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

Supporting Information

for

Theoretical Investigation of the Relative Impacts of Water and Ammonia on the Tropospheric Conversion of N_2O_5 to HNO_3

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Proof for same value of termolecular rate constant (k_t) of three different reaction channels for NH_3 catalyzed hydrolysis:

In presence of a catalyst (Y), there are three possibilities; in first case, N_2O_5 first reacts with X to form N_2O_5-X complex and then it reacts with Y. In the second case first X binds with Y to form X-Y complex and then it reacts with N_2O_5 and in the third case N_2O_5 first reacts with Y to form N_2O_5-Y complex and then it reacts with X. Scheme for this reaction can be written as follows-

$$\text{(Path 1)} \quad \mathrm{N_2O_5 + X + Y} \underset{k_r^{\mathrm{N_2O_5+X}}}{\overset{k_f^{\mathrm{N_2O_5+X}}}{\rightleftharpoons}} \mathrm{N_2O_5\text{–}X + Y} \underset{k_r^{\mathrm{N_2O_5-X+Y}}}{\overset{k_f^{\mathrm{N_2O_5-X+Y}}}{\rightleftharpoons}} \mathrm{N_2O_5\text{-}X\text{-}Y} \xrightarrow{k_{uni}^{\mathrm{N_2O_5-X+Y}}} \mathrm{P\text{-}Y}$$

$$\text{(Path2)} \quad \mathrm{N_2O_5 + X + Y} \underset{k_r^{\mathrm{X+Y}}}{\overset{k_f^{\mathrm{X+Y}}}{\rightleftharpoons}} \mathrm{N_2O_5 + X\text{-}Y} \underset{k_r^{\mathrm{N_2O_5+X-Y}}}{\overset{k_f^{\mathrm{N_2O_5+X-Y}}}{\rightleftharpoons}} \mathrm{N_2O_5\text{-}X\text{-}Y} \xrightarrow{k_{uni}^{\mathrm{N_2O_5+X-Y}}} \mathrm{P\text{-}Y}$$

$$\text{(Path 3)} \quad \mathrm{N_2O_5 + Y + X} \underset{k_r^{\mathrm{N_2O_5+Y}}}{\overset{k_f^{\mathrm{N_2O_5+Y}}}{\rightleftharpoons}} \mathrm{N_2O_5\text{–}Y + X} \underset{k_r^{\mathrm{N_2O_5-Y+X}}}{\overset{k_f^{\mathrm{N_2O_5-Y+X}}}{\rightleftharpoons}} \mathrm{N_2O_5\text{-}X\text{-}Y} \xrightarrow{k_{uni}^{\mathrm{N_2O_5-X+Y}}} \mathrm{P\text{-}Y}$$

For Path 1-

$$K_{eq}^{\mathrm{N_2O_5+X}} = \frac{\left[\mathrm{N_2O_5 - X}\right]}{\left[\mathrm{N_2O_5}\right]\left[\mathrm{X}\right]} \tag{1}$$

and

$$K_{eq}^{\mathrm{N_2O_5-X+Y}} = \frac{\left[\mathrm{N_2O_5 - X - Y}\right]}{\left[\mathrm{N_2O_5 - X}\right]\left[\mathrm{Y}\right]} \tag{2}$$

Therefore,

$$K_{eq}^{\mathrm{N_2O_5+X}} \times K_{eq}^{\mathrm{N_2O_5-X+Y}} = \frac{\left[\mathrm{N_2O_5 - X - Y}\right]}{\left[\mathrm{N_2O_5}\right]\left[\mathrm{X}\right]\left[\mathrm{Y}\right]} \tag{3}$$

Similarly, for Path 2-

$$K_{eq}^{\mathrm{X+Y}} \times K_{eq}^{\mathrm{N_2O_5+X-Y}} = \frac{\left[\mathrm{X - Y}\right]}{\left[\mathrm{X}\right]\left[\mathrm{Y}\right]} \times \frac{\left[\mathrm{N_2O_5 + X - Y}\right]}{\left[\mathrm{N_2O_5}\right]\left[\mathrm{X - Y}\right]} = \frac{\left[\mathrm{N_2O_5 - X - Y}\right]}{\left[\mathrm{N_2O_5}\right]\left[\mathrm{X}\right]\left[\mathrm{Y}\right]} \tag{4}$$

Similarly, for Path 3-

$$K_{eq}^{\mathrm{N_2O_5+Y}} \times K_{eq}^{\mathrm{N_2O_5-Y+X}} = \frac{\left[\mathrm{N_2O_5-Y}\right]}{\left[\mathrm{N_2O_5}\right]\left[\mathrm{Y}\right]} \times \frac{\left[\mathrm{N_2O_5-X-Y}\right]}{\left[\mathrm{N_2O_5-Y}\right]\left[\mathrm{X}\right]} = \frac{\left[\mathrm{N_2O_5-X-Y}\right]}{\left[\mathrm{N_2O_5}\right]\left[\mathrm{X}\right]\left[\mathrm{Y}\right]} \tag{5}$$

