Chemical loss processes of isocyanic acid, HNCO, in the atmosphere

— Supporting information —

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Additional modifications to chemical mechanism in EMAC

a. Gas phase

Table 1: Reactions added to MOM supplementing reactions presented in main text

Reaction	Rate coefficient	Reference
$\text{NH}_2\text{CHO} + \text{OH} \rightarrow \text{HNCO} + \text{HO}_2 + \text{H}_2\text{O}$	4.47×10^{-12}	Bunkan et al., 2016
$\text{CH}_3\text{NO}_2 + \text{OH} \rightarrow \text{HCHO} + \text{NO}_2 + \text{H}_2\text{O}$	$5.8 \times 10^{-13} \times \exp(-1102/T)$	Calvert et al., 2008
$\text{CH}_3\text{NO}_2 + h\nu \rightarrow \text{CH}_3 + \text{NO}_2$	-	Taylor et al., 1980
$\text{CH}_3\text{NH}_2 + \text{OH} \rightarrow \text{CH}_2\text{NH} + \text{H}_2\text{O} + \text{HO}_2$	1.97×10^{-11}	Nielsen et al., 2012
$(\text{CH}_3)_2\text{NH} + \text{OH} \rightarrow \text{CH}_2\text{NCH}_3 + \text{HO}_2$	6.71×10^{-11}	Nielsen et al., 2012
$(\text{CH}_3)_2\text{NH} + \text{OH} \rightarrow \text{CH}_3\text{NHCH}_2 + \text{H}_2\text{O}$	6.71×10^{-11}	Nielsen et al., 2012
$\text{CH}_3\text{NHCH}_2 \rightarrow \text{CH}_2\text{NCH}_3 + \text{HO}_2$	1.0×10^6	Nielsen et al., 2012
$\text{CH}_3\text{NHCH}_2 \rightarrow \text{CH}_3\text{NHCH}_2\text{O}_2$	1.0×10^6	Nielsen et al., 2012
$\text{CH}_3\text{NHCH}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{NHCHO} + \text{NO}_2 + \text{HO}_2$	$2.54 \times 10^{12} \times \exp(360/T)$	Nielsen et al., 2012
$\text{CH}_3\text{NHCH}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_2\text{NH} + \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$2.54 \times 10^{12} \times \exp(360/T)$	Nielsen et al., 2012
$(\text{CH}_3)_3\text{N} + \text{OH} \rightarrow (\text{CH}_3)_2\text{NCH}_2\text{O}_2 + \text{H}_2\text{O}$	4.50×10^{-11}	Nielsen et al., 2012
$(\text{CH}_3)_2\text{NCH}_2\text{O}_2 + \text{NO} \rightarrow (\text{CH}_3)_2\text{NCHO} + \text{NO}_2 + \text{HO}_2$	$2.54 \times 10^{12} \times \exp(360/T)$	Nielsen et al., 2012
$(\text{CH}_3)_2\text{NCH}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_2\text{NCH}_3 + \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$2.54 \times 10^{12} \times \exp(360/T)$	Nielsen et al., 2012

b. Aqueous phase

Table 2: Reactions added to aqueous phase mechanism in the submodel SCAV of EMAC

Reaction	Rate coefficient	Reference
$\text{HNCO} + \text{H}^+ \rightarrow \text{NH}_3 + \text{CO}_2 + \text{H}^+$	$4.4 \times 10^7 \times \exp(-6000/T)$	Borduas et al., 2016b
$\text{HNCO} \rightarrow \text{NH}_3 + \text{CO}_2$	$8.9 \times 10^6 \times \exp(-6770/T)$	Borduas et al., 2016b
$\text{NCO}^- \rightarrow \text{NH}_3 + \text{HCO}_3^-$	$7.2 \times 10^8 \times \exp(-10900/T)$	Borduas et al., 2016b
$\text{NH}_2\text{CHO} + \text{OH} \rightarrow \text{HNCO} + \text{H}_2\text{O} + \text{HO}_2$	5.0×10^8	Barnes et al., 2010
$\text{CN}^- + \text{OH} \rightarrow \text{HNCO} + \text{HO}_2$	7.35×10^9	Behar 1974
$\text{HCN} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{product}$	6.00×10^7	Buechler et al., 1976

HNCO + OH potential energy surface

a. M06-2X/aug-cc-pVTZ PES and reaction diagram

Figure 1: OH addition and hydrogen abstraction pathways of the HNCO + OH reaction calculated at the M06-2X/ aug-cc-pVTZ level of theory

Figure 2: Diagram of the HNCO + OH reaction

b. Geometries obtained using M06-2X/aug-cc-pVTZ

Bond lengths in Ångstrom, angles in degrees

HNCO + Cl potential energy surface

a. CCSD(T)/aVTZ//B3LYP/aVTZ extended PES and reaction diagram

Figure 3: Detailed potential energy surface of the HNCO + Cl reaction based on ZPE-corrected CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ energies. The intermediates are depicted below.

Figure 4: Diagram of the $\text{HNCO} + \text{Cl}$ reaction

b. Geometries obtained using B3LYP/aug-cc-pVTZ

Bond lengths in Ångstrom, angles in degrees

IS8

IS9

T0/3

T3P4

T0P1

T1P8

T1/7

T4P7

T3P4

T0/1

T1/2

T1P3

T7/2

T2P9

T0/5

T5/6

T5/8

T6P5

T6/9

T9P6

T8P9

T8P2

PR9

PR1

PR2

PR3

PR4

PR5

PR6

PR7

PR8

c. Geometries obtained using M06-2X/aug-cc-pVTZ

Bond lengths in Ångstrom, angles in degrees

RA	COM	T0P1	PR1

T0/5	IS5	ClC(=O)NHOO	

d. Energetic and entropic data

Table 3: Gibbs free energies (ΔG^0) and entropies (ΔS^0) for the Cl + HNCO reaction products at the CCSD(T)//B3LYP/aug-cc-pVTZ level of theory

Species	(ΔG^0) (298.15 K) (kcal mol ⁻¹)	(ΔS^0) (298.15 K) (cal mol ⁻¹ K ⁻¹)
PR1 (HCl + NCO)	6.9	3.7
PR2 (OH + NCCl)	39.6	3.9
PR3 (HNCl + CO)	21.9	10.0
PR4 (OCl + HNC)	69.2	7.0
PR5 (NH + ClCO)	118.7	9.3
PR6 (HCCl + NO)	94.1	10.2
PR7 (HCN + OCl)	92.6	-0.5
PR8 (OCNCl + H)	56.8	-0.7
PR9 (HOCN + Cl)	24.3	0.7
PR10 (ClOCN + H)	92.6	-0.5
PR11 (HCO + NCl)	118.3	9.8
PR12 (HC(O)N + Cl)	88.7	1.7
PR13 (HC(O)Cl + NCl)	125.62	2.2
PR14 (HCON + Cl)	158.9	0.6
PR15 (ClC(O)N + H)	102.0	-1.1
PR16 (CCl + HNO)	124.7	10.1

Table 4: Comparison of calculated heats of reaction (kcal mol^{-1}) of the products of the $\text{HNCO} + \text{Cl}$ reaction, against available literature data at 298.15 K. Levels of theory used are B3LYP/aug-cc-pVTZ (designated as B3LYP) and CCSD(T)/aug-cc-pVTZ (CCSD(T)). Literature data is from NIST (webbook.nist.gov).

Species	B3LYP	CCSD(T)	Literature
PR1 ($\text{HCl} + \text{NCO}$)	7.6	8.01	8.7
PR2 ($\text{OH} + \text{NCCl}$)	49.6	39.6	
PR3 ($\text{HNCI} + \text{CO}$)	26.3	24.7	
PR4 ($\text{OCl} + \text{HNC}$)	70.0	84.5	
PR5 ($\text{NH} + \text{ClCO}$)	127.3	121.4	123.4
PR6 ($\text{HCCl} + \text{NO}$)	129.2	127.6	
PR7 ($\text{ClO} + \text{HCN}$)	56.6	52.4	
PR8 ($\text{OCNCl} + \text{H}$)	58.2	56.8	
PR9 ($\text{HOCN} + \text{Cl}$)	28.4	24.3	21.4
PR10 ($\text{ClOCN} + \text{H}$)	96.7	92.4	
PR11 ($\text{HCO} + \text{NCl}$)	120.4	118.3	
PR12 ($\text{HC(O)N} + \text{Cl}$)	95.1	84.5	
PR13 ($\text{HC(O)Cl} + \text{NCl}$)	136.9	126.3	
PR14 ($\text{HCON} + \text{Cl}$)	165.5	159.0	
PR15 ($\text{ClC(O)N} + \text{H}$)	109.9	101.9	
PR16 ($\text{CCl} + \text{HNO}$)	129.2	127.6	

Table 5: Theoretical predication of relative energies ΔE (kcal/mol) for reactants, intermediates, transition states and products of the $\text{Cl} + \text{HNCO}$ reaction. Levels of theory used are $\text{B3LYP}/\text{aug-cc-pVTZ}$ (designated as B3LYP) and $\text{CCSD(T)}/\text{aug-cc-pVTZ}//\text{B3LYP}$ (CCSD(T))

Species	B3LYP	CCSD(T)
RA(HNCO+Cl)	0.0	0.0
IS1	26.1	26.1
IS2	41.3	40.7
IS3	58.8	58.1
IS4	55.6	54.2
IS5	3.9	3.6
IS6	70.7	86.2
IS7	26.5	25.9
IS8	12.5	10.7
IS9	87.3	33.9
T0P1	6.7	11.7
T0/1	30.6	35.2
T1P3	39.0	36.8
T1/2	93.3	91.3
T1/7	55.2	56.4
T2P9	43.6	45.1
T1P8	62.1	62.8
T2/7	76.3	76.7
T0/3	58.6	60.7
T3/4	75.3	79.7
T3P4	78.4	79.9
T0/5	5.7	8.5
T5/8	65.6	43.3
T5/6	99.9	99.4
T6P5	104.2	122.9
T6/9	114.8	109.5
T9P6	105.4	106.2
T8P2	47.9	44.5
T8P9	28.3	28.4
PR1 (HCl + NCO)	7.2	7.7
PR2 (OH + NCCl)	45.3	40.2
PR3 (HNCl + CO)	28.7	24.3
PR4 (Ocl + HNC)	71.7	70.9
PR5 (NH + ClCO)	129.3	120.8
PR6 (HCCl + NO)	101.0	96.6
PR7 (ClO + HCl)	96.1	82.0
PR8 (OCNCl + H)	57.6	56.2
PR9 (HOCN + Cl)	28.5	24.5
PR10 (ClOCN+H)	96.1	82.0
PR11 (HCO+NCl)	122.8	120.7
PR12 (HC(O)N+Cl)	90.9	84.5
PR13 (HC(O)Cl+N)	137.6	126.3
PR14 (HCON+Cl)	165.6	159.1
PR15 (ClC(O)N+H)	109.2	101.3
PR16 (CCl+HNO)	131.7	127.3

HNCO + NO₃ potential energy surface

a. M06-2X/aug-cc-pVTZ PES and reaction diagram

Figure 5: NO₃ addition and hydrogen abstraction pathways of the HNCO + NO₃ reaction calculated at the M06-2X/ aug-cc-pVTZ level of theory

Figure 6: Diagram of the HNCO + NO₃ reaction

b. Geometries obtained using M06-2X/aug-cc-pVTZ

Bond lengths in Ångstrom, angles in degrees

HNCO + O₃ potential energy surface

a. CCSD(T)/aVTZ//M06-2X/aVTZ extended PES and reaction diagram

Figure 7: Detailed potential energy surface of the HNCO + O₃ reaction based on ZPE-corrected CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ energies. The intermediates are depicted below.

b. Geometries obtained using M06-2X/aug-cc-pVTZ

Bond lengths in Ångstrom, angles in degrees

T3/4

T4P4

T4/5

T5P9

T5P11

T5/6

T6P3

T3/7

T7/8

T8P6

T8P7

T8P8

T8P13

T3P7

T7/9

T7P8

T7/10

T10P14

T9P10

T9/12

T9P15

T9/11

T11P3

PR1

c. Energetic and entropic data

Table 6: Gibbs free energies (ΔG_0) and entropies (ΔS_0) for the $O_3 + HNCO$ reaction products at the CCSD(T)//M06-2X /aug-cc-pVTZ level of theory

Species	(ΔG^0) (298.15 K)	(ΔS^0) (298.15 K)
	(kcal mol ⁻¹)	(cal mol ⁻¹ K ⁻¹)
PR1 (HN(O)CO + O ₂)	41.7	-3.1
PR2 (HNC(=O)O + O ₂)	34.5	-5.5
PR3 (cy_NC(=O)OO + OH)	22.8	-5.2
PR4 (HONCO + O ₂)	5.6	-2.4
PR5 (HO3 + NCO)	29.5	1.8
PR6 (HN(O)O + CO ₂)	-60.3	-2.3
PR7 (HNOO + CO ₂)	-41.7	-5.4
PR8 (HNO + CO ₃)	-21.7	-1.6
PR9 (NC(=O)O + HO ₂)	15.7	2.9
PR10 (HO ₂ + CO + NO)	-23.3	34.7
PR11 (HNC(=O)O + O ₂)	12.7	-5.8
PR12 (HO ₂ + ONCO)	13.2	4.2
PR13 (HNO + O ₂ + CO)	-21.8	32.8
PR14 (HOC(=O)O + NO)	-74.4	-0.4
PR15 (HO ₂ + CO + NO)	-82.1	26.7

Table 7: Comparison of calculated heats of reaction (kcal mol^{-1}) of the products of the $\text{O}_3 + \text{HNCO}$ reaction, against available literature data at 298.15 K. Levels of theory used are M06-2X/aug-cc-pVTZ (designated as M06-2X) and CCSD(T)/aug-cc-pVTZ (CCSD(T))

Species	M06-2X	CCSD(T)	Reference ^{a,b,c}
PR1 ($\text{HN(O)CO} + \text{O}_2$)	34.4	40.8	
PR2 ($\text{HNC(=O)O} + \text{O}_2$)	37.1	41.0	
PR3 ($\text{cy_NC(=O)OO} + \text{OH}$)	14.0	21.2	
PR4 ($\text{HONCO} + \text{O}_2$)	-2.1	4.9	
PR5 ($\text{HO}_3 + \text{NCO}$)	29.5	30.1	30.4
PR6 ($\text{HN(O)O} + \text{CO}_2$)	-61.0	-56.1	
PR7 ($\text{HNOO} + \text{CO}_2$)	-45.6	-43.3	
PR8 ($\text{HNO} + \text{CO}_3$)	-27.9	-22.2	
PR9 ($\text{NC(=O)O} + \text{HO}_2$)	5.9	16.6	
PR10 ($\text{HO}_2 + \text{CO} + \text{NO}$)	-19.8	-13.0	-11.3
PR11 ($\text{HNC(=O)O} + \text{O}_2$)	6.4	11.0	
PR12 ($\text{HO}_2 + \text{ONCO}$)	1.3	14.5	
PR13 ($\text{HNO} + \text{O}_2 + \text{CO}$)	-18.5	-12.0	-10.4
PR14 ($\text{HOC(=O)O} + \text{NO}$)	-84.5	-74.5	
PR15 ($\text{HO}_2 + \text{CO} + \text{NO}$)	-82.0	-74.1	-72.9

^a Ruscic, B. and Bross, D. H.: Active Thermochemical Tables (ATcT) values based on ver. 1.122g of the Thermochemical Network (2019); available at ATcT.anl.gov, Argonne National Laboratory Active Thermochemical Tables [online] Available from: <http://atct.anl.gov/>, 2019.

^b Ruscic, B., Pinzon, R. E., von Laszewski, G., Kodeboyina, D., Burcat, A., Leahy, D., Montoya, D. and Wagner, A. F.: Active Thermochemical Tables: thermochemistry for the 21st century, in SciDAC 2005: Scientific Discovery Through Advanced Computing, vol. 16, edited by A. Mezzacappa, pp. 561–570, Iop Publishing Ltd, Bristol., 2005.

