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Supplement of

Atmospheric chemical loss processes of isocyanic acid (HNCO): a combined theoretical kinetic and global modelling study

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Contents

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 and branching ratio	Reference
$NH_2CHO + OH \rightarrow HNCO + HO_2 + H_2O$	4.47×10^{-12}	Bunkan et al., 2016
$CH_3NO_2 + OH \rightarrow HCHO + NO_2 + H_2O$	$5.8\times10^{-13}\times\exp(-1102/T)$	Calvert et al., 2008
$CH_3NO_2 + hv \rightarrow CH_3 + NO_2$	-	Taylor et al., 1980
$CH_3NH_2 + OH \rightarrow CH_2NH + H_2O + HO_2$	1.97×10^{-11}	Nielsen et al., 2012
$(CH_3)_2NH + OH \rightarrow CH_2NCH_3 + HO_2$	$0.42\times6.71\times10^{-11}$	Nielsen et al., 2012
$(CH_3)_2NH + OH \rightarrow CH_3NHCH_2 + H_2O$	$0.58\times6.71\times10^{-11}$	Nielsen et al., 2012
$CH_3NHCH_2 \rightarrow CH_2NCH_3 + HO_2$	$0.55\times1.0\times10^{6}$	Nielsen et al., 2012
$CH_3NHCH_2 \rightarrow CH_3NHCH_2O_2$	$0.45\times1.0\times10^{6}$	Nielsen et al., 2012
$CH_3NHCH_2O_2 + NO \rightarrow CH_3NHCHO + NO_2 + HO_2$	$0.5\times2.54\times10^{12}\times\exp(360/T)$	Nielsen et al., 2012
$CH_3NHCH_2O_2 + NO \rightarrow CH_2NH + HCHO + NO_2+HO_2$	$0.5\times2.54\times10^{12}\times\exp(360/T)$	Nielsen et al., 2012
$(CH_3)_3N + OH \rightarrow (CH_3)_2NCH_2O_2 + H_2O$	4.50×10^{-11}	Nielsen et al., 2012
$(CH_3)_2NCH_2O_2 + NO \rightarrow (CH_3)_2NCHO + NO_2 + HO_2$	$0.4\times2.54\times10^{12}\times\exp(360/T)$	Nielsen et al., 2012
$(CH_3)_2NCH_2O_2 + NO \rightarrow CH_2NCH_3 + HCHO + NO_2 + HO_2$	$0.6\times2.54\times10^{12}\times\exp(360/T)$	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
$HNCO + H^+ \rightarrow NH_3 + CO_2 + H^+$	$4.4\times10^{7}\times\exp(-6000/T)$	Borduas et al., 2016b
$HNCO \rightarrow NH_3 + CO2$	$8.9\times10^{6}\times\exp(-6770/T)$	Borduas et al., 2016b
$NCO^- \rightarrow NH_3 + HCO_3^-$	$7.2\times10^{8}\times\exp(-10900/T)$	Borduas et al., 2016b
$NH_2CHO + OH \rightarrow HNCO + H_2O + HO_2$	5.0×10^{8}	Barnes et al., 2010
$CN^- + OH \rightarrow HNCO + HO_2$	7.35×10^{9}	Behar 1974
$HCN + OH \rightarrow H_2O + product$	6.00×10^{7}	Buechler et al., 1976

HNCO + OH potential energy surface

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

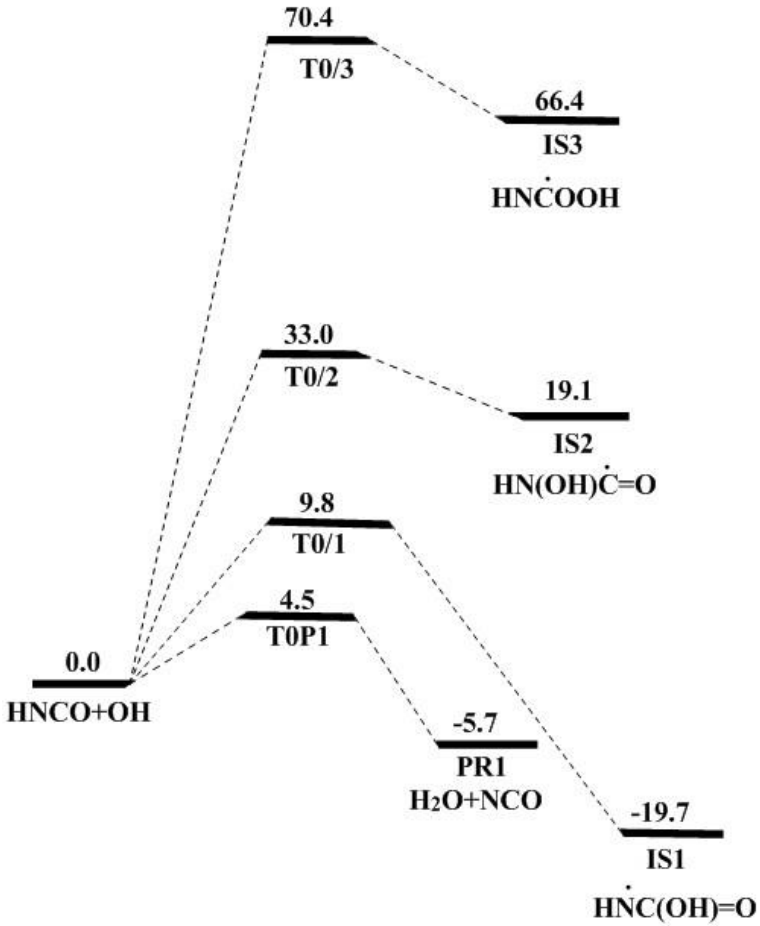


Figure 1: OH addition and hydrogen abstraction pathways of the HNCO + OH reaction calculated at the M06-2X/ aug-cc-pVTZ level of theory

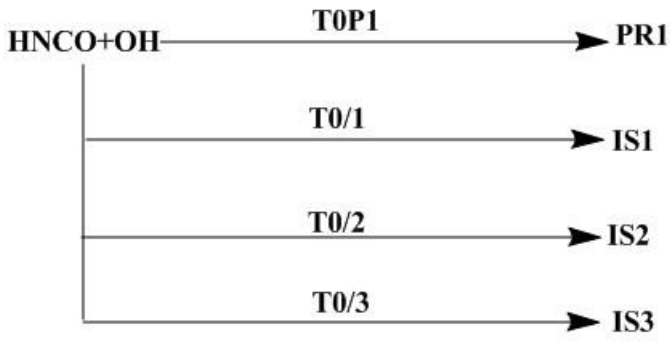
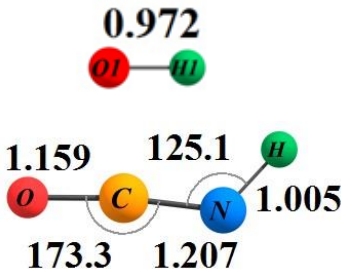


Figure 2: Diagram of the HNCO + OH reaction

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

Bond lengths in Ångstrom, angles in degrees



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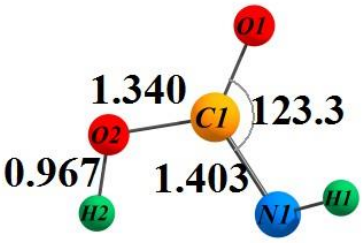

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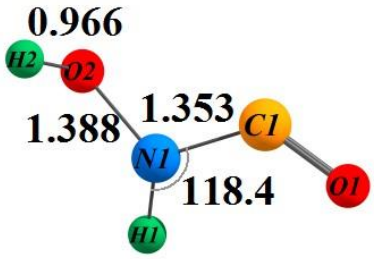

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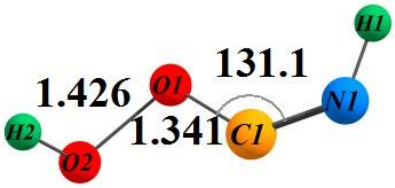

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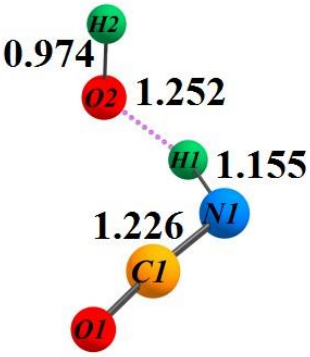

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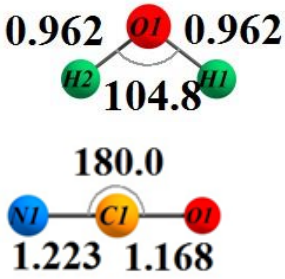

