.00000500

C	-2.57971200	-0.74725800	0.00000200
H	-2.57827000	-1.84010800	-0.00018800
H	-3.13533600	-0.40966100	0.88251700
H	-3.13547500	-0.40934900	-0.88230300

<frequencies>

80.6871	188.3299	200.7563	299.7762	411.8951	476.2188
498.3532	536.5331	538.4232	660.7372	729.1331	790.5287
854.9251	914.1984	916.2326	978.2060	980.6873	1026.5595
1062.0637	1100.0374	1168.4705	1190.9868	1283.5473	1342.4626
1364.9388	1420.6247	1443.1963	1487.7592	1489.5612	1497.5816
1561.8455	1600.0128	3038.6543	3094.1164	3129.6657	3178.0820
3193.9998	3200.2472	3217.7108			

Rotational constants (GHZ): 3.70019 1.83694 1.23697

m-Nitrotoluene R7 decomposition NO



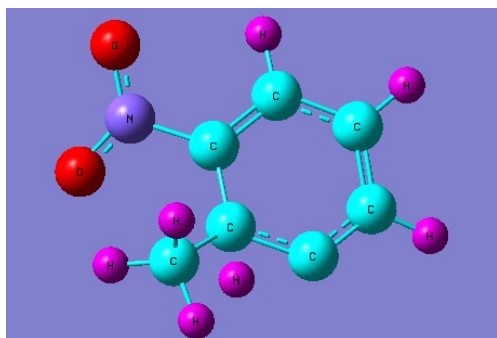
N	0.00000000	0.00000000	-0.61228500
O	0.00000000	0.00000000	0.53574900

<frequencies>

1979.6462

Rotational constants (GHZ): 51.35640 0 0

TS8-9



C	2.54880300	-0.23731300	0.30713300
C	1.89632300	1.01156400	0.12346900
C	1.92161400	-1.39953300	-0.09596300
C	0.50560400	-1.43140500	-0.20501800

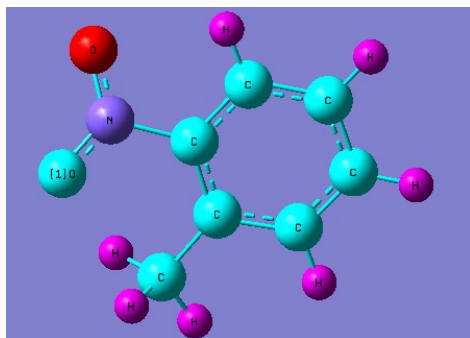
C	0.46664700	1.01832500	0.01041300
C	-0.21275200	-0.28299900	-0.05385900
N	-1.66333800	-0.38958000	0.12662600
C	-0.21358000	2.24575000	-0.58950000
O	-2.19340200	0.43400700	0.86661800
O	-2.25358100	-1.28695400	-0.46491800
H	2.47627800	-2.32071000	-0.24681100
H	-0.01491100	-2.37300500	-0.32980000
H	0.78760200	1.32053600	1.13346600
H	3.58681800	-0.26004800	0.62409000
H	0.43809300	3.10819000	-0.44844700
H	-0.34086200	2.08781100	-1.66383500
H	-1.18974700	2.44152300	-0.14869200

<frequencies>

-835.8940	67.6428	98.2542	171.0197	210.2490	222.5305
319.9178	379.0685	401.1665	455.5693	523.5968	566.5395
609.8204	699.7315	744.0128	801.4538	822.1599	855.4333
913.5695	941.6520	970.9540	1005.1893	1061.4539	1071.3496
1130.1537	1162.0805	1198.3052	1207.9263	1346.2337	1362.9888
1378.2845	1409.1745	1416.4900	1488.7697	1494.9976	1506.4480
1568.7470	1624.3271	2281.1515	3046.2758	3115.4522	3145.7775
3151.1233	3166.9664	3203.2460			

Rotational constants (GHZ): 2.23698 1.21093 0.85656

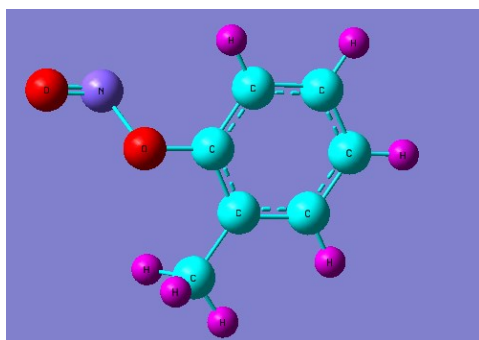
o-Nitrotoluene R9



C	1.82497900	0.97534900	0.05286200
C	0.42343400	0.98435200	0.05410800
C	2.56167000	-0.20174500	-0.03083700
C	1.91137200	-1.43262300	-0.09794700
C	0.52469400	-1.46827600	-0.07645600
C	-0.19531600	-0.27567000	-0.01436300
N	-1.66867600	-0.40713600	-0.01964300
C	-0.30034300	2.30370800	0.15222200
O	-2.14625300	-1.45540900	0.39831400
O	-2.32984800	0.52959100	-0.45271400

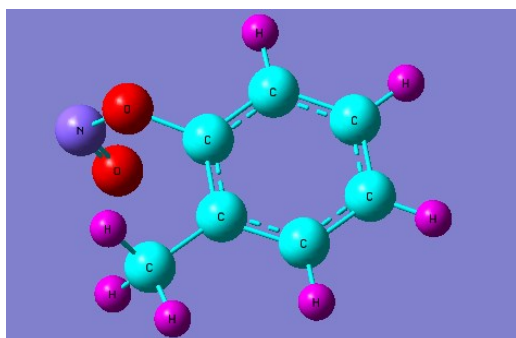
H	2.34449500	1.92457900	0.12189000
H	3.64477800	-0.15686200	-0.03815100
H	2.47622000	-2.35465800	-0.16138800
H	-0.01715000	-2.40347400	-0.10975500
H	0.40871900	3.09058000	0.41485700
H	-0.77784900	2.56271600	-0.79468200
H	-1.09261200	2.28304700	0.90239500
Rotational constants (GHZ):	2.25888	1.25113	0.82631