Table 8: Theoretical predication of relative energies ΔE (kcal/mol) for reactants, intermediates, transition states and products of the $O_3 + HNCO$ reaction. Levels of theory used are M06-2X/aug-cc-pVTZ (designated as M06-2X) and CCSD(T)/aug-cc-pVTZ (CCSD(T))

Species	M06-2X	CCSD(T)
RA(HNCO+O ₃)	0.0	0.0
IS1	13.0	28.3
IS2	20.7	17.8
IS3	-23.8	-8.1
IS4	21.8	35.7
IS5	31.4	32.1
IS6	25.7	36.2
IS7	-18.7	-8.2
IS8	-44.9	-34.9
IS9	-45.3	-30.7
IS10	-36.5	-21.4
IS11	13.6	27.1
IS12	9.5	13.0
T0P5	27.6	35.0
T0/1	37.9	41.8
T1P2	75.4	86.2
T0/2	43.2	45.9
T2P11	25.9	29.9
T0P1	62.4	67.2
T7P1	31.7	44.2
T0/3	29.4	34.8
T3/4	37.1	50.3
T4P4	15.4	44.6
T4/5	39.2	47.7
T5P9	50.1	46.7
T5P11	30.1	37.1
T5/6	40.1	47.5
T6P3	50.3	39.9
T3P7	-1.5	9.0
T3/7	10.6	19.1
T7P8	-4.0	7.25
T7/8	8.7	23.7
T8P6	-44.4	-32.8
T8P7	-20.4	-9.3
T8P8	-7.1	-1.8
T7/9	-10.4	-0.4
T7/10	21.1	35.0
T8P13	37.4	43.8
T9/11	35.3	40.7
T9/12	14.3	26.0
T9P10	1.3	9.6
T9P15	-8.3	-22.1
T11P3	57.1	42.3

T10P14	-0.5	10.1
PR1 (HN(O)CO + O ₂)	34.3	40.6
PR2 (HNC(=O)O + O ₂)	28.3	34.5
PR3 (cy_NC(=O)OO + OH)	14.0	26.3
PR4 (HONCO + O ₂)	-2.4	4.6
PR5 (HO ₃ + NCO)	29.6	32.7
PR6 (HN(O)O + CO ₂)	-60.8	-53.7
PR7 (HNOO + CO ₂)	-45.3	-38.0
PR8 (HNO + CO ₃)	-27.9	-17.1
PR9 (NC(=O)O + HO ₂)	5.9	21.6
PR10 (HO ₂ + CO + NO)	-21.2	-9.4
PR11 (HNC(=O)O + O ₂)	6.7	11.3
PR12 (HO ₂ + ONCO)	1.0	19.2
PR13 (HNO + O ₂ + CO)	-19.9	-8.4
PR14 (HOC(=O)O + NO)	-84.4	-69.5
PR15 (HO ₂ + CO + NO)	-83.3	-70.4

Raw quantum chemical data

HNCO + OH : M06-2X/aug-cc-pVTZ geometry
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Fragments
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H2O

E (CCSD(T)/Aug-CC-pVDZ) (Hartree): -76.27379178
E (CCSD/Aug-CC-pVDZ) (Hartree): -76.26857150
T1 diagnostic: 0.012291
E (MP2/Aug-CC-pVDZ) (Hartree): -76.26080866
E (MP3/Aug-CC-pVDZ) (Hartree): -76.26554049
E (RHF/Aug-CC-pVDZ) (Hartree): -76.04130375
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -76.34229785
E (CCSD/Aug-CC-pVTZ) (Hartree): -76.33365392
T1 diagnostic: 0.010020
E (MP2/Aug-CC-pVTZ) (Hartree): -76.32896290
E (MP3/Aug-CC-pVTZ) (Hartree): -76.33161488
E (RHF/Aug-CC-pVTZ) (Hartree): -76.06047622
E (CCSD(T)/Aug-CC-pVQZ) (Hartree): -76.36356927
E (CCSD/Aug-CC-pVQZ) (Hartree): -76.35418141
T1 diagnostic: 0.009322
E (MP2/Aug-CC-pVQZ) (Hartree): -76.35189638
E (MP3/Aug-CC-pVQZ) (Hartree): -76.35263788
E (RHF/Aug-CC-pVQZ) (Hartree): -76.06585061
E (RM062X/Aug-CC-pVTZ) (Hartree): -76.43010625
Point group : C2V
Electronic state : 1-A1
Cartesian coordinates (Angs):
H 0.000000 0.762173 -0.466394
H -0.000000 -0.762173 -0.466394
O 0.000000 -0.000000 0.116598
Rotational constants (GHz): 830.6570700 431.6138700 284.0302400
Vibrational harmonic frequencies (cm-1):
1621.7919 3864.9482 3966.9566
Zero-point correction (Hartree): 0.021537

HNCO

E (CCSD(T)/Aug-CC-pVDZ) (Hartree): -168.30258465
E (CCSD/Aug-CC-pVDZ) (Hartree): -168.28124890
T1 diagnostic: 0.018038
E (MP2/Aug-CC-pVDZ) (Hartree): -168.27834689
E (MP3/Aug-CC-pVDZ) (Hartree): -168.27384035
E (RHF/Aug-CC-pVDZ) (Hartree): -167.79177923
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -168.44532616
E (CCSD/Aug-CC-pVTZ) (Hartree): -168.41561675
T1 diagnostic: 0.017532
E (MP2/Aug-CC-pVTZ) (Hartree): -168.41955710
E (MP3/Aug-CC-pVTZ) (Hartree): -168.41062749
E (RHF/Aug-CC-pVTZ) (Hartree): -167.83284283
E (CCSD(T)/Aug-CC-pVQZ) (Hartree): -168.48867842
E (CCSD/Aug-CC-pVQZ) (Hartree): -168.45707212
T1 diagnostic: 0.017338
E (MP2/Aug-CC-pVQZ) (Hartree): -168.46658212
E (MP3/Aug-CC-pVQZ) (Hartree): -168.45326510
E (RHF/Aug-CC-pVQZ) (Hartree): -167.84366530
E (RM062X/Aug-CC-pVTZ) (Hartree): -168.68730418
Electronic state : 1-A
Cartesian coordinates (Angs):
N 1.154202 -0.122224 0.000000
C -0.045116 0.016799 0.000000
O -1.204025 0.015866 -0.000000
H 1.823480 0.627848 0.000002
Rotational constants (GHz): 879.6416200 11.1877300 11.0472300
Vibrational harmonic frequencies (cm-1):
565.6997 656.9786 786.0660
1369.4348 2362.7298 3698.6854
Zero-point correction (Hartree): 0.021505

NCO

E (CCSD(T)/Aug-CC-pVDZ) (Hartree): -167.62691510
E (CCSD/Aug-CC-pVDZ) (Hartree): -167.60765916
T1 diagnostic: 0.026290
E (MP2/Aug-CC-pVDZ) (Hartree): -167.58945819
E (MP3/Aug-CC-pVDZ) (Hartree): -167.59640402
E (PMP2/Aug-CC-pVDZ) (Hartree): -167.59849852

E(PMP3/Aug-CC-pVDZ) (Hartree): -167.60212188
 E(PUHF/Aug-CC-pVDZ) (Hartree): -167.16611850
 E(UHF/Aug-CC-pVDZ) (Hartree): -167.15459686
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -167.76182535
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -167.73450406
 T1 diagnostic: 0.025897
 E(MP2/Aug-CC-pVTZ) (Hartree): -167.72247683
 E(MP3/Aug-CC-pVTZ) (Hartree): -167.72587006
 E(PMP2/Aug-CC-pVTZ) (Hartree): -167.73164060
 E(PMP3/Aug-CC-pVTZ) (Hartree): -167.73164486
 E(PUHF/Aug-CC-pVTZ) (Hartree): -167.20496466
 E(UHF/Aug-CC-pVTZ) (Hartree): -167.19327287
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -167.80302538
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -167.77384889
 T1 diagnostic: 0.025899
 E(MP2/Aug-CC-pVQZ) (Hartree): -167.76694762
 E(MP3/Aug-CC-pVQZ) (Hartree): -167.76640616
 E(PMP2/Aug-CC-pVQZ) (Hartree): -167.77617939
 E(PMP3/Aug-CC-pVQZ) (Hartree): -167.77220396
 E(PUHF/Aug-CC-pVQZ) (Hartree): -167.21556437
 E(UHF/Aug-CC-pVQZ) (Hartree): -167.20379254
 E(UM062X/Aug-CC-pVTZ) (Hartree): -168.00175758
 Point group : C*v
 Cartesian coordinates (Angs):
 N 0.000000 0.000000 -1.259810
 C 0.000000 0.000000 -0.037198
 O 0.000000 0.000000 1.130232
 Rotational constants (GHz): 0.0000000 11.8429381 11.8429381
 Vibrational harmonic frequencies (cm-1):
 533.0069 (PI) 614.6584 (PI) 1326.9293 (SG)
 2040.1488 (SG)
 Zero-point correction (Hartree): 0.010285

OH

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E(CCS(D)/Aug-CC-pVDZ) (Hartree): -75.58402897
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -75.58066382
 T1 diagnostic: 0.012130
 E(MP2/Aug-CC-pVDZ) (Hartree): -75.56556301
 E(MP3/Aug-CC-pVDZ) (Hartree): -75.57786050
 E(PMP2/Aug-CC-pVDZ) (Hartree): -75.56732488
 E(PMP3/Aug-CC-pVDZ) (Hartree): -75.57892297
 E(PUHF/Aug-CC-pVDZ) (Hartree): -75.40650834
 E(UHF/Aug-CC-pVDZ) (Hartree): -75.40358239
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -75.64558463
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -75.63969553
 T1 diagnostic: 0.010033
 E(MP2/Aug-CC-pVTZ) (Hartree): -75.62633093
 E(MP3/Aug-CC-pVTZ) (Hartree): -75.63789591
 E(PMP2/Aug-CC-pVTZ) (Hartree): -75.62832174
 E(PMP3/Aug-CC-pVTZ) (Hartree): -75.63903909
 E(PUHF/Aug-CC-pVTZ) (Hartree): -75.42490811
 E(UHF/Aug-CC-pVTZ) (Hartree): -75.42155521
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -75.66449303
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -75.65800936
 T1 diagnostic: 0.009515
 E(MP2/Aug-CC-pVQZ) (Hartree): -75.64661096
 E(MP3/Aug-CC-pVQZ) (Hartree): -75.65671803
 E(PMP2/Aug-CC-pVQZ) (Hartree): -75.64862588
 E(PMP3/Aug-CC-pVQZ) (Hartree): -75.65786011
 E(PUHF/Aug-CC-pVQZ) (Hartree): -75.42993312
 E(UHF/Aug-CC-pVQZ) (Hartree): -75.42654255
 E(UM062X/Aug-CC-pVTZ) (Hartree): -75.73381015
 Point group : C*v
 Cartesian coordinates (Angs):
 O 0.000000 0.000000 0.108007
 H 0.000000 0.000000 -0.864057
 Rotational constants (GHz): 0.0000000 564.1304540 564.1304540
 Vibrational harmonic frequencies (cm-1):
 3767.8625 (SG)
 Zero-point correction (Hartree): 0.008584

Adducts

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HNC_OH_O (HNC(OH)O)

E(CCS(D)/Aug-CC-pVDZ) (Hartree): -243.92382876
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -243.89930153
 T1 diagnostic: 0.024293
 E(MP2/Aug-CC-pVDZ) (Hartree): -243.87662636
 E(MP3/Aug-CC-pVDZ) (Hartree): -243.88756468
 E(PMP2/Aug-CC-pVDZ) (Hartree): -243.88095809
 E(PMP3/Aug-CC-pVDZ) (Hartree): -243.89045477
 E(PUHF/Aug-CC-pVDZ) (Hartree): -243.22614352
 E(UHF/Aug-CC-pVDZ) (Hartree): -243.22051292
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -244.12846223
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -244.09269439

T1 diagnostic: 0.022869
 E(MP2/Aug-CC-pVTZ) (Hartree): -244.07895732
 E(MP3/Aug-CC-pVTZ) (Hartree): -244.08473400
 E(PMP2/Aug-CC-pVTZ) (Hartree): -244.08346168
 E(PMP3/Aug-CC-pVTZ) (Hartree): -244.08772099
 E(PUHF/Aug-CC-pVTZ) (Hartree): -243.28345339
 E(UHF/Aug-CC-pVTZ) (Hartree): -243.27757772
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -244.19131662
 E(CCSD/Aug-CC-pVQZ) (Hartree): -244.15292312
 T1 diagnostic: 0.022449
 E(MP2/Aug-CC-pVQZ) (Hartree): -244.14672930
 E(MP3/Aug-CC-pVQZ) (Hartree): -244.14678585
 E(PMP2/Aug-CC-pVQZ) (Hartree): -244.15127448
 E(PMP3/Aug-CC-pVQZ) (Hartree): -244.14978746
 E(PUHF/Aug-CC-pVQZ) (Hartree): -243.29922308
 E(UHF/Aug-CC-pVQZ) (Hartree): -243.29329855
 E(UM062X/Aug-CC-pVTZ) (Hartree): -244.45951097
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	0.743463	-1.106842	-0.077404
C	0.046336	0.104153	0.008487
O	0.584355	1.174896	-0.020002
H	1.608817	-1.002616	0.455638
O	-1.282325	-0.037661	0.030718
H	-1.507315	-0.972286	-0.050459

 Rotational constants (GHz): 12.1530700 11.2949100 5.8946200
 Vibrational harmonic frequencies (cm-1):

300.4381	467.4051	532.8139
596.1793	710.4215	942.0890
1108.7750	1237.2313	1383.4561
1796.0740	3481.9335	3838.1229

 Zero-point correction (Hartree): 0.037350

HNCOOH

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -243.78233506
 E(CCSD/Aug-CC-pVDZ) (Hartree): -243.75491909
 T1 diagnostic: 0.026100
 E(MP2/Aug-CC-pVDZ) (Hartree): -243.73146131
 E(MP3/Aug-CC-pVDZ) (Hartree): -243.74087503
 E(PMP2/Aug-CC-pVDZ) (Hartree): -243.73530097
 E(PMP3/Aug-CC-pVDZ) (Hartree): -243.74364239
 E(PUHF/Aug-CC-pVDZ) (Hartree): -243.06089368
 E(UHF/Aug-CC-pVDZ) (Hartree): -243.05626195
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -243.98861061
 E(CCSD/Aug-CC-pVTZ) (Hartree): -243.94932749
 T1 diagnostic: 0.025325
 E(MP2/Aug-CC-pVTZ) (Hartree): -243.93572757
 E(MP3/Aug-CC-pVTZ) (Hartree): -243.93923855
 E(PMP2/Aug-CC-pVTZ) (Hartree): -243.93964602
 E(PMP3/Aug-CC-pVTZ) (Hartree): -243.94204334
 E(PUHF/Aug-CC-pVTZ) (Hartree): -243.11981582
 E(UHF/Aug-CC-pVTZ) (Hartree): -243.11508675
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -244.05073026
 E(CCSD/Aug-CC-pVQZ) (Hartree): -244.00869547
 T1 diagnostic: 0.025161
 E(MP2/Aug-CC-pVQZ) (Hartree): -244.00290066
 E(MP3/Aug-CC-pVQZ) (Hartree): -244.00047998
 E(PMP2/Aug-CC-pVQZ) (Hartree): -244.00685193
 E(PMP3/Aug-CC-pVQZ) (Hartree): -244.00329641
 E(PUHF/Aug-CC-pVQZ) (Hartree): -243.13527996
 E(UHF/Aug-CC-pVQZ) (Hartree): -243.13051368
 E(UM062X/Aug-CC-pVTZ) (Hartree): -244.32029053
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	1.813840	-0.146658	0.011359
C	0.608771	-0.337989	0.012316
O	-0.421905	0.511006	-0.001847
H	2.186714	0.801214	-0.040014
O	-1.646548	-0.211644	-0.111112
H	-1.988594	-0.141571	0.790283

 Rotational constants (GHz): 63.3231200 4.7501100 4.4807800
 Vibrational harmonic frequencies (cm-1):

150.3017	198.5905	334.4188
568.7742	641.7866	822.9540
1026.4883	1087.9781	1427.1535
1908.5495	3461.5976	3811.7931

 Zero-point correction (Hartree): 0.035176

HN_OH_CO (HN(OH)CO)

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -243.85940138
 E(CCSD/Aug-CC-pVDZ) (Hartree): -243.83350296
 T1 diagnostic: 0.020302
 E(MP2/Aug-CC-pVDZ) (Hartree): -243.81648757
 E(MP3/Aug-CC-pVDZ) (Hartree): -243.82183243
 E(PMP2/Aug-CC-pVDZ) (Hartree): -243.81865224
 E(PMP3/Aug-CC-pVDZ) (Hartree): -243.82300490

E(PUHF/Aug-CC-pVDZ) (Hartree): -243.14380357
 E(UHF/Aug-CC-pVDZ) (Hartree): -243.14024635
 E(CCSd(T)/Aug-CC-pVTZ) (Hartree): -244.06455049
 E(CCSd/Aug-CC-pVTZ) (Hartree): -244.02691558
 T1 diagnostic: 0.019122
 E(MP2/Aug-CC-pVTZ) (Hartree): -244.01957063
 E(MP3/Aug-CC-pVTZ) (Hartree): -244.01903430
 E(PMP2/Aug-CC-pVTZ) (Hartree): -244.02183232
 E(PMP3/Aug-CC-pVTZ) (Hartree): -244.02023660
 E(PUHF/Aug-CC-pVTZ) (Hartree): -243.20150770
 E(UHF/Aug-CC-pVTZ) (Hartree): -243.19780057
 E(CCSd(T)/Aug-CC-pVQZ) (Hartree): -244.12770089
 E(CCSd/Aug-CC-pVQZ) (Hartree): -244.08736004
 T1 diagnostic: 0.018637
 E(MP2/Aug-CC-pVQZ) (Hartree): -244.08779258
 E(MP3/Aug-CC-pVQZ) (Hartree): -244.08137288
 E(PMP2/Aug-CC-pVQZ) (Hartree): -244.09007903
 E(PMP3/Aug-CC-pVQZ) (Hartree): -244.08257494
 E(PUHF/Aug-CC-pVQZ) (Hartree): -243.21743084
 E(UHF/Aug-CC-pVQZ) (Hartree): -243.21368737
 E(UM062X/Aug-CC-pVTZ) (Hartree): -244.39804484
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	0.424721	0.402442	0.106287
C	-0.680317	-0.356372	0.010537
O	-1.813431	-0.010756	-0.018064
H	0.399400	1.365332	-0.210956
O	1.645538	-0.204754	-0.146319
H	2.052605	-0.320112	0.718790

 Rotational constants (GHz): 67.5754300 4.6229100 4.4025200
 Vibrational harmonic frequencies (cm-1):

223.6267	340.4888	385.1750
511.6656	623.8900	1116.2621
1243.7149	1415.2825	1440.5571
1901.1431	3529.1986	3838.4925

