A corrected benzene nitration three-step mechanism derived by DFT calculation and MO theory

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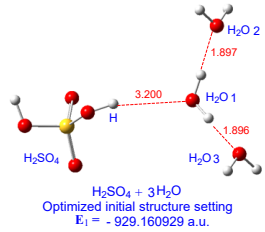
NOTE: The system energies in the figures are obtained by the DFT calculation at the LC-wHPBE/6-311++G(d,p) and have included the zero-point correction and the thermal correction to Gibbs free energy.

S1. The atom coordinate tables of structures 1-4 in Figure 2

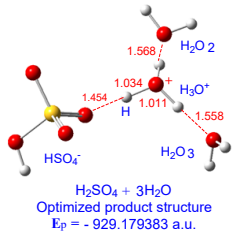
Structure 1



Basis set: LC-wHPBE/6-311++g(d,p)
scrf=(H_2O)
Zero-point correction= 0.110217 Hartree
Thermal correction to Gibbs Free Energy= 0.061063 Hartree
Sum of electronic and zero-point energies= -929.221992 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	16	0	2.019356	0.034859	-0.110892
2	8	0	1.685835	-1.017216	-1.028273
3	8	0	1.132572	-0.119429	1.199821
4	8	0	3.430338	-0.214064	0.546094
5	8	0	-3.758781	2.330238	0.290411
6	1	0	-3.264957	2.905265	0.882070
7	1	0	-4.212146	2.918716	-0.320117
8	8	0	2.028231	1.398079	-0.543670
9	1	0	3.564445	-1.139648	0.802936
10	1	0	0.197041	-0.254052	0.982536
11	8	0	-2.475802	-0.007320	-0.759598
12	1	0	-2.963265	-0.768085	-0.407909
13	1	0	-2.915597	0.777884	-0.398758
14	8	0	-3.898356	-2.273644	0.268886
15	1	0	-3.451718	-2.864358	0.882162
16	1	0	-4.366812	-2.847020	-0.344591

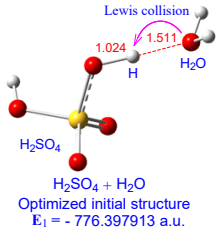
Structure 2



Basis set: LC-wHPBE/6-311++g(d,p)
scrf=(H_2O)
Zero-point correction= 0.112556 Hartree
Thermal correction to Gibbs Free Energy= 0.067821 Hartree
Sum of electronic and zero-point energies= -929.247204 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	16	0	-1.694790	-0.031916	-0.101777
2	8	0	-1.913767	1.189922	-0.862238
3	8	0	-0.357491	-0.056794	0.553324
4	8	0	-2.725499	-0.001948	1.146677
5	8	0	3.243526	-2.104965	0.242555
6	1	0	2.885406	-2.959493	-0.019787
7	1	0	4.183811	-2.129039	0.036666
8	8	0	-2.032724	-1.273354	-0.771824
9	1	0	-2.596910	0.801983	1.667732
10	1	0	0.960838	-0.024837	-0.057942
11	8	0	1.914271	-0.009870	-0.457214
12	1	0	2.406524	0.840149	-0.218281
13	1	0	2.442102	-0.828152	-0.189038
14	8	0	3.217907	2.133887	0.090841
15	1	0	3.113620	2.544838	0.955333
16	1	0	3.184050	2.845138	-0.557279

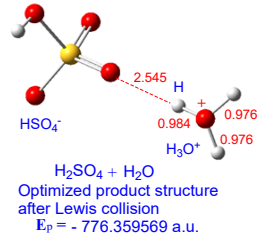
Structure 3



Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction= 0.063165 Hartree
Thermal correction to Gibbs Free Energy= 0.029666 Hartree
Sum of electronic and zero-point energies= -778.426532 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	16	0	-0.600639	0.114898	0.074467
2	8	0	-0.281860	-0.102004	1.462127
3	8	0	0.547279	-0.434221	-0.825052
4	8	0	-1.778181	-0.850409	-0.370930
5	8	0	-1.014218	1.419684	-0.357131
6	1	0	-1.630825	-1.763126	-0.080868
7	1	0	1.487561	-0.248722	-0.463725
8	8	0	2.889482	0.017429	0.033325
9	1	0	3.393452	-0.738445	0.353334
10	1	0	3.472262	0.510653	-0.553873