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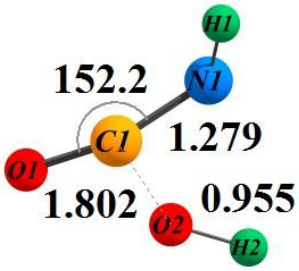

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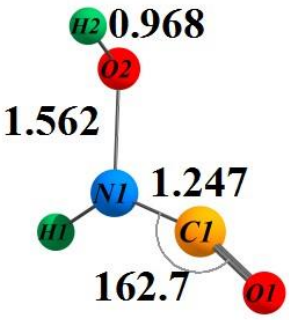

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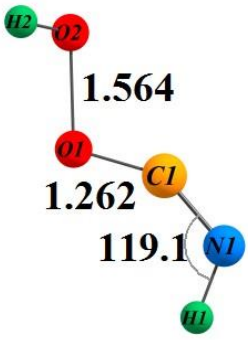


T0/3

HNCO + Cl potential energy surface

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

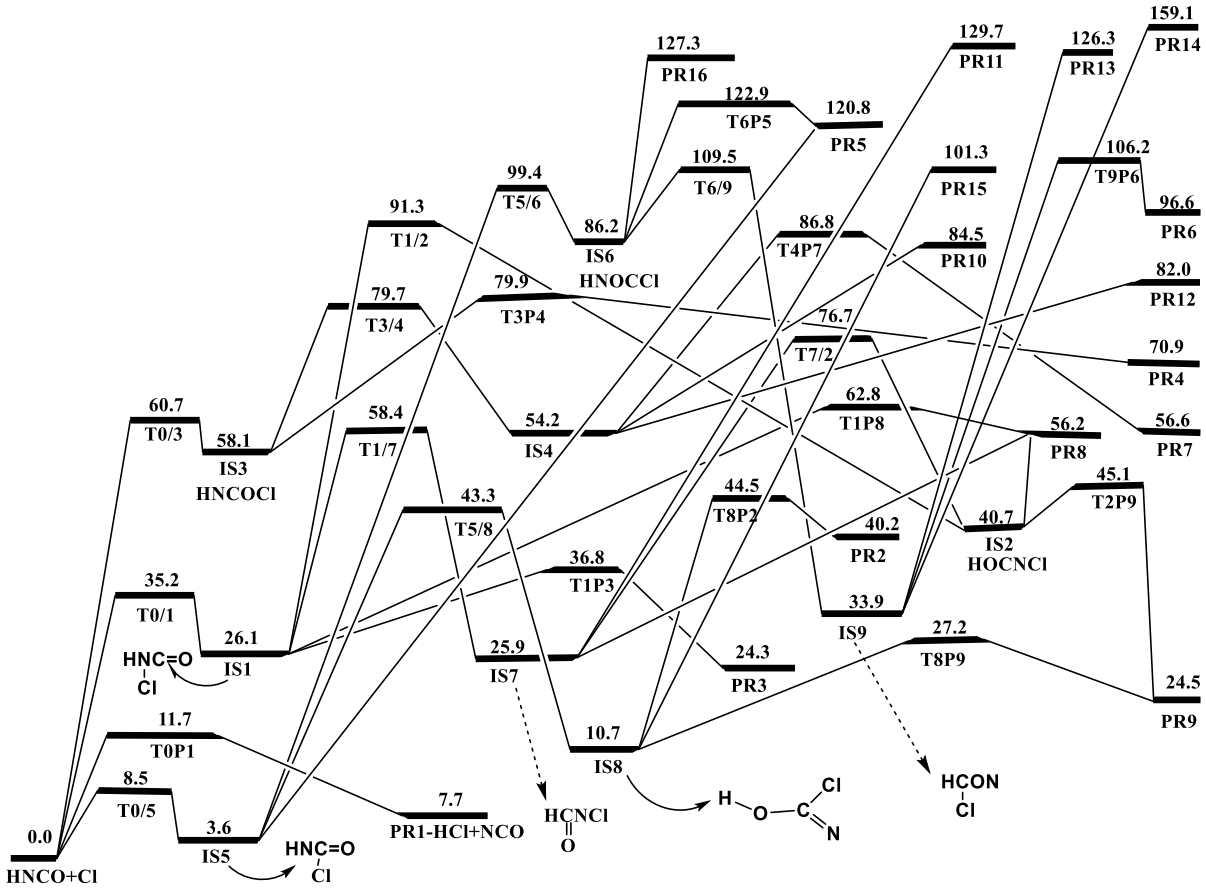


Figure 3: Detailed potential energy surface of the HNCO + Cl reaction based on ZPE-corrected CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ energies. The intermediates are depicted below.

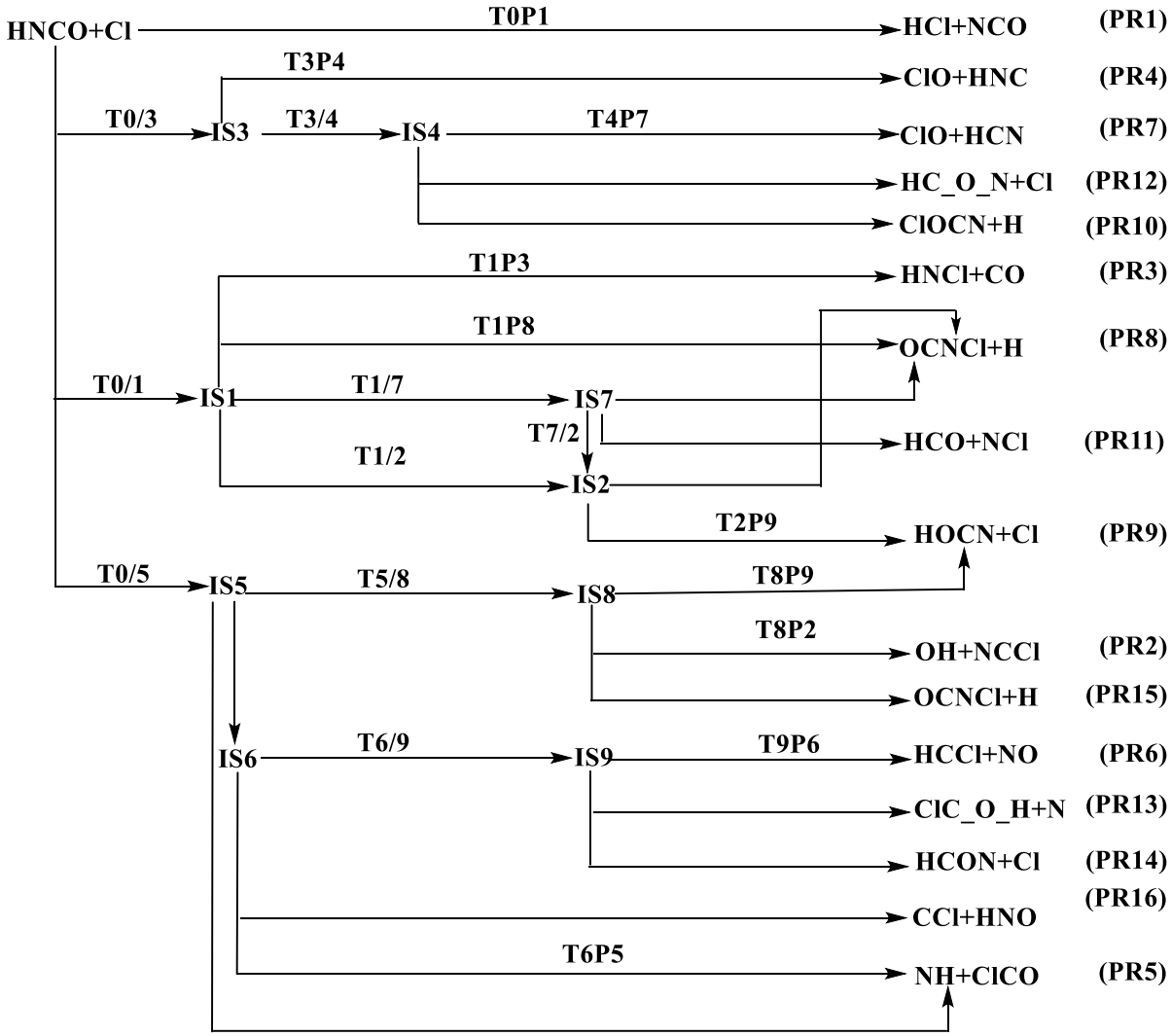
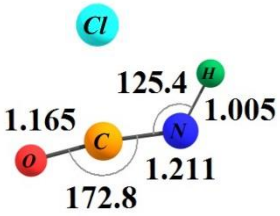


