Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Atmospheric Formation of NO_3 Radical from Gas-Phase Reaction of HNO_3 Acid with NH_2 Radical. Proton-Coupled Electron-Transfer versus Hydrogen Atom Transfer Mechanisms.

Josep M. Anglada,[a] Santiago Olivella[a] and Albert Solé[b]*

a) Departament de Química Biològica i Modelització Molecular, (IQAC – CSIC), Jordi Girona, 18-26, E-08034 Barcelona, Catalonia, Spain. E-mail: anglada@iqac.csic.es.

b) Departament de Química Física i Institut de Química Teòrica i Computacional (IQTCUB). Universitat de Barcelona, Martí i Franqués, 1, E-08028 Barcelona, Catalonia, Spain

Supporting information

This supporting information contains a Figure containing the most relevant geometrical parameters of the different stationary points optimized in this works, tables including the absolute energies, and the Cartesian coordinates of the stationary points investigated.

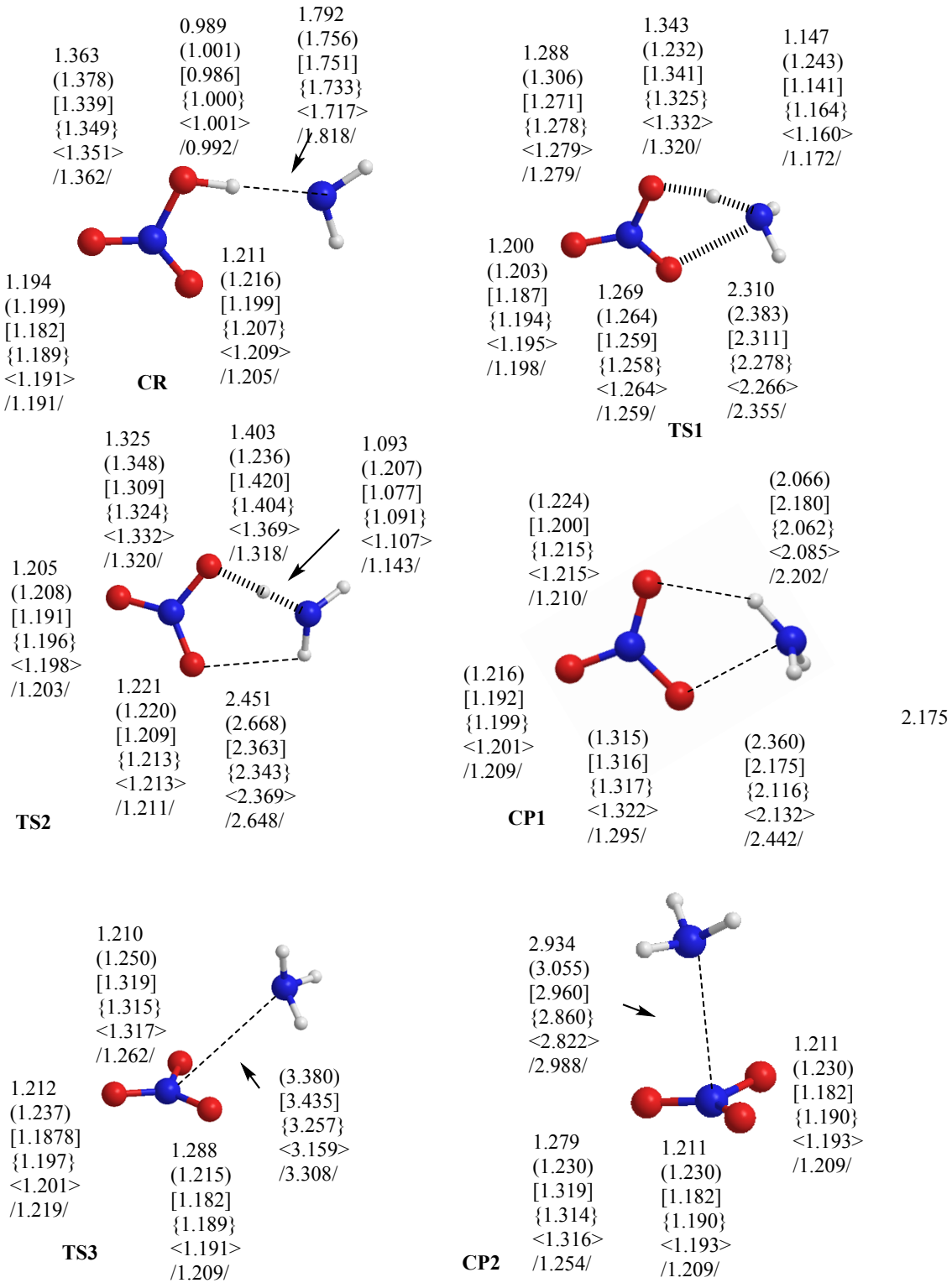

Figure S1: Selected geometrical parameters for the stationary points computed using the 6-311+G(2df,2p) basis set.. Plain text stands for QCISD; values in parenthesis stand for B3LYP; values in square brackets stand for BH&HLYP; values inbraces stand for M05-2X; values in angla brackets stand for M06-2X; values in slashes stand for M05.

Table S1: Absolute energies (in hartree) computed at the geometry optimized at B3LYP level of theory

Compound	B3LYP/ 6-311+G(2df,2p)	HF/ aug-cc-pVTZ	CCSD(T)/ aug-cc-pVTZ	HF/ aug-cc-pVQZ	CCSD(T)/ aug-cc-pVQZ
