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

Supporting Information

CH_3NO as a Potential Intermediate for Early Atmospheric HCN: A Quantum Chemical Insight

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Supporting Note 1:

Methodology for CBS Extrapolation: We have used the method proposed by Varandas and Pansini for CBS extrapolation.[1] For this, single point energy calculations have been carried out at CCSD(T) level of theory using aug-cc-pVDZ (≡ DZ), aug-cc-pVTZ (≡ TZ) basis sets and with HF/aug-cc-pVQZ (≡ HF/QZ) level of theory. In this method, energy extrapolation to CBS limit is done by separately extrapolating the correlation energy (Corr) and Hartree-Fock energy (HF) as shown below:

$$\mathrm{CBS(Corr)} = \frac{x_1^3 E_{x+1} - \mathrm{x}_2^3 E_x}{x_1^3 - \mathrm{x}_2^3} \qquad (1)$$

In Equation-1, E_X is the correlation energy at CCSD(T) level of theory employing a basis set whose cardinality is X, i.e., X = 2 for DZ basis and X = 3 for TZ basis. To extrapolate correlation energy, we have used DZ and TZ basis. Recommended values for x_1 and x_2 at DZ basis are 2.71 and 1.91 respectively.[1] Similarly, extrapolation of Hartree-Fock energy follows the following equation:

$$\mathrm{CBS(HF)} = \frac{x_1^5 E_{x+1} - \mathrm{x}_2^5 E_x}{x_1^5 - \mathrm{x}_2^5} \qquad (2)$$

In Equation-2, recommended values for x_1 and x_2 at TZ basis are 4 and 3 respectively. In the present study, HF energies of all molecular species were extrapolated by using energies obtain at TZ and QZ basis sets, on the other hand, correlation energys of all molecular species were extrapolated by using energies obtained at DZ and TZ basis sets. Potential energy diagram (see Figure 1) have been drawn on the basis of CCSD(T)/CBS//MP2/aug-cc-pVTZ level of calculation. That means single point CCSD(T) calculations have been carried out by using MP2/aug-cc-pVTZ level optimized geometries and ZPE corrections are taken from MP2/aug-cc-pVTZ level of calculations. The similar method has recently been employed successfully by Sarkar et al.[2-4] Total electronic energies of various species could be found in Table S2.

Table S1. Calculated zero point vibrational energy (zpe) corrected electronic energies (E_{zpe}), zero point vibrational energies, total electronic energies without zpe correction (E) of various molecules, complexes, intermediates and transitions States at the M06-2X level in conjunction with 6-311++G(3df,3pd) basis set as well as at the CCSD(T)/6-311++G(3df,3pd) level of theory.

Molecules/Complexes/ Intermediates/ Transitions States	**M06-2X/ 6-311++G(3df,3pd)**	**M06-2X/ 6-311++G(3df,3pd)**	**CCSD(T)/ 6-311++G(3df,3pd)**
	E_{zpe}	**zpe**	**E**
CH_3NO	-169.740352	0.043781	-169.5458242
(CH_2NOH)-I	-169.754162	0.044818	-169.5580378
(CH_2NOH)-II	-169.761269	0.045249	-169.5660905
HCN	-93.404403	0.016589	-93.2752787
$CH_3N(OH)_2$	-246.129539	0.073533	-245.8677976
H_2O	-76.405308	0.021732	-76.3374378
NH_3	-56.516498	0.034474	-56.4766835
HCl	-460.794798	0.006857	-460.3306738
HCOOH	-189.729164	0.034447	-189.5061268
HNO_3	-280.859627	0.027611	-280.5236721
H_2SO_4	-700.248532	0.040294	-699.4493013
$CH_3NO\cdots CH_3NO$	-339.484427	0.089577	-339.0969075
$CH_3NO\cdots H_2O$	-246.150710	0.068093	-245.8906795
$CH_3NO\cdots NH_3$	-226.260515	0.080424	-226.0276478
$CH_3NO\cdots HCl$	-630.539479	0.052902	-629.8832355
$CH_3NO\cdots HCOOH$	-359.478644	0.080345	-359.0626254
$CH_3NO\cdots HNO_3$	-450.610561	0.073517	-450.081448
$CH_3NO\cdots H_2SO_4$	-870.002118	0.086301	-869.0107673
$HCN\cdots H_2O$	-169.816264	0.040315	-169.6213481
$HCN\cdots CH_3N(OH)_2$	-339.544071	0.091432	-339.1531996
$HCN\cdots CH_3NO\cdots H_2O$	-339.563344	0.086277	-339.1745839
$(CH_2NOH\cdots H_2O)$-I	-246.167255	0.069511	-245.9061365
$(CH_2NOH\cdots H_2O)$-II	-246.171701	0.069821	-245.9114833
$HCN\cdots H_2O\cdots H_2O$	-246.232061	0.065714	-245.9712746
$(CH_2NOH\cdots NH_3)$-I	-226.280523	0.082189	-226.0473938
$(CH_2NOH\cdots NH_3)$-II	-226.281084	0.081997	-226.0487893
$HCN\cdots NH_3\cdots H_2O$	-226.33537	0.077845	-226.1043033
$(CH_2NOH\cdots HCl)$-I	-630.554066	0.053861	-629.896596
$(CH_2NOH\cdots HCl)$-II	-630.562414	0.053955	-629.9051793
$HCN\cdots HCl\cdots H_2O$	-630.620020	0.049994	-629.962238
$(CH_2NOH\cdots HCOOH)$-I	-359.498500	0.082241	-359.0817471
$(CH_2NOH\cdots HCOOH)$-II	-359.500976	0.081535	-359.0854534
$HCN\cdots HCOOH\cdots H_2O$	-359.558909	0.077893	-359.1422755
$(CH_2NOH\cdots HNO_3)$-I	-450.628872	0.074809	-450.098462
$(CH_2NOH\cdots HNO_3)$-II	-450.633190	0.074473	-450.1040995
$HCN\cdots HNO_3\cdots H_2O$	-450.694985	0.071175	-450.1637793
$(CH_2NOH\cdots H_2SO_4)$-I	-870.019298	0.087200	-869.0253297
$(CH_2NOH\cdots H_2SO_4)$-II	-870.024704	0.087289	-869.0337387
$HCN\cdots H_2SO_4\cdots H_2O$	-870.090298	0.083209	-869.0955588
(INT)-I	-339.491065	0.093739	-339.1010638
(INT)-II	-339.495504	0.094186	-339.1065761
TS-1	-169.645762	0.038355	-169.446604
TS-2	-169.749088	0.043957	-169.5527627
TS-3	-169.666266	0.037441	-169.4672161

TS-4	-339.429149	0.086941	-339.0376247
TS-5	-339.486688	0.092958	-339.0966273
TS-6	-339.414894	0.086237	-339.0420736
TS-7	-339.481284	0.085589	-339.088887
TS-8	-246.098087	0.064875	-245.8280954
TS-9	-246.161387	0.068868	-245.9000344
TS-10	-246.103709	0.062094	-245.8347973
TS-11	-226.221171	0.078341	-225.9816623
TS-12	-226.270197	0.080648	-226.0362718
TS-13	-226.211714	0.076490	-225.9751494
TS-14	-630.497003	0.051682	-629.8329928
TS-15	-630.550203	0.052917	-629.892372
TS-16	-630.509290	0.050176	-629.8484644
TS-17	-359.448437	0.074861	-359.021406
TS-18	-359.491616	0.080469	-359.0745194
TS-19	-359.446559	0.073444	-359.0216143
TS-20	-450.574458	0.067860	-450.03383
TS-21	-450.624311	0.073408	-450.0932029
TS-22	-450.578826	0.066411	-450.0411191
TS-23	-869.971973	0.081089	-868.9705058
TS-24	-870.016852	0.086390	-869.0236269
TS-25	-869.974588	0.078997	-868.976314

Table S2. Calculated electronic energies by using CCSD(T) and HF methods in conjunction with aug-cc-pVDZ (≡ DZ), aug-cc-pVTZ (≡ TZ) and aug-cc-pVQZ (≡ QZ) basis sets. Single point CCSD(T) calculations have been carried out by using MP2/aug-cc-pVTZ level optimized geometries MP2/aug-cc-pVTZ level calculated zero point vibrational energies (zpe) of various species have also been tabulated in the last column.

Species	**DZ**		**TZ**		**QZ**	**CCSD(T)/ CBS**	**MP2**
	E_{HF}	$E_{CCSD(T)}$	E_{HF}	$E_{CCSD(T)}$	E_{HF}		**ZPE**
CH_3NO	-168.855438	-169.413779	-168.893845	-169.557747	-168.904449	-169.628515	0.043495
TS-1	-168.725698	-169.314391	-168.763194	-169.458631	-168.773519	-169.529671	0.038210
(CH_2NOH)-I	-168.864413	-169.423825	-168.903948	-169.569709	-168.914609	-169.640976	0.044034
TS-2	-168.860390	-169.419135	-168.899709	-169.564652	-168.910225	-169.635648	0.043150
(CH_2NOH)-II	-168.873568	-169.432021	-168.912850	-169.577668	-168.923468	-169.648889	0.044497
TS-3	-168.750787	-169.336650	-168.788402	-169.480336	-168.798550	-169.550781	0.036334
$HCN^{\cdots}H_2O$	-168.934632	-169.487277	-168.974442	-169.632117	-168.985071	-169.702633	0.038984
HCN	-92.885650	-93.204347	-92.906678	-93.281062	-92.912064	-93.318124	0.015774
H_2O	-76.041141	-76.273855	-76.060282	-76.342325	-76.065648	-76.3759358	0.02141

Table S3. Calculated total electronic energies without zpe correction (E), zero point vibrational energies of various molecules and transitions States at the CASSCF level in conjunction with 6-311++G(3df,3pd) basis set as well as at the CASPT2/6-311++G(3df,3pd) level of theory. Active space of 10 electrons in 10 orbital's have been used for CASSCF and CASPT2 calculations.