Figure 4: Diagram of the HNCO + Cl reaction

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

Bond lengths in Ångstrom, angles in degrees



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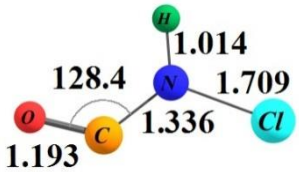

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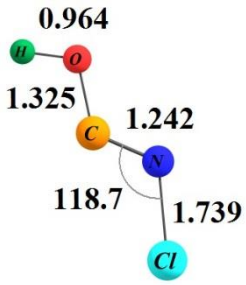

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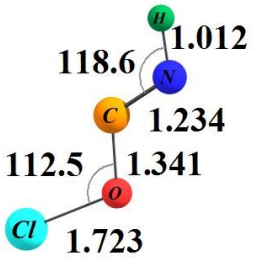

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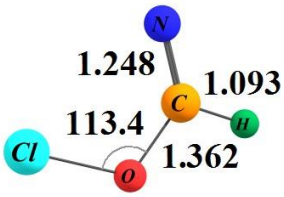

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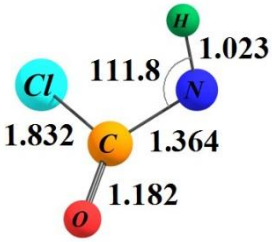

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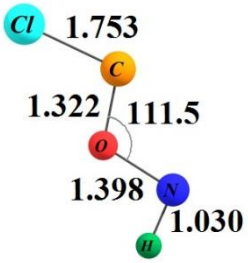

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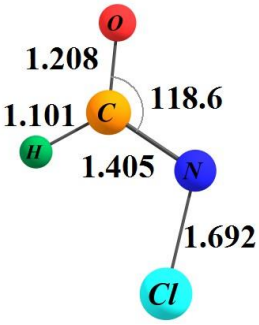

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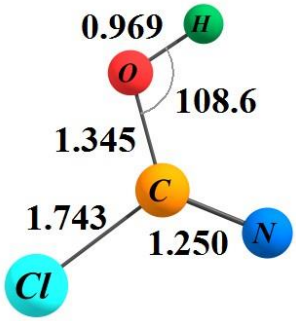

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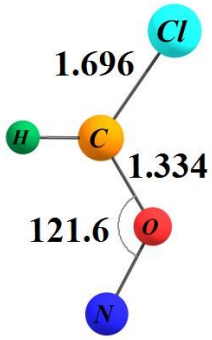

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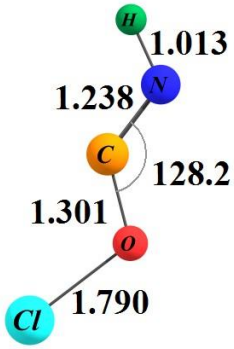

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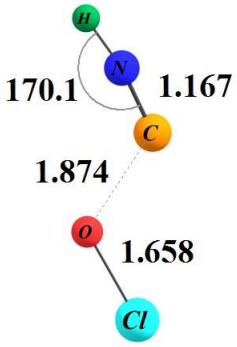

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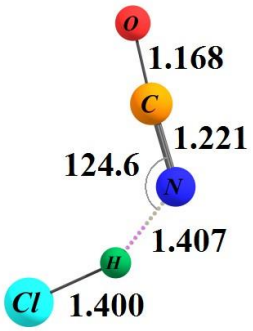

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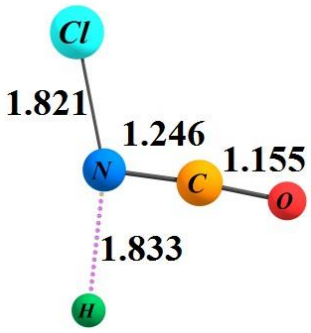

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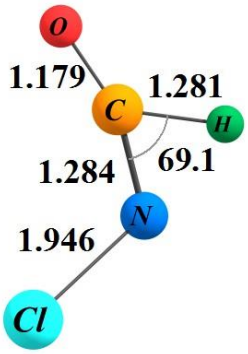

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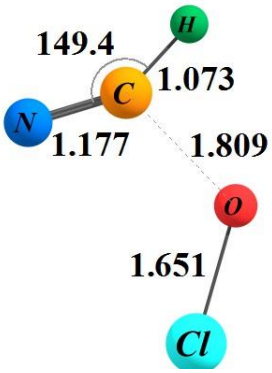

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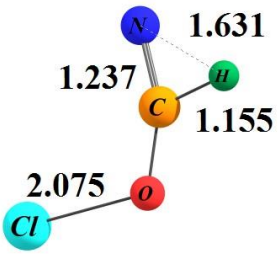

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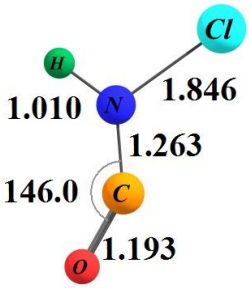

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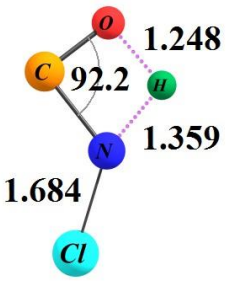

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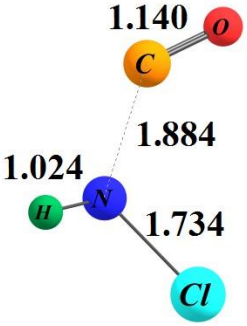

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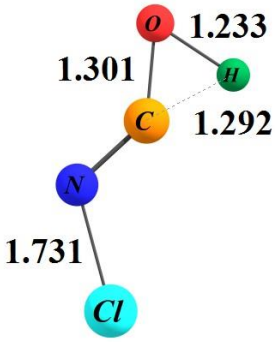

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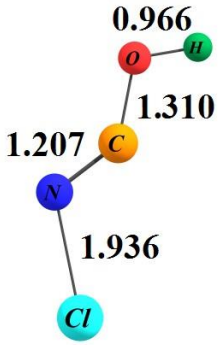

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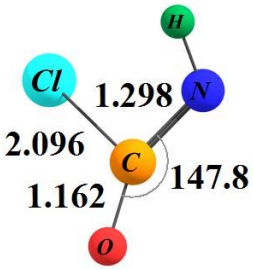

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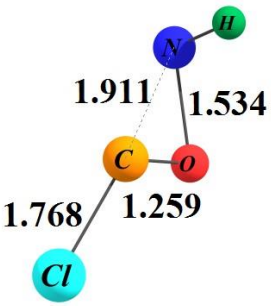

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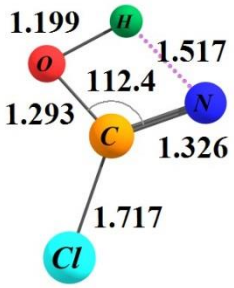

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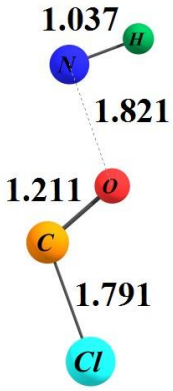

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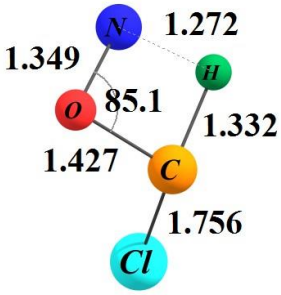

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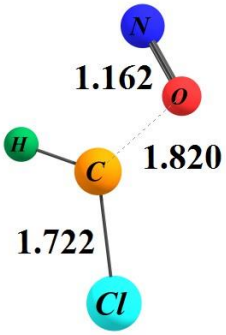

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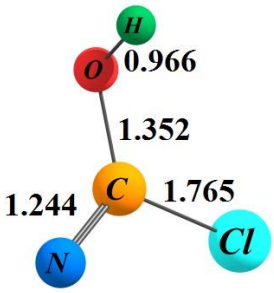

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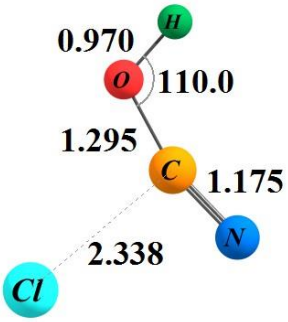

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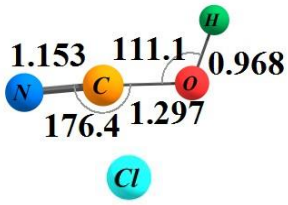

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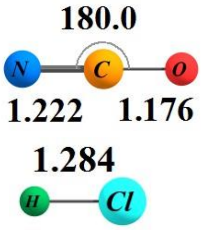

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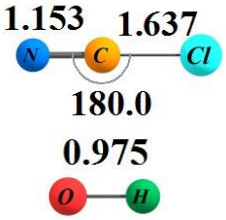