o-Nitrotoluene R10



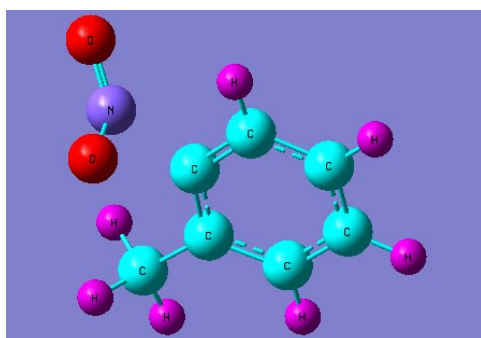
C	0.08958800	-0.09755100	0.21153700
C	-0.80116100	0.96823200	0.01808100
C	-0.33532800	-1.42368700	0.22242300
C	-2.14823700	0.64724600	-0.16522300
C	-2.59051800	-0.67545700	-0.17242000
C	-1.68238000	-1.71328600	0.01842900
H	0.38341000	-2.21415700	0.40040200
H	-2.86108100	1.45205300	-0.31148000
O	1.42021500	0.21973500	0.44114100
N	2.34756300	-0.54074500	-0.43386600
O	3.44769000	-0.30845400	-0.15317200
H	-2.01818600	-2.74368200	0.02296500
C	-0.31380000	2.39426000	0.01637400
H	0.16509000	2.65166600	0.96494500
H	0.43065600	2.55865200	-0.76754800
H	-1.14308000	3.08380900	-0.14918600
H	-3.64196500	-0.89191600	-0.32199100
Rotational constants (GHZ):	2.46458	0.97848	0.72007

o-Nitrotoluene R11



C	-0.15036300	-0.22614400	-0.46466300
C	0.43559600	0.99327800	-0.09490200
C	0.55563100	-1.42622600	-0.42400400
C	1.77402800	0.96143000	0.30740100
C	2.49438200	-0.23097800	0.35164300
C	1.88581500	-1.42948600	-0.01494600
H	0.05795200	-2.33958900	-0.72806100
H	2.25867600	1.89091700	0.58748800
O	-1.45979900	-0.23618100	-0.92591500
N	-2.53233000	-0.47951200	0.10641900
O	-2.13884100	-0.63747700	1.18403000
H	2.44165800	-2.35939100	0.01266300
C	-0.34707100	2.28007200	-0.14273800
H	-0.86115800	2.39483100	-1.09981500
H	-1.11251900	2.31167200	0.63931500
H	0.31159400	3.13761100	0.00359500
H	3.53112100	-0.22187800	0.66822500
Rotational constants (GHZ): 2.21092 1.16855 0.89096			

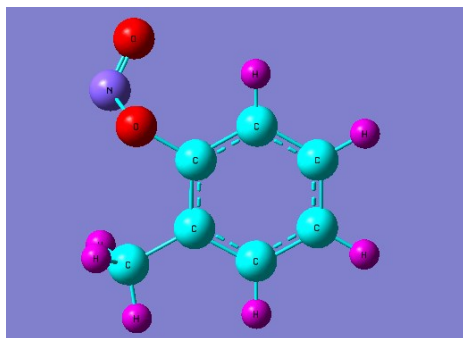
o-Nitrotoluene TS9-10



C	0.17083100	-0.17975100	0.10378600
C	-0.56136100	1.00073600	-0.02920200
C	-2.53151700	-0.44184800	-0.13204600
C	-1.74325400	-1.57772800	0.02145600
C	-0.35844500	-1.45831200	0.15240000
C	-1.93949500	0.82485400	-0.15567700

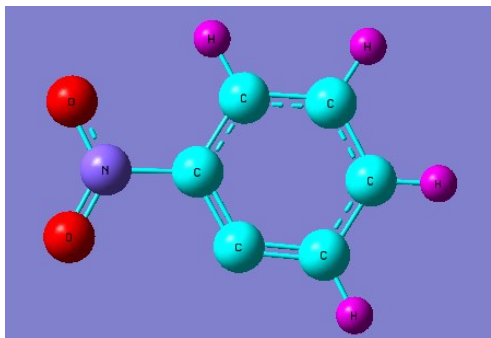
H	-2.55964700	1.70666700	-0.27737200
H	-2.19243500	-2.56356200	0.04398000
O	2.71779100	-0.76528700	-0.74668500
N	1.85237100	-0.10456200	-0.24236900
O	1.70409800	-0.06743500	1.05812300
H	-3.60601600	-0.53451500	-0.23282700
C	0.10664600	2.34147200	-0.03866000
H	0.28421600	-2.32102900	0.26272900
H	-0.60487800	3.13209300	-0.27926200
H	0.56021700	2.56012300	0.93233300
H	0.91640300	2.35739500	-0.77684400
Rotational constants (GHZ):	2.28474	1.16669	0.85124

o-Nitrotoluene TS10-11



C	0.14174200	-0.08463000	0.41270700
C	-0.70505600	0.97337500	0.02961800
C	-0.31142400	-1.40666400	0.42218200
C	-2.01500200	0.65348800	-0.33482600
C	-2.47339700	-0.66420700	-0.33258900
C	-1.62082800	-1.69785400	0.04809100
H	0.36741700	-2.18656800	0.74600700
H	-2.68904400	1.45365600	-0.62328700
O	1.42822200	0.18873500	0.81824400
N	2.45857900	0.13524900	-0.42890700
O	2.81911100	-0.93039700	-0.61487400
H	-1.97353000	-2.72280200	0.06352400
C	-0.21050300	2.39680100	0.03680900
H	0.23583800	2.65046000	1.00146100
H	0.56220800	2.55821500	-0.72045400
H	-1.02857000	3.09109100	-0.16334500
H	-3.49622100	-0.87935000	-0.62045900
Rotational constants (GHZ):	2.18502	1.09925	0.79855

o-Nitrotoluene R9 decomposition C6H4NO2



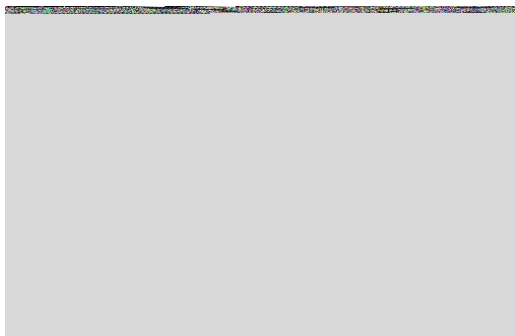
C	-1.82363900	-1.25789200	0.00000000
C	-0.45499200	-1.18777700	0.00000000
C	-2.51552300	-0.03628800	0.00000000
C	-1.82034600	1.17556700	0.00000000
C	-0.42821100	1.19929700	0.00000000
C	0.26008900	-0.01530800	0.00000000
N	1.73434300	-0.04498900	0.00000000
O	2.32482200	1.02742200	0.00000000
O	2.26828900	-1.14535900	0.00000000
H	-2.35402600	-2.20315500	0.00000000
H	-3.60009400	-0.03893200	0.00000000
H	-2.36876000	2.10964300	0.00000000
H	0.13332500	2.12528000	0.00000000