HNO_3	-280.99675	-279.56269	-280.54488	-279.58163	-280.61844
NH_2	-55.90398	-55.58793	-55.79984	-55.59126	-55.81307
CR	-336.91676	-335.16505	-336.36161	-335.18713	-336.44829
TS1	-336.90870	-335.13769	-336.34659	-335.15961	-336.43352
CP1	-336.92075	-335.12908	-336.34721	-335.15145	-336.43429
TS2	-336.90452	-335.13322	-336.34048	--	--
TS3	-336.91467	-335.14074	-336.34942	-335.16333	-336.43612
CP2	-336.91708	-335.10251	-336.35615	-335.12506	-336.44305
NO_3	-280.32651	-278.87800	-279.86908	-278.89701	-279.94108
NH_3	-56.58647	-56.22031	-56.48050	-56.22396	-56.49568

Table S2: Absolute energies (in hartree) computed at the geometry optimized at BH&HLYP level of theory

Compound	BH&HLYP/ 6-311+G(2df,2p)	HF/ aug-cc-pVTZ	CCSD(T)/ aug-cc-pVTZ	HF/ aug-cc-pVQZ	CCSD(T)/ aug-cc-pVQZ
HNO_3	-280.83621	-279.56936	-280.54207	-279.58863	-280.61640
NH_2	-55.87094	-55.58836	-55.79962	-55.59172	-55.81293
CR	-336.72489	-335.17145	-336.35882	-335.19386	-336.44628
TS1	-336.70666	-335.138526	-336.34261	-335.16075	-336.43029
CP1	-336.71462	-335.13950	-336.34884	-335.16203	-336.43644
TS2	-336.70960	-335.15635	-336.34720	-335.17902	-336.43440
CP2	-336.71235	-335.15878	-336.3510	-335.18148	-336.43813
NH_3	-56.54516	-56.22076	-56.48018	-56.22444	-56.49545
NO_3 (D_{3h})	-280.15194	-278.88456	-279.86575	-278.90387	-279.93844
NO_3 (2S1L)	-280.16195	-278.93462	-279.86411	-278.95375	-279.93628
NO_3 (2L1S)	-280.15779	-278.90821	-279.86538	-278.92747	-279.93779

Table S3: Absolute energies (in hartree) computed at the geometry optimized at QCISD level of theory