Molecules/Complexes/ Intermediates/ Transitions States	CASSCF (10, 10)/ 6-311++G(3df,3pd) E	CASSCF (10, 10)/ 6-311++G(3df,3pd) zpe	CASPT2 (10, 10)/ 6-311++G(3df,3pd) E
CH_3NO	-169.061856	0.044287	-169.498478
(CH_2NOH)-I	-169.073712	0.045214	-169.512148
(CH_2NOH)-II	-169.082894	0.045622	-169.520669
HCN	-93.0285531	0.016422	-93.249493
H_2O	-76.1104646	0.02163	-76.3202899
$HCN\cdots H_2O$	-169.1415188	0.039388	-169.57819
TS-1	-168.943643	0.038797	-169.400876
TS-2	-169.069786	0.044389	-169.506733
TS-3	-168.961592	0.038191	-169.417195

Table S4. TST/Eckart and CVT/SCT methods computed rate constants (k, sec^{-1}) of each unimoleulcar steps and overall rate constants for the unimolecular rearrangement of isolated decomposition of CH_3NO at the CCSD(T)/6-311++G(3df,3pd) level of calculation. The values given in the first bracket correspond to CVT/SCT computed rate constants.

T (K)	k_{TS-1}	k_{TS-2}	k_{TS-3}	k_{uni}^{iso}
298.15	7.10×10^{-23} (9.34×10^{-21})	6.54×10^{10}	6.23×10^{-24} (9.08×10^{-26})	6.23×10^{-24} (9.08×10^{-26})
318	1.49×10^{-21} (5.51×10^{-20})	8.99×10^{10}	1.94×10^{-22} (6.19×10^{-24})	1.94×10^{-22} (6.19×10^{-24})
343	4.50×10^{-20} (5.47×10^{-19})	1.28×10^{11}	9.89×10^{-21} (9.14×10^{-22})	9.89×10^{-21} (9.14×10^{-22})
358	2.99×10^{-19} (2.22×10^{-18})	1.54×10^{11}	9.36×10^{-20} (1.52×10^{-20})	9.36×10^{-20} (1.52×10^{-20})

Table S5. The CCSD(T)/6-311++G(3df,3pd) level calculated equilibrium constants (K_{eq}, $cm^3molecule^{-1}sec^{-1}$) for the formation of $CH_3NO\cdots CH_3NO$ complex. TST/Eckart and CVT/SCT methods computed rate constants (k, sec^{-1}) of each unimoleulcar steps and overall rate constants for unimolecular rearrangement for the bimolecular decomposition of CH_3NO at the CCSD(T)/6-311++G(3df,3pd) level of calculation. The values given in the first bracket correspond to CVT/SCT computed rate constants.

T (K)	$K_{eq}^{CH_3NO\cdot\cdot CH_3NO}$	k_{TS-4}	k_{TS-5}	k_{TS-6}	k_{uni}^{bi}
298.15	1.78×10^{-25}	4.09×10^{-15} (2.34×10^{-15})	1.55×10^{11}	3.09×10^{-13} (4.55×10^{-14})	4.04×10^{-15} (2.23×10^{-15})
318	1.57×10^{-25}	9.32×10^{-14} (6.51×10^{-14})	2.02×10^{11}	1.39×10^{-11} (2.24×10^{-12})	9.26×10^{-14} (6.33×10^{-14})
343	1.39×10^{-25}	3.21×10^{-12} (2.57×10^{-12})	2.70×10^{11}	9.10×10^{-10} (1.62×10^{-10})	3.20×10^{-12} (2.53×10^{-12})
358	1.31×10^{-25}	2.20×10^{-11} (1.85×10^{-11})	3.16×10^{11}	8.50×10^{-9} (1.59×10^{-9})	2.20×10^{-11} (1.83×10^{-11})

Table S6. The CCSD(T)/6-311++G(3df,3pd) level calculated equilibrium constants (K_{eq}, $cm^3molecule^{-1}sec^{-1}$) for the formation of $CH_3NO\cdots H_2O$ complex. TST/Eckart and CVT/SCT methods computed rate constants (k, sec^{-1}) of each unimoleulcar steps and overall rate constants for unimolecular rearrangement for the H_2O assisted decomposition of CH_3NO at the CCSD(T)/6-311++G(3df,3pd) level of calculation. The values given in the first bracket correspond to CVT/SCT computed rate constants.

T (K)	$K_{eq}^{CH_3NO\cdot\cdot H_2O}$	k_{TS-8}	k_{TS-9}	k_{TS-10}	k_{uni}^{HO}
298.15	7.80×10^{-23}	8.09×10^{-15} (3.24×10^{-13})	6.36×10^{9}	2.90×10^{-18} (4.26×10^{-19})	2.90×10^{-18} (4.26×10^{-19})
318	6.02×10^{-23}	8.71×10^{-14} (2.02×10^{-12})	9.16×10^{9}	5.40×10^{-17} (1.67×10^{-17})	5.40×10^{-17} (1.67×10^{-17})
343	4.60×10^{-23}	1.63×10^{-12} (1.90×10^{-11})	1.37×10^{10}	1.95×10^{-15} (1.08×10^{-15})	1.95×10^{-15} (1.08×10^{-15})
358	4.01×10^{-23}	8.82×10^{-12} (7.09×10^{-11})	1.70×10^{10}	1.55×10^{-14} (1.06×10^{-14})	1.55×10^{-14} (1.06×10^{-14})

Table S7. The CCSD(T)/6-311++G(3df,3pd) level calculated equilibrium constants (K_{eq}, $cm^3molecule^{-1}sec^{-1}$) for the formation of $CH_3NO\cdots NH_3$ complex. TST/Eckart and CVT/SCT methods computed rate constants (k, sec^{-1}) of each unimoleulcar steps and overall rate constants for unimolecular rearrangement for the NH_3 assisted decomposition of CH_3NO at the CCSD(T)/6-311++G(3df,3pd) level of calculation. The values given in the first bracket correspond to CVT/SCT computed rate constants.

T (K)	$K_{eq}^{CH_3NO\cdot\cdot NH_3}$	k_{TS-11}	k_{TS-12}	k_{TS-13}	$k_{uni}^{NH_3}$
298.15	5.20×10^{-24}	3.24×10^{-9} (1.93×10^{-9})	2.39×10^{8}	1.29×10^{-20} (1.04×10^{-19})	1.29×10^{-20} (1.04×10^{-19})
318	4.59×10^{-24}	4.52×10^{-8} (2.63×10^{-8})	4.67×10^{8}	1.00×10^{-18} (4.98×10^{-18})	1.00×10^{-18} (4.98×10^{-18})
343	4.08×10^{-24}	8.28×10^{-7} (4.72×10^{-7})	9.79×10^{8}	1.20×10^{-16} (4.02×10^{-16})	1.20×10^{-16} (4.02×10^{-16})
358	3.85×10^{-24}	3.93×10^{-6} (2.22×10^{-6})	1.46×10^{9}	1.54×10^{-15} (4.38×10^{-15})	1.54×10^{-15} (4.38×10^{-15})

Table S8. The CCSD(T)/6-311++G(3df,3pd) level calculated equilibrium constants (K_{eq}, $cm^3molecule^{-1}sec^{-1}$) for the formation of $CH_3NO\cdots HCl$ complex. TST/Eckart and CVT/SCT methods computed rate constants (k, sec^{-1}) of each unimoleulcar steps and overall rate constants for unimolecular rearrangement for the HCl assisted decomposition of CH_3NO at the CCSD(T)/6-311++G(3df,3pd) level of calculation. The values given in the first bracket correspond to CVT/SCT computed rate constants.

T (K)	$K_{eq}^{CH_3NO\cdot\cdot HCl}$	k_{TS-14}	k_{TS-15}	k_{TS-16}	k_{uni}^{HCl}
298.15	2.60×10^{-23}	1.94×10^{-11} (1.72×10^{-10})	1.29×10^{11}	3.93×10^{-13} (2.27×10^{-13})	3.93×10^{-13} (2.27×10^{-13})
318	2.00×10^{-23}	3.59×10^{-10} (1.68×10^{-9})	1.65×10^{11}	1.17×10^{-11} (6.85×10^{-12})	1.17×10^{-11} (6.82×10^{-12})
343	1.52×10^{-23}	9.01×10^{-9} (2.63×10^{-8})	2.15×10^{11}	4.85×10^{-10} (2.88×10^{-10})	4.85×10^{-10} (2.88×10^{-10})
358	1.32×10^{-23}	5.07×10^{-8} (1.23×10^{-7})	2.49×10^{11}	3.55×10^{-9} (2.12×10^{-9})	3.55×10^{-9} (2.12×10^{-9})

Table S9. The CCSD(T)/6-311++G(3df,3pd) level calculated equilibrium constants (K_{eq}, $cm^3molecule^{-1}sec^{-1}$) for the formation of $CH_3NO^{\cdots}HCOOH$ complex. TST/Eckart and CVT/SCT methods computed rate constants (k, sec^{-1}) of each unimoleulcar steps and overall rate constants for unimolecular rearrangement for the HCOOH assisted decomposition of CH_3NO at the CCSD(T)/6-311++G(3df,3pd) level of calculation. The values given in the first bracket correspond to CVT/SCT computed rate constants.