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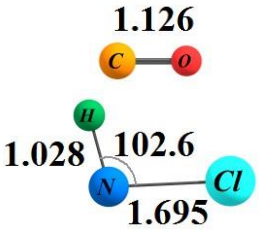

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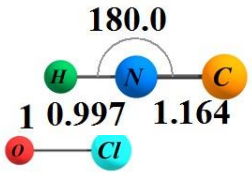

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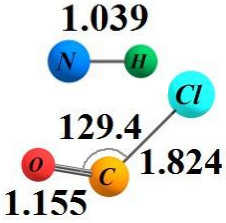

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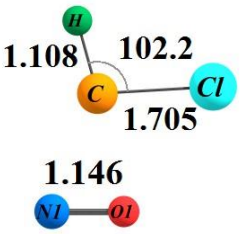

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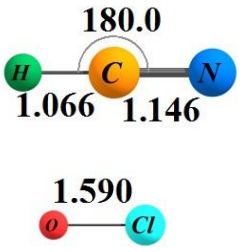

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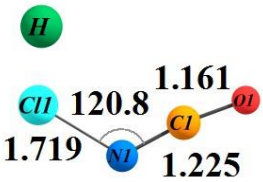

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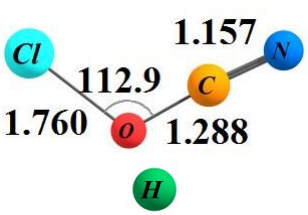

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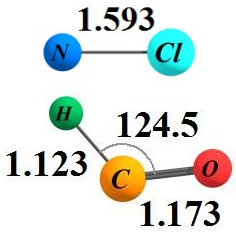

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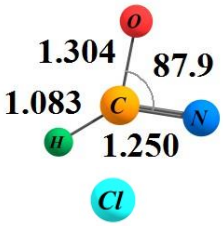

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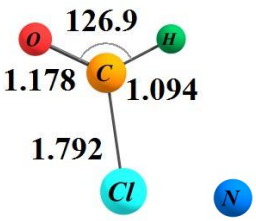

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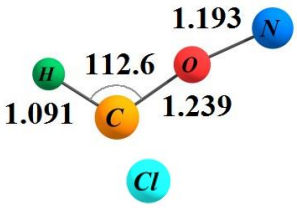

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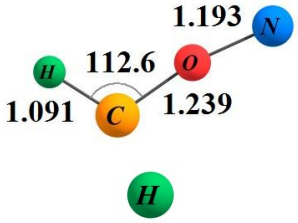

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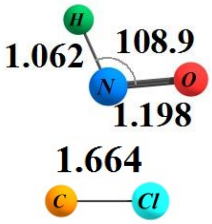
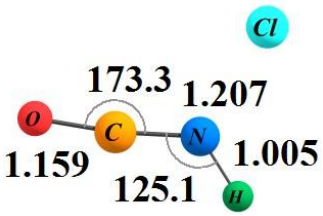


PR16

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

Bond lengths in Ångstrom, angles in degrees



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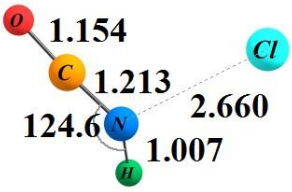

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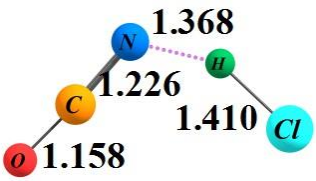

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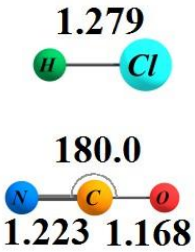

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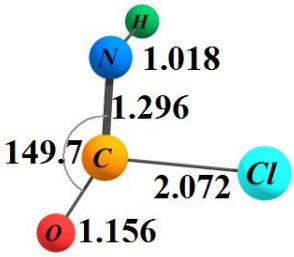
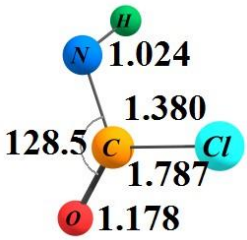


T0/5



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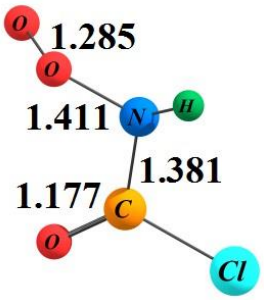


ClC(=O)NHOO

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

Table 5: Theoretical predication of relative energies ΔE (kcal/mol) for reactants, intermediates, transition states and products of the Cl + HNCO reaction. Levels of theory used are B3LYP/aug-cc-pVTZ (designated as B3LYP) and CCSD(T)/aug-cc-pVTZ//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 + NO_3 potential energy surface

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

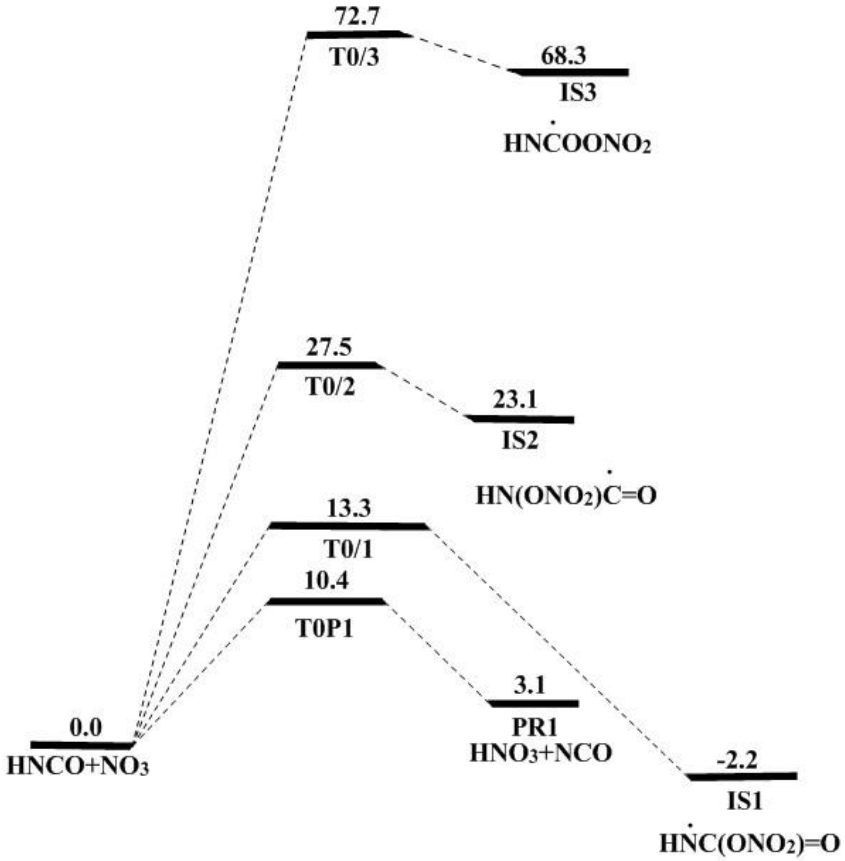


Figure 5: NO_3 addition and hydrogen abstraction pathways of the HNCO + NO_3 reaction calculated at the M06-2X/ aug-cc-pVTZ level of theory

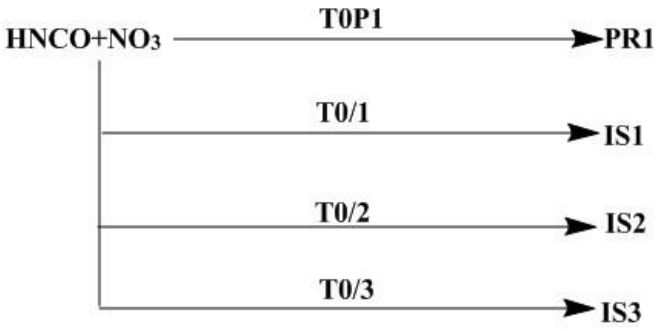
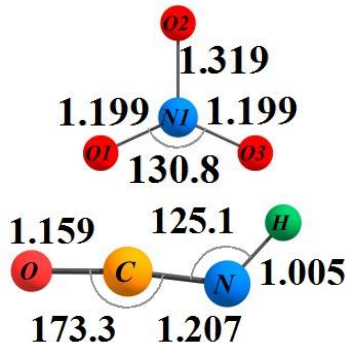


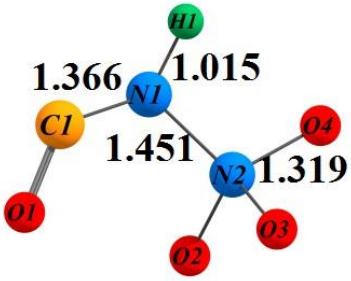
Figure 6: Diagram of the HNCO + NO_3 reaction