 Zero-point correction (Hartree): 0.037748

Transition states

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TS.HNCO+OH.H2O+NCO

E(CCSd(T)/Aug-CC-pVDZ) (Hartree): -243.87640877
 E(CCSd/Aug-CC-pVDZ) (Hartree): -243.84637161
 T1 diagnostic: 0.041435
 E(MP2/Aug-CC-pVDZ) (Hartree): -243.82696477
 E(MP3/Aug-CC-pVDZ) (Hartree): -243.82907020
 E(PMP2/Aug-CC-pVDZ) (Hartree): -243.83016369
 E(PMP3/Aug-CC-pVDZ) (Hartree): -243.83107480
 E(PUHF/Aug-CC-pVDZ) (Hartree): -243.15841045
 E(UHF/Aug-CC-pVDZ) (Hartree): -243.15345576
 E(CCSd(T)/Aug-CC-pVTZ) (Hartree): -244.08081628
 E(CCSd/Aug-CC-pVTZ) (Hartree): -244.03918090
 T1 diagnostic: 0.039727
 E(MP2/Aug-CC-pVTZ) (Hartree): -244.02932519
 E(MP3/Aug-CC-pVTZ) (Hartree): -244.02604766
 E(PMP2/Aug-CC-pVTZ) (Hartree): -244.03269815
 E(PMP3/Aug-CC-pVTZ) (Hartree): -244.02812029
 E(PUHF/Aug-CC-pVTZ) (Hartree): -243.21704552
 E(UHF/Aug-CC-pVTZ) (Hartree): -243.21179389
 E(CCSd(T)/Aug-CC-pVQZ) (Hartree): -244.14280122
 E(CCSd/Aug-CC-pVQZ) (Hartree): -244.09850032
 T1 diagnostic: 0.039304
 E(MP2/Aug-CC-pVQZ) (Hartree): -244.09648655
 E(MP3/Aug-CC-pVQZ) (Hartree): -244.08722632
 E(PMP2/Aug-CC-pVQZ) (Hartree): -244.09988037
 E(PMP3/Aug-CC-pVQZ) (Hartree): -244.08929603
 E(PUHF/Aug-CC-pVQZ) (Hartree): -243.23263004
 E(UHF/Aug-CC-pVQZ) (Hartree): -243.22734742
 E(UM062X/Aug-CC-pVTZ) (Hartree): -244.41296055
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	-0.094447	0.925704	0.027832
H	-1.165667	0.532358	-0.191323
C	0.846001	0.151877	0.000427
O	1.803466	-0.501425	-0.003313
O	-1.948555	-0.423785	-0.103876
H	-2.088502	-0.521868	0.851450

 Rotational constants (GHz): 24.4700100 3.9486100 3.4420400
 Vibrational harmonic frequencies (cm-1):

i1687.0870	111.8064	199.5012
421.0194	616.6612	643.1380
739.1833	1086.3718	1324.9759
1545.1352	2262.3379	3789.7463

 Zero-point correction (Hartree): 0.029024

TS.HNCO+OH.HNC_OH_O (TS.HNCO+OH.HNC(OH)O)

E(CCS(D(T)/Aug-CC-pVDZ) (Hartree): -243.87677763
E(CCS(D(Aug-CC-pVDZ) (Hartree): -243.84725316
T1 diagnostic: 0.029780
E(MP2/Aug-CC-pVDZ) (Hartree): -243.82584727
E(MP3/Aug-CC-pVDZ) (Hartree): -243.83068568
E(PMP2/Aug-CC-pVDZ) (Hartree): -243.83432126
E(PMP3/Aug-CC-pVDZ) (Hartree): -243.83622672
E(PUHF/Aug-CC-pVDZ) (Hartree): -243.16450794
E(UHF/Aug-CC-pVDZ) (Hartree): -243.15356505
E(CCS(D(T)/Aug-CC-pVTZ) (Hartree): -244.08076434
E(CCS(D(Aug-CC-pVTZ) (Hartree): -244.03965645
T1 diagnostic: 0.028672
E(MP2/Aug-CC-pVTZ) (Hartree): -244.02776550
E(MP3/Aug-CC-pVTZ) (Hartree): -244.02715647
E(PMP2/Aug-CC-pVTZ) (Hartree): -244.03640530
E(PMP3/Aug-CC-pVTZ) (Hartree): -244.03280683
E(PUHF/Aug-CC-pVTZ) (Hartree): -243.22231964
E(UHF/Aug-CC-pVTZ) (Hartree): -243.21115223
E(CCS(D(T)/Aug-CC-pVQZ) (Hartree): -244.14299039
E(CCS(D(Aug-CC-pVQZ) (Hartree): -244.09916704
T1 diagnostic: 0.028459
E(MP2/Aug-CC-pVQZ) (Hartree): -244.09500706
E(MP3/Aug-CC-pVQZ) (Hartree): -244.08848149
E(PMP2/Aug-CC-pVQZ) (Hartree): -244.10369237
E(PMP3/Aug-CC-pVQZ) (Hartree): -244.09414998
E(PUHF/Aug-CC-pVQZ) (Hartree): -243.23796533
E(UHF/Aug-CC-pVQZ) (Hartree): -243.22674277
E(UM062X/Aug-CC-pVTZ) (Hartree): -244.40918730
Electronic state : 2-A
Cartesian coordinates (Angs):
N -0.247355 1.225121 0.108835
C 0.432564 0.170639 -0.020970
O 1.369730 -0.504604 -0.002494
H -0.895532 1.447530 -0.637603
O -1.176170 -0.781380 -0.098383
H -1.516845 -0.759339 0.808596
Rotational constants (GHz): 12.8674800 8.4791500 5.2517000
Vibrational harmonic frequencies (cm-1):
i592.4667 258.4603 368.8116
480.6795 541.8280 609.1365
837.0991 936.0857 1233.2469
2194.2622 3598.6215 3804.3947
Zero-point correction (Hartree): 0.033860

TS.HNCO+OH.HNCOOH

E(CCS(D(T)/Aug-CC-pVDZ) (Hartree): -243.77589344
E(CCS(D(Aug-CC-pVDZ) (Hartree): -243.74600542
T1 diagnostic: 0.044717
E(MP2/Aug-CC-pVDZ) (Hartree): -243.70055619
E(MP3/Aug-CC-pVDZ) (Hartree): -243.71559663
E(PMP2/Aug-CC-pVDZ) (Hartree): -243.72239276
E(PMP3/Aug-CC-pVDZ) (Hartree): -243.73245491
E(PUHF/Aug-CC-pVDZ) (Hartree): -243.06984628
E(UHF/Aug-CC-pVDZ) (Hartree): -243.04523126
E(CCS(D(T)/Aug-CC-pVTZ) (Hartree): -243.98133797
E(CCS(D(Aug-CC-pVTZ) (Hartree): -243.93945759
T1 diagnostic: 0.043971
E(MP2/Aug-CC-pVTZ) (Hartree): -243.90342200
E(MP3/Aug-CC-pVTZ) (Hartree): -243.91345485
E(PMP2/Aug-CC-pVTZ) (Hartree): -243.92578064
E(PMP3/Aug-CC-pVTZ) (Hartree): -243.93073760
E(PUHF/Aug-CC-pVTZ) (Hartree): -243.12918491
E(UHF/Aug-CC-pVTZ) (Hartree): -243.10400968
E(CCS(D(T)/Aug-CC-pVQZ) (Hartree): -244.04311992
E(CCS(D(Aug-CC-pVQZ) (Hartree): -243.99841112
T1 diagnostic: 0.043940
E(MP2/Aug-CC-pVQZ) (Hartree): -243.96997477
E(MP3/Aug-CC-pVQZ) (Hartree): -243.97422933
E(PMP2/Aug-CC-pVQZ) (Hartree): -243.99244577
E(PMP3/Aug-CC-pVQZ) (Hartree): -243.99158068
E(PUHF/Aug-CC-pVQZ) (Hartree): -243.14467688
E(UHF/Aug-CC-pVQZ) (Hartree): -243.11938158
E(UM062X/Aug-CC-pVTZ) (Hartree): -244.31155642
Electronic state : 2-A
Cartesian coordinates (Angs):
N -1.827379 -0.239308 0.027687
C -0.607169 -0.174829 0.001920
O 0.403230 0.572612 -0.045794
H -2.385121 0.616043 0.017677
O 1.677342 -0.327151 -0.060064
H 2.175214 0.144395 0.623854
Rotational constants (GHz): 56.2899800 4.6032400 4.2892900
Vibrational harmonic frequencies (cm-1):
i1173.0904 135.4402 272.2672
327.4267 606.7060 685.8963
908.7694 994.1114 1260.8447
1987.5535 3421.4460 3801.0214

Zero-point correction (Hartree): 0.032809

TS.HNCO+OH.HN_OH_CO (TS.HNCO+OH.HN(OH)CO)

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -243.83209726
E(CCSD/Aug-CC-pVDZ) (Hartree): -243.80301942
T1 diagnostic: 0.028702
E(MP2/Aug-CC-pVDZ) (Hartree): -243.78291892
E(MP3/Aug-CC-pVDZ) (Hartree): -243.78606807
E(PMP2/Aug-CC-pVDZ) (Hartree): -243.79152814
E(PMP3/Aug-CC-pVDZ) (Hartree): -243.79156463
E(PUHF/Aug-CC-pVDZ) (Hartree): -243.10557871
E(UHF/Aug-CC-pVDZ) (Hartree): -243.09470552
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -244.03837288
E(CCSD/Aug-CC-pVTZ) (Hartree): -243.99718277
T1 diagnostic: 0.027961
E(MP2/Aug-CC-pVTZ) (Hartree): -243.98704695
E(MP3/Aug-CC-pVTZ) (Hartree): -243.98420639
E(PMP2/Aug-CC-pVTZ) (Hartree): -243.99593536
E(PMP3/Aug-CC-pVTZ) (Hartree): -243.98987896
E(PUHF/Aug-CC-pVTZ) (Hartree): -243.16430656
E(UHF/Aug-CC-pVTZ) (Hartree): -243.15309912
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -244.10111173
E(CCSD/Aug-CC-pVQZ) (Hartree): -244.05713802
T1 diagnostic: 0.027825
E(MP2/Aug-CC-pVQZ) (Hartree): -244.05482845
E(MP3/Aug-CC-pVQZ) (Hartree): -244.04600301
E(PMP2/Aug-CC-pVQZ) (Hartree): -244.06377796
E(PMP3/Aug-CC-pVQZ) (Hartree): -244.05169759
E(PUHF/Aug-CC-pVQZ) (Hartree): -243.17992715
E(UHF/Aug-CC-pVQZ) (Hartree): -243.16864636
E(UM062X/Aug-CC-pVTZ) (Hartree): -244.37283905
Electronic state : 2-A
Cartesian coordinates (Angs):
N 0.413433 0.524216 0.077387
C -0.694245 -0.025343 -0.003000
O -1.862626 -0.206939 -0.015009
H 0.720615 1.468582 -0.107214
O 1.699234 -0.333478 -0.132226
H 1.857954 -0.662708 0.761388
Rotational constants (GHz): 51.2302800 4.4080000 4.1174500
Vibrational harmonic frequencies (cm-1):
i882.6904 194.5410 310.3632
352.8994 522.7920 669.5841
1125.8480 1183.7050 1250.7705
2177.7008 3552.7436 3826.8909
Zero-point correction (Hartree): 0.034555

HNCO + Cl : M06-2X/aug-cc-pVTZ geometry
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Fragments

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Cl

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E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -459.61222148
E(CCSD/Aug-CC-pVDZ) (Hartree): -459.60993098
T1 diagnostic: 0.006428
E(MP2/Aug-CC-pVDZ) (Hartree): -459.59214974
E(MP3/Aug-CC-pVDZ) (Hartree): -459.60854055
E(PMP2/Aug-CC-pVDZ) (Hartree): -459.59352697
E(PMP3/Aug-CC-pVDZ) (Hartree): -459.60915212
E(PUHF/Aug-CC-pVDZ) (Hartree): -459.47549404
E(UHF/Aug-CC-pVDZ) (Hartree): -459.47278114
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -459.67621572
E(CCSD/Aug-CC-pVTZ) (Hartree): -459.67005135
T1 diagnostic: 0.006592
E(MP2/Aug-CC-pVTZ) (Hartree): -459.64733174
E(MP3/Aug-CC-pVTZ) (Hartree): -459.66892113
E(PMP2/Aug-CC-pVTZ) (Hartree): -459.64932188
E(PMP3/Aug-CC-pVTZ) (Hartree): -459.66984266
E(PUHF/Aug-CC-pVTZ) (Hartree): -459.48966776
E(UHF/Aug-CC-pVTZ) (Hartree): -459.48596887
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -459.69474301
E(CCSD/Aug-CC-pVQZ) (Hartree): -459.68742578
T1 diagnostic: 0.007068
E(MP2/Aug-CC-pVQZ) (Hartree): -459.66563967
E(MP3/Aug-CC-pVQZ) (Hartree): -459.68684405
E(PMP2/Aug-CC-pVQZ) (Hartree): -459.66768698
E(PMP3/Aug-CC-pVQZ) (Hartree): -459.68779580
E(PUHF/Aug-CC-pVQZ) (Hartree): -459.49294399
E(UHF/Aug-CC-pVQZ) (Hartree): -459.48917948
E(UM062X/Aug-CC-pVTZ) (Hartree): -460.14120758
Point group : OH
Cartesian coordinates (Angs):

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Cl      0.000000      0.000000      0.000000
Zero-point correction (Hartree): 0.000000

HCl
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E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -460.27219722
E(CCSD/Aug-CC-pVDZ) (Hartree): -460.26823945
T1 diagnostic: 0.006710
E(MP2/Aug-CC-pVDZ) (Hartree): -460.25177347
E(MP3/Aug-CC-pVDZ) (Hartree): -460.26801920
E(RHF/Aug-CC-pVDZ) (Hartree): -460.09261749
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -460.34324107
E(CCSD/Aug-CC-pVTZ) (Hartree): -460.33472154
T1 diagnostic: 0.006078
E(MP2/Aug-CC-pVTZ) (Hartree): -460.31511908
E(MP3/Aug-CC-pVTZ) (Hartree): -460.33545761
E(RHF/Aug-CC-pVTZ) (Hartree): -460.10754718
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -460.36416565
E(CCSD/Aug-CC-pVQZ) (Hartree): -460.35437945
T1 diagnostic: 0.006303
E(MP2/Aug-CC-pVQZ) (Hartree): -460.33607995
E(MP3/Aug-CC-pVQZ) (Hartree): -460.35570430
E(RHF/Aug-CC-pVQZ) (Hartree): -460.11133250
E(RM062X/Aug-CC-pVTZ) (Hartree): -460.80750704
Point group : Cv
Electronic state : 1-SG
Cartesian coordinates (Angs):
H      0.000000      0.000000      -1.207931
Cl      0.000000      0.000000      0.071055
Rotational constants (GHz): 0.0000000 315.3843834 315.3843834
Vibrational harmonic frequencies (cm-1):
2988.5153 ( SG)
Zero-point correction (Hartree): 0.006808

HNCO
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E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -168.30258139
E(CCSD/Aug-CC-pVDZ) (Hartree): -168.28124581
T1 diagnostic: 0.018038
E(MP2/Aug-CC-pVDZ) (Hartree): -168.27834469
E(MP3/Aug-CC-pVDZ) (Hartree): -168.27383710
E(RHF/Aug-CC-pVDZ) (Hartree): -167.79177692
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -168.44532500
E(CCSD/Aug-CC-pVTZ) (Hartree): -168.41561572
T1 diagnostic: 0.017532
E(MP2/Aug-CC-pVTZ) (Hartree): -168.41955688
E(MP3/Aug-CC-pVTZ) (Hartree): -168.41062627
E(RHF/Aug-CC-pVTZ) (Hartree): -167.83284184
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -168.48867748
E(CCSD/Aug-CC-pVQZ) (Hartree): -168.45707130
T1 diagnostic: 0.017338
E(MP2/Aug-CC-pVQZ) (Hartree): -168.46658210
E(MP3/Aug-CC-pVQZ) (Hartree): -168.45326411
E(RHF/Aug-CC-pVQZ) (Hartree): -167.84366420
E(RM062X/Aug-CC-pVTZ) (Hartree): -168.68730197
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
H      1.224195      -1.490249      -0.000000
N      0.287949      -1.124328      -0.000000
C      -0.000000      0.048088      0.000000
O      -0.404979      1.134003      0.000000
Rotational constants (GHz): 880.1178000 11.1877600 11.0473300
Vibrational harmonic frequencies (cm-1):
560.3477 ( A') 656.2172 ( A'') 783.0612 ( A')
1369.4169 ( A') 2362.5435 ( A') 3698.8989 ( A')
Zero-point correction (Hartree): 0.021484

NCO
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E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -167.62690657
E(CCSD/Aug-CC-pVDZ) (Hartree): -167.60765264
T1 diagnostic: 0.026292
E(MP2/Aug-CC-pVDZ) (Hartree): -167.58944503
E(MP3/Aug-CC-pVDZ) (Hartree): -167.59639592
E(PMP2/Aug-CC-pVDZ) (Hartree): -167.59848982
E(PMP3/Aug-CC-pVDZ) (Hartree): -167.60211632
E(PUHF/Aug-CC-pVDZ) (Hartree): -167.16612650
E(UHF/Aug-CC-pVDZ) (Hartree): -167.15459901
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -167.76182169
E(CCSD/Aug-CC-pVTZ) (Hartree): -167.73450254
T1 diagnostic: 0.025900
E(MP2/Aug-CC-pVTZ) (Hartree): -167.72246818
E(MP3/Aug-CC-pVTZ) (Hartree): -167.72586701
E(PMP2/Aug-CC-pVTZ) (Hartree): -167.73163653
E(PMP3/Aug-CC-pVTZ) (Hartree): -167.73164444
E(PUHF/Aug-CC-pVTZ) (Hartree): -167.20497544
E(UHF/Aug-CC-pVTZ) (Hartree): -167.19327769