Structure 4

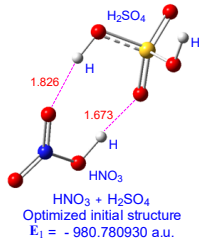


Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction= 0.060912 Hartree
Thermal correction to Gibbs Free Energy= 0.022171 Hartree
Sum of electronic and zero-point energies= -776.412776 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	16	0	-0.858050	0.123909	0.071734
2	8	0	-0.135849	-0.059519	1.298491
3	8	0	-0.039610	-0.552855	-1.111858
4	8	0	-2.140543	-0.791818	0.025735
5	8	0	-1.303348	1.423722	-0.323849
6	1	0	-1.968466	-1.692133	0.343043
7	1	0	0.915611	-0.435421	-0.992503
8	8	0	4.219869	0.034420	0.072853
9	1	0	4.656489	-0.805746	0.236478
10	1	0	4.778374	0.481602	-0.568501

S2. The atom coordinate tables of structures 1, 2 in Figure 5

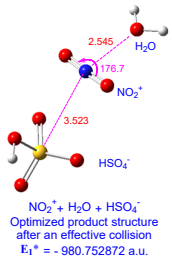
Structure 1



Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction= 0.068319 Hartree
Thermal correction to Gibbs Free Energy= 0.031410 Hartree
Sum of electronic and zero-point energies= -980.812340 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	7	0	2.517801	0.079474	0.020753
2	8	0	2.053307	-1.172443	0.066712
3	8	0	3.700345	0.190561	0.069561
4	8	0	1.710493	0.982919	-0.061061
5	1	0	1.060636	-1.125540	0.033988
6	16	0	-1.610592	-0.103639	-0.089321
7	8	0	-0.611481	-1.146472	-0.063514
8	8	0	-2.875272	-0.323486	-0.711188
9	8	0	-0.991759	1.179450	-0.747174
10	8	0	-1.794285	0.289784	1.427961
11	1	0	-0.032767	1.245717	-0.545662
12	1	0	-2.517673	0.922586	1.564524

Structure 2

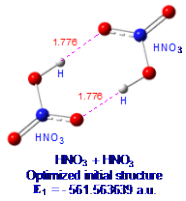


Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction= 0.064195 Hartree
Thermal correction to Gibbs Free Energy= 0.022425 Hartree
Sum of electronic and zero-point energies= -981.775297 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	7	0	1.778000	-0.243911	-0.150890
2	8	0	4.267145	0.268209	-0.005129
3	8	0	1.598890	0.829106	-0.349701
4	8	0	2.017636	-1.308227	0.028464
5	16	0	-1.703288	0.116687	0.253032
6	8	0	-1.375275	1.522218	0.026248
7	8	0	-2.368654	-0.424149	-1.133362
8	8	0	-2.697921	-0.111656	1.294698
9	8	0	-0.518667	-0.749161	0.355258
10	1	0	4.974754	-0.351638	0.193145
11	1	0	4.686574	1.131331	-0.063341
12	1	0	-3.186739	0.057237	-1.313722