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

Bond lengths in Ångstrom, angles in degrees



RA



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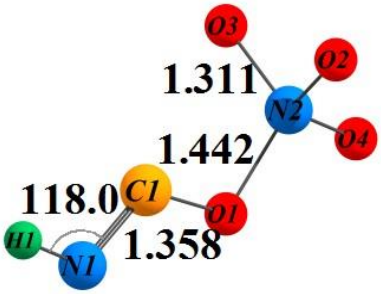

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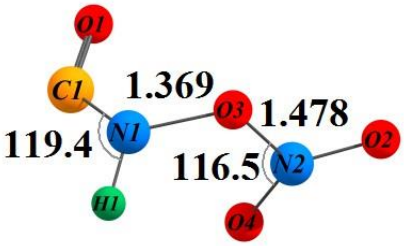

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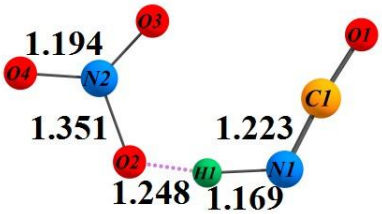

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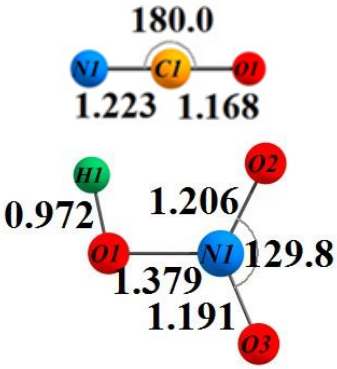

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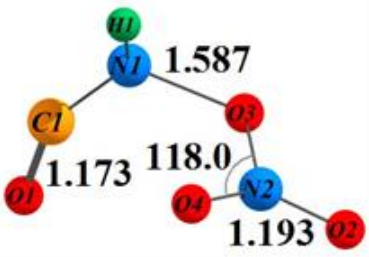
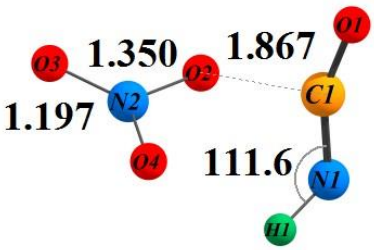


T0/3



T0/4

HNCO + O_3 potential energy surface

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

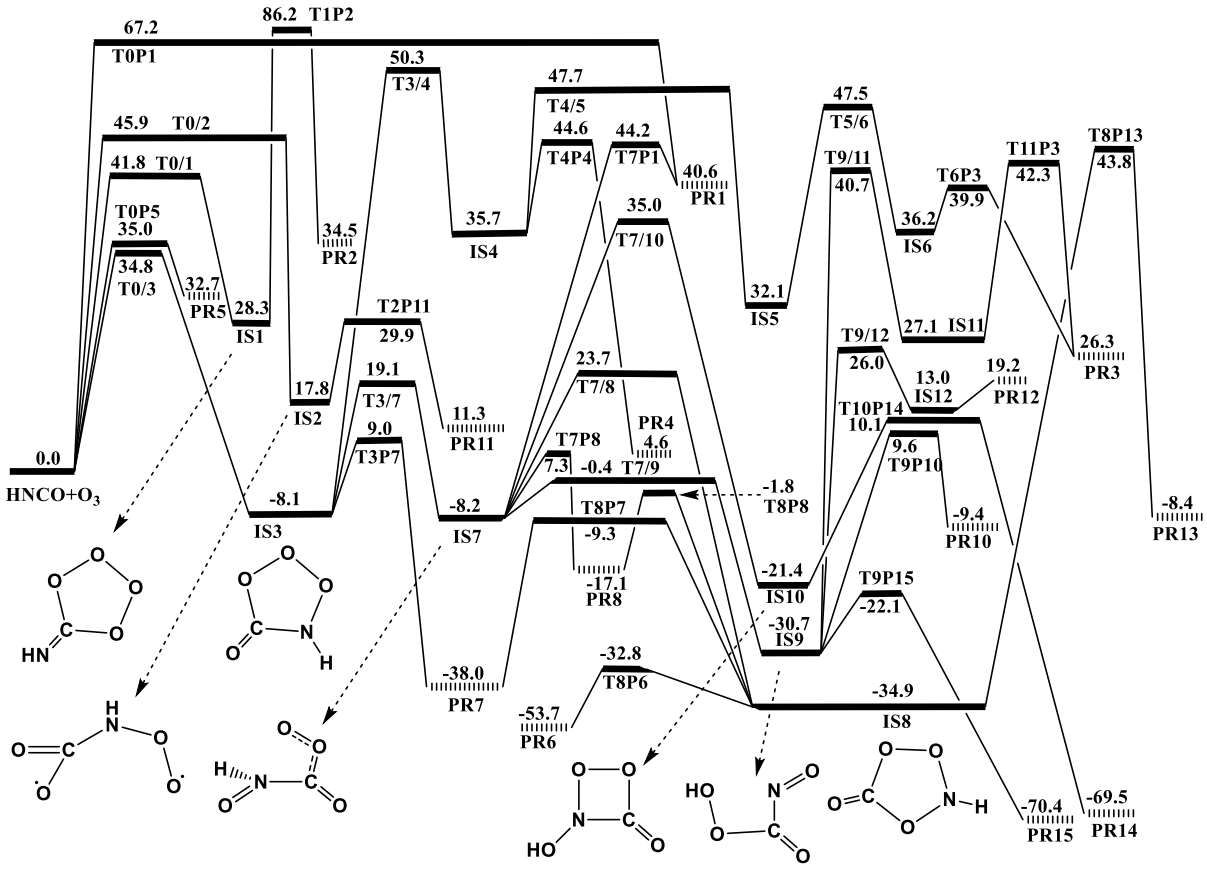


Figure 7: Detailed potential energy surface of the HNCO + O_3 reaction based on ZPE-corrected CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ energies. The intermediates are depicted below.

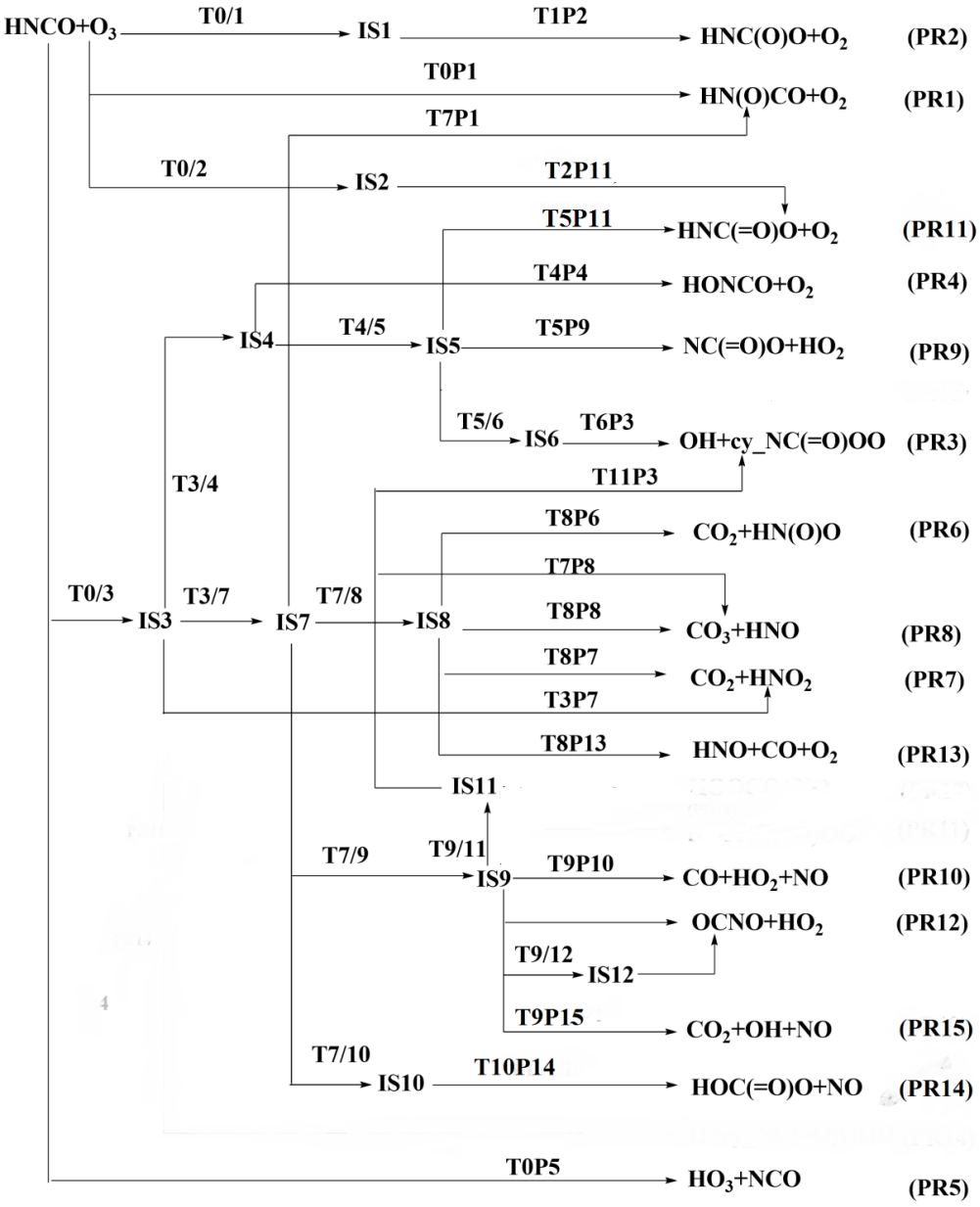
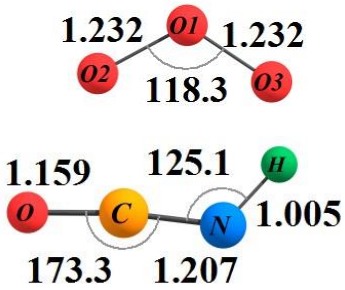