Compound	QCISD/ 6-311+G(2df,2p)	HF/ aug-cc-pVTZ	CCSD(T)/ aug-cc-pVTZ	HF/ aug-cc-pVQZ	CCSD(T)/ aug-cc-pVQZ
HNO_3	-280.46591	-279.56536	-280.54459	-279.58440	-280.61839
NH_2	-55.78411	-55.58807	-55.79983	-55.59140	-55.81308
CR	-336.26657	-335.16800	-336.36129	-335.19021	-336.44823
TS1	-336.24711	-335.13499	-336.34496	-335.15699	-336.43214
TS3	-336.25787	-335.15048	-336.34937	-335.17308	-336.43622
CP2	-336.26254	-335.15054	-336.35378	-335.17313	-336.44054
NH_3	-56.46136	-56.22042	-56.48052	-56.22407	-56.49571
NO_3 (D_{3h})	-279.78382	-278.87997	-279.86870	-278.89904	-279.94086
NO_3 (2S1L)	-279.79481	-278.92712	-279.86650	-278.94616	-279.93835
NO_3 (2L1S)	-279.78926	-278.90416	-279.86776	-278.92321	-279.93981

Table S4: Absolute energies (in hartree) computed at the geometry optimized at M05-2X level of theory

Compound	QCISD/ 6-311+G(2df,2p)	HF/ aug-cc-pVTZ	CCSD(T)/ aug-cc-pVTZ
HNO_3.	-280.94978	-279.56759	-280.54363
NH_2	-55.88580	-55.58823	-55.79976
NH_3	-56.56840	-56.22059	-56.48038
CR	-336.85395	-335.16919	-336.36038
TS1	-336.84209	-335.13636	-336.34417
TS2	-336.83306	-335.12482	-336.33618
CP1	-336.84990	-335.13309	-336.35019
TS3	-336.83885	-335.15419	-336.348523
CP2	-336.84201	-335.15700	-336.35241
NO_3 (D_{3h})	-280.26275	-278.88291	-279.86736
NO_3 (2S1L)	-280.26655	-278.93355	-279.86531
NO_3 (2L1S)	-280.26527	-278.90703	-279.86661

Table S5: Absolute energies (in hartree) computed at the geometry optimized at M06-2X level of theory

Compound	QCISD/ 6-311+G(2df,2p)	HF/ aug-cc-pVTZ	CCSD(T)/ aug-cc-pVTZ
HNO_3	-280.88361	-279.56703	-280.54393
NH_2	-55.86850	-55.58804	-55.79983
CR	-336.77089	-335.16824	-336.360707
TS1	-336.75614	-335.13510	-336.34457
TS2	-336.74827	-335.12507	-336.336617
CP1	-336.76524	-335.13382	-336.35067
TS3	-336.75491	-335.15293	-336.348782
CP2	-336.75826	-335.15609	-336.35275
NH_3	-56.54961	-56.22036	-56.48052
NO_3 (D_{3h})	-280.19724	-278.88224	-279.86779
NO_3 (2S1L)2	-280.20072	-278.93317	-279.86560
NO_3 (2L1S)	-280.20075	-278.90672	-279.86683

Table S6: Absolute energies (in hartree) computed at the geometry optimized at M05 level of theory

Compound	QCISD/ 6-311+G(2df,2p)	HF/ aug-cc-pVTZ	CCSD(T)/ aug-cc-pVTZ
HNO_3	-280.87669	-279.56629	-280.54415
NH_2	-55.86010	-55.58818	-55.79979
CR	-336.75352	-335.16904	-336.36081
TS1	-336.74064	-335.13774	-336.34402
TS2	-336.73596	-335.13104	-336.33597
CP1	-336.75150	-335.13575	-336.34551
TS3	-336.74699	-335.14818	-336.34940
CP2	-336.74958	-335.14935	-336.35302
NH_3	-56.53889	-56.22047	-56.48050
NO_3 (D_{3h})	-280.20449	-278.88291	-279.86736
NO_3 (2S1L)	-280.20457	-278.92584	-279.86582

NO_3 (2L1S)	-280.20449	-278.90703	-279.86661

Table S7: Cartesian coordinates of all the stationary points investigated in this work.