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E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -167.80302270
 E(CCSD/Aug-CC-pVQZ) (Hartree): -167.77384835
 T1 diagnostic: 0.025902
 E(MP2/Aug-CC-pVQZ) (Hartree): -167.76693975
 E(MP3/Aug-CC-pVQZ) (Hartree): -167.76640405
 E(PMP2/Aug-CC-pVQZ) (Hartree): -167.77617611
 E(PMP3/Aug-CC-pVQZ) (Hartree): -167.77220449
 E(PUHF/Aug-CC-pVQZ) (Hartree): -167.21557545
 E(UHF/Aug-CC-pVQZ) (Hartree): -167.20379764
 E(UM062X/Aug-CC-pVTZ) (Hartree): -168.00175757
 Point group : C*v
 Cartesian coordinates (Angs):
 N 0.000000 0.000000 -1.259735
 C 0.000000 0.000000 -0.037247
 O 0.000000 0.000000 1.130203
 Rotational constants (GHz): 0.0000000 11.8439475 11.8439475
 Vibrational harmonic frequencies (cm-1):
 532.8259 (PI) 614.5324 (PI) 1327.2296 (SG)
 2040.2979 (SG)
 Zero-point correction (Hartree): 0.010286

Adducts

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HNCC1O

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -627.91079551
 E(CCSD/Aug-CC-pVDZ) (Hartree): -627.88596678
 T1 diagnostic: 0.020530
 E(MP2/Aug-CC-pVDZ) (Hartree): -627.86017243
 E(MP3/Aug-CC-pVDZ) (Hartree): -627.87734760
 E(PMP2/Aug-CC-pVDZ) (Hartree): -627.86242980
 E(PMP3/Aug-CC-pVDZ) (Hartree): -627.87875690
 E(PUHF/Aug-CC-pVDZ) (Hartree): -627.25504247
 E(UHF/Aug-CC-pVDZ) (Hartree): -627.25151538
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -628.11725074
 E(CCSD/Aug-CC-pVTZ) (Hartree): -628.07962712
 T1 diagnostic: 0.019532
 E(MP2/Aug-CC-pVTZ) (Hartree): -628.05736701
 E(MP3/Aug-CC-pVTZ) (Hartree): -628.07491336
 E(PMP2/Aug-CC-pVTZ) (Hartree): -628.05979335
 E(PMP3/Aug-CC-pVTZ) (Hartree): -628.07639035
 E(PUHF/Aug-CC-pVTZ) (Hartree): -627.30784514
 E(UHF/Aug-CC-pVTZ) (Hartree): -627.30403301
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -628.18028414
 E(CCSD/Aug-CC-pVQZ) (Hartree): -628.13940542
 T1 diagnostic: 0.019233
 E(MP2/Aug-CC-pVQZ) (Hartree): -628.12386077
 E(MP3/Aug-CC-pVQZ) (Hartree): -628.13673622
 E(PMP2/Aug-CC-pVQZ) (Hartree): -628.12630958
 E(PMP3/Aug-CC-pVQZ) (Hartree): -628.13821508
 E(PUHF/Aug-CC-pVQZ) (Hartree): -627.32219808
 E(UHF/Aug-CC-pVQZ) (Hartree): -627.31835427
 E(UM062X/Aug-CC-pVTZ) (Hartree): -628.82407848
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 O 1.148609 -1.122831 0.023782
 N 1.057393 1.176217 -0.127494
 C 0.558457 -0.103751 -0.001324
 Cl -1.227290 -0.018981 -0.002037
 H 0.922561 1.694309 0.744767
 Rotational constants (GHz): 11.6787100 5.3326900 3.7009200
 Vibrational harmonic frequencies (cm-1):
 276.3917 346.4679 457.8337
 604.5605 658.2736 1037.3322
 1115.1290 1903.9291 3462.7109
 Zero-point correction (Hartree): 0.022469

HNC1CO

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -627.87076054
 E(CCSD/Aug-CC-pVDZ) (Hartree): -627.84567500
 T1 diagnostic: 0.019731
 E(MP2/Aug-CC-pVDZ) (Hartree): -627.82355213
 E(MP3/Aug-CC-pVDZ) (Hartree): -627.83579822
 E(PMP2/Aug-CC-pVDZ) (Hartree): -627.82575898
 E(PMP3/Aug-CC-pVDZ) (Hartree): -627.83699785
 E(PUHF/Aug-CC-pVDZ) (Hartree): -627.20484593
 E(UHF/Aug-CC-pVDZ) (Hartree): -627.20124831
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -628.08156646
 E(CCSD/Aug-CC-pVTZ) (Hartree): -628.04345225
 T1 diagnostic: 0.018870
 E(MP2/Aug-CC-pVTZ) (Hartree): -628.02512472
 E(MP3/Aug-CC-pVTZ) (Hartree): -628.03734726
 E(PMP2/Aug-CC-pVTZ) (Hartree): -628.02742052
 E(PMP3/Aug-CC-pVTZ) (Hartree): -628.03857493
 E(PUHF/Aug-CC-pVTZ) (Hartree): -627.26123357
 E(UHF/Aug-CC-pVTZ) (Hartree): -627.25749827

E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -628.14526549
 E(CCSD/Aug-CC-pVQZ) (Hartree): -628.10387436
 T1 diagnostic: 0.018467
 E(MP2/Aug-CC-pVQZ) (Hartree): -628.09241495
 E(MP3/Aug-CC-pVQZ) (Hartree): -628.09983458
 E(PMP2/Aug-CC-pVQZ) (Hartree): -628.09473433
 E(PMP3/Aug-CC-pVQZ) (Hartree): -628.10106225
 E(PUHF/Aug-CC-pVQZ) (Hartree): -627.27622735
 E(UHF/Aug-CC-pVQZ) (Hartree): -627.27245768
 E(UM062X/Aug-CC-pVTZ) (Hartree): -628.79192110
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	0.070682	0.471152	-0.025534
C	1.126466	-0.350678	-0.011114
H	0.159634	1.476968	0.053741
O	2.278003	-0.070216	0.012158
Cl	-1.508072	-0.124073	0.005554

 Rotational constants (GHz): 68.4372500 2.8418200 2.7290000
 Vibrational harmonic frequencies (cm-1):

79.6325	286.5276	437.3775
507.8972	906.1193	1229.6722
1341.8952	1884.4775	3545.6281

 Zero-point correction (Hartree): 0.023281

HNCOCl

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -627.81925657
 E(CCSD/Aug-CC-pVDZ) (Hartree): -627.79293620
 T1 diagnostic: 0.024842
 E(MP2/Aug-CC-pVDZ) (Hartree): -627.76533217
 E(MP3/Aug-CC-pVDZ) (Hartree): -627.78110515
 E(PMP2/Aug-CC-pVDZ) (Hartree): -627.76896903
 E(PMP3/Aug-CC-pVDZ) (Hartree): -627.78369047
 E(PUHF/Aug-CC-pVDZ) (Hartree): -627.14697118
 E(UHF/Aug-CC-pVDZ) (Hartree): -627.14251767
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -628.02945748
 E(CCSD/Aug-CC-pVTZ) (Hartree): -627.99004904
 T1 diagnostic: 0.024486
 E(MP2/Aug-CC-pVTZ) (Hartree): -627.96644218
 E(MP3/Aug-CC-pVTZ) (Hartree): -627.98193546
 E(PMP2/Aug-CC-pVTZ) (Hartree): -627.97022208
 E(PMP3/Aug-CC-pVTZ) (Hartree): -627.98460763
 E(PUHF/Aug-CC-pVTZ) (Hartree): -627.20310242
 E(UHF/Aug-CC-pVTZ) (Hartree): -627.19847540
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -628.09234067
 E(CCSD/Aug-CC-pVQZ) (Hartree): -628.04960159
 T1 diagnostic: 0.024391
 E(MP2/Aug-CC-pVQZ) (Hartree): -628.03288502
 E(MP3/Aug-CC-pVQZ) (Hartree): -628.04349862
 E(PMP2/Aug-CC-pVQZ) (Hartree): -628.03670425
 E(PMP3/Aug-CC-pVQZ) (Hartree): -628.04618843
 E(PUHF/Aug-CC-pVQZ) (Hartree): -627.21781166
 E(UHF/Aug-CC-pVQZ) (Hartree): -627.21314037
 E(UM062X/Aug-CC-pVTZ) (Hartree): -628.73800888
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	2.230960	0.016153	0.000075
H	2.912786	-0.732335	0.000017
C	1.042338	-0.293556	0.000008
O	0.039600	0.596248	0.000083
Cl	-1.476490	-0.140552	-0.000074

 Rotational constants (GHz): 63.8396400 3.0201100 2.8836800
 Vibrational harmonic frequencies (cm-1):

115.1707	283.2697	509.9345
651.8376	792.2196	957.8781
1161.5138	1822.4680	3592.7023

 Zero-point correction (Hartree): 0.022524

Transition states

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TS.HNCO+Cl.HCl+NCO

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -627.89122699
 E(CCSD/Aug-CC-pVDZ) (Hartree): -627.86447772
 T1 diagnostic: 0.027862
 E(MP2/Aug-CC-pVDZ) (Hartree): -627.83565345
 E(MP3/Aug-CC-pVDZ) (Hartree): -627.85215352
 E(PMP2/Aug-CC-pVDZ) (Hartree): -627.84439346
 E(PMP3/Aug-CC-pVDZ) (Hartree): -627.85766445
 E(PUHF/Aug-CC-pVDZ) (Hartree): -627.23064752
 E(UHF/Aug-CC-pVDZ) (Hartree): -627.21937647
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -628.09755192
 E(CCSD/Aug-CC-pVTZ) (Hartree): -628.05756114
 T1 diagnostic: 0.027168
 E(MP2/Aug-CC-pVTZ) (Hartree): -628.03250374
 E(MP3/Aug-CC-pVTZ) (Hartree): -628.04917496
 E(PMP2/Aug-CC-pVTZ) (Hartree): -628.04136194

E(PMP3/Aug-CC-pVTZ) (Hartree): -628.05474096
 E(PUHF/Aug-CC-pVTZ) (Hartree): -627.28338540
 E(UHF/Aug-CC-pVTZ) (Hartree): -627.27194483
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -628.15968091
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -628.11644606
 T1 diagnostic: 0.026792
 E(MP2/Aug-CC-pVQZ) (Hartree): -628.09812154
 E(MP3/Aug-CC-pVQZ) (Hartree): -628.11005328
 E(PMP2/Aug-CC-pVQZ) (Hartree): -628.10704285
 E(PMP3/Aug-CC-pVQZ) (Hartree): -628.11563944
 E(PUHF/Aug-CC-pVQZ) (Hartree): -627.29741195
 E(UHF/Aug-CC-pVQZ) (Hartree): -627.28589721
 E(UM062X/Aug-CC-pVTZ) (Hartree): -628.80562943
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 N -0.598765 1.068778 0.000040
 C -1.411294 0.150445 -0.000019
 O -2.233770 -0.665122 -0.000072
 H 0.728758 0.744631 0.000059
 Cl 1.752972 -0.223987 0.000021
 Rotational constants (GHz): 19.7103300 2.3320000 2.0852800
 Vibrational harmonic frequencies (cm-1):
 i1200.1648 89.9257 385.7978
 422.5687 619.3701 645.0230
 1234.8766 1348.7962 2137.3940
 Zero-point correction (Hartree): 0.015682

TS.HNCO+Cl.HNCClO

E(CCS(D)/Aug-CC-pVDZ) (Hartree): -627.90145327
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -627.87371363
 T1 diagnostic: 0.027968
 E(MP2/Aug-CC-pVDZ) (Hartree): -627.84856911
 E(MP3/Aug-CC-pVDZ) (Hartree): -627.86209735
 E(PMP2/Aug-CC-pVDZ) (Hartree): -627.85508783
 E(PMP3/Aug-CC-pVDZ) (Hartree): -627.86640122
 E(PUHF/Aug-CC-pVDZ) (Hartree): -627.23844719
 E(UHF/Aug-CC-pVDZ) (Hartree): -627.22990453
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -628.10871220
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -628.06770704
 T1 diagnostic: 0.027260
 E(MP2/Aug-CC-pVTZ) (Hartree): -628.04611547
 E(MP3/Aug-CC-pVTZ) (Hartree): -628.05995852
 E(PMP2/Aug-CC-pVTZ) (Hartree): -628.05316565
 E(PMP3/Aug-CC-pVTZ) (Hartree): -628.06463020
 E(PUHF/Aug-CC-pVTZ) (Hartree): -627.29178549
 E(UHF/Aug-CC-pVTZ) (Hartree): -627.28259331
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -628.17141825
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -628.12709127
 T1 diagnostic: 0.026797
 E(MP2/Aug-CC-pVQZ) (Hartree): -628.11227108
 E(MP3/Aug-CC-pVQZ) (Hartree): -628.12146359
 E(PMP2/Aug-CC-pVQZ) (Hartree): -628.11940350
 E(PMP3/Aug-CC-pVQZ) (Hartree): -628.12617315
 E(PUHF/Aug-CC-pVQZ) (Hartree): -627.30580219
 E(UHF/Aug-CC-pVQZ) (Hartree): -627.29651268
 E(UM062X/Aug-CC-pVTZ) (Hartree): -628.81589008
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 N 0.734479 1.287760 -0.121418
 C 0.795582 0.000933 0.021703
 O 1.413462 -0.975980 0.016133
 H 0.341536 1.784654 0.675425
 Cl -1.268475 -0.176278 -0.004987
 Rotational constants (GHz): 11.6517300 4.8549300 3.4568000
 Vibrational harmonic frequencies (cm-1):
 i506.0835 351.7867 416.7688
 457.4830 604.2081 951.3182
 1137.7169 2119.0894 3540.9621
 Zero-point correction (Hartree): 0.021823

TS.HNCO+Cl.HNClCO

E(CCS(D)/Aug-CC-pVDZ) (Hartree): -627.85424253
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -627.82737184
 T1 diagnostic: 0.028762
 E(MP2/Aug-CC-pVDZ) (Hartree): -627.80306103
 E(MP3/Aug-CC-pVDZ) (Hartree): -627.81570831
 E(PMP2/Aug-CC-pVDZ) (Hartree): -627.80667665
 E(PMP3/Aug-CC-pVDZ) (Hartree): -627.81790532
 E(PUHF/Aug-CC-pVDZ) (Hartree): -627.18017620
 E(UHF/Aug-CC-pVDZ) (Hartree): -627.17510707
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -628.06431547
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -628.02414402
 T1 diagnostic: 0.028110
 E(MP2/Aug-CC-pVTZ) (Hartree): -628.00384687
 E(MP3/Aug-CC-pVTZ) (Hartree): -628.01641242
 E(PMP2/Aug-CC-pVTZ) (Hartree): -628.00754998

E(PMP3/Aug-CC-pVTZ) (Hartree): -628.01864920
 E(PUHF/Aug-CC-pVTZ) (Hartree): -627.23559239
 E(UHF/Aug-CC-pVTZ) (Hartree): -627.23039303
 E(CCS(D)/T)/Aug-CC-pVQZ) (Hartree): -628.12739577
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -628.08386200
 T1 diagnostic: 0.028439
 E(MP2/Aug-CC-pVQZ) (Hartree): -628.07041661
 E(MP3/Aug-CC-pVQZ) (Hartree): -628.07809640
 E(PMP2/Aug-CC-pVQZ) (Hartree): -628.07413253
 E(PMP3/Aug-CC-pVQZ) (Hartree): -628.08032758
 E(PUHF/Aug-CC-pVQZ) (Hartree): -627.25001152
 E(UHF/Aug-CC-pVQZ) (Hartree): -627.24478905
 E(UM062X/Aug-CC-pVTZ) (Hartree): -628.77757623
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 N 0.119302 0.584078 -0.003340
 H -0.005870 1.586415 0.010454
 C 1.150096 -0.130437 -0.000612
 O 2.330955 -0.230820 0.001057
 Cl -1.551615 -0.179164 0.000479
 Rotational constants (GHz): 53.4607900 2.7005800 2.5707300
 Vibrational harmonic frequencies (cm-1):
 i1019.5189 114.5305 269.4452
 463.6429 725.6795 997.8335
 1214.9774 2066.3541 3548.4561
 Zero-point correction (Hartree): 0.021417