Figure 8: Diagram of the HNCO + O_3 reaction

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

Bond lengths in Ångstrom, angles in degrees



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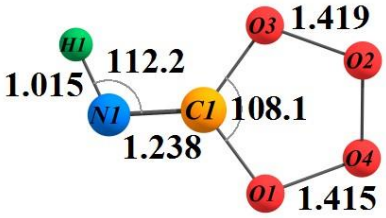

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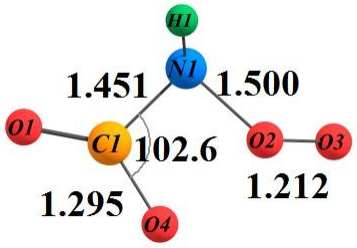

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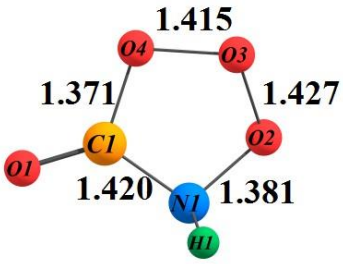

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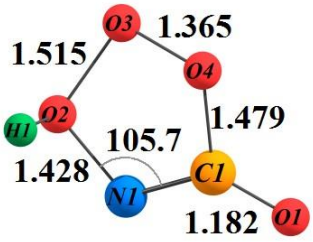

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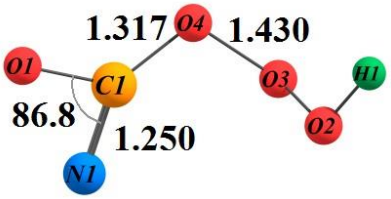

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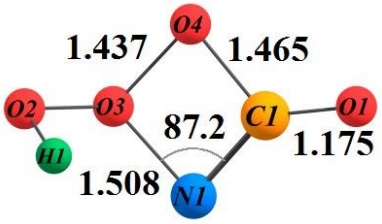

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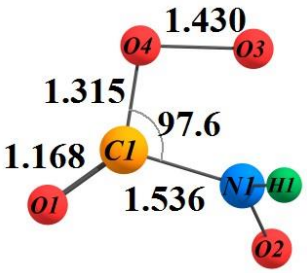

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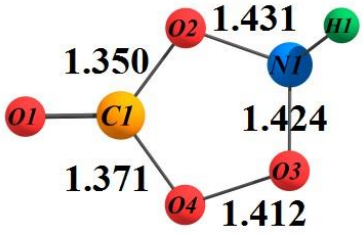

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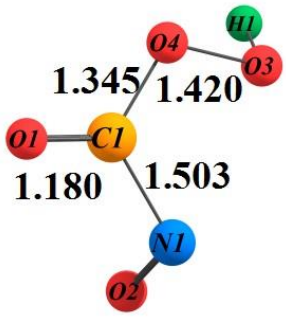

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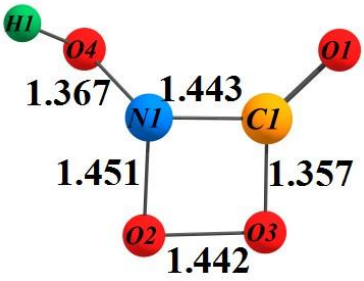
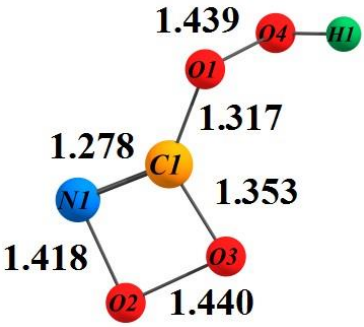


IS10



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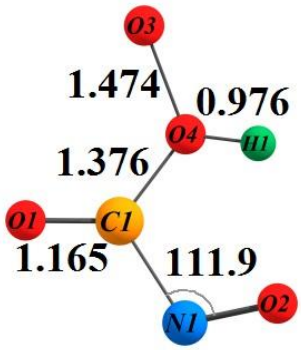

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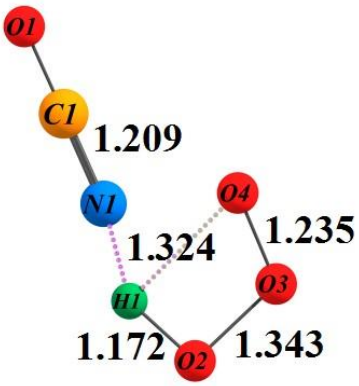
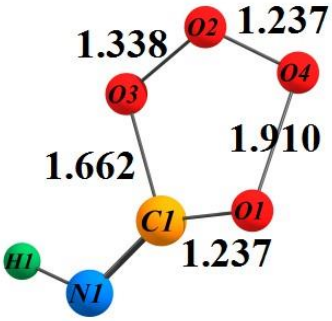
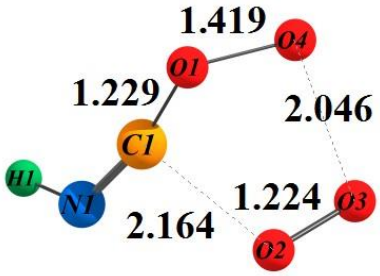


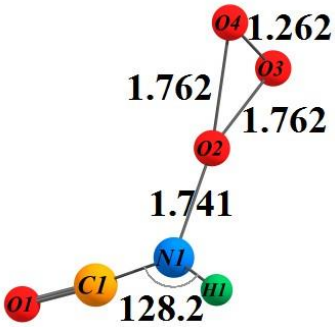
T0P5



T0/1



T1P2



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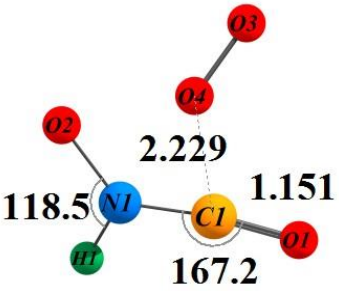

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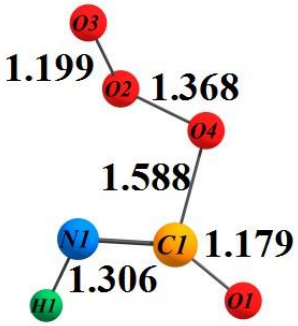

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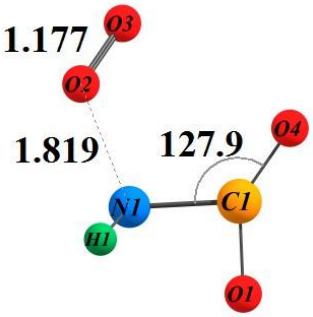

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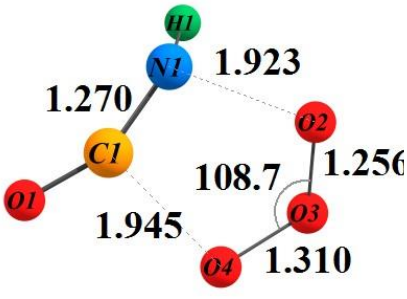