<frequencies>

57.1110	161.9784	217.7133	378.6074	412.9369	450.2685
530.7625	616.3983	644.6080	685.2669	712.1352	767.8400
857.5783	865.2658	964.5112	987.0613	996.6380	1032.6031
1112.6196	1148.4749	1182.1255	1255.7439	1337.8176	1370.0571
1455.8191	1462.7463	1566.7312	1602.2654	1635.6356	3169.7909
3184.0029	3192.9029	3205.7916			

Rotational constants (GHZ): 4.15701 1.27702 0.97691

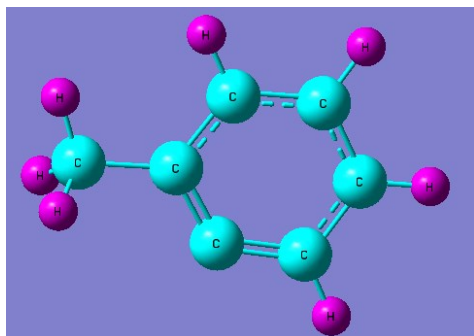
o-Nitrotoluene R9 decomposition CH3



C	0.00000200	-0.00000300	-0.00001400
H	1.00967800	-0.38513000	0.00002700
H	-0.17130100	1.06696700	0.00002700

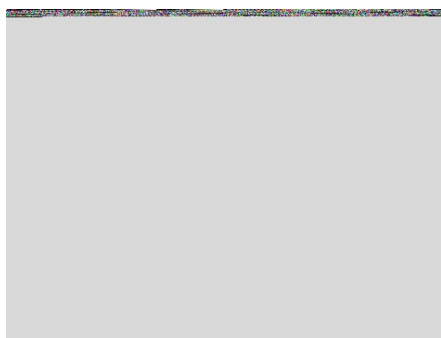
H	-0.83838700	-0.68182100	0.00002700		
<frequencies>					
536.9517	1402.2722	1402.3867	3102.9360	3282.7699	3282.8919
Rotational constants (GHZ):					
	286.28026	286.26962	143.13747		

o-Nitrotoluene R9 decomposition C6H4CH3



C	-0.24042700	1.15294300	-0.00006800		
C	-0.94540100	-0.06342300	-0.00009400		
C	1.15551400	1.18214000	0.00002900		
C	1.89338900	0.00017700	0.00006300		
C	1.22361200	-1.23354100	0.00000400		
C	-0.14757700	-1.19029900	-0.00007200		
C	-2.45341100	-0.12317300	0.00006700		
H	-0.79954200	2.08434900	-0.00013500		
H	1.66870900	2.13718600	0.00003600		
H	2.97782600	0.02714200	0.00009200		
H	1.77310800	-2.16865300	-0.00001900		
H	-2.88453800	0.87979600	-0.00090000		
H	-2.82497500	-0.65530500	-0.88002200		
H	-2.82478000	-0.65345800	0.88137700		
<frequencies>					
39.3901	202.0045	329.0149	415.7491	485.3841	517.5905
632.5691	680.7166	739.1825	793.5703	844.2716	930.9913
976.2356	980.6804	1000.3800	1043.0816	1057.2385	1131.4557
1173.9996	1218.2083	1272.9858	1320.8294	1411.3853	1437.8718
1473.5410	1483.6505	1498.6669	1571.7816	1632.9106	3030.3633
3083.2201	3105.7828	3147.4698	3160.0071	3172.5912	3185.2849
Rotational constants (GHZ):					
	5.93815	2.49666	1.77698		

o-Nitrotoluene R9 decomposition NO2

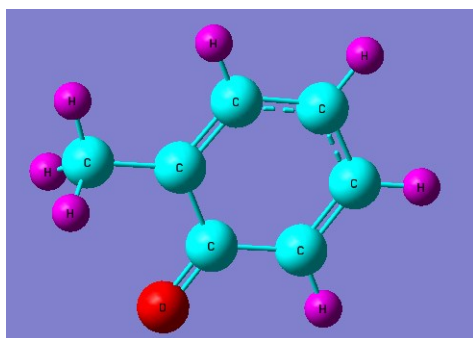


N	0.00000000	0.00000000	0.32194100
O	0.00000000	-1.09996700	-0.14084900
O	0.00000000	1.09996700	-0.14084900

<frequencies>

764.6896	1391.2897	1701.4273	
Rotational constants (GHZ):	242.27262	13.05707	12.38935

o-Nitrotoluene R10 decomposition C6H4CH3O



C	0.37602200	0.88200700	-0.00000200
C	0.70277900	-0.54795700	-0.00000300
C	-1.02682500	1.25753600	0.00000200
C	-0.32977200	-1.46723600	-0.00000400
C	-1.67370300	-1.06111500	0.00000100
C	-2.01604500	0.30649900	0.00000300
H	-1.24664100	2.31876600	0.00000200
H	-0.09961500	-2.52792200	-0.00001000
O	1.27743700	1.74919100	-0.00000300
H	-3.06037800	0.59828400	0.00000300
C	2.14551900	-0.94732400	0.00000200
H	2.66040100	-0.53672800	-0.87349000
H	2.66029700	-0.53708300	0.87372400
H	2.25595200	-2.03297000	-0.00020200
H	-2.45737100	-1.81032800	-0.00000100

<frequencies>

102.4181	145.7792	244.3805	300.8385	424.8173	452.1270
495.9954	538.3138	575.4100	692.4975	721.1125	788.4664