T (K)	$K_{eq}^{CH_3NO\cdot\cdot HCOOH}$	k_{TS-17}	k_{TS-18}	k_{TS-19}	k_{uni}^{HCOOH}
298.15	3.02×10^{-23}	2.80×10^{-4} (6.98×10^{-4})	3.32×10^{10}	6.06×10^{-14} (2.49×10^{-14})	6.06×10^{-14} (2.49×10^{-14})
318	1.87×10^{-23}	1.23×10^{-3} (3.03×10^{-3})	5.00×10^{10}	1.59×10^{-12} (7.02×10^{-13})	1.59×10^{-12} (7.02×10^{-13})
343	1.11×10^{-23}	7.30×10^{-3} (1.67×10^{-2})	7.86×10^{10}	6.25×10^{-11} (2.89×10^{-11})	6.25×10^{-11} (2.89×10^{-11})
358	8.48×10^{-24}	2.00×10^{-2} (4.32×10^{-2})	1.00×10^{11}	4.55×10^{-10} (2.14×10^{-10})	4.55×10^{-10} (2.14×10^{-10})

Table S10. The CCSD(T)/6-311++G(3df,3pd) level calculated equilibrium constants (K_{eq}, $cm^3molecule^{-1}sec^{-1}$) for the formation of $CH_3NO^{\cdots}HNO_3$ complex. TST/Eckart and CVT/SCT methods computed rate constants (k, sec^{-1}) of each unimoleulcar steps and overall rate constants for unimolecular rearrangement for the HNO_3 assisted decomposition of CH_3NO at the CCSD(T)/6-311++G(3df,3pd) level of calculation. The values given in the first bracket correspond to CVT/SCT computed rate constants.

T (K)	$K_{eq}^{CH_3NO\cdot\cdot HNO_3}$	k_{TS-20}	k_{TS-21}	k_{TS-22}	$k_{uni}^{HNO_3}$
298.15	5.81×10^{-23}	3.87×10^{-7} (3.10×10^{-6})	1.24×10^{11}	3.27×10^{-13} (1.85×10^{-13})	3.27×10^{-13} (1.85×10^{-13})
318	3.28×10^{-23}	2.73×10^{-6} (1.61×10^{-5})	1.66×10^{11}	7.58×10^{-12} (5.20×10^{-12})	7.58×10^{-12} (5.20×10^{-12})
343	1.77×10^{-23}	2.75×10^{-5} (1.13×10^{-4})	2.30×10^{11}	2.68×10^{-10} (2.10×10^{-10})	2.68×10^{-10} (2.10×10^{-10})
358	1.28×10^{-23}	9.99×10^{-5} (3.44×10^{-4})	2.74×10^{11}	1.87×10^{-9} (1.53×10^{-9})	1.87×10^{-9} (1.53×10^{-9})

Table S11. The CCSD(T)/6-311++G(3df,3pd) level calculated equilibrium constants (K_{eq}, $cm^3molecule^{-1}sec^{-1}$) for the formation of $CH_3NO^{\cdots}H_2SO_4$ complex. TST/Eckart and CVT/SCT methods computed rate constants (k, sec^{-1}) of each unimoleulcar steps and overall rate constants for unimolecular rearrangement for the H_2SO_4 assisted decomposition of CH_3NO at the CCSD(T)/6-311++G(3df,3pd) level of calculation. The values given in the first bracket correspond to CVT/SCT computed rate constants.

T (K)	$K_{eq}^{CH_3NO\cdot\cdot H_2SO_4}$	k_{TS-23}	k_{TS-24}	k_{TS-25}	$k_{uni}^{H_2SO_4}$
298.15	2.19×10^{-21}	1.84×10^{-4} (9.09×10^{-4})	2.55×10^{12}	1.35×10^{-10} (1.94×10^{-11})	1.35×10^{-10} (1.94×10^{-11})
318	9.70×10^{-22}	1.20×10^{-3} (4.28×10^{-3})	2.76×10^{12}	2.53×10^{-9} (4.41×10^{-10})	2.53×10^{-9} (4.41×10^{-10})
343	4.02×10^{-22}	9.99×10^{-3} (2.63×10^{-2})	3.00×10^{12}	6.80×10^{-8} (1.39×10^{-8})	6.80×10^{-8} (1.39×10^{-8})
358	2.50×10^{-22}	3.17×10^{-2} (7.26×10^{-2})	3.14×10^{12}	4.04×10^{-7} (8.78×10^{-8})	4.04×10^{-7} (8.78×10^{-8})

Figure S1. Images of CASSCF(10,10)/6-311++G(3df,3pd) level optimized active space orbital's of CH_3NO molecule.

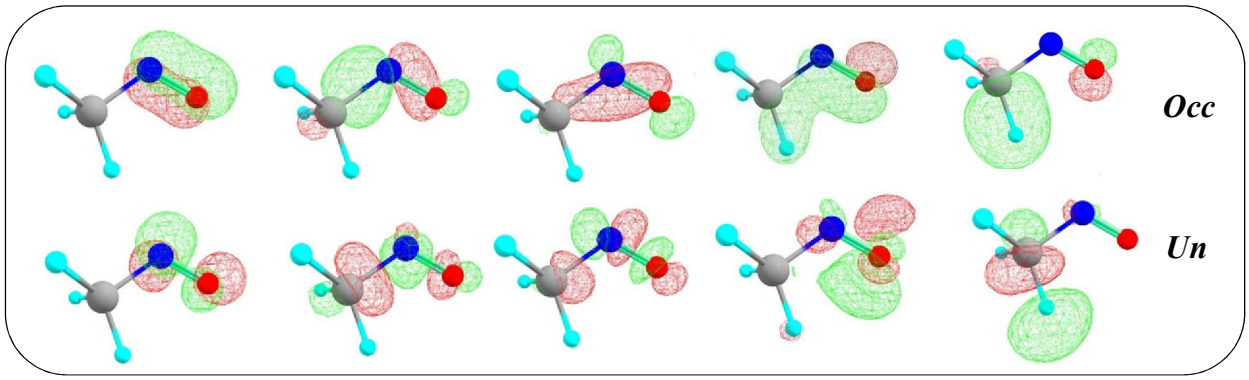


Figure S2. Temperature and pressure dependent Bartis-Widom phenomenological rate coefficients for CH_3NO to HCN conversion via (A) unimolecular, (B) bimolecular decomposition pathways and via (C) H_2O, (D) NH_3, (E) HCl, (F) HCOOH, (G) HNO_3, (H) H_2SO_4 assistance.