Geometries optimized at B3LYP/6-311+G(2df,2p)

HNO_3

N	0.000000	0.154713	0.000000
O	-0.266837	-1.230038	0.000000
O	1.168014	0.462155	0.000000
O	-0.978490	0.836034	0.000000
H	0.618501	-1.628203	0.000000

NH_2

N	0.000000	0.000000	0.141287
H	0.000000	0.806177	-0.494506
H	0.000000	-0.806177	-0.494506

CR

O	2.027114	-0.207949	0.000138
N	0.860957	0.072451	0.000003
O	0.349039	1.175093	-0.000034
O	0.005548	-1.008425	-0.000149
H	-0.919496	-0.625299	-0.000295
N	-2.566367	-0.016996	0.000026
H	-2.694503	0.998003	-0.000450
H	-3.501739	-0.430649	0.000904

TS1

O	-0.007808	1.911151	0.000000
N	0.000000	0.707809	0.000000
O	1.065550	0.028555	0.000000
O	-1.123684	0.041909	0.000000
H	-0.707697	-1.118263	0.000000
N	0.031246	-2.117783	0.000000
H	0.508259	-2.432417	0.838398
H	0.508259	-2.432417	-0.838398

TS2

O	-1.934873	-0.303939	0.025770
N	-0.781560	0.055643	0.003504
O	-0.368233	1.203208	-0.007717
O	0.123052	-0.943626	-0.011244
H	1.249738	-0.489850	-0.241086
N	2.342721	-0.002278	-0.082198
H	2.280889	0.973365	0.204434
H	2.981681	-0.502212	0.533047

CP1

O	0.444123	1.889946	0.000000
N	0.000000	0.758282	0.000000
O	0.912518	-0.188765	0.000000
O	-1.183572	0.444879	0.000000
H	-0.906536	-1.601994	0.000000
N	-0.164990	-2.287981	0.000000
H	0.338460	-2.429295	0.857928

H	0.338460	-2.429295	-0.857928

TS3

O	-0.026127	0.052947	-0.032427
N	0.099035	0.021604	1.175744
O	1.226554	0.053402	1.714058
O	-0.858508	-0.035653	1.957129
H	3.262345	-1.821449	0.034017
N	2.326587	-2.184517	-0.087627
H	1.862948	-1.658834	-0.817005
H	2.384025	-3.156153	-0.362387

CP2

O	-0.081020	0.416238	0.028914
N	0.217451	-0.017732	1.140726
O	1.139784	0.493869	1.773813
O	-0.418854	-0.951706	1.627117
H	3.129142	-1.788896	0.141879
N	2.174443	-1.988543	-0.131917
H	2.139072	-1.954755	-1.143776
H	1.976571	-2.943103	0.143635

NO_3

N	0.000000	0.000000	0.000000
O	0.000000	1.231447	0.000000
O	1.066465	-0.615724	0.000000

O -1.066465 -0.615724 0.000000

NH_3

N 0.000000 0.110832 0.000000

H 0.471489 -0.258677 0.816567

H -0.942978 -0.258470 0.000000

H 0.471489 -0.258677 -0.816567

Geometries optimized at BH&HLYP/6-311+G(2df,2p)

HNO_3

N 0.000000 0.141825 0.000000

O -0.283453 -1.190215 0.000000

O 1.157727 0.426542 0.000000

O -0.946169 0.841592 0.000000

H 0.575160 -1.616130 0.000000

NH_2

N 0.000000 0.000000 0.138762

H 0.000000 0.800792 -0.485667

H 0.000000 -0.800792 -0.485667

NH_3

N 0.000000 0.107292 0.000000

H 0.468663 -0.251341 0.810745

H -0.937326 -0.248362 0.000000

H 0.468663 -0.251341 -0.810745

NO_3 D3h, $^2A'_2$

N 0.000000 0.000000 0.000000

O 0.000000 1.208811 0.000000

O	1.046861	-0.604405	0.000000
O	-1.046861	-0.604405	0.000000

NO_3 C_{2v}, $^2B_2$ (2S1L)