853.2735	858.5234	952.0071	977.6363	993.8449	1038.6604
1044.7153	1127.6198	1165.0128	1172.4671	1273.4023	1321.6654
1407.0675	1415.9925	1449.1265	1465.9112	1474.0037	1498.8836
1542.6035	1595.4210	3031.5235	3079.4685	3113.0230	3158.7169
3169.0182	3185.7580	3195.8530			
Rotational constants (GHZ):					
	3.30459	2.25492	1.35136		

o-Nitrotoluene R10 decomposition NO



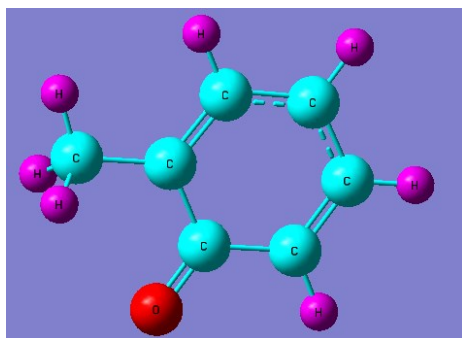
N	0.00000000	0.00000000	-0.61228500
O	0.00000000	0.00000000	0.53574900

<frequencies>

1979.6462

Rotational constants (GHZ):	51.35640	0	0
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o-Nitrotoluene R11 decomposition C6H4CH3O



C	-0.37602400	0.88200200	0.00000000
C	-0.70277800	-0.54796200	-0.00000200
C	1.02682100	1.25753900	0.00000000
C	0.32977400	-1.46723500	-0.00000200
C	1.67370500	-1.06111000	0.00000400
C	2.01604500	0.30650400	-0.00000200
H	1.24663400	2.31877000	-0.00000200
H	0.09962100	-2.52792200	-0.00000500
O	-1.27744500	1.74918400	0.00000100
H	3.06037700	0.59829100	-0.00000300
C	-2.14551200	-0.94732600	-0.00000100

H	-2.66037300	-0.53680600	-0.87354300
H	-2.25594900	-2.03297000	-0.00010800
H	-2.66031700	-0.53699400	0.87366300
H	2.45737500	-1.81032100	0.00000400

<frequencies>

102.4258	145.7766	244.3834	300.8397	424.8153	452.1261
495.9959	538.3152	575.4067	692.4940	721.1163	788.4648
853.2730	858.5496	952.0084	977.6366	993.8511	1038.6410
1044.7161	1127.6310	1165.0184	1172.4545	1273.4034	1321.6660
1407.0657	1415.9955	1449.1538	1465.9079	1474.0012	1498.8839
1542.5868	1595.4177	3031.5157	3079.4551	3113.0347	3158.7166
3168.9959	3185.7513	3195.8524			

Rotational constants (GHZ): 3.30460 2.25492 1.35136

o-Nitrotoluene R11 decomposition NO



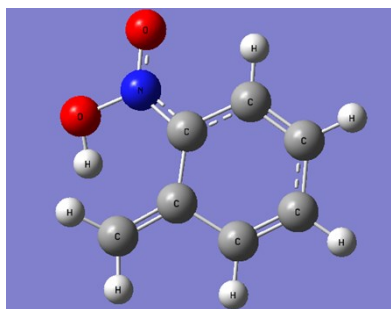
N	0.00000000	0.00000000	-0.61228500
O	0.00000000	0.00000000	0.53574900

<frequencies>

1979.6462

Rotational constants (GHZ): 51.35640 0 0

o-Nitrotoluene R12



C	-2.55388700	-0.21685700	-0.18317300
C	-1.88141400	0.95586800	-0.18614100
C	-1.86531500	-1.46068400	0.04796300
C	-0.51764200	-1.48078100	0.18283900
C	0.24315600	-0.25956500	0.10291000

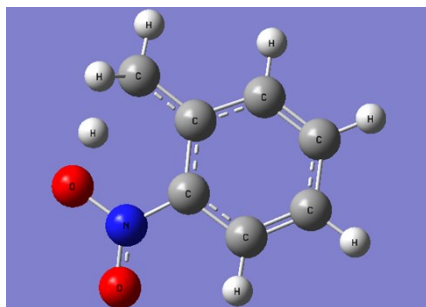
N	1.57648100	-0.41256300	-0.02398600
C	-0.44724400	1.04202800	0.07474600
O	2.20474800	-1.46515200	0.03397600
O	2.37713200	0.70614400	-0.29193100
H	-3.62683500	-0.22567300	-0.33756300
H	-2.42765600	-2.38556000	0.08800300
H	0.02988900	-2.40378700	0.30977000
H	-2.40919900	1.89286500	-0.32200000
C	0.09253300	2.27099200	0.32312000
H	-0.54385400	3.14442100	0.25711900
H	1.09029000	2.43781100	0.70353800
H	1.77582000	1.39392700	-0.64091200

<frequencies>

93.0460	117.5062	206.5741	267.2715	362.6101	380.3396
400.6578	452.7626	488.3746	538.9408	562.5143	594.7721
635.6758	688.7045	710.5515	724.5217	780.7972	836.6434
859.2218	878.5299	971.7046	976.5025	985.4417	989.1647
1024.6819	1161.7334	1189.1018	1247.1489	1275.1909	1333.4546
1359.2573	1411.0180	1460.3625	1475.9487	1570.6981	1590.5382
1607.1081	1672.5535	3158.0169	3169.5431	3184.1934	3193.9911
3225.5701	3242.9440	3552.8856			

Rotational constants (GHZ): 2.27514 1.24218 0.81748

o-Nitrotoluene TS9-12



C	1.77910800	1.06158300	-0.18053600
C	0.61476100	-1.46174500	0.22059400
C	2.54624100	-0.07205000	-0.16627600
C	1.96822800	-1.34954700	0.06955800
C	-0.19280200	-0.29314600	0.19251200
N	-1.55684900	-0.47403600	-0.00795100
C	0.37410400	1.02832800	0.08950600
O	-2.32601900	0.59887200	-0.11158700
O	-2.07112400	-1.57008000	-0.19257400
H	-1.07727300	2.35850800	0.98464700
H	2.23819500	2.03179100	-0.33047600

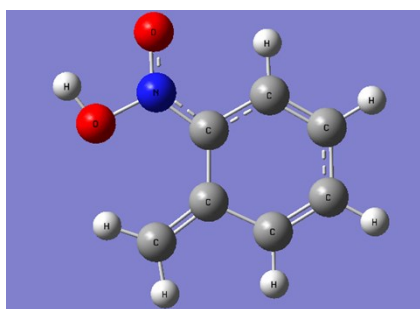
H	3.61736200	0.00591700	-0.31695700
H	2.59616000	-2.23116000	0.10220200
C	-0.40280300	2.21000400	0.14251300
H	0.07865300	3.12360900	-0.18936300
H	-1.62930100	1.47986700	-0.30524400
H	0.13027500	-2.42117300	0.33691800