S3. The atom coordinate tables of structures 1 and 2 in Figure 6

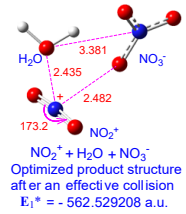
Structure 1



Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction= 0.056302 Hartree
Thermal correction to Gibbs Free Energy= 0.021148 Hartree
Sum of electronic and zero-point energies = -561.584787 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	8	0	-3.202738	-0.162023	-0.024023
2	8	0	-1.230349	-0.999077	0.109241
3	8	0	-1.520246	1.158288	-0.091238
4	1	0	-0.538331	1.074732	-0.032401
5	7	0	2.019335	0.081351	0.003474
6	8	0	1.520271	-1.158267	-0.091410
7	8	0	3.202726	0.162071	-0.024085
8	8	0	1.230315	0.999059	0.109409
9	1	0	0.538352	-1.074763	-0.032607
10	7	0	-2.019342	-0.081328	0.003484

Structure 2

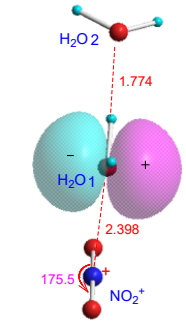


Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction= 0.053097 Hartree
Thermal correction to Gibbs Free Energy= 0.015969 Hartree
Sum of electronic and zero-point energies= -561.545177 Hartree

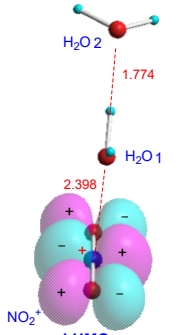
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	7	0	-1.784695	-0.542876	0.085440
2	8	0	-1.066462	1.783576	0.119187
3	8	0	-1.933954	-0.600882	-1.009977
4	8	0	-1.728808	-0.577921	1.190195
5	8	0	1.561803	1.047193	0.145077
6	1	0	-0.095614	1.637635	0.109062
7	1	0	-1.253232	2.432946	-0.563736
8	7	0	1.681594	-0.177842	-0.067479
9	8	0	2.795619	-0.680650	-0.170286
10	8	0	0.659645	-0.883885	-0.174813

S4. The atom coordinate tables of structures 1- 4 in Figure 8

Structure 1 and 2



1

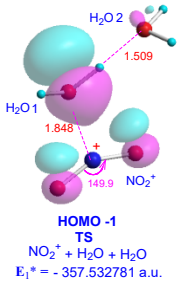


2

Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction= 0.060575 Hartree
Thermal correction to Gibbs Free Energy= 0.025902 Hartree
Sum of electronic and zero-point energies= -357.567712 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	7	0	1.610130	0.307128	-0.020985
2	8	0	-0.453233	-0.914041	-0.043528
3	8	0	1.080285	1.275222	0.051903
4	8	0	2.214688	-0.616194	-0.093122
5	1	0	-0.558616	-1.867845	-0.083283
6	8	0	-2.976576	0.177459	0.091192
7	1	0	-3.318187	0.660222	-0.667353
8	1	0	-3.217435	0.697969	0.863328
9	1	0	-1.353173	-0.533381	0.002562

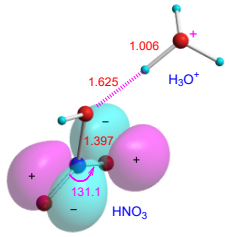
Structure 3



Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction= 0.061317 Hartree
Thermal correction to Gibbs Free Energy= 0.029723 Hartree
Sum of electronic and zero-point energies= -357.562504 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	7	0	1.127125	0.221176	0.014229
2	8	0	-0.272836	-0.929667	-0.348977
3	8	0	0.702781	1.254789	-0.173724
4	8	0	2.004244	-0.445020	0.281046
5	1	0	-0.173028	-1.757867	0.144384
6	8	0	-2.544333	0.069303	0.167182
7	1	0	-2.967011	0.587296	-0.526183
8	1	0	-2.687634	0.539318	0.995535
9	1	0	-1.181052	-0.512212	-0.117550

Structure 4



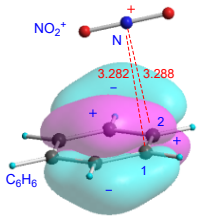
HOMO
$HNO_3 + H_3O^+$
Optimized product structure
E_P = - 357.541639 a.u.

Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction= 0.064506 Hartree
Thermal correction to Gibbs Free Energy= 0.033370 Hartree
Sum of electronic and zero-point energies= -357.575009 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	7	0	1.008937	0.118072	0.004475
2	8	0	-0.071013	-0.741068	-0.210490
3	8	0	0.730799	1.262192	-0.118809
4	8	0	2.040114	-0.410410	0.267859
5	1	0	0.247448	-1.648180	-0.052074
6	8	0	-2.598601	-0.069607	0.054280
7	1	0	-2.965749	0.327621	-0.755384
8	1	0	-2.778248	0.496204	0.826131
9	1	0	-1.618747	-0.275853	-0.039894

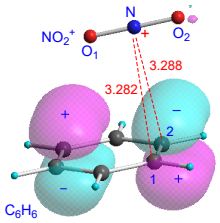
S5. The atom coordinate tables of structures 1-6 in Figure 10

Structure 1-3



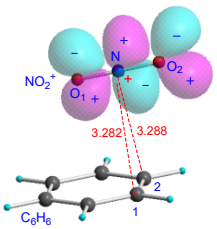
HOMO
$C_6H_6 + NO_2^+$
Optimized initial structure
E_{HOMO} = - 0.378236 a.u.
E_1 = - 436.701413 a.u.

1



HOMO -1
$C_6H_6 + NO_2^+$
Optimized initial structure
E_{HOMO-1} = - 0.379370 a.u.
E_1 = - 436.701413 a.u.

2



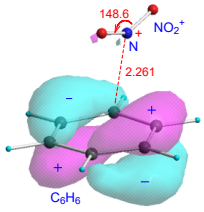
LUMO
$C_6H_6 + NO_2^+$
Optimized initial structure
E_{HOMO} = - 0.078832 a.u.
E_1 = - 436.701413 a.u.

3

Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction= 0.114942 Hartree
Thermal correction to Gibbs free energy= 0.078442 Hartree
Sum of electronic and zero-point Energies= -436.779855 Hartree

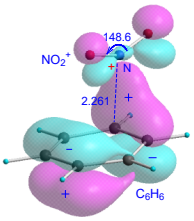
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	8	0	2.778689	0.473739	-0.027530
2	6	0	-0.608060	1.295705	-0.687192
3	6	0	-0.609932	1.292588	0.702316
4	6	0	-1.160054	0.220792	1.393126
5	6	0	-1.708962	-0.845117	0.695149
6	6	0	-1.707031	-0.842082	-0.692736
7	6	0	-1.156232	0.226957	-1.384402
8	1	0	-0.188850	2.131191	1.247040
9	1	0	-1.162357	0.218955	2.477711
10	1	0	-2.140147	-1.681439	1.234638
11	1	0	-2.135740	-1.676499	-1.237134
12	1	0	-1.155865	0.230148	-2.468997
13	7	0	2.112177	-0.409457	-0.013765
14	8	0	1.453151	-1.297858	0.000327
15	1	0	-0.186145	2.137058	-1.227049

Structures 4 and 5



TS
HOMO
$C_6H_6 + NO_2^+$
E_{HOMO} = - 0.410595 a.u.
E_1* = - 436.690750 a.u.

4



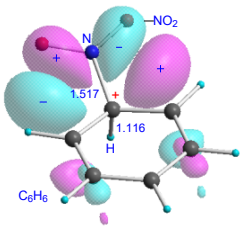
TS
HOMO -1
$C_6H_6 + NO_2^+$
E_{HOMO-1} = - 0.413096 a.u.
E_1* = - 436.690750 a.u.