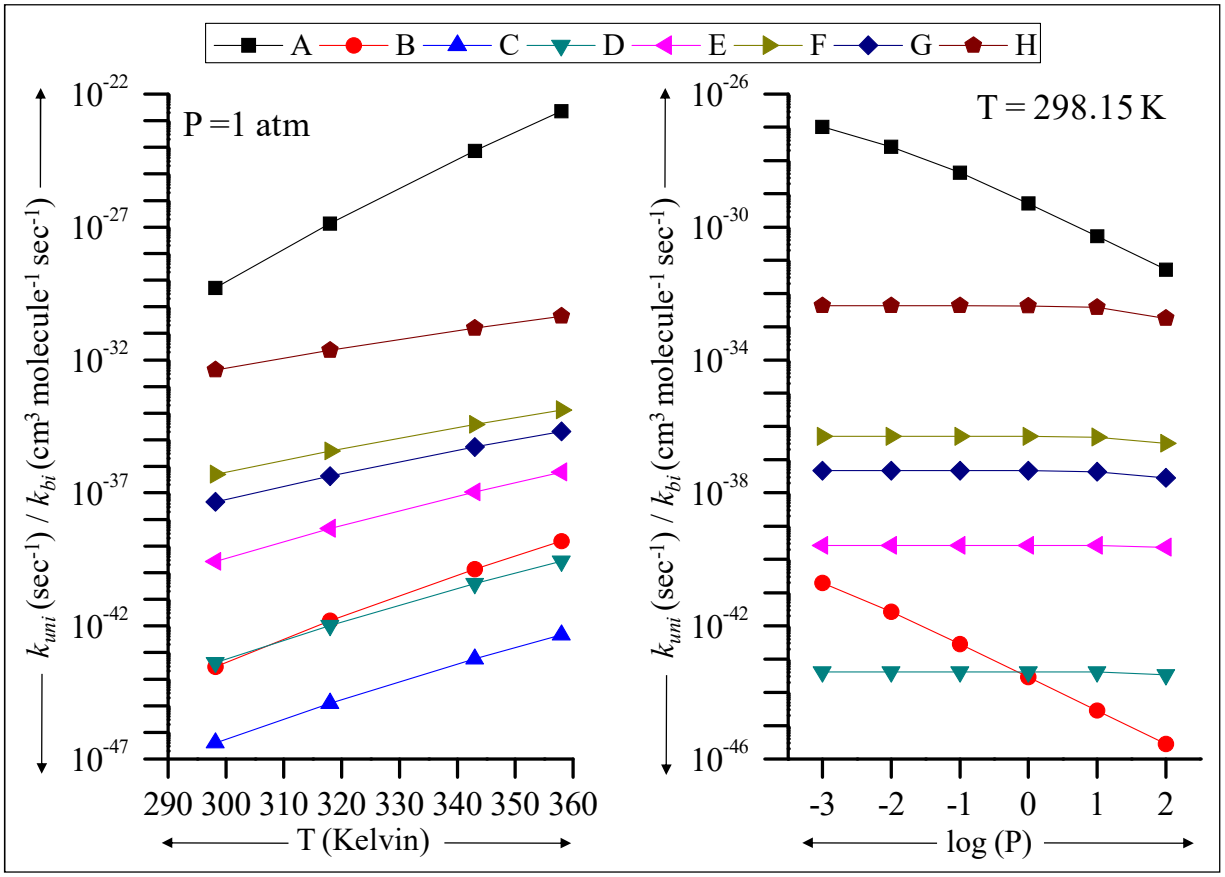
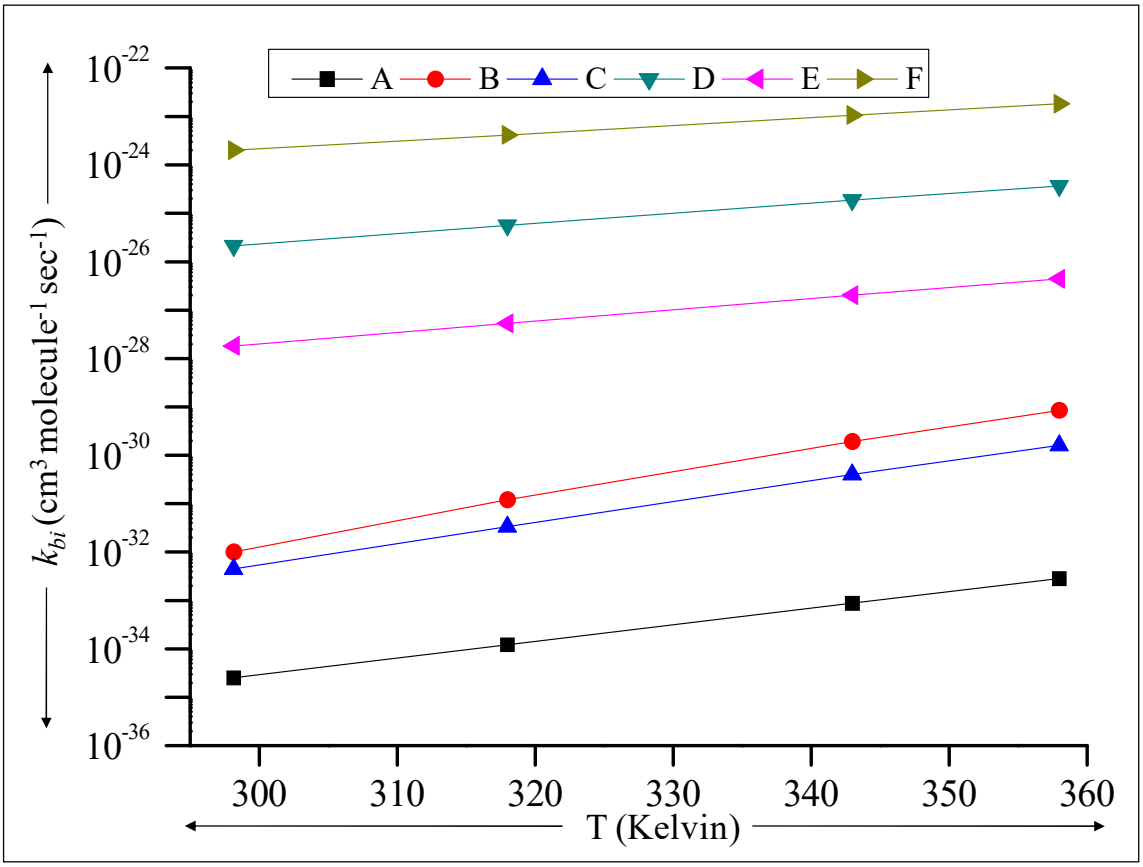


Figure S3. CVT/SCT computed rate coefficients for CH_3NO to (CH_2NOH)-I conversion via (A) H_2O, (B) NH_3, (C) HCl, (D) HCOOH, (E) HNO_3 and (F) H_2SO_4 assisted decomposition pathways.



Cartesian coordinates of M06-2X/6-311++G(3df,3pd) level's optimized geometries.

CH_3NO	C,0,0.002560313,-0.000343391,-0.0017985589 H,0,-0.0015829687,-0.0032534197,1.0875808997 H,0,1.0125428579,0.0038854942,-0.4057504818 H,0,-0.5731338009,0.8639665295,-0.331203362 O,0,-0.1084552154,-1.927520701,-1.1289316784 N,0,-0.7414462536,-1.1986670779,-0.4338140011
(CH_2NOH)-I	C,0,-0.0645849987,0.9022005774,0.7431025338 H,0,-0.564132294,1.209859854,1.6497250101 H,0,0.8877503907,0.0813038858,-1.1447495676 H,0,0.625220221,1.5861640421,0.2459834718 O,0,0.3172396337,-0.6389712895,-0.835151099 N,0,-0.3166149529,-0.2551010698,0.3102646508
(CH_2NOH)-II	C,0,-0.0672132757,0.8781114469,0.7311735756 H,0,-0.5555471524,1.2074801793,1.6362407668 H,0,0.0446615246,-1.4870240068,-1.0366527139 H,0,0.6252383894,1.5248791091,0.2004696558 O,0,0.3374487845,-0.5964464451,-0.8319145306 N,0,-0.3425411904,-0.2844711434,0.3286676262
HCN	C,0,0.,0.,-0.0002368384 H,0,0.,0.,1.0657278922 N,0,0.,0.,-1.1420910538
$CH_3N(OH)_2$	O,0,0.022187099,-0.6349551521,-1.3350954985 H,0,0.5893203574,-0.148068526,-1.954935511 H,0,-0.0904240751,1.1812067267,0.5314009456 O,0,0.7406626566,0.9112956469,0.1302633632 N,0,0.5857520631,-0.4731061348,-0.070443865 C,0,1.9436425036,-0.994362503,-0.1007391072 H,0,2.3814077826,-0.8621993184,0.8837180188 H,0,1.8857687075,-2.0490213811,-0.348860661 H,0,2.5464479053,-0.4614393581,-0.845103685
H_2O	H,0,3.5570575294,0.136514371,-0.9314714521 H,0,3.0079175243,-0.1598070934,-2.3185225289 O,0,2.7410569464,-0.0220772776,-1.408463019
NH_3	N,0,-0.0161871708,0.0282959422,-0.0113732791 H,0,0.0058122228,-0.0105204612,1.0004515514 H,0,0.9451709677,-0.0105589485,-0.3280288621 H,0,-0.4633914289,-0.8237132348,-0.3277158788
HCl	H,0,0.,0.,0.0207330095 Cl,0,0.,0.,1.2973990905
HCOOH	H,0,0.3141193059,-0.6541984014,-0.4392162473 O,0,1.9452166723,0.3133577541,0.8854556155 C,0,1.7404730528,0.5480221777,-0.2642022199

	O,0,0.7879822176,-0.0280637538,-1.0035108062
	H,0,2.3024937514,1.2672062233,-0.8687993421
HNO_3	O,0,0.838059596,0.7036362107,-0.6661995475
	N,0,1.5115735716,-0.1929135149,-0.2397518849
	O,0,0.9681908254,-0.9058235916,0.8039528014
	H,0,0.1106685203,-0.4795375584,0.9519198915
	O,0,2.5832684867,-0.5662585458,-0.5796242606
H_2SO_4	O,0,3.1193249909,-0.5559319147,-0.3565766031
	S,0,4.1058418679,-0.0398509533,0.5127787692
	O,0,3.3887530062,0.6901794206,1.7097114658
	H,0,2.5175985994,0.2976104161,1.8553452047
	O,0,5.1429147942,0.8245710705,0.0974388141
	O,0,4.7483657465,-1.2881518037,1.226118996
	H,0,5.6051579949,-1.0429052355,1.5996403532
$CH_3NO\cdots CH_3NO$	C,0,0.0618593761,0.1073900223,0.0073816641
	N,0,0.4250871023,-0.4313533674,1.3275325473
	O,0,1.3800800303,-1.143910859,1.3091584804
	H,0,-0.9841137773,-0.146827138,-0.1600341073
	H,0,0.1360564601,1.1918827502,0.0887354765
	H,0,0.7159552093,-0.2778936905,-0.7712067392
	O,0,2.7816430883,1.413395081,0.3832289443
	N,0,3.5842368816,1.0603629423,1.1904423796
	C,0,4.2311798549,-0.2199952456,0.8636966406
	H,0,5.3045183589,-0.0332839862,0.8506015788
	H,0,4.0167768523,-0.8937341258,1.6929026786
	H,0,3.8652193574,-0.6192276201,-0.0793119366
$CH_3NO\cdots H_2O$	C,0,0.0192372228,-0.0078770387,-0.0156083378
	H,0,0.0256334863,-0.013661194,1.0742717676
	H,0,1.0245357154,-0.0029304574,-0.4309945618
	H,0,3.2035306489,-1.6476787792,-2.3051855832
	H,0,-0.5611491688,0.8590803128,-0.3306728952
	O,0,2.6081536174,-1.1359166098,-1.7557916843
	H,0,1.7833332922,-1.6330559362,-1.7211283464
	O,0,-0.1542901019,-1.9471567616,-1.1300497246
	N,0,-0.7520061694,-1.1913621925,-0.4267726405
$CH_3NO\cdots NH_3$	C,0,-1.0931088618,1.0089510295,-0.0159488538
	H,0,-1.5027027152,0.6540227335,0.9274862882
	H,0,-0.2891815232,1.7260131457,0.1467247057
	H,0,2.213968247,-0.0177875622,-0.0274698441
	H,0,-1.8489518183,1.4665166326,-0.6525204102
	H,0,1.5656139769,-0.422652806,1.4014652317
	O,0,-0.4846731219,-1.1355548654,-0.2005882142
	N,0,-0.4931398376,-0.0946430396,-0.7810823504
	N,0,1.9764930615,0.3484890909,0.8874100901
	H,0,2.8475335926,0.5823566409,1.347687357
$CH_3NO\cdots HCl$	C,0,0.0342298531,0.0090173554,-0.0257529924