TS.HNCO+Cl.HNCOCl

E(CCS(D)/T)/Aug-CC-pVDZ) (Hartree): -627.81525783
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -627.78722485
 T1 diagnostic: 0.036320
 E(MP2/Aug-CC-pVDZ) (Hartree): -627.75025656
 E(MP3/Aug-CC-pVDZ) (Hartree): -627.76884155
 E(PMP2/Aug-CC-pVDZ) (Hartree): -627.76169245
 E(PMP3/Aug-CC-pVDZ) (Hartree): -627.77728087
 E(PUHF/Aug-CC-pVDZ) (Hartree): -627.14636933
 E(UHF/Aug-CC-pVDZ) (Hartree): -627.13318093
 E(CCS(D)/T)/Aug-CC-pVTZ) (Hartree): -628.02313037
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -627.98187847
 T1 diagnostic: 0.035675
 E(MP2/Aug-CC-pVTZ) (Hartree): -627.94881603
 E(MP3/Aug-CC-pVTZ) (Hartree): -627.96748882
 E(PMP2/Aug-CC-pVTZ) (Hartree): -627.96052811
 E(PMP3/Aug-CC-pVTZ) (Hartree): -627.97613574
 E(PUHF/Aug-CC-pVTZ) (Hartree): -627.20079411
 E(UHF/Aug-CC-pVTZ) (Hartree): -627.18730280
 E(CCS(D)/T)/Aug-CC-pVQZ) (Hartree): -628.08546760
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -628.04082319
 T1 diagnostic: 0.035697
 E(MP2/Aug-CC-pVQZ) (Hartree): -628.01477985
 E(MP3/Aug-CC-pVQZ) (Hartree): -628.02853381
 E(PMP2/Aug-CC-pVQZ) (Hartree): -628.02640123
 E(PMP3/Aug-CC-pVQZ) (Hartree): -628.03709087
 E(PUHF/Aug-CC-pVQZ) (Hartree): -627.21499731
 E(UHF/Aug-CC-pVQZ) (Hartree): -627.20160703
 E(UM062X/Aug-CC-pVTZ) (Hartree): -628.73214784
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 N 2.282495 -0.058189 0.000092
 H 2.836872 -0.906779 0.000007
 C 1.056965 -0.183169 0.000024
 O 0.090294 0.646267 0.000091
 Cl -1.522263 -0.162178 -0.000089
 Rotational constants (GHz): 57.2747400 2.8805400 2.7426000
 Vibrational harmonic frequencies (cm-1):
 i1240.3388 218.9565 270.9608
 650.4230 714.8489 852.1748
 1016.2749 1851.1572 3560.1427
 Zero-point correction (Hartree): 0.020811

 HNCO + NO3 : M06-2X/aug-cc-pVTZ geometry
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Fragments
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HNCO

E(CCS(D)/T)/Aug-CC-pVDZ) (Hartree): -168.30258465
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -168.28124890
 T1 diagnostic: 0.018038
 E(MP2/Aug-CC-pVDZ) (Hartree): -168.27834689
 E(MP3/Aug-CC-pVDZ) (Hartree): -168.27384035

E(RHF/Aug-CC-pVDZ) (Hartree): -167.79177923
 E(CCSd(T)/Aug-CC-pVTZ) (Hartree): -168.44532616
 E(CCSd/Aug-CC-pVTZ) (Hartree): -168.41561675
 T1 diagnostic: 0.017532
 E(MP2/Aug-CC-pVTZ) (Hartree): -168.41955710
 E(MP3/Aug-CC-pVTZ) (Hartree): -168.41062749
 E(RHF/Aug-CC-pVTZ) (Hartree): -167.83284283
 E(CCSd(T)/Aug-CC-pVQZ) (Hartree): -168.48867842
 E(CCSd/Aug-CC-pVQZ) (Hartree): -168.45707212
 T1 diagnostic: 0.017338
 E(MP2/Aug-CC-pVQZ) (Hartree): -168.46658212
 E(MP3/Aug-CC-pVQZ) (Hartree): -168.45326510
 E(RHF/Aug-CC-pVQZ) (Hartree): -167.84366530
 E(RM062X/Aug-CC-pVTZ) (Hartree): -168.68730418
 Electronic state : 1-A
 Cartesian coordinates (Angs):

N	1.154202	-0.122224	0.000000
C	-0.045116	0.016799	0.000000
O	-1.204025	0.015866	-0.000000
H	1.823480	0.627848	0.000002

 Rotational constants (GHz): 879.6416200 11.1877300 11.0472300
 Vibrational harmonic frequencies (cm-1):

565.6997	656.9786	786.0660
1369.4348	2362.7298	3698.6854

 Zero-point correction (Hartree): 0.021505

HNO3

 E(CCSd(T)/Aug-CC-pVDZ) (Hartree): -280.30992814
 E(CCSd/Aug-CC-pVDZ) (Hartree): -280.27671910
 T1 diagnostic: 0.018872
 E(MP2/Aug-CC-pVDZ) (Hartree): -280.28216767
 E(MP3/Aug-CC-pVDZ) (Hartree): -280.26419787
 E(RHF/Aug-CC-pVDZ) (Hartree): -279.50039771
 E(CCSd(T)/Aug-CC-pVTZ) (Hartree): -280.54402187
 E(CCSd/Aug-CC-pVTZ) (Hartree): -280.49739612
 T1 diagnostic: 0.018110
 E(MP2/Aug-CC-pVTZ) (Hartree): -280.51317150
 E(MP3/Aug-CC-pVTZ) (Hartree): -280.48824374
 E(RHF/Aug-CC-pVTZ) (Hartree): -279.56681902
 E(CCSd(T)/Aug-CC-pVQZ) (Hartree): -280.61798362
 E(CCSd/Aug-CC-pVQZ) (Hartree): -280.56824782
 T1 diagnostic: 0.017859
 E(MP2/Aug-CC-pVQZ) (Hartree): -280.59216705
 E(MP3/Aug-CC-pVQZ) (Hartree): -280.56115931
 E(RHF/Aug-CC-pVQZ) (Hartree): -279.58592174
 E(RM062X/Aug-CC-pVTZ) (Hartree): -280.89733052
 Electronic state : 1-A
 Cartesian coordinates (Angs):

H	1.716795	0.178522	0.000001
O	1.098616	-0.568576	0.000001
N	-0.140829	0.035612	0.000000
O	-0.136825	1.236669	-0.000000
O	-1.053165	-0.721569	-0.000001

 Rotational constants (GHz): 13.3089300 12.4524700 6.4332300
 Vibrational harmonic frequencies (cm-1):

505.5130	621.6476	706.5789
825.2542	983.4229	1358.6868
1416.0974	1808.8840	3782.0136

 Zero-point correction (Hartree): 0.027356

NCO

 E(CCSd(T)/Aug-CC-pVDZ) (Hartree): -167.62797128
 E(CCSd/Aug-CC-pVDZ) (Hartree): -167.60844012
 T1 diagnostic: 0.026892
 E(MP2/Aug-CC-pVDZ) (Hartree): -167.59017232
 E(MP3/Aug-CC-pVDZ) (Hartree): -167.59683207
 E(PMP2/Aug-CC-pVDZ) (Hartree): -167.59948361
 E(PMP3/Aug-CC-pVDZ) (Hartree): -167.60276840
 E(PUHF/Aug-CC-pVDZ) (Hartree): -167.16572546
 E(UHF/Aug-CC-pVDZ) (Hartree): -167.15393031
 E(CCSd(T)/Aug-CC-pVTZ) (Hartree): -167.76225014
 E(CCSd/Aug-CC-pVTZ) (Hartree): -167.73461730
 T1 diagnostic: 0.026506
 E(MP2/Aug-CC-pVTZ) (Hartree): -167.72258397
 E(MP3/Aug-CC-pVTZ) (Hartree): -167.72563789
 E(PMP2/Aug-CC-pVTZ) (Hartree): -167.73202135
 E(PMP3/Aug-CC-pVTZ) (Hartree): -167.73163223
 E(PUHF/Aug-CC-pVTZ) (Hartree): -167.20420545
 E(UHF/Aug-CC-pVTZ) (Hartree): -167.19223761
 E(CCSd(T)/Aug-CC-pVQZ) (Hartree): -167.80328045
 E(CCSd/Aug-CC-pVQZ) (Hartree): -167.77378740
 T1 diagnostic: 0.026521
 E(MP2/Aug-CC-pVQZ) (Hartree): -167.76689329
 E(MP3/Aug-CC-pVQZ) (Hartree): -167.76599684
 E(PMP2/Aug-CC-pVQZ) (Hartree): -167.77640225
 E(PMP3/Aug-CC-pVQZ) (Hartree): -167.77201636

E(PUHF/Aug-CC-pVQZ) (Hartree): -167.21474443
 E(UHF/Aug-CC-pVQZ) (Hartree): -167.20269276
 E(UM062X/Aug-CC-pVT2) (Hartree): -168.00175758
 Point group : C_v
 Cartesian coordinates (Angs):
 N 0.000000 0.000000 -1.259810
 C 0.000000 0.000000 -0.037198
 O 0.000000 0.000000 1.130232
 Rotational constants (GHz): 0.0000000 11.8429381 11.8429381
 Vibrational harmonic frequencies (cm⁻¹):
 533.0069 (PI) 614.6584 (PI) 1326.9293 (SG)
 2040.1488 (SG)
 Zero-point correction (Hartree): 0.010285

NO3

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -279.63880313
 E(CCSD/Aug-CC-pVDZ) (Hartree): -279.60369390
 T1 diagnostic: 0.040113
 E(MP2/Aug-CC-pVDZ) (Hartree): -279.59508373
 E(MP3/Aug-CC-pVDZ) (Hartree): -279.58333011
 E(PMP2/Aug-CC-pVDZ) (Hartree): -279.59729565
 E(PMP3/Aug-CC-pVDZ) (Hartree): -279.58485291
 E(PUHF/Aug-CC-pVDZ) (Hartree): -278.87110190
 E(UHF/Aug-CC-pVDZ) (Hartree): -278.86753216
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -279.86543977
 E(CCSD/Aug-CC-pVTZ) (Hartree): -279.81759238
 T1 diagnostic: 0.039912
 E(MP2/Aug-CC-pVTZ) (Hartree): -279.81685032
 E(MP3/Aug-CC-pVTZ) (Hartree): -279.80057579
 E(PMP2/Aug-CC-pVTZ) (Hartree): -279.82105102
 E(PMP3/Aug-CC-pVTZ) (Hartree): -279.80355269
 E(PUHF/Aug-CC-pVTZ) (Hartree): -278.93836722
 E(UHF/Aug-CC-pVTZ) (Hartree): -278.93320112
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -279.93748312
 E(CCSD/Aug-CC-pVQZ) (Hartree): -279.88655503
 T1 diagnostic: 0.037108
 E(MP2/Aug-CC-pVQZ) (Hartree): -279.89561241
 E(MP3/Aug-CC-pVQZ) (Hartree): -279.87267534
 E(PMP2/Aug-CC-pVQZ) (Hartree): -279.89804323
 E(PMP3/Aug-CC-pVQZ) (Hartree): -279.87427648
 E(PUHF/Aug-CC-pVQZ) (Hartree): -278.95617416
 E(UHF/Aug-CC-pVQZ) (Hartree): -278.95221601
 E(UM062X/Aug-CC-pVT2) (Hartree): -280.21367243
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 N -0.000003 0.087298 0.000018
 O -1.085665 0.581007 -0.000006
 O 0.000028 -1.238446 -0.000004
 O 1.085639 0.581053 -0.000006
 Rotational constants (GHz): 14.2607200 13.4036900 6.9094600
 Vibrational harmonic frequencies (cm⁻¹):
 330.1049 677.6175 816.5198
 862.2603 1378.4575 1670.6793
 Zero-point correction (Hartree): 0.013067

Adducts

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HNCONO2

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -447.83468679
 E(CCSD/Aug-CC-pVDZ) (Hartree): -447.77549766
 T1 diagnostic: 0.025098
 E(MP2/Aug-CC-pVDZ) (Hartree): -447.77207128
 E(MP3/Aug-CC-pVDZ) (Hartree): -447.75075071
 E(PMP2/Aug-CC-pVDZ) (Hartree): -447.77572976
 E(PMP3/Aug-CC-pVDZ) (Hartree): -447.75333899
 E(PUHF/Aug-CC-pVDZ) (Hartree): -446.51667265
 E(UHF/Aug-CC-pVDZ) (Hartree): -446.51216620
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -448.20395521
 E(CCSD/Aug-CC-pVTZ) (Hartree): -448.12308628
 T1 diagnostic: 0.032066
 E(MP2/Aug-CC-pVTZ) (Hartree): -448.12639062
 E(MP3/Aug-CC-pVTZ) (Hartree): -448.09954983
 E(PMP2/Aug-CC-pVTZ) (Hartree): -448.13648150
 E(PMP3/Aug-CC-pVTZ) (Hartree): -448.10702951
 E(PUHF/Aug-CC-pVTZ) (Hartree): -446.62930714
 E(UHF/Aug-CC-pVTZ) (Hartree): -446.61786079
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -448.31799009
 E(CCSD/Aug-CC-pVQZ) (Hartree): -448.23194010
 T1 diagnostic: 0.032119
 E(MP2/Aug-CC-pVQZ) (Hartree): -448.24856992
 E(MP3/Aug-CC-pVQZ) (Hartree): -448.21166999
 E(PMP2/Aug-CC-pVQZ) (Hartree): -448.25890139
 E(PMP3/Aug-CC-pVQZ) (Hartree): -448.21932756
 E(PUHF/Aug-CC-pVQZ) (Hartree): -446.65854174
 E(UHF/Aug-CC-pVQZ) (Hartree): -446.64683372

E(UM062X/Aug-CC-pVTZ) (Hartree): -448.79629090
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	-2.757495	0.298347	-0.145477
C	-1.602251	-0.042522	-0.359750
O	-0.798307	-0.575633	0.587582
H	-3.299825	0.710171	-0.894335
N	1.319140	0.180919	-0.014666
O	0.410265	-0.959951	0.013442
O	2.380458	-0.163579	-0.401242
O	0.880311	1.222925	0.321948

 Rotational constants (GHz): 8.5695600 1.6797800 1.5081300
 Vibrational harmonic frequencies (cm-1):

82.9604	96.5466	186.9753
363.3217	377.1206	469.2427
636.1642	656.5788	750.6646
784.8460	856.6373	892.3273
1064.6767	1138.2196	1402.3818
1846.0096	1851.0918	3596.2795

 Zero-point correction (Hartree): 0.038847

HN_CO_NO3

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -447.76835173
 E(CCSD/Aug-CC-pVDZ) (Hartree): -447.71304249
 T1 diagnostic: 0.047193
 E(MP2/Aug-CC-pVDZ) (Hartree): -447.66653071
 E(MP3/Aug-CC-pVDZ) (Hartree): -447.67274132
 E(PMP2/Aug-CC-pVDZ) (Hartree): -447.67249384
 E(PMP3/Aug-CC-pVDZ) (Hartree): -447.67646134
 E(PUHF/Aug-CC-pVDZ) (Hartree): -446.50570535
 E(UHF/Aug-CC-pVDZ) (Hartree): -446.49656152
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -448.13053096
 E(CCSD/Aug-CC-pVTZ) (Hartree): -448.05382276
 T1 diagnostic: 0.045372
 E(MP2/Aug-CC-pVTZ) (Hartree): -448.02384648
 E(MP3/Aug-CC-pVTZ) (Hartree): -448.02125753
 E(PMP2/Aug-CC-pVTZ) (Hartree): -448.03007606
 E(PMP3/Aug-CC-pVTZ) (Hartree): -448.02510184
 E(PUHF/Aug-CC-pVTZ) (Hartree): -446.60759149
 E(UHF/Aug-CC-pVTZ) (Hartree): -446.59803703
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -448.24286886
 E(CCSD/Aug-CC-pVQZ) (Hartree): -448.16105421
 T1 diagnostic: 0.044852
 E(MP2/Aug-CC-pVQZ) (Hartree): -448.14455877
 E(MP3/Aug-CC-pVQZ) (Hartree): -448.13223172
 E(PMP2/Aug-CC-pVQZ) (Hartree): -448.15083931
 E(PMP3/Aug-CC-pVQZ) (Hartree): -448.13608043
 E(PUHF/Aug-CC-pVQZ) (Hartree): -446.63651358
 E(UHF/Aug-CC-pVQZ) (Hartree): -446.62688475
 E(UM062X/Aug-CC-pVTZ) (Hartree): -448.71962621

Electronic state : 4-A

Cartesian coordinates (Angs):

N	-0.384171	0.961601	-0.202182
C	-1.671425	0.598486	0.025383
O	-2.173123	-0.460608	0.109653
H	-0.054355	1.873792	0.082741
N	0.691783	-0.004732	-0.073050
O	0.516326	-1.026977	-0.911695
O	0.792143	-0.638502	1.093561
O	1.855856	0.605737	-0.080070

 Rotational constants (GHz): 5.8233600 2.2909400 2.1002500
 Vibrational harmonic frequencies (cm-1):

75.2213	171.2716	284.2731
315.6095	422.3125	448.5183
523.9130	538.7488	601.2211
740.0396	834.2998	911.2036
1002.4201	1073.6435	1148.7603
1412.2611	1949.9249	3615.5994

 Zero-point correction (Hartree): 0.036608

HNCONO3

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -447.71948766
 E(CCSD/Aug-CC-pVDZ) (Hartree): -447.66302906
 T1 diagnostic: 0.048308
 E(MP2/Aug-CC-pVDZ) (Hartree): -447.61083942
 E(MP3/Aug-CC-pVDZ) (Hartree): -447.62118579
 E(PMP2/Aug-CC-pVDZ) (Hartree): -447.61774234
 E(PMP3/Aug-CC-pVDZ) (Hartree): -447.62600374
 E(PUHF/Aug-CC-pVDZ) (Hartree): -446.45484460
 E(UHF/Aug-CC-pVDZ) (Hartree): -446.44569926
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -448.08253458
 E(CCSD/Aug-CC-pVTZ) (Hartree): -448.00488096
 T1 diagnostic: 0.046578
 E(MP2/Aug-CC-pVTZ) (Hartree): -447.96946120
 E(MP3/Aug-CC-pVTZ) (Hartree): -447.97097428
 E(PMP2/Aug-CC-pVTZ) (Hartree): -447.97670530