<frequencies>

-1366.8354	126.4681	145.2356	223.6803	327.4127	417.3602
442.1148	501.9927	516.1747	559.1750	575.4491	643.6522
670.1014	724.4204	750.8249	777.4138	807.9065	855.7455
876.0957	966.0026	979.9720	994.6791	1000.1979	1042.3320
1109.3118	1170.7704	1189.9094	1211.1428	1264.3215	1328.1785
1375.8825	1392.7018	1451.5382	1484.8787	1491.7317	1526.2234
1565.4521	1641.6676	1652.4994	3094.2529	3169.1035	3181.9107
3186.2719	3194.7143	3221.2209			

Rotational constants (GHZ): 2.31307 1.28529 0.83818

o-Nitrotoluene R13



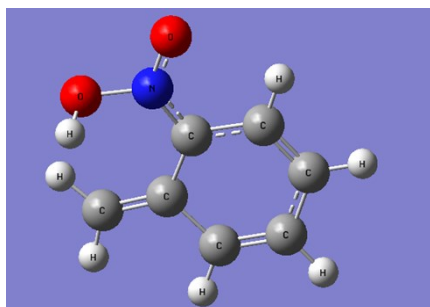
C	2.59559400	-0.24227400	-0.00020900
C	1.94060600	0.93824700	-0.00022500
C	1.85927100	-1.48033100	0.00006400
C	0.50603300	-1.47783700	0.00022200
C	-0.23534700	-0.23845600	0.00011400
N	-1.56231500	-0.38461700	-0.00001100
C	0.48262300	1.05268500	0.00005200
O	-2.21932300	-1.44766100	0.00001900
O	-2.33716200	0.78533600	-0.00031700
H	3.67911100	-0.26616200	-0.00037500
H	2.39510500	-2.42216400	0.00012500
H	-0.06452000	-2.39535300	0.00037500
H	2.49390400	1.87051100	-0.00038800
C	-0.04968800	2.30397900	0.00034800
H	0.62717000	3.15038500	0.00029600
H	-1.10466700	2.51086600	0.00071900
H	-3.23256900	0.40675500	-0.00048400

<frequencies>

59.2124	115.3469	214.3722	271.9657	335.7376	379.9261
399.7458	407.4468	490.2991	539.0051	555.2146	558.8256
610.9197	659.9336	695.4733	713.3130	775.8846	836.7051
861.5166	906.5206	971.9127	985.6788	987.9653	996.8986
1028.5192	1159.7050	1191.0463	1245.2707	1274.7162	1288.5624
1345.3391	1410.4730	1459.9501	1476.0441	1580.3992	1600.4521
1651.5463	1679.0774	3162.0282	3169.4402	3181.5569	3192.7636
3226.0397	3302.7150	3718.0888			

Rotational constants (GHZ): 2.31202 1.22611 0.80121

o-Nitrotoluene TS12-13



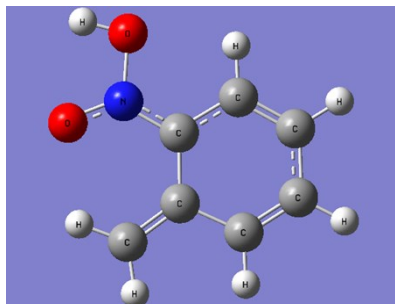
C	-1.91076100	0.95184900	0.09712900
C	-0.51526800	-1.47896600	-0.09550900
C	-2.58074300	-0.22005400	0.10152800
C	-1.86658500	-1.46507500	-0.02004700
C	0.24708000	-0.25256600	-0.05599500
N	1.57687700	-0.42029000	0.00742200
C	-0.45694400	1.04841800	-0.03931300
O	2.38943800	0.74693900	0.08324100
O	2.20139100	-1.48456300	-0.02218900
H	1.11588800	2.49104500	-0.36224800
H	-2.44939000	1.89004600	0.16628500
H	-3.66131100	-0.23073400	0.18442000
H	-2.41682100	-2.39825600	-0.04280900
C	0.07365100	2.29421100	-0.17831100
H	-0.59728200	3.14484300	-0.16173100
H	2.26185300	1.08235900	0.98630200
H	0.03971600	-2.40318900	-0.16748000

<frequencies>

-346.2078	80.0020	107.9417	212.7996	270.8689	378.7260
392.2195	406.4828	486.4975	530.0721	547.8834	561.8465
623.2570	668.9391	689.4171	702.4446	777.9169	837.5317
858.8136	898.1296	955.3129	970.3134	989.3581	997.2593
1025.6066	1161.2807	1190.8684	1239.4476	1260.5161	1307.2892
1344.3589	1406.3141	1454.5366	1474.0602	1562.1326	1581.3418

1595.7369	1677.5518	3161.6853	3169.9949	3182.2877	3193.2076
3226.6640	3283.4452	3704.7057			
Rotational constants (GHZ):			2.27850	1.23280	0.80541

o-Nitrotoluene R14

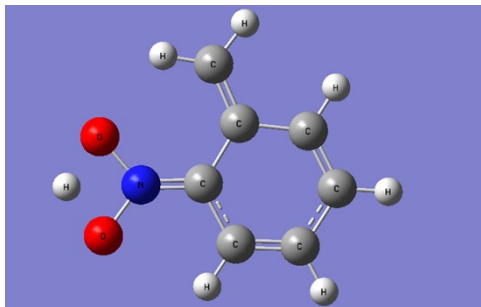


C	2.57410100	-0.36983500	-0.00008000
C	1.99934000	0.85342400	-0.00009600
C	1.75843000	-1.55600100	0.00007300
C	0.40557800	-1.47200800	0.00012100
C	-0.24539700	-0.18637200	0.00004400
N	-1.57450200	-0.12432700	-0.00004100
C	0.55475000	1.05158200	0.00000400
O	-2.24915600	-1.37392900	-0.00014400
O	-2.31585300	0.87707800	0.00004800
H	3.65345500	-0.46736200	-0.00014900
H	2.23405400	-2.52968700	0.00016100
H	-0.20744100	-2.36043800	0.00025900
H	2.61119000	1.74850300	-0.00016800
C	0.06188700	2.31974400	0.00006600
H	0.76281700	3.14701700	0.00000000
H	-0.99141300	2.54054200	0.00017700
H	-3.17322800	-1.07668500	-0.00001500