5

Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction = 0.114179 Hartree
Thermal correction to Gibbs free energy = 0.081498 Hartree
Sum of electronic and zero-point Energies = -436.772248 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	8	0	-1.048255	-0.199595	1.390490
2	6	0	0.550924	-1.296687	-0.845424
3	6	0	1.506524	-1.226035	0.134081
4	6	0	1.898344	0.019723	0.654251
5	6	0	1.352350	1.195880	0.183067
6	6	0	0.352106	1.136004	-0.774282
7	6	0	-0.078140	-0.117292	-1.267378
8	1	0	1.973553	-2.128930	0.509329
9	1	0	2.655588	0.052051	1.429614
10	1	0	1.679892	2.151873	0.571806
11	1	0	-0.101685	2.043224	-1.158329
12	1	0	-0.819618	-0.152573	-2.057905
13	7	0	-1.527339	0.198427	0.438977
14	8	0	-2.457767	0.589718	-0.093258
15	1	0	0.248807	-2.248289	-1.265135

Structure 6



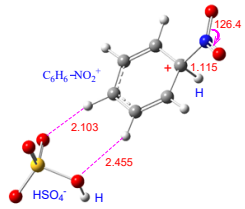
HOMO -1
σ-complex of $C_6H_6 + NO_2^+$
An optimized product structure
E_σ = - 436.717861 a.u.

Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction = 0.115483 Hartree
Thermal correction to Gibbs free energy = 0.082383 Hartree
Sum of electronic and zero-point Energies = -436.800244 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	8	0	-2.236466	1.072259	-0.166961
2	6	0	-0.255077	-0.000002	0.388725
3	6	0	0.451137	1.254456	0.128202
4	6	0	1.789779	1.235203	-0.070784
5	6	0	2.448006	0.000008	-0.174478
6	6	0	1.789793	-1.235194	-0.070752
7	6	0	0.451151	-1.254459	0.128231
8	1	0	-0.115243	2.177258	0.173903
9	1	0	2.343850	2.155467	-0.198502
10	1	0	3.515391	0.000011	-0.373122
11	1	0	2.343877	-2.155454	-0.198442
12	1	0	-0.115215	-2.177267	0.173957
13	7	0	-1.712491	-0.000006	-0.033064
14	8	0	-2.236421	-1.072273	-0.167125
15	1	0	-0.308069	0.000010	1.503518

S6. The atom coordinate tables of structure 1-6 in Figure 11

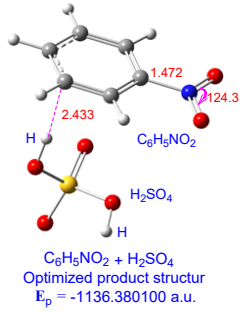
Structure 1



Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction = 0. 143723 Hartree
Thermal correction to Gibbs free energy = 0.097369 Hartree
Sum of electronic and zero-point Energies = -1136.408338 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	7	0	4.220807	-0.474391	0.176801
2	8	0	5.053236	0.343235	0.463318
3	8	0	4.330752	-1.666643	0.273663
4	6	0	2.621888	1.439270	-0.054380
5	6	0	1.334430	1.853362	-0.032123
6	6	0	0.304872	0.910733	-0.195685
7	6	0	0.546255	-0.460570	-0.387345
8	6	0	1.821199	-0.911802	-0.412114
9	6	0	2.923837	0.050488	-0.404691
10	1	0	3.453239	2.116152	0.104472
11	1	0	1.091776	2.891067	0.154745
12	1	0	-0.734492	1.238653	-0.144461
13	1	0	-0.294633	-1.138258	-0.466827
14	1	0	2.063556	-1.962859	-0.516425
15	1	0	3.148937	0.140031	-1.493349
16	16	0	-3.546938	-0.039320	0.160617
17	8	0	-2.836141	1.222407	-0.082206
18	8	0	-3.396360	-0.558708	1.514219
19	8	0	-4.912373	-0.047561	-0.361368
20	8	0	-2.736487	-1.161042	-0.722294
21	1	0	-2.881444	-0.995458	-1.662970