	H,0,0.0435779471,0.0151131958,1.0638063216
	H,0,2.5260785949,-0.0187570568,-1.80804741
	H,0,-0.9866683882,0.2171697447,-0.3446856344
	O,0,1.2805416864,-1.484259416,-1.1407183447
	N,0,0.3253367089,-1.3730246892,-0.4358444712
	H,0,0.7450884592,0.7189423908,-0.4430395494
	Cl,0,3.1762831767,1.052628777,-2.1012154509
$CH_3NO^{\cdots}HCOOH$	C,0,-1.719622515,0.1532681227,-0.9469367247
	N,0,-1.8571666565,-0.577292627,0.3160595926
	O,0,-1.103666069,-0.2297250063,1.1743905022
	H,0,-1.0604535839,1.0133567242,-0.8517843408
	H,0,-1.3123806895,-0.5630191025,-1.6614393575
	H,0,-2.7242297413,0.4269214462,-1.2639938803
	O,0,1.2351136237,-0.5666907816,-0.9724755484
	C,0,1.8888495706,0.2229125264,-0.3542892351
	O,0,1.4692276707,0.8996809318,0.7055541446
	H,0,0.5547609697,0.6231935746,0.9102443458
	H,0,2.9236644206,0.4861071914,-0.5977344982
$CH_3NO^{\cdots}HNO_3$	C,0,-2.0953451839,-0.072558805,-0.8559563382
	N,0,-2.2605628923,0.6420126291,0.4130268207
	O,0,-1.4622177628,0.3558130719,1.2539098366
	H,0,-3.0850108402,-0.403604662,-1.1638843602
	H,0,-1.7469233943,0.6728095454,-1.5726750924
	H,0,-1.386224178,-0.8940183994,-0.7779865
	O,0,0.8431266243,0.7046008353,-0.6732359972
	N,0,1.5114631156,-0.1979603203,-0.233554197
	O,0,0.9712308354,-0.9051247181,0.7937576346
	H,0,0.0998158286,-0.4802365297,0.9660657938
	O,0,2.5861238476,-0.5621756472,-0.5827366007
$CH_3NO^{\cdots}H_2SO_4$	C,0,0.2419199742,0.2072397963,0.1368420006
	N,0,0.2074136669,-0.8006249639,1.1966833715
	O,0,1.0762630521,-0.7033607798,2.01191356
	H,0,-0.7718390762,0.5915085333,0.0392244946
	H,0,0.9725132208,0.9896616711,0.3284645768
	H,0,0.4925942405,-0.3338225362,-0.7766375914
	O,0,3.1236172709,-0.5488873089,-0.3653917263
	S,0,4.1055460028,-0.0281146626,0.5150081492
	O,0,3.3951241025,0.700474885,1.6941336704
	H,0,2.5294982055,0.2661559577,1.8809748327
	O,0,5.1476442414,0.8216255577,0.0775312106
	O,0,4.7430243587,-1.2868806646,1.2178666209
	H,0,5.5835035624,-1.0388533088,1.6243343605
$HCN^{\cdots}H_2O$	C,0,-0.1576694317,-0.0045726035,-0.2742668974
	H,0,0.8462567065,-0.0117687596,-0.6580089212
	H,0,3.5572071953,0.1372469248,-0.9274280494
	H,0,3.0052659823,-0.1605903601,-2.3215767069
	O,0,2.743559001,-0.0220269153,-1.4094517902
	N,0,-1.2252192136,0.0038451083,0.1328393333

$HCN^{\cdots}CH_3N(OH)_2$	C,0,-2.1999635872,-0.0817473859,0.4345095887 N,0,-2.2436884898,0.8890880917,1.036038239 O,0,0.0297679544,-0.6518483242,-1.346593414 H,0,0.5553838463,-0.1128508093,-1.9591520291 H,0,-2.1252178332,-0.9740955247,-0.1469039175 H,0,-0.085349744,1.1801581005,0.5383607333 O,0,0.7386164141,0.9066279882,0.1123442097 N,0,0.5921670743,-0.4699893557,-0.0734662197 C,0,1.9484604545,-0.9980837657,-0.0958792784 H,0,2.379130306,-0.8600233049,0.8908755032 H,0,1.890460419,-2.0542074279,-0.3376321382 H,0,2.5561301854,-0.4704342823,-0.838655277
$HCN^{\cdots}CH_3NO^{\cdots}H_2O$	C,0,0.0035741176,-0.0025768262,0.008880155 N,0,-0.0058157163,0.0050656492,1.1516720958 O,0,1.8434993343,0.0267818099,-2.3774403297 H,0,3.261149957,1.1506883594,1.6033701195 H,0,0.0513883347,0.0050230565,-1.0615565058 H,0,2.2792365142,0.0871916342,1.1350718118 O,0,3.1732019617,0.4162859034,0.9932093852 N,0,2.3743338143,-0.7125597237,-1.6046796558 C,0,3.812568915,-0.8820870846,-1.821356602 H,0,4.2834453953,-0.5388177103,-0.9002137138 H,0,3.9933900217,-1.9521362299,-1.9161108465 H,0,4.1474803504,-0.3263058378,-2.6941349137
$(CH_2NOH^{\cdots}H_2O)$-I	C,0,0.0089570657,-0.0088864252,-0.0025533272 H,0,0.0008450315,0.0040855913,1.0865043745 H,0,2.4851490994,-0.0202107011,3.2886145321 H,0,1.9022674272,-1.4332856717,3.3433610766 H,0,-0.8678756333,0.2960552061,-0.555110906 O,0,1.8142167314,-0.5863591672,2.9001466471 H,0,1.9446240597,-0.6871355579,0.9737204945 O,0,2.1188075705,-0.7559845812,0.0181638672 N,0,1.0121950083,-0.369387039,-0.6814510814
$(CH_2NOH^{\cdots}H_2O)$-II	C,0,0.0323154339,0.0004881155,0.0145319547 H,0,0.0912660974,0.0771834054,1.0961647227 H,0,2.2844839707,0.00684981,1.6927589949 H,0,2.7592316438,0.6565551409,3.0000269942 H,0,-0.7797183014,0.4568878994,-0.5327710856 O,0,2.0466772942,0.66117188,2.35987846 H,0,2.4918055433,-1.5607266607,-0.5181575854 O,0,1.898303984,-1.152408204,0.1158936351 N,0,0.8968399527,-0.600567538,-0.6787338737
$HCN^{\cdots}H_2O^{\cdots}H_2O$	C,0,0.022076037,0.0141777982,0.0479248914 H,0,0.0135573208,0.0212772689,2.8893860325 H,0,1.9752396547,-0.0596106639,1.5957464131 H,0,-1.3133359005,-0.4342449893,3.5300670853 H,0,-0.850309772,0.0138941227,0.67530478

	O,0,-0.9505531108,0.0390854854,2.7807166477
	H,0,2.4065678931,0.7603800588,2.8149213397
	O,0,1.8676978039,0.0119503898,2.5510083997
	N,0,1.0015002382,0.009436454,-0.5418989014
$(CH_2NOH^{\cdots}NH_3)$-I	C,0,-0.0066436147,-0.0380445561,0.0029036893
	N,0,-0.0012254438,0.0383255894,1.265143389
	O,0,1.2135204439,0.1065330279,1.8737121278
	N,0,3.6624532565,0.0316189346,0.3102445998
	H,0,0.9030230272,-0.0492396815,-0.595083351
	H,0,3.849463526,-0.7216453143,-0.34063247
	H,0,4.2880796503,-0.0948150756,1.0975618286
	H,0,-0.971448999,-0.0934682071,-0.4798289991
	H,0,1.9352718994,0.0763495418,1.2097723436
	H,0,3.9286669589,0.8968730727,-0.1442481383
$(CH_2NOH^{\cdots}NH_3)$-II	C,0,0.0000465028,0.001418544,0.0002900359
	H,0,-0.001802874,-0.0238457755,1.0872198907
	H,0,1.9311677141,-0.0436987673,2.3840597309
	H,0,1.5287194138,-0.6674077691,3.8393574887
	H,0,-0.9188763339,0.0857064628,-0.5620962993
	H,0,2.9088142066,-0.2092434805,-0.5020956763
	O,0,2.1843586018,-0.1688863729,0.1255486175
	N,0,1.0589159073,-0.0611437455,-0.682500238
	N,0,1.3111507535,0.0685725891,3.1790812203
	H,0,1.5519107519,0.9450641587,3.625149822
$HCN^{\cdots}NH_3^{\cdots}H_2O$	C,0,0.0156320316,-0.0351818319,-0.0131153567
	N,0,-0.1040115224,0.0036440612,1.1206282516
	O,0,0.8328903996,0.0843160826,4.1363987667
	N,0,-1.2310591419,0.617915064,6.2079029717
	H,0,-1.0562975073,1.5327658392,6.6047303653
	H,0,0.0911079912,0.2710922255,4.7294287359
	H,0,-2.2243802357,0.5491475743,6.0265846188
	H,0,0.129560148,-0.0716213081,-1.0728189045
	H,0,0.4581855316,0.063694422,3.2523137263
	H,0,-1.0038908758,-0.0676051154,6.917608544
$(CH_2NOH^{\cdots}HCl)$-I	C,0,0.0143573324,0.0152565136,-0.0078109275
	H,0,0.0173051947,0.0289579773,1.0718903214
	H,0,0.2016804918,-0.0153896415,-2.2730237783
	H,0,-0.926977969,0.1199805962,-0.5484759293
	O,0,1.1095671906,-0.1402066958,-1.9546612113
	N,0,1.1276403957,-0.1245853754,-0.5812219922
	H,0,2.2287869139,1.4434133615,-2.4213450731
	Cl,0,2.6252009501,2.6138981674,-2.7790821045
$(CH_2NOH^{\cdots}HCl)$-II	C,0,0.0052020734,-0.0238109838,-0.026510126
	H,0,-0.0215570127,-0.0379570752,1.0529162333
	H,0,1.972097815,0.0521551685,-2.2385754878
	H,0,-0.9120901316,-0.0396424167,-0.6076927745
	O,0,1.0567870166,0.0180731639,-1.9482973511