<frequencies>

90.4564	121.8980	212.1788	266.3508	274.8375	378.1533
394.2424	418.5137	486.3585	514.4549	546.1345	557.3133
608.7343	670.4974	707.8172	718.6514	772.8536	835.7649
839.1281	913.2531	956.2261	971.1843	983.0823	995.4803
1024.3787	1187.0635	1194.8607	1245.9814	1276.4639	1290.7057
1357.7198	1420.5397	1449.5723	1478.1028	1568.7418	1589.0871
1663.4670	1678.2395	3155.2525	3168.4448	3180.7346	3192.4719
3236.1998	3293.7406	3740.4766			
Rotational constants (GHZ):			2.30325	1.23447	0.80371

o-Nitrotoluene TS13-14



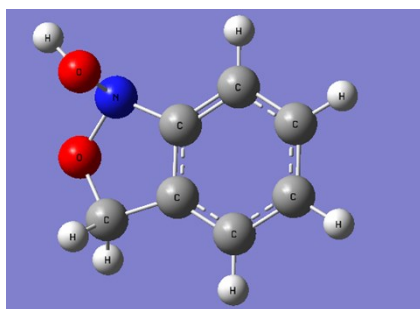
C	-2.60751800	-0.29513500	0.00006000
C	-1.99281500	0.90759600	0.00002400
C	-1.83411300	-1.51387200	0.00006600
C	-0.48159700	-1.48107800	0.00003600
C	0.21299000	-0.21481600	-0.00000100
N	1.52664500	-0.25373900	-0.00002100
C	-0.54131200	1.05368800	-0.00001300
O	2.39991100	0.74958800	-0.00005500
O	2.31170000	-1.33095000	-0.00001800
H	-3.68942400	-0.35610400	0.00008600
H	-2.34777200	-2.46805700	0.00009400
H	0.11602900	-2.38201400	0.00004100
H	-2.57318800	1.82330100	0.00001900
C	0.00970000	2.29373200	-0.00005700
H	-0.64468200	3.15782800	-0.00006100
H	1.07471200	2.46059600	-0.00008600
H	3.09291400	-0.30916300	-0.00004800

<frequencies>

90.4564	121.8980	212.1788	266.3508	274.8375	378.1533
394.2424	418.5137	486.3585	514.4549	546.1345	557.3133
608.7343	670.4974	707.8172	718.6514	772.8536	835.7649
839.1281	913.2531	956.2261	971.1843	983.0823	995.4803
1024.3787	1187.0635	1194.8607	1245.9814	1276.4639	1290.7057
1357.7198	1420.5397	1449.5723	1478.1028	1568.7418	1589.0871
1663.4670	1678.2395	3155.2525	3168.4448	3180.7346	3192.4719
3236.1998	3293.7406	3740.4766			

Rotational constants (GHZ): 2.38913 1.19273 0.79556

o-Nitrotoluene R15



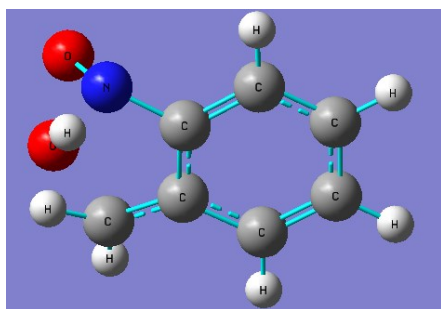
C	-2.54259000	0.33866600	0.17419900
C	-1.52704000	1.29517500	0.24954400
C	-2.24792500	-0.99930900	-0.10281700
C	-0.93140600	-1.41284500	-0.31049000
C	0.05865800	-0.44587100	-0.23878000
N	1.47127100	-0.66593200	-0.41179800
C	-0.21711800	0.88565800	0.03513000
H	-3.57277800	0.63857300	0.32786200
H	-3.05141400	-1.72443100	-0.15962200
H	-0.68647000	-2.44646900	-0.51987400
H	-1.76320700	2.33066400	0.46777400
C	1.09125400	1.61801600	0.04513000
H	1.40514100	1.90742600	1.05495300
H	1.12078800	2.49068500	-0.61012100
O	2.01002900	0.65277700	-0.52578100
O	1.91741300	-1.21904500	0.85204300
H	2.72650500	-1.68172000	0.60002400

<frequencies>

111.4238	149.7229	214.8707	324.9032	373.2415	417.0426
447.8251	492.5647	555.0935	565.6730	626.9212	718.6753
740.2387	758.2092	809.0332	827.0417	858.8118	877.5002
916.6116	953.4153	954.7253	991.8336	1031.9656	1039.7938
1119.4731	1178.4500	1190.1205	1191.1422	1237.3389	1288.7421
1335.0617	1361.1758	1375.8598	1492.5954	1496.8439	1505.6026
1637.1086	1653.9835	3017.7245	3088.5318	3168.0175	3178.0525
3189.9648	3202.1101	3801.0221			

Rotational constants (GHZ): 2.67241 1.24564 0.92407

o-Nitrotoluene TS13-15



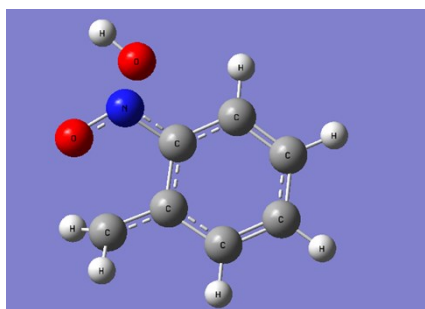
C	-2.59070500	0.16431500	0.08421200
C	-1.67608900	1.19821000	0.11865400
C	-2.16498300	-1.16635600	-0.04121300
C	-0.80089700	-1.45890400	-0.07767600
C	0.12083600	-0.43660500	0.03896700
N	1.51449500	-0.69951400	-0.10103100
C	-0.27186200	0.95114100	0.05354600
O	2.05275700	-0.32250700	-1.17023300
O	2.24526300	-0.20545300	1.09070900
H	-3.65021900	0.38460500	0.14779400
H	-2.89070000	-1.96784000	-0.10544600
H	-0.44801900	-2.47795700	-0.17815200
H	-2.01651800	2.22034800	0.23772900
C	0.67053900	1.94713500	-0.17234200
H	1.71596900	1.81929500	0.06018500
H	0.34668900	2.91957800	-0.52315700
H	2.23614100	-0.97136600	1.67955700