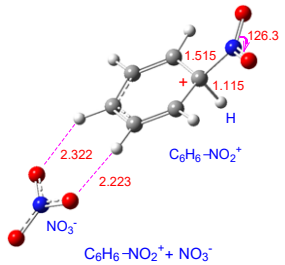
Structure 2



Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction = 0.144955 Hartree
Thermal correction to Gibbs free energy = 0.100429 Hartree
Sum of electronic and zero-point Energies = -1136. 480529 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	6	0	1.506308	-1.770449	1.205775
2	6	0	1.904291	-2.406443	0.035976
3	6	0	2.174869	-1.669123	-1.107121
4	6	0	2.046433	-0.291098	-1.092261
5	6	0	1.649686	0.318555	0.082245
6	6	0	1.377295	-0.390831	1.237678
7	1	0	1.303012	-2.348138	2.099920
8	1	0	2.004710	-3.485672	0.018442
9	1	0	1.072406	0.127824	2.137111
10	8	0	1.173020	2.303861	1.145085
11	8	0	1.687067	2.386347	-0.928651
12	1	0	2.485486	-2.168346	-2.017091
13	1	0	2.245837	0.304813	-1.973117
14	1	0	-0.674665	-1.531326	0.145981
15	7	0	1.491909	1.781243	0.101213
16	16	0	-2.255305	-0.087107	-0.016848
17	8	0	-2.137527	0.169190	1.386162
18	8	0	-1.376474	1.035480	-0.714366
19	8	0	-1.484114	-1.421020	-0.384651
20	8	0	-3.522855	-0.187215	-0.671467
21	1	0	-1.507532	1.057669	-1.675608

Structure 3

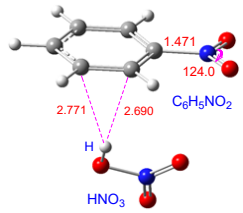


C_6H_6-NO_2^+ + NO_3^-
A optimized initial structur
E_I = - 717.088022 a.u.

Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction = 0.131048 Hartree
Thermal correction to Gibbs free energy = 0.086615 Hartree
Sum of electronic and zero-point Energies = -717.174637 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	7	0	-3.404706	-0.647939	-0.048238
2	8	0	-4.340540	0.066420	-0.287746
3	8	0	-3.396110	-1.848626	-0.093480
4	6	0	-2.060405	1.462866	0.135799
5	6	0	-0.855441	2.057208	-0.020299
6	6	0	0.299501	1.258439	-0.080067
7	6	0	-0.276738	-0.141832	0.016136
8	6	0	-0.912782	-0.769305	0.170103
9	6	0	-2.122071	0.024175	0.397452
10	1	0	-2.986846	2.024611	0.151539
11	1	0	-0.779549	3.129535	-0.141869
12	1	0	1.268633	1.724470	-0.234175
13	1	0	1.208444	-0.691867	-0.081723
14	1	0	-1.000183	-1.848850	0.210412
15	1	0	-2.194611	0.002126	1.510247
16	8	0	3.408077	0.824463	-0.287850
17	7	0	3.979291	-0.258392	-0.066280
18	8	0	3.338865	-1.321123	-0.152344
19	8	0	5.178806	-0.277645	0.239420

Structure 4

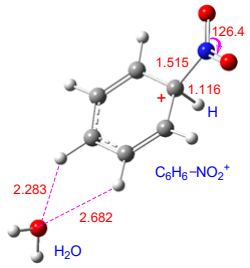


$C_6H_5NO_2$ + HNO_3
Optimized product structur
E_P = - 717.167531 a.u.

Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction = 0.132783 Hartree
Thermal correction to Gibbs Free Energy = 0.088259 Hartree
Sum of electronic and zero-point Energies = -717.255790 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	7	0	0.951054	1.838954	0.040937
2	8	0	0.766864	2.383171	1.106716
3	8	0	0.931641	2.412210	-1.025030
4	6	0	1.340984	-0.259328	1.253051
5	6	0	1.576914	-1.623621	1.243456
6	6	0	1.673467	-2.305497	0.040558
7	6	0	1.539391	-1.628727	-1.164859
8	6	0	1.309581	-0.263646	-1.173334
9	6	0	1.212589	0.391524	0.041513
10	1	0	1.256572	0.293597	2.179295
11	1	0	1.683385	-2.154778	2.181824
12	1	0	1.854860	-3.374299	0.039577
13	1	0	1.618129	-2.164279	-2.103652
14	1	0	1.205476	0.287449	-2.098940
15	1	0	-1.173928	-1.220091	-0.778873
16	7	0	-2.570166	-0.207152	-0.047312
17	8	0	-2.018774	0.757984	-0.500962
18	8	0	-1.974074	-1.411692	-0.257176
19	8	0	-3.584191	-0.260980	0.574336

Structure 5

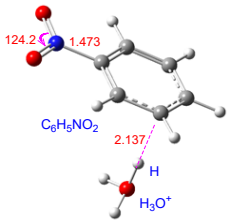


C_6H_6-NO_2^+ + H_2O
Optimized initial structure
E_i = - 513.105180 a.u.

Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction = 0.138466 Hartree
Thermal correction to Gibbs free energy = 0.097976 Hartree
Sum of electronic and zero-point Energies = -513.203156 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	7	0	-2.392736	-0.306854	-0.063687
2	8	0	-3.151108	0.611964	-0.218058
3	8	0	-2.649167	-1.472761	-0.196508
4	6	0	-0.569605	1.407254	0.083625
5	6	0	0.748382	1.683688	-0.050137
6	6	0	1.673277	0.627145	-0.045862
7	6	0	1.301235	-0.719995	0.088876
8	6	0	-0.007873	-1.035168	0.221595
9	6	0	-0.988070	0.038454	0.387093
10	1	0	-1.331484	2.177397	0.051440
11	1	0	1.086970	2.699817	-0.202601
12	1	0	2.731800	0.835505	-0.178009
13	1	0	2.065934	-1.483798	0.041137
14	1	0	-0.356311	-2.058948	0.291395
15	1	0	-1.080450	0.080687	1.498316
16	8	0	4.563209	-0.527445	-0.161216
17	1	0	5.190829	-0.524699	0.566970
18	1	0	5.086335	-0.729922	-0.941834

Structure 6



$C_6H_5NO_2$ + H_3O^+
Optimized product structure
E_p= - 513.140748 a.u.

Basis set: LC-wHPBE/6-311++g(d,p)
scrf=($HCONH_2$)
Zero-point correction = 0.142204 Hartree
Thermal correction to Gibbs Free Energy = 0.104733 Hartree
Sum of electronic and zero-point Energies = -513.245481 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	*y*	*z*
1	6	0	1.427250	-0.015211	1.239405
2	6	0	1.865968	1.126650	0.576865
3	6	0	1.023505	1.797640	-0.298882
4	6	0	-0.261638	1.335398	-0.514089
5	6	0	-0.674974	0.197456	0.154258
6	6	0	0.140100	-0.491871	1.028567
7	1	0	2.075505	-0.519526	1.948363
8	1	0	2.869815	1.497331	0.751838
9	1	0	-0.224941	-1.374952	1.536350
10	8	0	-2.370105	-1.327378	0.473023
11	8	0	-2.765482	0.346824	-0.798172
12	1	0	1.367857	2.686790	-0.812693
13	1	0	-0.937448	1.842494	-1.190202
14	1	0	2.303903	-1.034611	-0.421819
15	7	0	-2.042469	-0.299347	-0.074630
16	8	0	2.717773	-1.593711	-1.127410
17	1	0	2.851035	-2.509428	-0.817569
18	1	0	2.185222	-1.578741	-1.945264