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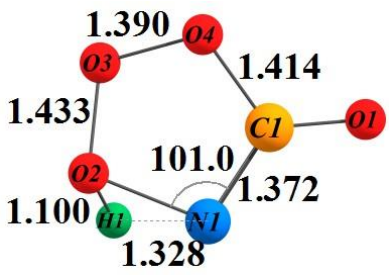

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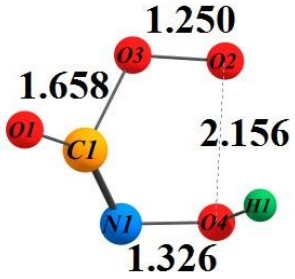

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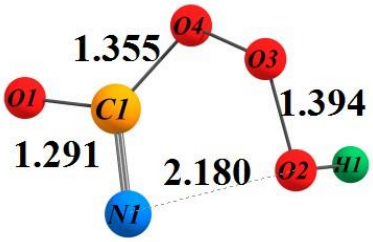

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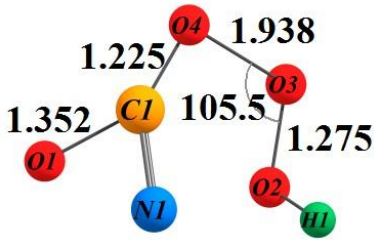

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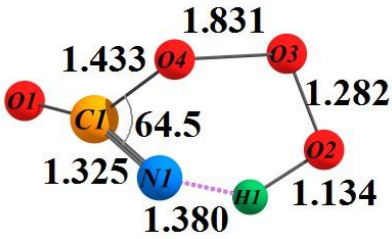

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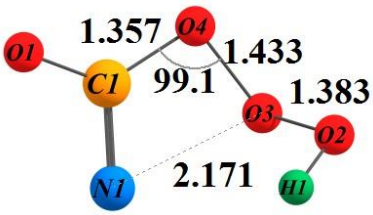

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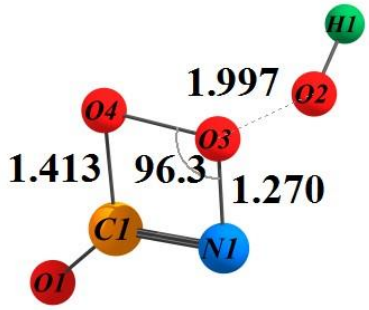

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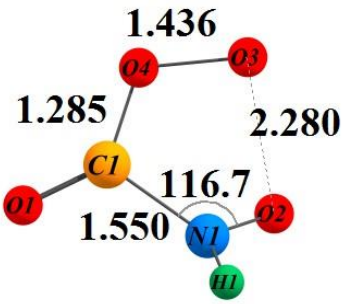

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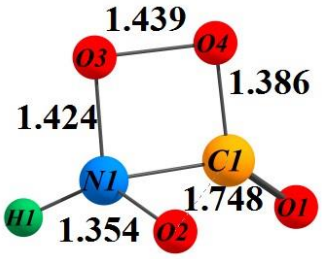

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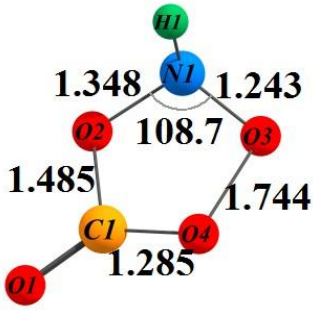

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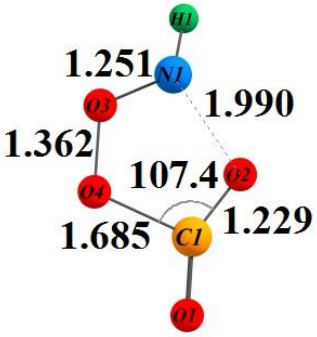

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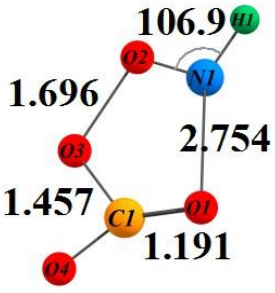

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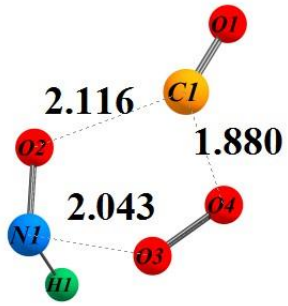

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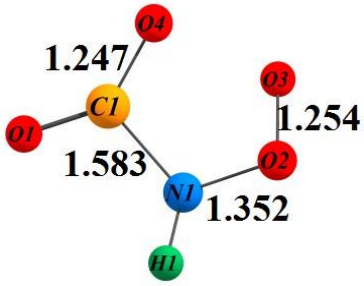

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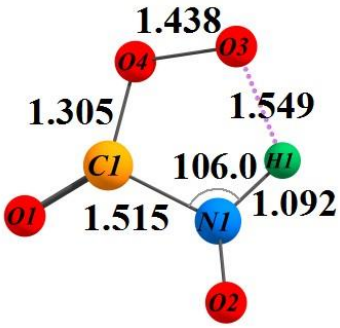

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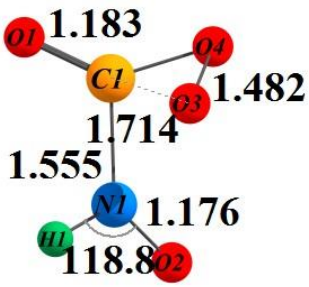

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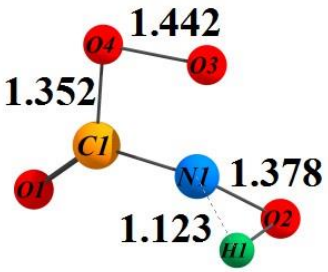

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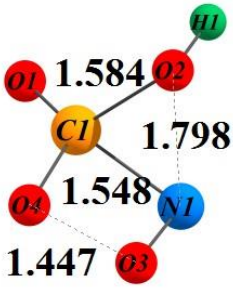

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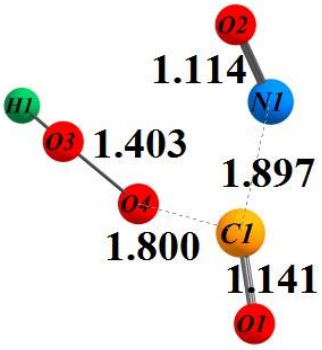

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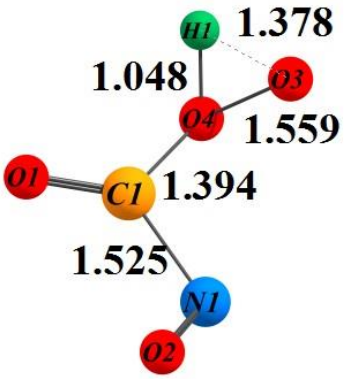

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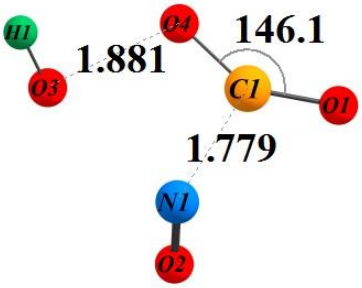

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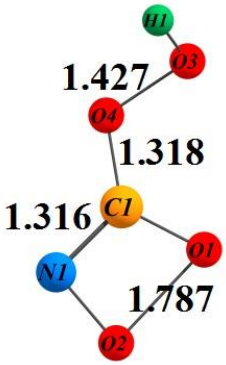

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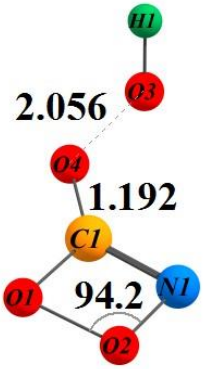

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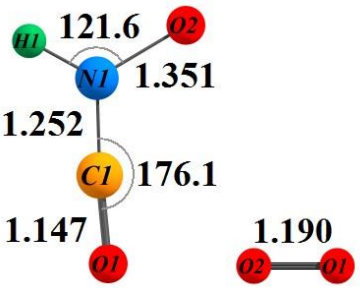

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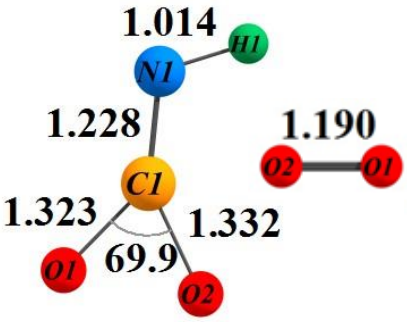