E(PMP3/Aug-CC-pVTZ) (Hartree): -447.97599035
 E(PUHF/Aug-CC-pVTZ) (Hartree): -446.55823885
 E(UHF/Aug-CC-pVTZ) (Hartree): -446.54864135
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -448.19416759
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -448.11141030
 T1 diagnostic: 0.046141
 E(MP2/Aug-CC-pVQZ) (Hartree): -448.08945257
 E(MP3/Aug-CC-pVQZ) (Hartree): -448.08119131
 E(PMP2/Aug-CC-pVQZ) (Hartree): -448.09676384
 E(PMP3/Aug-CC-pVQZ) (Hartree): -448.08623184
 E(PUHF/Aug-CC-pVQZ) (Hartree): -446.58686172
 E(UHF/Aug-CC-pVQZ) (Hartree): -446.57718416
 E(UM062X/Aug-CC-pVTZ) (Hartree): -448.67121076
 Electronic state : 4-A
 Cartesian coordinates (Angs):

N	2.667881	-0.132886	0.011696
C	1.487555	0.181169	0.067340
O	0.473604	-0.688004	-0.146387
H	3.369909	0.572135	0.202021
N	-0.794964	-0.010742	-0.053140
O	-0.874473	1.024623	-0.844577
O	-1.050496	0.534385	1.108466
O	-1.724342	-0.952723	-0.156996

 Rotational constants (GHz): 6.6207900 1.9483000 1.8589500
 Vibrational harmonic frequencies (cm-1):

96.4498	173.0601	211.8487
294.7894	411.7617	431.5474
517.5092	573.0284	670.2045
674.5736	808.0994	907.9057
924.7908	966.8306	1055.2107
1176.4688	1865.6046	3586.7681

 Zero-point correction (Hartree): 0.034962

HNC_O_ONO2

 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -447.94832392
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -447.89290147
 T1 diagnostic: 0.022259
 E(MP2/Aug-CC-pVDZ) (Hartree): -447.88988692
 E(MP3/Aug-CC-pVDZ) (Hartree): -447.87073151
 E(PMP2/Aug-CC-pVDZ) (Hartree): -447.89263145
 E(PMP3/Aug-CC-pVDZ) (Hartree): -447.87252243
 E(PUHF/Aug-CC-pVDZ) (Hartree): -446.65738325
 E(UHF/Aug-CC-pVDZ) (Hartree): -446.65347647
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -448.31706238
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -448.24040623
 T1 diagnostic: 0.021370
 E(MP2/Aug-CC-pVTZ) (Hartree): -448.25402507
 E(MP3/Aug-CC-pVTZ) (Hartree): -448.22437808
 E(PMP2/Aug-CC-pVTZ) (Hartree): -448.25692364
 E(PMP3/Aug-CC-pVTZ) (Hartree): -448.22623760
 E(PUHF/Aug-CC-pVTZ) (Hartree): -446.76209278
 E(UHF/Aug-CC-pVTZ) (Hartree): -446.75793113
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -448.42953025
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -448.34864327
 T1 diagnostic: 0.038117
 E(MP2/Aug-CC-pVQZ) (Hartree): -448.35002173
 E(MP3/Aug-CC-pVQZ) (Hartree): -448.32397019
 E(PMP2/Aug-CC-pVQZ) (Hartree): -448.36764194
 E(PMP3/Aug-CC-pVQZ) (Hartree): -448.33776349
 E(PUHF/Aug-CC-pVQZ) (Hartree): -446.80913087
 E(UHF/Aug-CC-pVQZ) (Hartree): -446.78966266
 E(UM062X/Aug-CC-pVTZ) (Hartree): -448.90882469
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	-2.333561	-0.545724	-0.124297
C	-1.110459	0.101049	-0.000263
O	-0.948077	1.281000	0.057406
H	-2.938819	-0.248089	0.644571
N	1.197157	-0.145941	-0.002173
O	-0.105784	-0.818213	-0.056135
O	1.630512	0.123252	-1.063727
O	1.617899	-0.025608	1.092744

 Rotational constants (GHz): 6.3354100 1.9693700 1.9394400
 Vibrational harmonic frequencies (cm-1):

56.2533	104.8318	185.0609
211.4836	381.0355	571.1414
593.2440	695.0646	702.8288
823.8631	853.2956	994.6111
1087.1537	1285.2453	1429.9387
1829.4751	1850.6685	3471.4383

 Zero-point correction (Hartree): 0.039017

OCN_H_ONO2

 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -447.90744407
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -447.84962528
 T1 diagnostic: 0.021784

E(MP2/Aug-CC-pVDZ) (Hartree): -447.85265821
 E(MP3/Aug-CC-pVDZ) (Hartree): -447.82659963
 E(PMP2/Aug-CC-pVDZ) (Hartree): -447.85509292
 E(PMP3/Aug-CC-pVDZ) (Hartree): -447.82790131
 E(PUHF/Aug-CC-pVDZ) (Hartree): -446.59663831
 E(UHF/Aug-CC-pVDZ) (Hartree): -446.59271211
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -448.27566368
 E(CCSD/Aug-CC-pVTZ) (Hartree): -448.19626493
 T1 diagnostic: 0.028753
 E(MP2/Aug-CC-pVTZ) (Hartree): -448.20675557
 E(MP3/Aug-CC-pVTZ) (Hartree): -448.17476340
 E(PMP2/Aug-CC-pVTZ) (Hartree): -448.21563389
 E(PMP3/Aug-CC-pVTZ) (Hartree): -448.18118264
 E(PUHF/Aug-CC-pVTZ) (Hartree): -446.70733666
 E(UHF/Aug-CC-pVTZ) (Hartree): -446.69710149
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -448.39062739
 E(CCSD/Aug-CC-pVQZ) (Hartree): -448.30609762
 T1 diagnostic: 0.028749
 E(MP2/Aug-CC-pVQZ) (Hartree): -448.32981074
 E(MP3/Aug-CC-pVQZ) (Hartree): -448.28785958
 E(PMP2/Aug-CC-pVQZ) (Hartree): -448.33892683
 E(PMP3/Aug-CC-pVQZ) (Hartree): -448.29445417
 E(PUHF/Aug-CC-pVQZ) (Hartree): -446.73695388
 E(UHF/Aug-CC-pVQZ) (Hartree): -446.72645958
 E(UM062X/Aug-CC-pVTZ) (Hartree): -448.86994197
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	-0.925881	0.949977	0.300677
C	-1.841371	-0.037257	0.189420
O	-1.902514	-0.926618	-0.580818
H	-0.840380	1.461634	1.165351
N	1.163888	-0.114496	0.061872
O	2.109801	-0.191725	-0.636093
O	0.220434	0.901700	-0.446897
O	0.850099	-0.669164	1.058843

 Rotational constants (GHz): 5.9077000 2.0240300 1.9181300
 Vibrational harmonic frequencies (cm-1):

83.9815	87.7485	242.4385
304.6657	434.4910	510.6740
526.2356	686.7446	789.2816
840.9261	848.8429	1051.4098
1118.2884	1400.9113	1467.2479
1846.8035	1934.4903	3630.6724

 Zero-point correction (Hartree): 0.040565

 Transition states
 =====
 TS.HN_CO_NO3.HNCONO3

 IRC pathway available
 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -447.71626493
 E(CCSD/Aug-CC-pVDZ) (Hartree): -447.65699461
 T1 diagnostic: 0.047928
 E(MP2/Aug-CC-pVDZ) (Hartree): -447.60658475
 E(MP3/Aug-CC-pVDZ) (Hartree): -447.61367308
 E(PMP2/Aug-CC-pVDZ) (Hartree): -447.62003564
 E(PMP3/Aug-CC-pVDZ) (Hartree): -447.62383390
 E(PUHF/Aug-CC-pVDZ) (Hartree): -446.44995473
 E(UHF/Aug-CC-pVDZ) (Hartree): -446.43415028
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -448.07887058
 E(CCSD/Aug-CC-pVTZ) (Hartree): -447.99840413
 T1 diagnostic: 0.046298
 E(MP2/Aug-CC-pVTZ) (Hartree): -447.96496710
 E(MP3/Aug-CC-pVTZ) (Hartree): -447.96299287
 E(PMP2/Aug-CC-pVTZ) (Hartree): -447.97827284
 E(PMP3/Aug-CC-pVTZ) (Hartree): -447.97300892
 E(PUHF/Aug-CC-pVTZ) (Hartree): -446.55294012
 E(UHF/Aug-CC-pVTZ) (Hartree): -446.53722591
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -448.19024300
 E(CCSD/Aug-CC-pVQZ) (Hartree): -448.10467088
 T1 diagnostic: 0.045976
 E(MP2/Aug-CC-pVQZ) (Hartree): -448.08460211
 E(MP3/Aug-CC-pVQZ) (Hartree): -448.07283676
 E(PMP2/Aug-CC-pVQZ) (Hartree): -448.09802275
 E(PMP3/Aug-CC-pVQZ) (Hartree): -448.08292476
 E(PUHF/Aug-CC-pVQZ) (Hartree): -446.58153865
 E(UHF/Aug-CC-pVQZ) (Hartree): -446.56569512
 E(UM062X/Aug-CC-pVTZ) (Hartree): -448.66809056
 Electronic state : 4-A
 Cartesian coordinates (Angs):

N	-2.721579	0.061092	0.025259
C	-1.500662	-0.081773	0.022743
O	-0.533874	0.765421	-0.061156
H	-3.295926	-0.768552	0.119737
N	0.859402	-0.029047	-0.032234
O	0.865638	-0.983479	-0.890029
O	1.083737	-0.614337	1.083480

O 1.751391 0.961755 -0.158215
 Rotational constants (GHz): 6.4524000 1.8835500 1.7874600
 Vibrational harmonic frequencies (cm-1):
 i638.6682 76.9447 192.9219
 230.8149 327.9030 373.4452
 469.0494 546.8272 621.8592
 661.2569 710.5062 872.8815
 933.5951 1001.6425 1074.9399
 1173.7211 1872.7839 3567.9279
 Zero-point correction (Hartree): 0.033510

TS.HNCO+NO3.HN_CO_NO3

IRC pathway available

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -447.76324348

E(CCSD/Aug-CC-pVDZ) (Hartree): -447.70497742

T1 diagnostic: 0.048993

E(MP2/Aug-CC-pVDZ) (Hartree): -447.65994248

E(MP3/Aug-CC-pVDZ) (Hartree): -447.66251019

E(PMP2/Aug-CC-pVDZ) (Hartree): -447.66881732

E(PMP3/Aug-CC-pVDZ) (Hartree): -447.66842366

E(PUHF/Aug-CC-pVDZ) (Hartree): -446.49337479

E(UHF/Aug-CC-pVDZ) (Hartree): -446.48142843

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -448.12572772

E(CCSD/Aug-CC-pVTZ) (Hartree): -448.04598262

T1 diagnostic: 0.047413

E(MP2/Aug-CC-pVTZ) (Hartree): -448.01748858

E(MP3/Aug-CC-pVTZ) (Hartree): -448.01123102

E(PMP2/Aug-CC-pVTZ) (Hartree): -448.02674129

E(PMP3/Aug-CC-pVTZ) (Hartree): -448.01736901

E(PUHF/Aug-CC-pVTZ) (Hartree): -446.59627183

E(UHF/Aug-CC-pVTZ) (Hartree): -446.58382402

E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -448.23779972

E(CCSD/Aug-CC-pVQZ) (Hartree): -448.15293674

T1 diagnostic: 0.046977

E(MP2/Aug-CC-pVQZ) (Hartree): -448.13792598

E(MP3/Aug-CC-pVQZ) (Hartree): -448.12187813

E(PMP2/Aug-CC-pVQZ) (Hartree): -448.14724641

E(PMP3/Aug-CC-pVQZ) (Hartree): -448.12803783

E(PUHF/Aug-CC-pVQZ) (Hartree): -446.62503474

E(UHF/Aug-CC-pVQZ) (Hartree): -446.61250016

E(UM062X/Aug-CC-pVTZ) (Hartree): -448.71493483

Electronic state : 4-A

Cartesian coordinates (Angs):

N -0.529247 0.925686 -0.118820
 C -1.745074 0.510892 0.021737
 O -2.408703 -0.454413 0.085945
 H -0.220318 1.861990 0.103323
 N 0.793681 -0.029074 -0.053147
 O 0.577435 -1.112890 -0.800707
 O 1.081322 -0.526621 1.122279
 O 1.854912 0.693471 -0.286264

Rotational constants (GHz): 5.8814300 1.9952900 1.8374000

Vibrational harmonic frequencies (cm-1):

i666.3535 42.5926 142.5663
 240.8409 292.7199 355.1398
 391.2660 507.6311 536.5005
 607.5437 704.5381 904.8785
 934.3876 1081.1172 1171.2339
 1243.7209 2033.9099 3623.1896

Zero-point correction (Hartree): 0.033748

TS.HNCO+NO3.HNC_O_ONO2

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -447.92324708

E(CCSD/Aug-CC-pVDZ) (Hartree): -447.86355987

T1 diagnostic: 0.029199

E(MP2/Aug-CC-pVDZ) (Hartree): -447.85997336

E(MP3/Aug-CC-pVDZ) (Hartree): -447.83640850

E(PMP2/Aug-CC-pVDZ) (Hartree): -447.86712231

E(PMP3/Aug-CC-pVDZ) (Hartree): -447.84118406

E(PUHF/Aug-CC-pVDZ) (Hartree): -446.62200765

E(UHF/Aug-CC-pVDZ) (Hartree): -446.61270241

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -448.29074922

E(CCSD/Aug-CC-pVTZ) (Hartree): -448.20931431

T1 diagnostic: 0.028168

E(MP2/Aug-CC-pVTZ) (Hartree): -448.22276651

E(MP3/Aug-CC-pVTZ) (Hartree): -448.18846245

E(PMP2/Aug-CC-pVTZ) (Hartree): -448.23037490

E(PMP3/Aug-CC-pVTZ) (Hartree): -448.19353743

E(PUHF/Aug-CC-pVTZ) (Hartree): -446.72553910

E(UHF/Aug-CC-pVTZ) (Hartree): -446.71568752

E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -448.40533058

E(CCSD/Aug-CC-pVQZ) (Hartree): -448.31882795

T1 diagnostic: 0.027763

E(MP2/Aug-CC-pVQZ) (Hartree): -448.34583160

E(MP3/Aug-CC-pVQZ) (Hartree): -448.30145743

E(PMP2/Aug-CC-pVQZ) (Hartree): -448.35352362

E(PMP3/Aug-CC-pVQZ) (Hartree): -448.30657471
 E(PUHF/Aug-CC-pVQZ) (Hartree): -446.75486771
 E(UHF/Aug-CC-pVQZ) (Hartree): -446.74492411
 E(UM062X/Aug-CC-pVTZ) (Hartree): -448.88247734
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	-1.526240	1.045070	-0.570242
C	-1.453230	-0.096502	0.012972
O	-1.851016	-1.018372	0.569351
H	-0.883559	1.733458	-0.172599
N	1.186958	0.015407	0.032640
O	0.190168	-0.401018	-0.779455
O	2.239437	-0.501039	-0.177380
O	0.918650	0.848205	0.869730

 Rotational constants (GHz): 5.9327800 1.9461700 1.8006700
 Vibrational harmonic frequencies (cm-1):

i654.3013	61.8303	80.6348
218.8012	351.0109	415.1662
544.4675	608.7446	689.5620
724.5802	828.0938	949.2871
991.1491	1167.0884	1357.2151
1706.5101	2183.2506	3483.8702

 Zero-point correction (Hartree): 0.037274

TS.HNCO+NO3.HNCOONO2

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -447.82771064
 E(CCSD/Aug-CC-pVDZ) (Hartree): -447.76594976
 T1 diagnostic: 0.038074
 E(MP2/Aug-CC-pVDZ) (Hartree): -447.73981763
 E(MP3/Aug-CC-pVDZ) (Hartree): -447.72532444
 E(PMP2/Aug-CC-pVDZ) (Hartree): -447.76014779
 E(PMP3/Aug-CC-pVDZ) (Hartree): -447.74073410
 E(PUHF/Aug-CC-pVDZ) (Hartree): -446.52299449
 E(UHF/Aug-CC-pVDZ) (Hartree): -446.50001310
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -448.19634354
 E(CCSD/Aug-CC-pVTZ) (Hartree): -448.11273690
 T1 diagnostic: 0.042515
 E(MP2/Aug-CC-pVTZ) (Hartree): -448.09375724
 E(MP3/Aug-CC-pVTZ) (Hartree): -448.07410674
 E(PMP2/Aug-CC-pVTZ) (Hartree): -448.12155087
 E(PMP3/Aug-CC-pVTZ) (Hartree): -448.09583193
 E(PUHF/Aug-CC-pVTZ) (Hartree): -446.63647192
 E(UHF/Aug-CC-pVTZ) (Hartree): -446.60562779
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -448.30992974
 E(CCSD/Aug-CC-pVQZ) (Hartree): -448.22113198
 T1 diagnostic: 0.043740
 E(MP2/Aug-CC-pVQZ) (Hartree): -448.21270023
 E(MP3/Aug-CC-pVQZ) (Hartree): -448.18453917
 E(PMP2/Aug-CC-pVQZ) (Hartree): -448.24301501
 E(PMP3/Aug-CC-pVQZ) (Hartree): -448.20847499
 E(PUHF/Aug-CC-pVQZ) (Hartree): -446.66844358
 E(UHF/Aug-CC-pVQZ) (Hartree): -446.63495559
 E(UM062X/Aug-CC-pVTZ) (Hartree): -448.78719036
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	2.773889	0.349330	-0.244432
C	1.622629	-0.069751	-0.229917
O	0.864174	-0.613513	0.633305
H	3.141205	0.751528	-1.099107
N	-1.323335	0.171797	-0.015485
O	-0.471550	-0.965974	-0.043033
O	-0.878948	1.191833	0.391312
O	-2.392534	-0.109960	-0.444331