	N,0,1.1470970834,0.0091996962,-0.5592270814
	H,0,0.0421773688,-1.5598932892,-2.4092363838
	Cl,0,-0.7471872759,-2.5789714377,-2.4527421513
HCN···HCl···H_2O	C,0,0.063897819,0.0091552355,-0.0337330948
	H,0,0.1562728999,0.0306346289,1.0294276187
	H,0,1.7459959546,-0.0371840664,-2.2457038759
	H,0,3.073671379,0.1682047953,-0.5598600358
	O,0,2.7120246099,-0.02578604,-2.2207806205
	N,0,-0.0195603501,-0.0129721867,-1.1719450734
	H,0,2.985829446,0.7091699718,-2.7741516124
	Cl,0,3.2744149293,0.3195960388,0.7340698307
(CH_2NOH···HCOOH)-I	C,0,-1.8773748075,0.514179581,-0.8245858318
	N,0,-1.6987248494,-0.6038928019,-0.2664096429
	O,0,-0.8796064151,-0.5956727642,0.8443588792
	H,0,-1.4255266,1.4393328415,-0.470799224
	H,0,0.7324441962,-1.1867075523,0.090975837
	H,0,-2.514653483,0.5209208307,-1.6972307888
	O,0,1.5990165526,-1.0573227421,-0.3467791505
	C,0,1.8828115019,0.2295161844,-0.3830801886
	O,0,1.1981350337,1.112783885,0.0627619185
	H,0,-0.4712713375,0.2858515263,0.9288419607
	H,0,2.8419652079,0.4061350116,-0.8794677688
(CH_2NOH···HCOOH)-II	C,0,-1.8575699026,0.4181639903,-0.5527546904
	N,0,-2.0413420147,-0.236390093,0.5091263875
	O,0,-0.970171631,-1.0983048717,0.7639645177
	H,0,-0.9653964356,0.3142243923,-1.1643857795
	H,0,0.693720636,-0.3590154775,0.7364567157
	H,0,-2.6443123992,1.1095337506,-0.8188358294
	O,0,1.5998251051,0.0033027642,0.8213632244
	C,0,1.9962078718,0.5034945226,-0.3377662125
	O,0,1.3445817624,0.5343202708,-1.3420082642
	H,0,-1.2262572052,-1.546433976,1.574010861
	H,0,3.0159522131,0.8962547273,-0.2606159303
HCN···HCOOH···H_2O	C,0,-2.096471794,0.9005760886,-0.6946153781
	N,0,-2.433865937,0.3926982297,0.2703683716
	O,0,-0.2446178352,-1.5383608313,0.898848994
	H,0,0.3076274515,-0.6705398656,-0.428966346
	H,0,0.4093898797,-1.1208910511,1.4753407115
	H,0,-1.7652088099,1.3645055967,-1.5967293106
	O,0,1.9459275574,0.3165896395,0.8833004053
	C,0,1.7334270085,0.5474023578,-0.2759739049
	O,0,0.789308137,-0.0171904744,-1.0080726357
	H,0,-1.0975774122,-1.1637830669,1.1456512614
	H,0,2.3139947541,1.2700623771,-0.8605601687
(CH_2NOH···HNO_3)-I	C,0,-2.3235775091,-0.425349323,-0.6787462243
	N,0,-2.0438242423,0.6899010531,-0.1616416482
	O,0,-1.2745485773,0.6407471185,0.9888608381

H,0,-2.9220426287,-0.4050676074,-1.5780454874
H,0,0.2881908265,1.0509272422,0.3194472659
H,0,-1.9910009902,-1.3777269494,-0.2680001074
O,0,1.166138587,1.0944538616,-0.1325198853
N,0,1.5220837708,-0.1885828279,-0.3655120973
O,0,0.7664441832,-1.0493614186,0.0302079846
H,0,-1.0475885223,-0.2845211892,1.1823525699
O,0,2.5509281025,-0.33201996,-0.9378252087

$(CH_2NOH^{\cdots}HNO_3)$-II

C,0,-2.3623424859,-0.4875515745,-0.397931501
N,0,-2.4601952506,0.0696505078,0.7282326096
O,0,-1.4239615197,0.9894548565,0.9294124975
H,0,-3.124387455,-1.2171535018,-0.6306621931
H,0,0.1761555335,0.3347254809,0.7768288382
H,0,-1.5660375078,-0.2587065382,-1.0996959558
O,0,1.0837460659,-0.0458694907,0.8600291084
N,0,1.5514908638,-0.1803098662,-0.4057061909
O,0,0.7985473088,0.1300704651,-1.2950671962
H,0,-1.6263251419,1.3782575366,1.784876247
O,0,2.6613135889,-0.5958878757,-0.4892862636

$HCN^{\cdots}HNO_3^{\cdots}H_2O$

C,0,-1.8950164235,-1.2124449708,-0.7629408922
N,0,-2.1262689326,-0.43349679,0.0378032374
O,0,-0.7739695141,1.7940587473,1.3778717548
H,0,-1.6582592987,-1.9358424492,-1.5122489151
H,0,-0.3415237695,1.4146275011,2.1487286148
H,0,0.1708687478,1.3934615611,0.1481659264
O,0,0.9451065,-0.5272805917,0.853749557
N,0,0.8988813663,-0.2747199247,-0.3234967191
O,0,0.590276647,0.9837171412,-0.6740164035
H,0,-1.5050398549,1.1899528231,1.1797623693
O,0,1.0884695322,-1.0288780475,-1.2344575297

$(CH_2NOH^{\cdots}H_2SO_4)$-I

C -2.70597 0.42397 -0.42503
N -2.09941 -0.66086 -0.20897
O -1.56109 -0.83696 1.04154
H -2.82699 1.19335 0.33444
H -0.43575 -0.90207 -1.00094
H -3.10687 0.57322 -1.41739
O 0.49613 -0.70775 -1.24945
S 1.16039 0.31766 -0.28636
O 0.19155 1.23758 0.19578
H -1.41428 0.0339 1.44315
O 2.34864 0.74712 -0.92036
O 1.542 -0.56416 0.96214
H 2.35615 -1.05109 0.77918

$(CH_2NOH^{\cdots}H_2SO_4)$-II

C,0,-2.9063751923,0.2623166406,-0.4385458711
N,0,-2.9884515218,-0.9371784068,-0.06065312
O,0,-1.8736882512,-1.2984304732,0.7138514904
H,0,-2.0716542196,0.908805391,-0.1817943513
H,0,-0.4014318336,-1.0333007054,-0.0217416436