N	0.000000	0.000000	-0.089900
O	0.000000	1.077305	-0.577118
O	0.000000	-1.077305	-0.577118
O	0.000000	0.000000	1.232898

NO_3 C_{2v}, $^2B_2$ (2L1S)

N	0.000000	0.000000	0.076925
O	0.000000	0.000000	1.248815
O	0.000000	0.998613	-0.658062
O	0.000000	-0.998613	-0.658062

CR

O	-0.251312	2.098473	-0.057676
N	-0.002218	0.943891	-0.112380
O	0.972364	0.421508	-0.576315
O	-0.930467	0.133458	0.411426
H	-0.597435	-0.788097	0.297619
N	-0.017937	-2.428080	0.091917
H	-0.345135	-3.361288	0.307014
H	0.882535	-2.523815	-0.361606

TS1

O	0.047357	1.882257	0.000000
N	0.000000	0.695733	0.000000
O	1.031122	-0.010971	0.000000

8	-1.115272	0.087004	0.000000
H	-0.697288	-1.187604	0.000000
N	0.008671	-2.083374	0.000000
H	0.465465	-2.382620	0.842849
H	0.465465	-2.382620	-0.842849

CP1

O	0.136160	1.925020	-0.003723
N	-0.046427	0.747301	0.001231
O	1.060674	0.036369	-0.000438
O	-1.105936	0.183015	0.007301
H	-0.479585	-1.905425	-0.005129
N	0.507437	-2.066842	-0.001166
H	0.864953	-2.468932	0.840369
H	0.872005	-2.471476	-0.838446

TS2

O	0.002872	0.018346	0.002844
N	0.000704	0.006459	1.184939
O	1.184721	0.020816	1.765587
O	-0.900981	-0.006631	1.956050
H	3.393384	-1.953259	-0.169428
N	2.400970	-2.084895	-0.106099
H	1.977387	-1.658931	-0.909703
H	2.217802	-3.070557	-0.142689

CP2

O	0.697398	-0.961750	-0.758016
N	0.712098	0.013680	-0.090796
O	0.790078	-0.213685	1.206295

O	0.689851	1.158290	-0.385334
H	-2.692916	0.588888	0.712218
N	-2.244064	-0.014896	0.048200
H	-2.657248	-0.925298	0.134445
H	-2.457397	0.330595	-0.869751

Geometries optimized at QCISD/6-311+G(2df,2p)

HNO_3

N	0.000000	0.147570	0.000000
O	-0.280955	-1.210716	0.000000
O	1.170713	0.438477	0.000000
O	-0.964604	0.844563	0.000000
H	0.598768	-1.611577	0.000000

NH_2

N	0.000000	0.000000	0.141274
H	0.000000	0.802427	-0.494460
H	0.000000	-0.802427	-0.494460

CR

O	-2.023162	-0.177139	-0.000370
N	-0.855723	0.073169	-0.000047
O	-0.316161	1.157826	-0.000080
O	-0.035663	-1.015730	0.000261
H	0.881869	-0.646362	0.000389
N	2.562131	-0.024572	0.000245
H	2.664189	0.991333	-0.000454
H	3.508975	-0.404808	0.000196

TS1

O	0.058481	1.896274	0.000000

N	0.000000	0.698195	0.000000
O	1.042634	-0.024624	0.000000
O	-1.134416	0.088784	0.000000
H	-0.698549	-1.181417	0.000000
N	0.004007	-2.087705	0.000000
H	0.468452	-2.387745	0.846819
H	0.468452	-2.387745	-0.846819

TS2

O	-2.167811	-0.083779	0.064667
N	-0.964730	0.046424	-0.007575
O	-0.282236	-1.044674	-0.054475
O	-0.348900	1.087735	-0.040831
H	2.306557	0.721468	-0.217254
N	2.853615	-0.094740	0.022166
H	3.653042	-0.110901	-0.596819
H	3.209778	0.053388	0.957047