From the equation 3, 4 and 5, it is clear that, the product of $K_{eq}^{\mathrm{N_2O_5+X}}$ and $K_{eq}^{\mathrm{N_2O_5-X+Y}}$ or $K_{eq}^{\mathrm{X+Y}}$ and $K_{eq}^{\mathrm{N_2O_5+X-Y}}$ or $K_{eq}^{\mathrm{N_2O_5+Y}}$ and $K_{eq}^{\mathrm{N_2O_5-Y+X}}$ for Path 1, Path 2 and Path 3 are also same, it gives same termolecular rate (k_t).

Table S1: Concentrations of water and ammonia (in molecules cm^{-3}) within 280 to 320 K at 0 km altitude

Species	Abundance	T(K)					
		280	290	298	300	310	320
H_2O[a]	20% RH	5.16×10^{16}	9.56×10^{16}	1.55×10^{17}	1.72×10^{17}	2.92×10^{17}	4.70×10^{17}
	100% RH	2.58×10^{17}	4.78×10^{17}	7.73×10^{17}	8.58×10^{17}	1.46×10^{17}	2.35×10^{17}
NH_3[b]	0.1 ppbv	2.62×10^{9}	2.53×10^{9}	2.46×10^{9}	2.44×10^{9}	2.36×10^{9}	2.29×10^{9}
	10 ppbv	2.62×10^{11}	2.53×10^{11}	2.46×10^{11}	2.44×10^{11}	2.36×10^{11}	2.29×10^{11}
	2900 ppbv	7.61×10^{13}	7.34×10^{13}	7.14×10^{13}	7.10×10^{13}	6.87×10^{13}	6.66×10^{13}

[a]-Reference 1
[b]-References 2-5

Table S2: Concentrations of water and ammonia (molecules cm^{-3}) from 0 to 15 km altitudes in troposphere

Altitude(km)	H_2O[a]	NH_3[b]
0	5.2×10^{17}	2.5×10^{11}
5	2.4×10^{16}	7.6×10^{9}
10	4.9×10^{15}	8.5×10^{8}
15	2.0×10^{13}	1.2×10^{8}

[a]-Reference 1
[b]-References 6-8

Table S3: Equilibrium constants (cm^3 $molecule^{-1}$), unimolecular rate coefficients (s^{-1}), bimolecular rate coefficients (cm^3 $molecule^{-1}$ s^{-1}) and termolecular rate coefficients (cm^6 $molecule^{-2}$ s^{-1}) for all the studied reaction channels at different temperatures