<frequencies>

-419.3503	142.4710	162.4627	223.9676	305.4947	342.4091
415.3485	450.9710	484.8694	524.7188	554.7383	585.8969
619.7910	724.4160	735.6618	750.2744	769.2495	831.1987
859.4896	926.0572	949.3725	969.1669	994.2126	1005.1134
1047.6615	1150.4840	1179.7808	1196.0340	1262.6882	1290.5682
1319.3693	1365.6132	1429.3721	1473.2882	1481.8051	1518.1052
1569.5393	1641.5492	3112.9368	3170.3633	3182.1351	3192.7255
3212.7945	3262.3887	3779.3080			

Rotational constants (GHZ): 2.52294 1.13826 0.91177

o-Nitrotoluene TS14-15



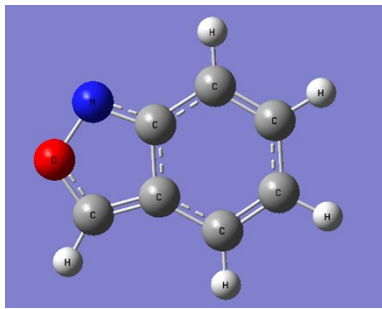
C	-2.54324900	0.03800200	0.19682900
C	-1.70225800	1.12481300	0.26791200
C	-2.04234700	-1.24055700	-0.13742800
C	-0.69832400	-1.42341500	-0.36972000
C	0.16021500	-0.31111000	-0.31113600
N	1.53365300	-0.42722700	-0.26446000
C	-0.32175800	1.00830100	-0.05420800
O	1.92068900	-1.43580000	0.70350000
O	2.19150100	0.66611500	-0.23007900
H	-3.60197400	0.16350900	0.39202800
H	-2.71656600	-2.08782200	-0.18062900
H	-0.28255900	-2.40331800	-0.56192500
H	-2.09922300	2.10473900	0.50612800
C	0.58818000	2.09132300	0.00074000
H	0.39366500	2.87373400	0.73284700
H	1.19140300	2.38615200	-0.84011100
H	2.83941000	-1.61307700	0.45757600

<frequencies>

-419.3503	142.4710	162.4627	223.9676	305.4947	342.4091
415.3485	450.9710	484.8694	524.7188	554.7383	585.8969
619.7910	724.4160	735.6618	750.2744	769.2495	831.1987
859.4896	926.0572	949.3725	969.1669	994.2126	1005.1134
1047.6615	1150.4840	1179.7808	1196.0340	1262.6882	1290.5682
1319.3693	1365.6132	1429.3721	1473.2882	1481.8051	1518.1052
1569.5393	1641.5492	3112.9368	3170.3633	3182.1351	3192.7255
3212.7945	3262.3887	3779.3080			

Rotational constants (GHZ): 2.35961 1.28364 0.87856

o-Nitrotoluene R15 decomposition to C6H4CH2NOH



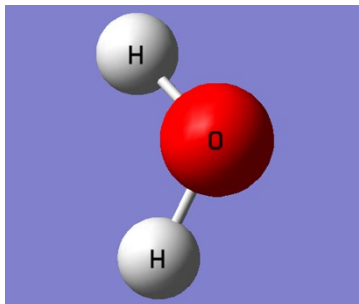
C	-2.11109100	0.72751300	-0.00000200
C	-0.95400000	1.45370200	0.00000000
C	-2.09885300	-0.70961600	0.00000500
C	-0.93857000	-1.42998400	0.00000000
C	0.28857200	-0.70138400	-0.00000200
N	1.52036600	-1.18941000	0.00000000
C	0.27857700	0.73944800	-0.00000200
H	-3.06780100	1.23657800	-0.00000200
H	-3.04957800	-1.23096100	0.00000300
H	-0.93034700	-2.51253700	-0.00000500
H	-0.96874400	2.53709600	-0.00000300
C	1.61384500	1.05664400	0.00000000
H	2.16613300	1.98278400	0.00001100
O	2.34211300	-0.06312900	0.00000100

<frequencies>

209.2307	249.2160	407.4144	438.8048	544.8526	552.5717
601.1845	614.4555	726.3120	752.1734	765.5934	797.7841
848.9108	894.8579	918.9135	934.0714	969.8697	991.5642
1003.1104	1142.0903	1160.9864	1181.9450	1260.9102	1281.5657
1381.0570	1408.0298	1424.8526	1490.8419	1553.6508	1590.9231
1679.9520	3170.0337	3180.1698	3193.8356	3203.7011	3261.9710

Rotational constants (GHZ): 3.95495 1.64973 1.16413

o-Nitrotoluene R15 decomposition to H2O

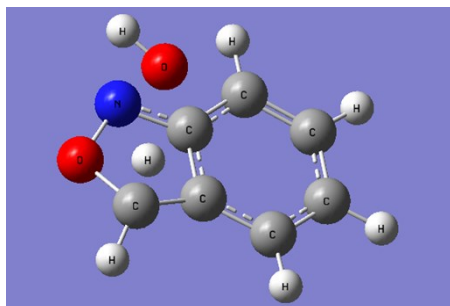


O	0.00000000	0.00000000	0.11706300
H	0.00000000	0.76356200	-0.46825300
H	0.00000000	-0.76356200	-0.46825300

<frequencies>

1602.6800	3817.0069	3922.1463
Rotational constants (GHZ):	824.07569	430.04420 282.57982

o-Nitrotoluene TS15-16



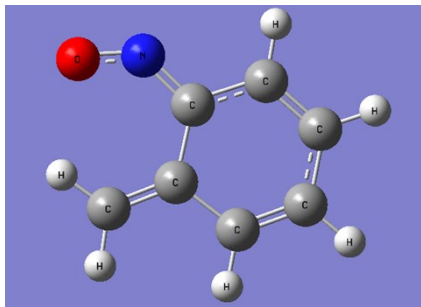
C	-2.42239200	0.55981200	0.26295300
C	-1.31502700	1.40515700	0.22320400
C	-2.31764300	-0.82130300	-0.00122500
C	-1.10151100	-1.39780900	-0.32248400
C	-0.00017500	-0.53648600	-0.40196000
N	1.28927400	-0.87710700	-0.71482200
C	-0.09429900	0.84570800	-0.12961200
H	-3.39412700	0.97251900	0.50911000
H	-3.20759600	-1.43674400	0.05307700
H	-0.99211000	-2.45801700	-0.50996400
H	-1.41199500	2.45716300	0.46231500
C	1.30660800	1.26847600	-0.13468800
H	1.68343300	0.84393600	0.89578000
H	1.63468300	2.26203300	-0.41924300
O	1.96057400	0.25191900	-0.91852300
O	1.76552600	-0.65305800	1.61550600
H	2.52062500	-1.23336900	1.45968500