CP2

O	-0.711301	1.078326	-0.607285
N	-0.736921	-0.000624	-0.057821
O	-0.823213	0.001882	1.218720
O	-0.707245	-1.081154	-0.603499
H	2.596935	-0.876118	0.345855
N	2.195516	0.001240	0.042028
H	2.615915	0.726367	0.608275
H	2.511061	0.153008	-0.907062

NH_3

N	0.000000	0.112590	0.000000

H	0.469269	-0.262703	0.812809
H	-0.938538	-0.262726	0.000000
H	0.469269	-0.262703	-0.812809

NO_3 D_{3h}, $^2A'_2$

N	0.000000	0.000000	0.000000
O	0.000000	1.226095	0.000000
O	1.061830	-0.613048	0.000000
O	-1.061830	-0.613048	0.000000

NO_3- C_{2v}, $^2B_2$ (2S1L)

N	0.000000	0.000000	-0.048723
O	0.000000	1.081110	-0.595636
O	0.000000	-1.081110	-0.595636
O	0.000000	0.000000	1.233906

NO_3- C_{2v}, $^2B_2$ (2L1S)

N	0.000000	0.000000	0.062548
O	0.000000	0.000000	1.255497
O	0.000000	1.023321	-0.655113
O	0.000000	-1.023321	-0.655113

Geometry optimized at M05-2X/6-311+G(2df,2p)

HNO_3

N	-0.001116	0.145516	0.000000
O	-0.288900	-1.198873	0.000000
O	1.163812	0.427649	0.000000
O	-0.951998	0.849573	0.000000

H	0.581467	-1.620251	0.000000

NH_2

N	0.000000	0.000000	0.137214
H	0.000000	0.802663	-0.492430
H	0.000000	-0.802663	-0.492430

NH_3

N	0.000088	0.101760	-0.000033
H	0.470428	-0.259089	0.815056
H	-0.940994	-0.259140	0.000040
H	0.470478	-0.259073	-0.815063

NO_3 D_{3h}, $^2A'_2$

N	0.000000	0.000000	-0.000102
O	0.000000	0.000000	1.216239
O	1.053457	0.000000	-0.608069
O	-1.053457	0.000000	-0.608069

NO_3 C_{2v}, $^2B_2$ (2S1L)

N	0.000000	0.000000	-0.085489
O	0.000000	1.083281	-0.579234
O	0.000000	-1.083281	-0.579234
O	0.000000	0.000000	1.233271

NO_3 C_{2v}, $^2B_2$ (2L1S)

N	0.000000	0.000000	0.073733

O	0.000000	0.000000	1.254654
O	0.000000	1.005586	-0.659585
O	0.000000	-1.005586	-0.659585

CR

O	-2.022799	-0.219616	-0.250325
N	-0.869061	0.031087	-0.110944
O	-0.362860	1.108169	0.087958
O	-0.034660	-1.025576	-0.186863
H	0.884269	-0.657047	-0.048941
N	2.437259	0.062857	0.219228
H	2.384797	1.070597	0.350577
H	3.413866	-0.205466	0.305694

TS1

O	0.062189	1.874469	-0.000007
N	-0.002361	0.682644	-0.000002
O	1.027079	-0.040663	0.000001
O	-1.132511	0.085947	-0.000001
H	-0.721331	-1.173176	0.000003
N	0.009643	-2.078873	0.000006
H	0.481406	-2.366290	0.844251
H	0.481406	-2.366254	-0.844252

TS2

O	-1.885136	-0.264496	0.082018
N	-0.733458	0.049433	0.000867
O	-0.297231	1.179928	-0.057719

O	0.130765	-0.953279	-0.028458
H	1.387109	-0.500737	-0.461737
N	2.260410	0.011471	-0.055004
H	2.017817	0.953750	0.227217
H	2.745975	-0.499001	0.670599

CP1

O	0.174452	1.799219	0.000057
N	-0.100222	0.631770	0.000120
O	0.937020	-0.179468	0.000307
O	-1.220773	0.162451	-0.000381
H	-0.760523	-1.847290	-0.000578
N	0.196225	-2.161788	-0.000111
H	0.553714	-2.547673	0.854077
H	0.554575	-2.547716	-0.853917