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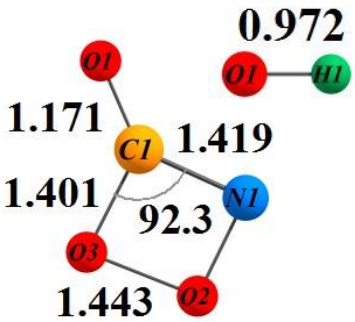

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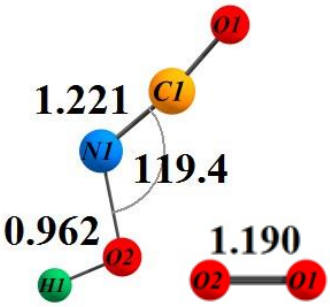

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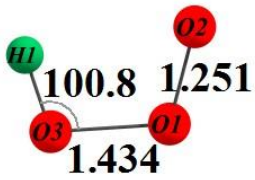

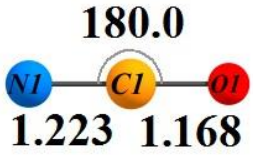

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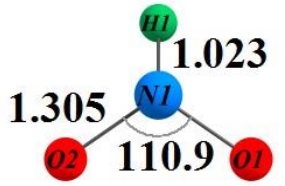

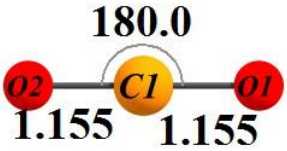

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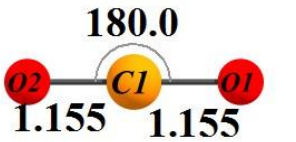

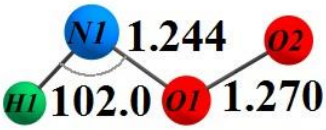

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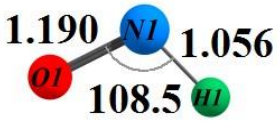

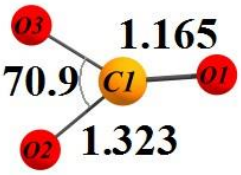

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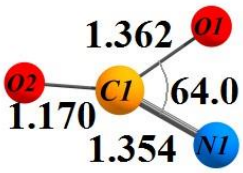

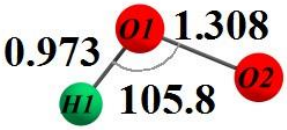

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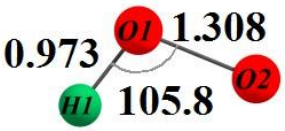

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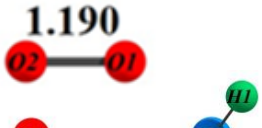

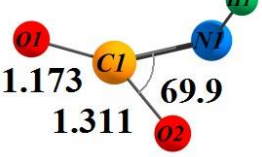

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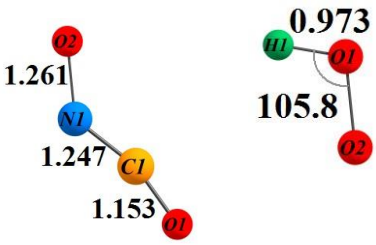

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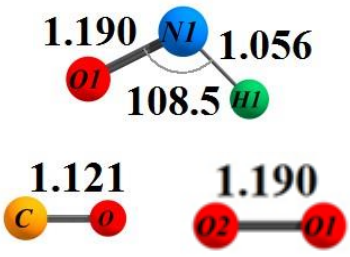

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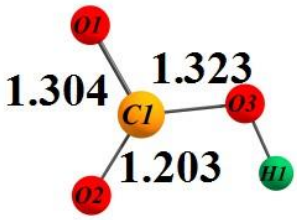

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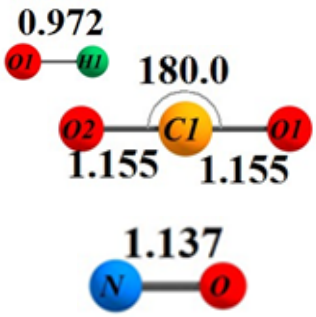

PR15

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^o) (298.15 K) (kcal mol^{-1})	(ΔS^o) (298.15 K) (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 O_3 + 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 (HN(O)CO + O_2)	34.4	40.8	
PR2 (HNC(=O)O + O_2)	37.1	41.0	
PR3 (cy_NC(=O)OO + OH)	14.0	21.2	
PR4 (HONCO + O_2)	-2.1	4.9	
PR5 (HO_3 + NCO)	29.5	30.1	30.4
PR6 (HN(O)O + CO_2)	-61.0	-56.1	
PR7 (HNOO + CO_2)	-45.6	-43.3	
PR8 (HNO + CO_3)	-27.9	-22.2	
PR9 (NC(=O)O + HO_2)	5.9	16.6	
PR10 (HO_2 + CO + NO)	-19.8	-13.0	-11.3
PR11 (HNC(=O)O + O_2)	6.4	11.0	
PR12 (HO_2 + ONCO)	1.3	14.5	
PR13 (HNO + O_2 + CO)	-18.5	-12.0	-10.4
PR14 (HOC(=O)O + NO)	-84.5	-74.5	
PR15 (HO_2 + CO + 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

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

Fragments
=========

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
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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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -167.76182535
E(CCSD/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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -167.80302538
E(CCSD/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(CCSD(T)/Aug-CC-pVDZ) (Hartree):  -75.58402897
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree):  -75.64558463
E(CCSD/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(CCSD(T)/Aug-CC-pVQZ) (Hartree):  -75.66449303
E(CCSD/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(CCSD(T)/Aug-CC-pVDZ) (Hartree): -243.92382876
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -244.12846223
E(CCSD/Aug-CC-pVTZ) (Hartree): -244.09269439
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     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
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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
=================

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)
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E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -243.87677763
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -244.08076434
E(CCSD/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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -244.14299039
E(CCSD/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(CCSD(T)/Aug-CC-pVDZ) (Hartree): -243.77589344
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -243.98133797
E(CCSD/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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -244.04311992
E(CCSD/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
```

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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
################################################################################

Fragments
=========

Cl
--
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
---
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 : C*V
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
----
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
---
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
=======

HNCClO
------
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

HNClCO
------
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
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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
=================

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
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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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -628.15968091
E(CCSD/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(CCSD(T)/Aug-CC-pVDZ) (Hartree): -627.90145327
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -628.10871220
E(CCSD/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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -628.17141825
E(CCSD/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(CCSD(T)/Aug-CC-pVDZ) (Hartree): -627.85424253
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -628.06431547
E(CCSD/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
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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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -628.12739577
E(CCSD/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(CCSD(T)/Aug-CC-pVDZ) (Hartree): -627.81525783
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -628.02313037
E(CCSD/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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -628.08546760
E(CCSD/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
################################################################################

Fragments
=========

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
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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
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E(PUHF/Aug-CC-pVQZ) (Hartree): -167.21474443
E(UHF/Aug-CC-pVQZ) (Hartree): -167.20269276
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

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-pVTZ) (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
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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
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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
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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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -448.19416759
E(CCSD/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(CCSD(T)/Aug-CC-pVDZ) (Hartree): -447.94832392
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -448.31706238
E(CCSD/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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -448.42953025
E(CCSD/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
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E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -447.90744407
E(CCSD/Aug-CC-pVDZ) (Hartree): -447.84962528
     T1 diagnostic:  0.021784
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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
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TS.HN_CO_NO3.HNCONO3
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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
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     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
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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
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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
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################################################################################
HNCO + O3 : M06-2X/aug-cc-pVTZ geometry
################################################################################

Fragments
=========

HNCO
----
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -168.30258903
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -168.44533015
E(CCSD/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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -168.48868126
E(CCSD/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(CCSD(T)/Aug-CC-pVDZ) (Hartree): -243.23568465
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -243.43870340
E(CCSD/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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -243.50138267
E(CCSD/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(CCSD(T)/Aug-CC-pVDZ) (Hartree): -167.62693028
E(CCSD/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
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E(UHF/Aug-CC-pVDZ) (Hartree): -167.15458842
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -167.76183039
E(CCSD/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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -167.80303120
E(CCSD/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(CCSD(T)/Aug-CC-pVDZ) (Hartree): -150.01974519
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -150.14024980
E(CCSD/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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -150.17820201
E(CCSD/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(CCSD(T)/Aug-CC-pVDZ) (Hartree): -149.96951201
E(CCSD/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(CCSD(T)/Aug-CC-pVTZ) (Hartree): -150.09177700
E(CCSD/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(CCSD(T)/Aug-CC-pVQZ) (Hartree): -150.13032570
E(CCSD/Aug-CC-pVQZ) (Hartree): -150.10602219
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     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
--
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

OC_O_N_H_OO
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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

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
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     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
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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
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     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):
     i572.5421                 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
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