 Rotational constants (GHz): 8.2482700 1.6415600 1.4872700
 Vibrational harmonic frequencies (cm-1):

i1276.1019	74.1346	81.0958
253.7342	319.1771	361.5089
558.2201	634.4485	701.7712
719.0916	792.0341	899.9476
988.9351	1056.5823	1390.0042
1804.1552	1904.3414	3562.9273

 Zero-point correction (Hartree): 0.036683

TS.HNCO+NO3.HNO3+NCO

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -447.92365964
 E(CCSD/Aug-CC-pVDZ) (Hartree): -447.85365836
 T1 diagnostic: 0.120771
 E(MP2/Aug-CC-pVDZ) (Hartree): -447.83549404
 E(MP3/Aug-CC-pVDZ) (Hartree): -447.82060313
 E(PMP2/Aug-CC-pVDZ) (Hartree): -447.84619369
 E(PMP3/Aug-CC-pVDZ) (Hartree): -447.82741244
 E(PUHF/Aug-CC-pVDZ) (Hartree): -446.62136780
 E(UHF/Aug-CC-pVDZ) (Hartree): -446.60784032
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -448.29164641
 E(CCSD/Aug-CC-pVTZ) (Hartree): -448.20001143
 T1 diagnostic: 0.108144

E(MP2/Aug-CC-pVTZ) (Hartree): -448.19962777
 E(MP3/Aug-CC-pVTZ) (Hartree): -448.17429081
 E(PMP2/Aug-CC-pVTZ) (Hartree): -448.21052750
 E(PMP3/Aug-CC-pVTZ) (Hartree): -448.18121597
 E(PUHF/Aug-CC-pVTZ) (Hartree): -446.72569306
 E(UHF/Aug-CC-pVTZ) (Hartree): -446.71191794
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -448.40533852
 E(CCSD/Aug-CC-pVQZ) (Hartree): -448.30933524
 T1 diagnostic: 0.103260
 E(MP2/Aug-CC-pVQZ) (Hartree): -448.32270412
 E(MP3/Aug-CC-pVQZ) (Hartree): -448.28734611
 E(PMP2/Aug-CC-pVQZ) (Hartree): -448.33368324
 E(PMP3/Aug-CC-pVQZ) (Hartree): -448.29430092
 E(PUHF/Aug-CC-pVQZ) (Hartree): -446.75504145
 E(UHF/Aug-CC-pVQZ) (Hartree): -446.74117411
 E(UM062X/Aug-CC-pVTZ) (Hartree): -448.88170942
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	-1.407432	1.169833	0.260627
C	-1.956590	0.108300	0.000399
O	-2.567458	-0.846103	-0.224116
H	-0.241296	1.224465	0.198501
N	1.384187	-0.187370	0.011315
O	0.922966	1.061707	-0.217704
O	0.590669	-1.049432	0.262667
O	2.571767	-0.260110	-0.083908

 Rotational constants (GHz): 6.9002700 1.5096500 1.2619700
 Vibrational harmonic frequencies (cm-1):

i1946.8251	45.3896	72.4187
96.0041	204.2822	377.7978
588.9523	622.5818	672.1903
721.7630	813.9969	915.3122
945.5214	1255.0150	1362.1822
1400.5051	1698.6268	2171.7913

 Zero-point correction (Hartree): 0.031813

 TS.HNCO+NO3.OCN_H_ONO2

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -447.89950221
 E(CCSD/Aug-CC-pVDZ) (Hartree): -447.83959913
 T1 diagnostic: 0.026509
 E(MP2/Aug-CC-pVDZ) (Hartree): -447.83631380
 E(MP3/Aug-CC-pVDZ) (Hartree): -447.81128996
 E(PMP2/Aug-CC-pVDZ) (Hartree): -447.84584321
 E(PMP3/Aug-CC-pVDZ) (Hartree): -447.81725656
 E(PUHF/Aug-CC-pVDZ) (Hartree): -446.58848884
 E(UHF/Aug-CC-pVDZ) (Hartree): -446.57639678
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -448.26829089
 E(CCSD/Aug-CC-pVTZ) (Hartree): -448.18634090
 T1 diagnostic: 0.025967
 E(MP2/Aug-CC-pVTZ) (Hartree): -448.20026303
 E(MP3/Aug-CC-pVTZ) (Hartree): -448.16420237
 E(PMP2/Aug-CC-pVTZ) (Hartree): -448.21010983
 E(PMP3/Aug-CC-pVTZ) (Hartree): -448.17035903
 E(PUHF/Aug-CC-pVTZ) (Hartree): -446.69305243
 E(UHF/Aug-CC-pVTZ) (Hartree): -446.68056857
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -448.38294999
 E(CCSD/Aug-CC-pVQZ) (Hartree): -448.29584621
 T1 diagnostic: 0.025809
 E(MP2/Aug-CC-pVQZ) (Hartree): -448.32334721
 E(MP3/Aug-CC-pVQZ) (Hartree): -448.27708364
 E(PMP2/Aug-CC-pVQZ) (Hartree): -448.33324380
 E(PMP3/Aug-CC-pVQZ) (Hartree): -448.28325237
 E(PUHF/Aug-CC-pVQZ) (Hartree): -446.72223346
 E(UHF/Aug-CC-pVQZ) (Hartree): -446.70968788
 E(UM062X/Aug-CC-pVTZ) (Hartree): -448.86066721
 Electronic state : 2-A
 Cartesian coordinates (Angs):

N	-0.973736	0.926014	0.396251
C	-1.854685	0.031639	0.132271
O	-2.204819	-0.809361	-0.598411
H	-0.796890	1.232188	1.340981
N	1.224962	-0.128510	0.031841
O	2.238771	-0.166526	-0.585161
O	0.403353	0.934154	-0.371532
O	0.833497	-0.833836	0.913698

 Rotational constants (GHz): 6.2592400 1.8134600 1.6972900
 Vibrational harmonic frequencies (cm-1):

i813.3798	49.4042	73.7675
214.0136	302.5979	464.2818
542.7230	572.4193	693.8503
779.8991	811.6935	913.0002
1154.2011	1257.5356	1392.5106
1770.0088	2091.3030	3650.1056

 Zero-point correction (Hartree): 0.038121

 HNCO + O3 : M06-2X/aug-cc-pVTZ geometry
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Fragments
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HNCO

E(CCS(D)/Aug-CC-pVDZ) (Hartree): -168.30258903
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -168.28125135
 T1 diagnostic: 0.018041
 E(MP2/Aug-CC-pVDZ) (Hartree): -168.27835301
 E(MP3/Aug-CC-pVDZ) (Hartree): -168.27384099
 E(RHF/Aug-CC-pVDZ) (Hartree): -167.79177355
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -168.44533015
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -168.41561850
 E(MP2/Aug-CC-pVTZ) (Hartree): -168.41956259
 E(MP3/Aug-CC-pVTZ) (Hartree): -168.41062722
 E(RHF/6-31G(d,p)) (Hartree): -167.76545219
 E(RHF/Aug-CC-pVTZ) (Hartree): -167.83283656
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -168.48868126
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -168.45707276
 T1 diagnostic: 0.017340
 E(MP2/Aug-CC-pVQZ) (Hartree): -168.46658688
 E(MP3/Aug-CC-pVQZ) (Hartree): -168.45326396
 E(RHF/Aug-CC-pVQZ) (Hartree): -167.84365842
 E(RM062X/Aug-CC-pVTZ) (Hartree): -168.68730523
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):

N	0.289904	-1.123860	0.000000
H	1.226714	-1.488086	0.000000
C	0.000000	0.048082	0.000000
O	-0.407005	1.133327	0.000000

 Rotational constants (GHz): 880.1140600 11.1871200 11.0467000
 Vibrational harmonic frequencies (cm-1):

563.8698 (A')	657.1801 (A'')	782.7913 (A')
1369.4249 (A')	2366.0466 (A')	3706.3649 (A')

 Zero-point correction (Hartree): 0.021519

HN_O_CO

E(CCS(D)/Aug-CC-pVDZ) (Hartree): -243.23568465
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -243.20564724
 T1 diagnostic: 0.024289
 E(MP2/Aug-CC-pVDZ) (Hartree): -243.19909173
 E(MP3/Aug-CC-pVDZ) (Hartree): -243.19254550
 E(RHF/Aug-CC-pVDZ) (Hartree): -242.51533725
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -243.43870340
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -243.39658695
 E(MP2/Aug-CC-pVTZ) (Hartree): -243.40004390
 E(MP3/Aug-CC-pVTZ) (Hartree): -243.38724333
 E(RHF/6-31G(d,p)) (Hartree): -242.46936665
 E(RHF/Aug-CC-pVTZ) (Hartree): -242.57275756
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -243.50138267
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -243.45650850
 T1 diagnostic: 0.022614
 E(MP2/Aug-CC-pVQZ) (Hartree): -243.46773727
 E(MP3/Aug-CC-pVQZ) (Hartree): -243.44907503
 E(RHF/Aug-CC-pVQZ) (Hartree): -242.58839770
 E(RM062X/Aug-CC-pVTZ) (Hartree): -243.77249424
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):

N	0.616198	-0.460388	0.000000
C	0.000000	0.629903	0.000000
O	-0.630978	1.587739	0.000000
H	1.634338	-0.478560	0.000000
O	-0.112488	-1.597506	0.000000

 Rotational constants (GHz): 48.3078300 5.4242000 4.8766300
 Vibrational harmonic frequencies (cm-1):

206.3218 (A')	424.8644 (A'')	551.2151 (A'')
671.7966 (A')	971.9498 (A')	1222.3629 (A')
1402.2747 (A')	2345.0872 (A')	3444.4356 (A')

 Zero-point correction (Hartree): 0.025607

NCO

E(CCS(D)/Aug-CC-pVDZ) (Hartree): -167.62693028
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -167.60767126
 T1 diagnostic: 0.026310
 E(MP2/Aug-CC-pVDZ) (Hartree): -167.58945443
 E(MP3/Aug-CC-pVDZ) (Hartree): -167.59640341
 E(PMP2/Aug-CC-pVDZ) (Hartree): -167.59851147
 E(PMP3/Aug-CC-pVDZ) (Hartree): -167.60213246
 E(PUHF/Aug-CC-pVDZ) (Hartree): -167.16612982

E(UHF/Aug-CC-pVDZ) (Hartree): -167.15458842
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -167.76183039
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -167.73450689
 E(MP2/Aug-CC-pVTZ) (Hartree): -167.72246615
 E(MP3/Aug-CC-pVTZ) (Hartree): -167.72586224
 E(PMP2/Aug-CC-pVTZ) (Hartree): -167.73164695
 E(PMP3/Aug-CC-pVTZ) (Hartree): -167.73164844
 E(PUHF/Aug-CC-pVTZ) (Hartree): -167.20497190
 E(UHF/6-31G(d,p)) (Hartree): -167.12855965
 E(UHF/Aug-CC-pVTZ) (Hartree): -167.19326003
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -167.80303120
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -167.77385078
 T1 diagnostic: 0.025921
 E(MP2/Aug-CC-pVQZ) (Hartree): -167.76693421
 E(MP3/Aug-CC-pVQZ) (Hartree): -167.76639553
 E(PMP2/Aug-CC-pVQZ) (Hartree): -167.77618313
 E(PMP3/Aug-CC-pVQZ) (Hartree): -167.77220480
 E(PUHF/Aug-CC-pVQZ) (Hartree): -167.21557056
 E(UHF/Aug-CC-pVQZ) (Hartree): -167.20377852
 E(UM062X/Aug-CC-pVTZ) (Hartree): -168.00176764
 Point group : C*v
 Cartesian coordinates (Angs):
 O 0.000000 0.000000 1.130345
 C 0.000000 0.000000 -0.037292
 N 0.000000 0.000000 -1.259859
 Rotational constants (GHz): 0.0000000 11.8412931 11.8412931
 Vibrational harmonic frequencies (cm-1):
 545.5037 (PI) 619.5696 (PI) 1329.1219 (SG)
 2052.4724 (SG)
 Zero-point correction (Hartree): 0.010358

O2 (triplet)

 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -150.01974519
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -150.00798962
 T1 diagnostic: 0.017239
 E(MP2/Aug-CC-pVDZ) (Hartree): -150.00188564
 E(MP3/Aug-CC-pVDZ) (Hartree): -149.99996195
 E(PMP2/Aug-CC-pVDZ) (Hartree): -150.00861128
 E(PMP3/Aug-CC-pVDZ) (Hartree): -150.00309471
 E(PUHF/Aug-CC-pVDZ) (Hartree): -149.65562305
 E(UHF/Aug-CC-pVDZ) (Hartree): -149.64482099
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -150.14024980
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -150.12182279
 E(MP2/Aug-CC-pVTZ) (Hartree): -150.11944130
 E(MP3/Aug-CC-pVTZ) (Hartree): -150.11498987
 E(PMP2/Aug-CC-pVTZ) (Hartree): -150.12652379
 E(PMP3/Aug-CC-pVTZ) (Hartree): -150.11821008
 E(PUHF/Aug-CC-pVTZ) (Hartree): -149.69197969
 E(UHF/6-31G(d,p)) (Hartree): -149.61689809
 E(UHF/Aug-CC-pVTZ) (Hartree): -149.68069574
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -150.17820201
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -150.15821114
 T1 diagnostic: 0.017206
 E(MP2/Aug-CC-pVQZ) (Hartree): -150.15935385
 E(MP3/Aug-CC-pVQZ) (Hartree): -150.15234763
 E(PMP2/Aug-CC-pVQZ) (Hartree): -150.16652801
 E(PMP3/Aug-CC-pVQZ) (Hartree): -150.15557503
 E(PUHF/Aug-CC-pVQZ) (Hartree): -149.70247961
 E(UHF/Aug-CC-pVQZ) (Hartree): -149.69108999
 E(UM062X/Aug-CC-pVTZ) (Hartree): -150.32481496
 Point group : D*H
 Electronic state : 3-SGG
 Cartesian coordinates (Angs):
 O 0.000000 0.000000 0.594953
 O 0.000000 0.000000 -0.594953
 Rotational constants (GHz): 0.0000000 44.6313876 44.6313876
 Vibrational harmonic frequencies (cm-1):
 1757.6183 (SGG)
 Zero-point correction (Hartree): 0.004004

O2 (singlet)

 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -149.96951201
 E(CCS(D)/Aug-CC-pVDZ) (Hartree): -149.95369083
 T1 diagnostic: 0.015546
 E(MP2/Aug-CC-pVDZ) (Hartree): -149.95020430
 E(MP3/Aug-CC-pVDZ) (Hartree): -149.94364960
 E(RHF/Aug-CC-pVDZ) (Hartree): -149.55943179
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -150.09177700
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -150.06904109
 T1 diagnostic: 0.014672
 E(MP2/Aug-CC-pVTZ) (Hartree): -150.07077477
 E(MP3/Aug-CC-pVTZ) (Hartree): -150.06086175
 E(RHF/Aug-CC-pVTZ) (Hartree): -149.59507488
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -150.13032570
 E(CCS(D)/Aug-CC-pVQZ) (Hartree): -150.10602219

T1 diagnostic: 0.014546
 E(MP2/Aug-CC-pVQZ) (Hartree): -150.11192750
 E(MP3/Aug-CC-pVQZ) (Hartree): -150.09907027
 E(RHF/Aug-CC-pVQZ) (Hartree): -149.60535832
 E(RM062X/Aug-CC-pVTZ) (Hartree): -150.26570483
 Point group : D*H
 Cartesian coordinates (Angs):
 O 0.000000 0.000000 0.593979
 O 0.000000 0.000000 -0.593979
 Rotational constants (GHz): 0.0000000 44.7778544 44.7778544
 Vibrational harmonic frequencies (cm-1):
 1749.4267 (SGG)
 Zero-point correction (Hartree): 0.003985

O3
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 E(CCSd(T)/Aug-CC-pVDZ) (Hartree): -224.96402704
 E(CCSd/Aug-CC-pVDZ) (Hartree): -224.93019226
 T1 diagnostic: 0.025459
 E(MP2/Aug-CC-pVDZ) (Hartree): -224.95076976
 E(MP3/Aug-CC-pVDZ) (Hartree): -224.91583494
 E(RHF/Aug-CC-pVDZ) (Hartree): -224.30230914
 E(CCSd(T)/Aug-CC-pVTZ) (Hartree): -225.14987055
 E(CCSd/Aug-CC-pVTZ) (Hartree): -225.10453547
 E(MP2/Aug-CC-pVTZ) (Hartree): -225.13397192
 E(MP3/Aug-CC-pVTZ) (Hartree): -225.09297033
 E(RHF/6-31G(d,p)) (Hartree): -224.25916614
 E(RHF/Aug-CC-pVTZ) (Hartree): -224.35728323
 E(CCSd(T)/Aug-CC-pVQZ) (Hartree): -225.20810633
 E(CCSd/Aug-CC-pVQZ) (Hartree): -225.16016260
 T1 diagnostic: 0.024377
 E(MP2/Aug-CC-pVQZ) (Hartree): -225.19606922
 E(MP3/Aug-CC-pVQZ) (Hartree): -225.15039623
 E(RHF/Aug-CC-pVQZ) (Hartree): -224.37274046
 E(RM062X/Aug-CC-pVTZ) (Hartree): -225.40547093
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):
 O 0.000000 0.421186 0.000000
 O 1.057275 -0.210593 0.000000
 O -1.057275 -0.210593 0.000000
 Rotational constants (GHz): 118.7400400 14.1328300 12.6296200
 Vibrational harmonic frequencies (cm-1):
 792.9313 (A') 1363.1357 (A') 1363.5294 (A')
 Zero-point correction (Hartree): 0.008018