TS3

O	0.017964	0.006044	-0.038047
N	0.064370	-0.039952	1.149096
O	1.253356	0.044583	1.704135
O	-0.815803	-0.138291	1.954144
H	3.322154	-1.913543	-0.050688
N	2.322304	-2.036907	-0.084323
H	1.981797	-1.624344	-0.938944
H	2.130717	-3.026240	-0.113873

CP2

O	0.633391	-0.973827	-0.752166
N	0.661866	0.011420	-0.085356
O	0.763671	-0.204316	1.206934
O	0.634200	1.160472	-0.394739
H	-2.664868	0.582254	0.718202
N	-2.194704	-0.013482	0.054238
H	-2.606902	-0.931572	0.118724
H	-2.388854	0.344875	-0.868576

Geometry optimized at M06-2X/6-311+G(2df,2p)

HNO_3

N	-0.000182	0.146465	0.000000
O	-0.289739	-1.199873	0.000000
O	1.166397	0.430804	0.000000
O	-0.954149	0.850145	0.000000
H	0.580938	-1.623927	0.000000

NH_2

N	0.000000	0.000000	0.140603
H	0.000000	0.804238	-0.494124
H	0.000000	-0.804238	-0.494124

CR

O	-1.919428	-0.220745	-0.075050
N	-0.757071	0.035887	-0.039673
O	-0.235159	1.125704	-0.085400
O	0.066308	-1.030696	0.065064

H	0.995023	-0.656278	0.077246
N	2.543300	0.086431	0.086999
H	2.497727	1.106674	0.063603
H	3.529994	-0.173941	0.088685

TS1

O	0.067360	1.875237	-0.000005
N	-0.005411	0.682494	-0.000002
O	1.027049	-0.046784	0.000002
O	-1.138254	0.088576	-0.000005
H	-0.725284	-1.177664	0.000003
N	0.012408	-2.072744	0.000007
H	0.483830	-2.365671	0.846980
H	0.483823	-2.365638	-0.846981

TS2

O	-1.890406	-0.270209	0.078096
N	-0.739480	0.051332	-0.002392
O	-0.301606	1.181796	-0.043897
O	0.126987	-0.958489	-0.052079
H	1.361929	-0.505747	-0.429881
N	2.272054	0.008679	-0.065639
H	2.042750	0.959346	0.216404
H	2.754022	-0.489638	0.677170

CP1

O	0.175299	1.803926	0.000007

N	-0.101303	0.634865	-0.000011
O	0.943195	-0.175458	0.000002
O	-1.220976	0.162335	-0.000036
H	-0.769767	-1.873701	0.000020
N	0.195235	-2.171844	-0.000006
H	0.538783	-2.581407	0.852954
H	0.538769	-2.581453	-0.852924

TS3

O	-0.024131	-0.073401	-0.056252
N	0.084895	-0.079232	1.129380
O	1.287121	0.116378	1.629389
O	-0.748241	-0.219970	1.982446
H	3.308452	-1.990457	0.026667
N	2.301076	-1.986334	-0.065729
H	2.071942	-1.545832	-0.947595
H	1.995746	-2.949804	-0.116804

CP2

O	0.634780	-0.978171	-0.751230
N	0.648604	0.010929	-0.085154
O	0.721548	-0.201550	1.211117
O	0.624676	1.161044	-0.399976
H	-2.627179	0.578840	0.728004
N	-2.170939	-0.013752	0.046236
H	-2.589958	-0.932298	0.117492
H	-2.403732	0.350781	-0.869228

NH_3

N	0.000061	0.110527	-0.000041
H	0.470347	-0.262017	0.814906
H	-0.940855	-0.262055	0.000072
H	0.470448	-0.261998	-0.814938

NO_3 D_{3h}, $^2A'_2$

N	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.218913
O	1.055376	0.000000	-0.609565
O	-1.055376	0.000000	-0.609565

NO_3 C_{2v}, $^2B_2$ (2S1L)