<frequencies>

-736.8462	109.0514	180.3392	245.8971	253.6975	294.7892
401.9424	425.9893	482.0113	540.6936	568.1765	609.0213
636.6198	737.2716	764.5332	781.5267	807.5928	878.9961
893.2234	932.8324	949.7765	967.5477	1004.7997	1027.1888
1053.2179	1113.3587	1139.2965	1184.0722	1238.0901	1256.9875
1289.5082	1330.3644	1381.4123	1396.5462	1465.7787	1512.7651
1610.6031	1641.7247	2177.6472	3175.1858	3184.5646	3187.9138
3196.3877	3211.0818	3828.6147			

Rotational constants (GHZ):	2.49239	1.16574	1.02337
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o-Nitrotoluene R14 decomposition to C6H4CH(O)N



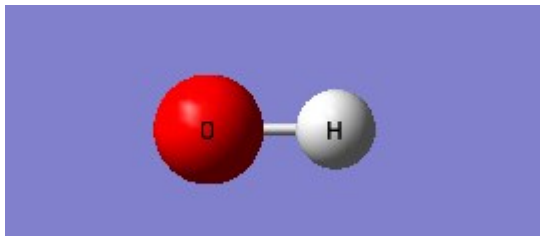
C	-2.28169100	0.34102100	0.00001100
C	-1.29866700	1.26994600	0.00001300
C	-1.97278800	-1.06985300	0.00000100
C	-0.68754100	-1.49322000	-0.00000700
C	0.39744800	-0.53988500	-0.00000500
N	1.61797000	-1.01753400	-0.00001300
C	0.11407900	0.91306600	0.00000500
O	2.71497400	-0.47429100	-0.00001400
H	-3.32039300	0.65093500	0.00001700
H	-2.78225400	-1.79004700	0.00000000
H	-0.43168100	-2.54560400	-0.00001400
H	-1.53912900	2.32741900	0.00002100
C	1.07837400	1.86653100	0.00000700
H	0.79883300	2.91366900	0.00001500
H	2.13376400	1.63505200	0.00000100

<frequencies>

96.1204	204.2228	235.3447	326.2170	403.3272	422.2641
440.1039	501.2998	569.4338	608.3314	608.8818	711.8378
719.2768	770.0195	835.5011	879.0607	894.5018	962.5534
978.7939	992.2006	1010.4746	1164.9138	1183.9127	1250.6147
1255.0653	1346.1054	1396.1545	1449.7475	1469.6718	1525.3359
1593.3071	1630.7025	1674.8307	3151.7160	3165.8424	3178.6127
3187.7016	3200.0418	3250.4385			

Rotational constants (GHZ): 3.13412 1.52056 1.02383

o-Nitrotoluene R14 decomposition to OH



O	0.00000000	0.00000000	0.10842800
H	0.00000000	0.00000000	-0.86742600

<frequencies>

3709.4917

Rotational constants (GHZ): 559.756863 0 0

Table S1. The enthalpies of formation at 298 K for all reactants, TSs and products of three nitrotoluene isomer systems in this work.

Molecules	$\Delta_f H_{298\text{ K}}^0$ (kcal/mol)
R1	0.82
R2	2.87
TS1-2	63.32
R3	2.24
TS2-3	10.43
R4	95.11
TS1-4	106.38
p-C ₆ H ₄ NO ₂	74.10
p-C ₆ H ₄ CH ₃	82.14
p-C ₆ H ₄ (O)CH ₃	7.97
TS4-5	95.27
R5	1.13
R6	1.00
TS5-6	62.77
R7	2.06
TS6-7	10.20
R8	90.00
TS5-8	103.28
m-C ₆ H ₄ NO ₂	70.75
m-C ₆ H ₄ CH ₃	81.66
m-C ₆ H ₄ (O)CH ₃	8.65
TS8-9	95.93
R9	3.19
R10	-0.07
TS9-10	60.35

R11	1.32
TS10-11	9.70
o-C ₆ H ₄ NO ₂	68.29
o-C ₆ H ₄ CH ₃	81.92
o-C ₆ H ₄ (O)CH ₃	6.83
NO	91.04
NO ₂	33.97
CH ₃	146.70
R12	41.60
TS9-12	47.29
R13	36.16
TS12-13	42.05
R14	32.33
TS13-14	53.84
R15	14.79
TS13-15	68.83
TS14-15	48.79
o-C ₆ H ₄ CH(O)N	56.24
o-H ₂ O	-57.77
TS15-16	50.35
o- C ₆ H ₄ CH ₂ NO	62.59
o-OH	9.31

Table S2. Calculated barrier width L (Å), as well as forward and reverse barrier heights (E_1 , E_{-1}) at the CCSD(T)/CBS level of theory (kcal/mol), and imaginary frequencies ν^* of the transition state (cm^{-1}).

	Imaginary frequency	E_1	E_{-1}	Barrier width
Rxn1-2	808.33	65.0	61.8	15.94
Rxn2-3	205.76	8.5	9.1	21.80

Rxn1-4	535.28	107.9	11.6	23.93
Rxn4-5	543.21	0.1	95.9	5.61
Rxn5-6	798.53	64.2	63.1	16.16
Rxn6-7	208.98	10.1	9.0	22.36
Rxn5-8	469.67	104.6	13.7	28.47
Rxn8-9	835.89	7.7	96.7	26.39
Rxn9-10	790.71	147.1	149.1	24.70
Rxn10-11	217.13	10.7	9.2	22.05
Rxn9-12	1366.84	47.9	8.5	15.42
Rxn12-13	346.21	0.9	6.8	22.30
Rxn13-14	1854.90	21.1	24.6	14.34
Rxn13-15	189.96	34.9	56.8	85.59
Rxn14-15	419.35	17.6	36.0	38.41
Rxn15-16	736.85	39.0	56.0-	43.01