	H,0,-3.7269968048,0.6182548404,-1.0448534956
	O,0,0.4628617793,-0.8849966518,-0.4863696981
	S,0,1.1216007861,0.4524919735,-0.0531764067
	O,0,0.1153956962,1.4231230893,0.1826470643
	H,0,-2.0626602461,-2.2019971922,0.9816352176
	O,0,2.2027889751,0.6819573886,-0.9360991495
	O,0,1.7071097933,0.1051244595,1.3727068899
	H,0,2.5746600392,-0.3065943536,1.2676620739
$HCN^{\cdots}H_2SO_4^{\cdots}H_2O$	C,0,-2.3732190004,1.0806163655,-0.7720063399
	N,0,-2.9167065708,0.1580479121,-0.3770365038
	O,0,-1.4141145901,-1.8718184432,1.0266669501
	H,0,-0.5605027109,-0.6755011775,1.3495980969
	H,0,-0.9498223992,-2.1954081127,0.244257406
	H,0,-1.8264198697,1.9302688606,-1.1219548178
	O,0,0.5341726141,-0.7208107404,-0.7819403109
	S,0,0.7670466728,0.3873253678,0.0791074384
	O,0,0.0243414397,0.1719731229,1.4046188107
	H,0,-2.2264092168,-1.4747107564,0.6778032436
	O,0,0.5286481214,1.7158712235,-0.378718009
	O,0,2.2776859694,0.2999208082,0.5103837381
	H,0,2.5890725405,1.1724855694,0.7824182977
(INT)-I	C,0,-2.4127310985,-0.2939227287,-0.4903528575
	N,0,-1.3699087122,0.1795096995,0.0380057325
	O,0,-0.2404127553,-0.4111857231,-0.4909968808
	H,0,-2.3853737382,-1.0558300202,-1.2638365368
	H,0,-3.3531433664,0.0972590034,-0.1316680108
	H,0,1.2880388133,0.9759931817,-1.661228757
	O,0,1.1714184447,1.3124498968,-0.75786515
	N,0,0.8919251597,0.2210520014,0.0533540087
	C,0,1.9499048801,-0.7681926467,-0.1007437409
	H,0,2.8720961517,-0.3055373628,0.2340382717
	H,0,1.710237234,-1.6233819369,0.5231161496
	H,0,2.0465229873,-1.0871963645,-1.1449642284
(INT)-II	C,0,-2.4556881866,-0.2836082968,-0.0667142923
	N,0,-1.3532726295,0.240848967,0.2520505689
	O,0,-0.2961367881,-0.5655534264,-0.0905021748
	H,0,-2.5238398231,-1.2542487676,-0.548400422
	H,0,-3.3452673169,0.2822391241,0.1662187982
	H,0,0.778999627,1.8275811508,-0.4112354928
	O,0,1.182309244,1.0100310937,-0.7183606856
	N,0,0.8889479992,0.0998010595,0.3047725768
	C,0,1.9080791982,-0.9359000754,0.2002171531
	H,0,2.8582133656,-0.4734152483,0.444651776
	H,0,1.6715633793,-1.7104925775,0.9222535525
	H,0,1.940641931,-1.348736003,-0.8095123579
TS-1	C,0,-0.1144040202,-0.0436622883,0.2451853079
	H,0,-0.2701260224,0.2230953466,1.28135072
	H,0,0.7761371336,-0.4341561444,-0.8132117309

H,0,-0.3842445129,0.7359413293,-0.4684869579
O,0,0.0966087653,-1.4950087613,-1.227226171
N,0,-0.5920223434,-1.2409464818,-0.2042961681

TS-2

C,0,-0.0367041132,0.9126378209,0.7953922878
H,0,-0.7046224793,1.2656956696,1.5700135183
H,0,0.4813380877,-0.0091980423,-1.4636328928
H,0,0.8312250346,1.5002956822,0.5043399724
O,0,0.6268439329,-0.586073148,-0.7064794408
N,0,-0.3132014625,-0.1979019823,0.269541555

TS-3

C,0,-0.1100307075,0.8550628465,0.8750812926
H,0,-0.4234041,1.3022200599,1.8145615779
H,0,0.6061465949,-1.1240010869,-0.8645534648
H,0,0.6159492404,0.6165260085,-0.3152013851
O,0,0.118939557,-0.2915212774,-0.9484251143
N,0,-0.765553505,-0.1157574106,0.4665214736

TS-4

C,0,0.4174577029,0.144283636,0.1684544837
N,0,0.5052298229,0.1684030254,1.50963344
O,0,1.5531113581,-0.3788746643,1.9490093848
H,0,0.9198039857,-0.652297754,-0.3746738688
H,0,-0.4816183279,0.5725638731,-0.2493359546
H,0,1.5053543242,0.9974702748,0.0380378146
O,0,2.5568609476,1.406182199,0.4475342781
N,0,3.0514739596,0.5877212744,1.2686833952
C,0,3.7305097808,-0.5247406197,0.6007760489
H,0,4.7295681304,-0.1502228324,0.3719508529
H,0,3.7975110467,-1.3526872338,1.2971632456
H,0,3.2332352692,-0.8109951786,-0.3241061203

TS-5

C,0,-2.3026073802,-0.2232604242,0.0915577154
N,0,-1.3342933601,0.294860992,-0.5292085791
O,0,-0.1560215987,-0.3755705295,-0.2432965527
H,0,-2.1856986333,-1.0729305037,0.7575346304
H,0,-3.2713254978,0.2261754318,-0.0682466039
H,0,0.2967959775,-1.0129694092,-2.2084890203
O,0,1.0619070087,-0.4309812449,-2.1458059613
N,0,0.8946443874,0.2647020547,-0.9135084345
C,0,2.0753007188,-0.0601019174,-0.1208735776
H,0,2.9345319929,0.3040482795,-0.6743381045
H,0,1.9933712525,0.4639419397,0.8265790113
H,0,2.1619691325,-1.1368976689,0.0349534769

TS-6

C -1.43003 -0.67353 -0.69452
N -1.15919 0.04874 0.22795
O 0.83025 -0.36686 -0.5875
H -0.42256 -0.99141 -1.27058
H -2.38697 -1.04537 -1.04975
H 2.14713 1.5842 -1.3575
O 2.50586 0.72308 -1.59752
N 2.07369 -0.1269 -0.56251

C 2.96139 -1.27998 -0.51221
H 3.97536 -0.93203 -0.35039
H 2.63116 -1.90153 0.31265
H 2.89768 -1.83261 -1.45328

TS-7

C,0,-2.1726098514,-0.0832595747,0.3297154185
N,0,-2.1403087781,0.9231208113,0.8712385958
O,0,0.0347320746,-0.7833467064,-1.2873013561
H,0,0.2647851764,0.5376977511,-1.1324017503
H,0,-2.1392364041,-1.0054506849,-0.2107027985
H,0,-0.0591061305,1.2126826244,0.3843394669
O,0,0.698708358,0.9173542646,-0.1537852156
N,0,0.5910837774,-0.7016873627,-0.0643556883
C,0,1.9992016559,-1.0886611381,-0.1214785992
H,0,2.4908716104,-0.7870173067,0.7982312827
H,0,1.9856033916,-2.1741678249,-0.198568446
H,0,2.4821701198,-0.6646698533,-1.0010829098

TS-8

C,0,-0.0003350063,0.0003130727,-0.0029933692
H,0,-0.0062096056,0.0009096341,1.088080103
H,0,1.4387018139,-0.0074132477,0.0834928748
H,0,3.0761463939,-0.7249151979,-0.1834635019
H,0,-0.5369088318,0.7851428369,-0.5126024874
O,0,2.4106541816,-0.6120888617,0.5045593553
H,0,1.7852093271,-1.4682734351,0.4816764862
O,0,0.5931706085,-2.1269254401,-0.0294990441
N,0,-0.0065049263,-1.192087901,-0.626664217

TS-9

C,0,0.0021948515,0.0000413917,0.0044923757
H,0,-0.0073524583,-0.0161101862,1.0916960673
H,0,2.250073124,-0.0071316004,1.660930929
H,0,2.6899697333,0.9423482724,2.7877022181
H,0,-0.7745443919,0.5151623818,-0.5459732381
O,0,1.9397477247,0.449705452,2.4527844378
H,0,1.4770297025,-1.953797588,0.4928424128
O,0,1.894747848,-1.1746983759,0.1090394302
N,0,0.9031074809,-0.5444168588,-0.6886733515

TS-10

C,0,0.0029557179,0.0044344673,0.0123580107
H,0,-0.0017567814,0.0029207304,1.4424301653
H,0,1.5898725656,-0.008086917,1.7739008351
H,0,0.4185836855,-0.8265838387,2.9283604686
H,0,-0.751261034,-0.0643563263,-0.7720466673
O,0,0.5820535899,-0.0031603021,2.460605392
H,0,2.8668895776,-0.5574159744,0.6081855844
O,0,2.2488275426,0.1510535057,0.8083572415
N,0,1.1322048188,-0.0045710092,-0.4775969025

TS-11

C,0,-0.086832047,-0.000541086,-0.0229276557
H,0,-0.3445239684,-0.1255993304,1.0306399713
H,0,1.4121831138,-0.0679383059,0.2622847117
H,0,3.1601481691,-0.6426460446,-0.0350528776

H,0,-0.4563894103,0.864986655,-0.5526584612
H,0,2.0235793141,-1.5614927803,0.7716195138
O,0,0.3888458141,-2.1510187445,-0.140931158
N,0,0.0857797967,-1.1076732006,-0.7641769538
N,0,2.4260108807,-0.62186074,0.6629354742
H,0,2.7669313346,-0.2448780097,1.5374281709

TS-12

C,0,-0.1377388911,-0.2130014867,-0.0134229138
H,0,-0.1152918149,-0.3899652442,1.0591539608
H,0,2.1253875545,0.2435037745,1.7289960182
H,0,2.2667601886,0.5699418876,3.3229548527
H,0,-1.0009233115,0.2425938535,-0.4820493829
H,0,1.6617145994,-1.9588261405,0.1321095777
O,0,1.9216969201,-1.0556956314,-0.0772766746
N,0,0.8264690083,-0.4891377633,-0.7773447192
N,0,1.6888118022,0.7291819961,2.5068549093
H,0,1.7431690246,1.7199498942,2.3031941617

TS-13

C,0,-1.2839279397,0.2437109646,-0.3844827177
H,0,-0.5031094775,0.8311415283,1.013264297
H,0,0.9716399919,0.2095638887,0.8133625469
H,0,0.3318925686,0.3629419575,2.4951320126
H,0,-2.2957485007,0.1600181408,-0.7905931802
H,0,1.405805643,-1.1706864507,-0.7334145704
O,0,1.0745746478,-0.3041265455,-0.490334347
N,0,-0.5367966647,-0.4427290408,-1.0782960283
N,0,0.4381819296,0.8180132454,1.5964843173
H,0,0.830754802,1.7452103116,1.70965467