N	0.000000	0.000000	-0.085476
O	0.000000	1.085286	-0.580550
O	0.000000	-1.085286	-0.580550
O	0.000000	0.000000	1.235891

NO_3 C_{2v}, $^2B_2$ (2L1S)

N	0.000000	0.000000	0.077553
O	0.000000	0.000000	1.259401
O	0.000000	1.004543	-0.663630
O	0.000000	-1.004543	-0.663630

Geometry optimized at M05/6-311+G(2df,2p)

HNO_3

N	0.002378	0.153406	0.000000
O	-0.290732	-1.205170	0.000000
O	1.167920	0.433177	0.000000
O	-0.956088	0.849829	0.000000
H	0.579786	-1.627628	0.000000

NH_2

N	0.000000	0.000000	0.140647
H	0.000000	0.801387	-0.492263
H	0.000000	-0.801387	-0.492263

CR

O	2.023360	-0.183736	0.000000
N	0.860679	0.072681	0.000000
O	0.327846	1.153653	0.000000
O	0.039024	-1.013910	0.000000
H	-0.886079	-0.657095	0.000000
N	-2.589388	-0.021417	0.000000
H	-2.675517	0.993679	0.000000
H	-3.539373	-0.387625	0.000000

TS1

O	0.034124	1.910808	0.000017
N	-0.002458	0.713351	0.000007
O	1.046659	0.018199	-0.000018
O	-1.117504	0.087354	0.000021
H	-0.693235	-1.162693	-0.000015
N	0.013096	-2.098213	-0.000022
H	0.462403	-2.425454	0.842354
H	0.462435	-2.425547	-0.842344

TS2

O	-1.957498	-0.314791	-0.021438
N	-0.810887	0.047711	-0.025817

O	-0.410987	1.190987	-0.051468
O	0.079332	-0.926968	-0.000946
H	1.286913	-0.469412	-0.266336
N	2.307219	0.003409	-0.062805
H	2.208685	0.960659	0.255426
H	2.923476	-0.514525	0.551166

CP1

O	0.474949	1.898895	-0.000010
N	-0.002040	0.787490	0.000011
O	0.880274	-0.161068	-0.000001
O	-1.178297	0.504773	0.000007
H	-0.923177	-1.682469	-0.000006
N	-0.179980	-2.360580	-0.000001
H	0.353363	-2.415630	0.848170
H	0.353370	-2.415633	-0.848169

TS3

O	-0.112204	-0.043100	-0.024717
N	0.071423	-0.017879	1.161596
O	1.242047	0.109861	1.614899
O	-0.782516	-0.095738	2.027315
H	3.322089	-1.966350	0.048628
N	2.329665	-2.092659	-0.081385
H	2.045250	-1.554781	-0.886614
H	2.161105	-3.068005	-0.278221

CP2

O	0.715346	-0.859632	-0.874585
N	0.737516	0.010853	-0.036133
O	0.779724	-0.350515	1.163490
O	0.737160	1.199463	-0.254644
H	-2.671567	0.716116	0.587701
N	-2.249616	-0.001780	0.015813
H	-2.632554	-0.884409	0.323758
H	-2.578208	0.145729	-0.928139

NH_3

N	0.000000	0.111741	0.000000
H	0.468970	-0.262415	0.812454
H	-0.937967	-0.262452	0.000000
H	0.468970	-0.262415	-0.812454

NO_3 D_{3h}, $^2A'_2$

N	0.000000	0.000000	-0.000270
O	0.000000	0.000000	1.222292
O	1.058968	0.000000	-0.611011
O	-1.058968	0.000000	-0.611011

NO_3 C_{2v}, $^2B_2$ (2S1L)

N	0.000000	0.000000	-0.040437
O	0.000000	1.076702	-0.590468
O	0.000000	-1.076702	-0.590468
O	0.000000	0.000000	1.216318

NO_3 C_{2v}, $^2B_2$ (2L1S)

N	0.000000	0.000000	-0.055564
O	0.000000	0.000000	1.153494
O	0.000000	1.046654	-0.701545
O	0.000000	-1.046654	-0.701545