Adducts
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cy_C_NH_OOOO

 E(CCSd(T)/Aug-CC-pVDZ) (Hartree): -393.23257589
 E(CCSd/Aug-CC-pVDZ) (Hartree): -393.18514800
 T1 diagnostic: 0.019538
 E(MP2/Aug-CC-pVDZ) (Hartree): -393.16993467
 E(MP3/Aug-CC-pVDZ) (Hartree): -393.16982322
 E(RHF/Aug-CC-pVDZ) (Hartree): -392.08454011
 E(CCSd(T)/Aug-CC-pVTZ) (Hartree): -393.56421032
 E(CCSd/Aug-CC-pVTZ) (Hartree): -393.49769124
 E(MP2/Aug-CC-pVTZ) (Hartree): -393.49839338
 E(MP3/Aug-CC-pVTZ) (Hartree): -393.48846082
 E(RHF/6-31G(d,p)) (Hartree): -392.02093361
 E(RHF/Aug-CC-pVTZ) (Hartree): -392.18068073
 E(CCSd(T)/Aug-CC-pVQZ) (Hartree): -393.66421183
 E(CCSd/Aug-CC-pVQZ) (Hartree): -393.59317121
 T1 diagnostic: 0.018153
 E(MP2/Aug-CC-pVQZ) (Hartree): -393.60599534
 E(MP3/Aug-CC-pVQZ) (Hartree): -393.58718362
 E(RHF/Aug-CC-pVQZ) (Hartree): -392.20527405
 E(RM062X/Aug-CC-pVTZ) (Hartree): -394.07807221
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 N 2.009276 -0.131572 0.002917
 H 2.464916 0.774423 0.036954
 C 0.775058 -0.034441 -0.003242
 O -0.060921 -1.103550 -0.167808
 O -1.283738 0.665231 -0.268091
 O 0.004223 1.090601 0.148365
 O -1.307088 -0.608128 0.282794
 Rotational constants (GHz): 9.1005400 3.9846800 2.8731400
 Vibrational harmonic frequencies (cm-1):
 173.3041 451.9977 465.0206
 694.4502 726.9493 797.1010
 802.0077 912.6836 942.0971
 980.4905 1025.4069 1043.3074
 1272.3421 1862.0364 3559.9118
 Zero-point correction (Hartree): 0.035788

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cy_N_H_C_O_OOO
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -393.29336201
E(CCSD/Aug-CC-pVDZ) (Hartree): -393.24730186
  T1 diagnostic: 0.019248
E(MP2/Aug-CC-pVDZ) (Hartree): -393.23472686
E(MP3/Aug-CC-pVDZ) (Hartree): -393.23124254
E(RHF/Aug-CC-pVDZ) (Hartree): -392.15347405
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -393.62318191
E(CCSD/Aug-CC-pVTZ) (Hartree): -393.55818073
E(MP2/Aug-CC-pVTZ) (Hartree): -393.56113073
E(MP3/Aug-CC-pVTZ) (Hartree): -393.54809819
E(RHF/6-31G(d,p)) (Hartree): -392.08933928
E(RHF/Aug-CC-pVTZ) (Hartree): -392.24768499
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -393.72378873
E(CCSD/Aug-CC-pVQZ) (Hartree): -393.65431251
  T1 diagnostic: 0.017762
E(MP2/Aug-CC-pVQZ) (Hartree): -393.66923453
E(MP3/Aug-CC-pVQZ) (Hartree): -393.64745748
E(RHF/Aug-CC-pVQZ) (Hartree): -392.27252394
E(RM062X/Aug-CC-pVTZ) (Hartree): -394.13765090
Electronic state : 1-A
Cartesian coordinates (Angs):
  N      -0.070709      1.128511      0.031724
  C       0.811905      0.016759     -0.021234
  O       1.990015      0.016242      0.004440
  H      -0.086374      1.532911      0.969066
  O      -1.311579      0.607948     -0.279911
  O      -1.253486     -0.705461      0.275587
  O       0.038788     -1.110360     -0.133082
Rotational constants (GHz):   8.7917500   3.9586600   2.8420600
Vibrational harmonic frequencies (cm-1):
  187.5161      392.8537      513.3355
  646.3573      722.7067      786.8801
  863.6550      878.6671      952.1559
  1029.4235     1099.5336     1200.9928
  1408.3970     1977.3872     3439.9504
Zero-point correction (Hartree): 0.036678

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OC_O_N_H_OO
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -393.25629555
E(CCSD/Aug-CC-pVDZ) (Hartree): -393.18873036
  T1 diagnostic: 0.035006
E(MP2/Aug-CC-pVDZ) (Hartree): -393.20425933
E(MP3/Aug-CC-pVDZ) (Hartree): -393.16099520
E(RHF/Aug-CC-pVDZ) (Hartree): -392.04555991
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -393.58035675
E(CCSD/Aug-CC-pVTZ) (Hartree): -393.49291826
E(MP2/Aug-CC-pVTZ) (Hartree): -393.52564973
E(MP3/Aug-CC-pVTZ) (Hartree): -393.47125663
E(RHF/6-31G(d,p)) (Hartree): -391.97753686
E(RHF/Aug-CC-pVTZ) (Hartree): -392.13686092
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -393.68021968
E(CCSD/Aug-CC-pVQZ) (Hartree): -393.58823743
  T1 diagnostic: 0.033554
E(MP2/Aug-CC-pVQZ) (Hartree): -393.63347143
E(MP3/Aug-CC-pVQZ) (Hartree): -393.56991710
E(RHF/Aug-CC-pVQZ) (Hartree): -392.16203706
E(RM062X/Aug-CC-pVTZ) (Hartree): -394.06519495
Electronic state : 1-A
Cartesian coordinates (Angs):
  C       0.987419      0.051038     -0.034199
  N      -0.047579     -0.965433     -0.049990
  H       0.010912     -1.645191      0.710555
  O       2.150525     -0.164691     -0.143843
  O      -1.112674     -0.012041      0.404086
  O      -2.045010      0.042428     -0.368664
  O       0.306863      1.146428      0.088991
Rotational constants (GHz):  11.7353900   2.8130200   2.3927000
Vibrational harmonic frequencies (cm-1):
  135.5822      256.7675      458.8756
  507.1398      601.0420      642.0171
  719.9268      824.4984      884.9283
  1009.1998     1232.3274     1335.4959
  1452.6617     1924.3081     3455.9903
Zero-point correction (Hartree): 0.035177

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Transition states
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TS.HNCO+O3.cy_C_NH_OOOO
-----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -393.21425434
E(CCSD/Aug-CC-pVDZ) (Hartree): -393.15060335
  T1 diagnostic: 0.038429
E(MP2/Aug-CC-pVDZ) (Hartree): -393.15547870

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E(MP3/Aug-CC-pVDZ) (Hartree): -393.12359387
 E(RHF/Aug-CC-pVDZ) (Hartree): -392.01073158
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -393.53998104
 E(CCSD/Aug-CC-pVTZ) (Hartree): -393.45626749
 E(MP2/Aug-CC-pVTZ) (Hartree): -393.47810321
 E(MP3/Aug-CC-pVTZ) (Hartree): -393.43547331
 E(RHF/6-31G(d,p)) (Hartree): -391.94343984
 E(RHF/Aug-CC-pVTZ) (Hartree): -392.10325578
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -393.64005897
 E(CCSD/Aug-CC-pVQZ) (Hartree): -393.55168392
 T1 diagnostic: 0.037145
 E(MP2/Aug-CC-pVQZ) (Hartree): -393.58592336
 E(MP3/Aug-CC-pVQZ) (Hartree): -393.53419946
 E(RHF/Aug-CC-pVQZ) (Hartree): -392.12850051
 E(RM062X/Aug-CC-pVTZ) (Hartree): -394.03578149
 Electronic state : 1-A
 Cartesian coordinates (Angs):

N	-2.068268	-0.128887	0.107236
H	-2.188556	-1.132308	0.187122
C	-0.883750	0.214754	-0.032124
O	-0.194667	1.225384	-0.218626
O	1.329088	-0.538218	-0.290278
O	0.150511	-1.084198	0.030757
O	1.461184	0.490281	0.385019

 Rotational constants (GHz): 8.7143200 3.5539500 2.6489200
 Vibrational harmonic frequencies (cm-1):

i641.4321	137.7413	333.7787
481.1350	527.5903	681.6602
683.5741	733.9279	826.6644
1015.7604	1084.3039	1214.5230
1306.8747	1875.3845	3572.2633

 Zero-point correction (Hartree): 0.032977

TS.HNCO+O3.cy_N_H_C_O_OOO

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -393.22437247
 E(CCSD/Aug-CC-pVDZ) (Hartree): -393.16215473
 T1 diagnostic: 0.037450
 E(MP2/Aug-CC-pVDZ) (Hartree): -393.17527172
 E(MP3/Aug-CC-pVDZ) (Hartree): -393.13731545
 E(RHF/Aug-CC-pVDZ) (Hartree): -392.02240764
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -393.55036463
 E(CCSD/Aug-CC-pVTZ) (Hartree): -393.46786571
 E(MP2/Aug-CC-pVTZ) (Hartree): -393.49810008
 E(MP3/Aug-CC-pVTZ) (Hartree): -393.44904786
 E(RHF/6-31G(d,p)) (Hartree): -391.95560007
 E(RHF/Aug-CC-pVTZ) (Hartree): -392.11467745
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -393.65053184
 E(CCSD/Aug-CC-pVQZ) (Hartree): -393.56334578
 T1 diagnostic: 0.036147
 E(MP2/Aug-CC-pVQZ) (Hartree): -393.60598779
 E(MP3/Aug-CC-pVQZ) (Hartree): -393.54778370
 E(RHF/Aug-CC-pVQZ) (Hartree): -392.13992146
 E(RM062X/Aug-CC-pVTZ) (Hartree): -394.04850529
 Electronic state : 1-A
 Cartesian coordinates (Angs):

N	0.314593	1.241803	-0.011267
H	0.196104	1.795062	0.826679
C	1.045997	0.204167	0.017336
O	2.054624	-0.370033	-0.020763
O	-1.466176	0.573237	-0.295167
O	-1.346726	-0.500825	0.345430
O	-0.326003	-1.166465	-0.135978

 Rotational constants (GHz): 8.0451000 3.3375700 2.4564200
 Vibrational harmonic frequencies (cm-1):

i643.5327	119.5269	271.6102
393.1549	463.2466	546.7089
641.8543	657.1761	809.7450
910.5677	1087.3114	1214.0559
1272.3605	2142.7675	3600.1179

 Zero-point correction (Hartree): 0.032191

TS.HNCO+O3.HN_O_CO+O2

 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -393.16933291
 E(CCSD/Aug-CC-pVDZ) (Hartree): -393.11130194
 T1 diagnostic: 0.030142
 E(MP2/Aug-CC-pVDZ) (Hartree): -393.10696261
 E(MP3/Aug-CC-pVDZ) (Hartree): -393.08271719
 E(RHF/Aug-CC-pVDZ) (Hartree): -391.99696427
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -393.49562738
 E(CCSD/Aug-CC-pVTZ) (Hartree): -393.41807532
 E(MP2/Aug-CC-pVTZ) (Hartree): -393.43045920
 E(MP3/Aug-CC-pVTZ) (Hartree): -393.39601167
 E(RHF/6-31G(d,p)) (Hartree): -391.93435226
 E(RHF/Aug-CC-pVTZ) (Hartree): -392.09173481
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -393.59493902
 E(CCSD/Aug-CC-pVQZ) (Hartree): -393.51284851

T1 diagnostic: 0.028433
 E(MP2/Aug-CC-pVQZ) (Hartree): -393.53756286
 E(MP3/Aug-CC-pVQZ) (Hartree): -393.49413683
 E(RHF/Aug-CC-pVQZ) (Hartree): -392.11652776
 E(RM062X/Aug-CC-pVTZ) (Hartree): -393.99287981
 Electronic state : 1-A
 Cartesian coordinates (Angs):

N	-0.992644	0.923071	-0.000157
C	-1.853225	0.056515	-0.000003
O	-2.578412	-0.831640	0.000258
H	-1.115518	1.921663	-0.001329
O	0.624660	0.279333	-0.000050
O	2.175961	-0.268432	0.631090
O	2.175714	-0.269543	-0.630992

 Rotational constants (GHz): 11.7530100 1.5175000 1.4416500
 Vibrational harmonic frequencies (cm-1):

i816.7682	60.8409	85.2170
115.8623	154.6666	313.1689
405.4050	610.2117	639.0544
642.9089	930.9578	1357.0847
1402.7476	2371.7850	3680.7108

 Zero-point correction (Hartree): 0.029094

TS.HNCO+O3.HO3+NCO

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -393.21947422
 E(CCSD/Aug-CC-pVDZ) (Hartree): -393.15650943
 T1 diagnostic: 0.037799
 E(MP2/Aug-CC-pVDZ) (Hartree): -393.16888505
 E(MP3/Aug-CC-pVDZ) (Hartree): -393.13055999
 E(RHF/Aug-CC-pVDZ) (Hartree): -392.02019818
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -393.54687307
 E(CCSD/Aug-CC-pVTZ) (Hartree): -393.46379739
 E(MP2/Aug-CC-pVTZ) (Hartree): -393.49295827
 E(MP3/Aug-CC-pVTZ) (Hartree): -393.44394106
 E(RHF/6-31G(d,p)) (Hartree): -391.95401143
 E(RHF/Aug-CC-pVTZ) (Hartree): -392.11451023
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -393.64691612
 E(CCSD/Aug-CC-pVQZ) (Hartree): -393.55922155
 T1 diagnostic: 0.036144
 E(MP2/Aug-CC-pVQZ) (Hartree): -393.60079263
 E(MP3/Aug-CC-pVQZ) (Hartree): -393.54259894
 E(RHF/Aug-CC-pVQZ) (Hartree): -392.13978898
 E(RM062X/Aug-CC-pVTZ) (Hartree): -394.04818822
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.575555	-0.219476	0.062467
N	0.498562	-0.684926	0.356175
H	-0.690004	-1.009522	-0.129684
O	2.634664	0.199420	-0.169607
O	-1.816945	-0.749291	-0.316422
O	-1.700933	0.457972	0.261511
O	-0.648444	0.982006	-0.117776

 Rotational constants (GHz): 12.0979700 1.9757100 1.7600700
 Vibrational harmonic frequencies (cm-1):

i1353.1295	54.7923	100.8968
334.2962	478.8113	556.3274
646.5053	673.3756	811.5787
1037.2417	1117.5813	1303.6615
1422.4970	1861.9079	2301.5000

 Zero-point correction (Hartree): 0.028935

TS.HNCO+O3.OC_O_N_H_OO

E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -393.20755552
 E(CCSD/Aug-CC-pVDZ) (Hartree): -393.14157943
 T1 diagnostic: 0.043962
 E(MP2/Aug-CC-pVDZ) (Hartree): -393.14492233
 E(MP3/Aug-CC-pVDZ) (Hartree): -393.11171907
 E(RHF/Aug-CC-pVDZ) (Hartree): -392.00473865
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -393.53298073
 E(CCSD/Aug-CC-pVTZ) (Hartree): -393.44737647
 E(MP2/Aug-CC-pVTZ) (Hartree): -393.46716648
 E(MP3/Aug-CC-pVTZ) (Hartree): -393.42366756
 E(RHF/6-31G(d,p)) (Hartree): -391.93659793
 E(RHF/Aug-CC-pVTZ) (Hartree): -392.09852017
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -393.63305004
 E(CCSD/Aug-CC-pVQZ) (Hartree): -393.54284944
 T1 diagnostic: 0.042860
 E(MP2/Aug-CC-pVQZ) (Hartree): -393.57493448
 E(MP3/Aug-CC-pVQZ) (Hartree): -393.52236092
 E(RHF/Aug-CC-pVQZ) (Hartree): -392.12401976
 E(RM062X/Aug-CC-pVTZ) (Hartree): -394.02679946
 Electronic state : 1-A
 Cartesian coordinates (Angs):

N	0.504538	1.246251	-0.077161
C	1.064212	0.066844	-0.034212
O	2.099559	-0.496818	-0.021080

H	1.171844	1.978391	0.154970	
O	-1.150520	-0.034262	0.423369	
O	-2.132367	0.032856	-0.260892	
O	-0.202783	-0.889677	-0.067594	
Rotational constants (GHz):		10.8757300	2.6912800	2.2367500
Vibrational harmonic frequencies (cm-1):				
	1572.5421	114.1327		217.5569
	346.5962	499.6931		615.8756
	695.1183	709.0945		768.5036
	975.3033	1145.3223		1217.5113
	1471.5528	1973.7783		3514.2273
Zero-point correction (Hartree): 0.032496				