TS-14

C,0,0.006762351,0.008025673,0.0017993366
H,0,-0.0083708988,-0.0093422235,1.0806013177
H,0,0.6105195522,-0.0734213216,-2.1743627089
H,0,-0.9342870854,0.2571413543,-0.4890094816
O,0,0.7739999501,-1.0467371907,-1.7861201424
N,0,0.6977751584,-1.0396514463,-0.5269418059
H,0,0.611928011,0.940731308,-0.557480213
Cl,0,0.9472076209,1.7044279639,-2.1511165764

TS-15

C,0,-0.0091313072,0.0166151195,0.032912305
N,0,0.1057933639,-0.18504758,1.2699891484
O,0,1.452872351,-0.1212774624,1.7043604456
Cl,0,0.922447382,-0.6085572773,4.8482623262
H,0,-1.0095402329,-0.0383291815,-0.3754268842
H,0,1.7054491919,0.8092034716,1.6783528564
H,0,0.8407655687,0.2302017486,-0.6108035446
H,0,1.1332218066,-0.5637378456,3.5769976252

TS-16

C,0,-0.0048119637,-0.0035224401,0.0095335743
H,0,-0.0094780537,0.0062056616,1.0982284622
H,0,1.4202027644,0.0080311505,-2.650081437
H,0,-0.8237339802,-0.6335451884,-0.6386319481
O,0,0.6068532406,0.4493328159,-2.382448438

	N,0,0.897108397,0.6000592064,-0.5286370853
	H,0,-0.1447659192,-0.2153121417,-2.4807624473
	Cl,0,-1.5769665148,-1.4018607304,-1.9867463778
TS-17	C,0,0.4953764028,-0.0002277895,0.0837003668
	N,0,0.3028405544,-0.6535652564,1.2473877094
	O,0,0.9360657181,-0.2219252557,2.2405740536
	H,0,0.7845347945,1.0497785567,0.134607612
	H,0,1.7405139833,-0.5027184637,-0.108175852
	H,0,-0.1729811592,-0.3034610338,-0.7083451576
	O,0,3.0068572265,-0.6650979655,-0.1390329141
	C,0,3.619635086,0.0477089072,0.6761915237
	O,0,3.1269297134,0.6341895257,1.6817585092
	H,0,2.0741891485,0.3523372616,1.932754822
	H,0,4.689909532,0.1985455135,0.5210393271
TS-18	C,0,-1.8433516477,0.4151934062,-0.8130862473
	N,0,-2.1178610053,-0.6106908615,-0.1338586289
	O,0,-1.0608982394,-0.9482648385,0.7629798239
	H,0,-0.9193384803,0.9768700154,-0.6934305538
	H,0,0.5673322256,-0.9698201047,0.0620647961
	H,0,-2.5931398879,0.7159015805,-1.5340116665
	O,0,1.4784020925,-0.9351823924,-0.3071157548
	C,0,1.8912972735,0.3179323703,-0.3430610718
	O,0,1.2479333355,1.2736818238,-0.0058305942
	H,0,-1.1376204996,-0.3410790039,1.5077896365
	H,0,2.9141922031,0.3829363247,-0.7298900492
TS-19	C,0,-1.5189520483,0.5142717138,-0.8551302993
	N,0,-1.9751556646,-0.1488931788,0.0713106587
	O,0,-0.718285795,-1.1813796582,0.616777369
	H,0,-0.1968485905,0.5949687632,-1.2877007134
	H,0,0.1963835081,-0.6215542595,0.6000245147
	H,0,-2.3166021413,1.1619190155,-1.2308812458
	O,0,1.411895155,0.0320915498,0.5067223787
	C,0,1.7345877056,0.5204789679,-0.5863664754
	O,0,0.9633843109,0.7528913702,-1.5612216664
	H,0,-0.9799684581,-1.3458483546,1.5286109412
	H,0,2.7867780182,0.7861780709,-0.7435594619
TS-20	C,0,0.4907623454,-0.0318218895,0.1215349369
	N,0,0.254557367,0.6210662402,1.2882602603
	O,0,1.0221747902,0.3564450933,2.2427448843
	H,0,-0.2507830468,0.175805865,-0.6341947297
	H,0,1.628778814,0.5052559664,-0.0820357828
	H,0,0.8618082242,-1.0546759052,0.1930941964
	O,0,2.9703265287,0.8173748468,0.0234249867
	N,0,3.6294280303,-0.1056679668,0.5990137701
	O,0,3.0420947037,-0.7751181394,1.5124024016
	H,0,1.9264384781,-0.2306244252,1.9281385914
	O,0,4.7542307653,-0.3425616855,0.2988184848

TS-21

C,0,-2.2999456039,-0.2626521039,-0.7216783615
N,0,-2.507295807,0.6657841798,0.1045909199
O,0,-1.3567165212,0.9326393422,0.9049977266
H,0,-3.1235924677,-0.504660337,-1.3805560455
H,0,0.0919298072,0.9587837793,0.0929036644
H,0,-1.3619953805,-0.8095303915,-0.7820728651
O,0,0.9564404674,0.9588315991,-0.403805971
N,0,1.4849525353,-0.2700924125,-0.2146580767
O,0,0.8274520062,-1.0507031136,0.4369088365
H,0,-1.3165889104,0.2316852223,1.5674967265
O,0,2.5443724745,-0.4513936643,-0.7194362641

TS-22

C,0,-1.7627175193,-0.568900917,-0.6153755791
N,0,-2.2790369576,-0.0541154799,0.359806229
O,0,-1.0685542563,1.1060585186,0.9900360728
H,0,-2.4447348103,-1.2862275813,-1.078661114
H,0,-0.1853857817,0.5969051078,0.9118068551
H,0,-0.5223159847,-0.3511543197,-1.0467542035
O,0,1.0703748775,-0.2168156986,0.6971219316
N,0,1.5011058949,-0.2944287847,-0.4750928965
O,0,0.6538637724,-0.1579216535,-1.4381820264
H,0,-1.3115093358,1.1610579825,1.9208610387
O,0,2.6479647909,-0.4885424141,-0.7285742477

TS-23

C,0,0.5690690371,0.1320433009,0.0714442864
N,0,0.339872925,-0.819498678,1.0118970205
O,0,1.0530859902,-0.793118145,2.0423709214
H,0,0.9153355525,1.1039433843,0.4228783967
H,0,1.6993699811,-0.2889194828,-0.312517688
H,0,-0.1671115974,0.1151014558,-0.717975908
O,0,3.06727892,-0.5466010781,-0.3809331021
S,0,3.8896560824,0.1060297725,0.6487026388
O,0,3.0127505082,0.6194769198,1.7216963228
H,0,1.8974936051,-0.0906237203,1.9760784285
O,0,4.8463625354,1.0497416738,0.1948816035
O,0,4.669902947,-1.1162861541,1.2771795667
H,0,5.5433392534,-0.8171531288,1.5590724626

TS-24

C,0,-2.8862765842,0.3025737475,-0.5652639074
N,0,-3.0685212098,-0.5748296338,0.3204013829
O,0,-1.8469832209,-0.9356770566,0.9694459437
H,0,-1.9201601517,0.7531906356,-0.7755716856
H,0,-0.5029576073,-0.949281258,0.0597169316
H,0,-3.7673047335,0.6053915581,-1.1163535708
O,0,0.3456751544,-0.7729385029,-0.4448611883
S,0,1.0490499825,0.4684750374,0.159723465
O,0,0.0703514464,1.2951211531,0.7780684077
H,0,-1.6965700105,-0.2573669938,1.6424842774
O,0,1.9514034996,0.9648491867,-0.8092839568
O,0,1.8798615589,-0.1413497712,1.3542596171
H,0,2.7105714964,-0.5042629821,1.0198625333

TS-25	C,0,-2.3409542699,0.6468519142,-0.3514982042 N,0,-2.8583234058,-0.3842142571,0.0305377851 O,0,-1.5490658679,-1.6342526679,0.2994530337 H,0,-1.0846789945,0.9996007415,-0.5237090056 H,0,-0.7544158853,-1.4358365374,-0.2895610847 H,0,-3.1302189223,1.386805672,-0.5303191044 O,0,0.5304882317,-0.9730186125,-1.0711689719 S,0,1.0923072735,0.2411641325,-0.5221464828 O,0,0.1204266297,1.3634539998,-0.6494795452 H,0,-1.2554835579,-1.4873954124,1.2072983669 O,0,2.4057403695,0.6128625499,-0.8988668614 O,0,1.0963083682,-0.0806574018,1.0479466826 H,0,1.6723680312,0.5485628792,1.4992383921

References:

1. A. Varandas and F. Pansini, *J. Chem. Phys*., 2014, 141, 224113.
2. S. Sarkar, S. Mallick, Deepak, P. Kumar and B. Bandyopadhyay, *Phys. Chem. Chem. Phys.*, 2017, 19, 27848.
3. S. Sarkar, S. Mallick, P. Kumar and B. Bandyopadhyay, *Phys. Chem. Chem. Phys.*, 2018, 20, 13437.
4. S. Sarkar, B. K. Oram and B. Bandyopadhyay, *Phys. Chem. Chem. Phys.*, 2019, 21, 16170.