Reactions	Catalysts	Channels	Rate Constants	T (K)													
				213	216	219	224	230	235	250	259	280	290	298	300	310	320
Hydrolysis	Uncat	A	$K_{eq}^{N_2O_5-H_2O}$	7.9×10^{-23}	7.2×10^{-23}	6.6×10^{-23}	5.7×10^{-23}	4.9×10^{-23}	4.3×10^{-23}	3.0×10^{-23}	2.5×10^{-23}	1.7×10^{-23}	1.5×10^{-23}	1.3×10^{-23}	1.3×10^{-23}	1.1×10^{-23}	1.0×10^{-23}
			$k_{uni}^{N_2O_5-H_2O}$	5.3×10^{-11}	1.0×10^{-10}	2.0×10^{-10}	5.7×10^{-10}	1.9×10^{-9}	4.9×10^{-9}	6.8×10^{-8}	2.8×10^{-7}	5.5×10^{-6}	2.0×10^{-5}	5.0×10^{-5}	6.3×10^{-5}	1.9×10^{-4}	5.3×10^{-4}
			$k_{bi}^{N_2O_5+H_2O}$	4.2×10^{-33}	7.5×10^{-33}	1.3×10^{-32}	3.3×10^{-32}	9.3×10^{-32}	2.1×10^{-31}	2.1×10^{-30}	7.2×10^{-30}	9.7×10^{-29}	2.9×10^{-28}	6.7×10^{-28}	8.2×10^{-28}	2.2×10^{-27}	5.4×10^{-27}
	H_2O-cat	C	K_{eq}^{1}-Path1	7.9×10^{-23}	7.2×10^{-23}	6.6×10^{-23}	5.7×10^{-23}	4.9×10^{-23}	4.3×10^{-23}	3.0×10^{-23}	2.5×10^{-23}	1.7×10^{-23}	1.5×10^{-23}	1.3×10^{-23}	1.3×10^{-23}	1.1×10^{-23}	1.0×10^{-23}
			K_{eq}^{2}-Path1	7.3×10^{-22}	6.1×10^{-22}	5.1×10^{-22}	3.9×10^{-22}	2.9×10^{-22}	2.2×10^{-22}	1.1×10^{-22}	7.9×10^{-23}	3.7×10^{-23}	2.7×10^{-23}	2.1×10^{-23}	2.0×10^{-23}	1.5×10^{-23}	1.2×10^{-23}
			k_{uni}-Path1	1.3×10^{-10}	2.5×10^{-10}	4.9×10^{-10}	1.4×10^{-9}	4.8×10^{-9}	1.3×10^{-8}	1.8×10^{-7}	7.6×10^{-7}	1.5×10^{-5}	5.5×10^{-5}	1.4×10^{-4}	1.8×10^{-4}	5.4×10^{-4}	1.5×10^{-3}
			k_r-Path1	7.4×10^{-54}	1.1×10^{-53}	1.7×10^{-53}	3.2×10^{-53}	6.7×10^{-53}	1.2×10^{-52}	6.2×10^{-52}	1.5×10^{-51}	9.9×10^{-51}	2.2×10^{-50}	4.0×10^{-50}	4.7×10^{-50}	9.5×10^{-50}	1.8×10^{-49}
		G	K_{eq}^{1}-Path2	7.5×10^{-21}	6.7×10^{-21}	6.1×10^{-21}	5.2×10^{-21}	4.3×10^{-21}	3.7×10^{-21}	2.5×10^{-21}	2.0×10^{-21}	1.3×10^{-21}	1.1×10^{-21}	9.5×10^{-22}	9.2×10^{-22}	7.9×10^{-22}	6.8×10^{-22}
			K_{eq}^{2}-Path2	7.7×10^{-24}	6.5×10^{-24}	5.6×10^{-24}	4.3×10^{-24}	3.3×10^{-24}	2.6×10^{-24}	1.4×10^{-24}	9.9×10^{-25}	5.0×10^{-25}	3.7×10^{-25}	3.0×10^{-25}	2.9×10^{-25}	2.2×10^{-25}	1.8×10^{-25}
			k_{uni}-Path2	1.3×10^{-10}	2.5×10^{-10}	4.9×10^{-10}	1.4×10^{-9}	4.8×10^{-9}	1.3×10^{-8}	1.8×10^{-7}	7.6×10^{-7}	1.5×10^{-5}	5.5×10^{-5}	1.4×10^{-4}	1.8×10^{-4}	5.4×10^{-4}	1.5×10^{-3}
			k_r-Path2	7.4×10^{-54}	1.1×10^{-53}	1.7×10^{-53}	3.2×10^{-53}	6.7×10^{-53}	1.2×10^{-52}	6.2×10^{-52}	1.5×10^{-51}	9.9×10^{-51}	2.2×10^{-50}	4.0×10^{-50}	4.7×10^{-50}	9.5×10^{-50}	1.8×10^{-49}
	NH_3-cat	D	K_{eq}^{1}-Path1	7.9×10^{-23}	7.2×10^{-23}	6.6×10^{-23}	5.7×10^{-23}	4.9×10^{-23}	4.3×10^{-23}	3.0×10^{-23}	2.5×10^{-23}	1.7×10^{-23}	1.5×10^{-23}	1.3×10^{-23}	1.3×10^{-23}	1.1×10^{-23}	1.0×10^{-23}
			K_{eq}^{2}-Path1	6.3×10^{-20}	5.0×10^{-20}	4.0×10^{-20}	2.8×10^{-20}	1.8×10^{-20}	1.3×10^{-20}	5.4×10^{-21}	3.3×10^{-21}	1.2×10^{-21}	7.9×10^{-22}	5.7×10^{-22}	5.3×10^{-22}	3.7×10^{-22}	2.6×10^{-22}
			k_{uni}-Path1	3.3×10^{-11}	6.6×10^{-11}	1.3×10^{-10}	3.9×10^{-10}	1.4×10^{-9}	3.7×10^{-9}	5.8×10^{-8}	2.6×10^{-7}	5.8×10^{-6}	2.2×10^{-5}	5.8×10^{-5}	7.4×10^{-5}	2.3×10^{-4}	6.8×10^{-4}
			k_r-Path1	1.6×10^{-52}	2.4×10^{-52}	3.4×10^{-52}	6.2×10^{-52}	1.2×10^{-51}	2.1×10^{-51}	9.5×10^{-51}	2.2×10^{-50}	1.2×10^{-49}	2.5×10^{-49}	4.4×10^{-49}	5.1×10^{-49}	9.8×10^{-49}	1.8×10^{-48}
		H	K_{eq}^{1}-Path2	3.4×10^{-20}	3.0×10^{-20}	2.6×10^{-20}	2.0×10^{-20}	1.6×10^{-20}	1.3×10^{-20}	7.4×10^{-21}	5.5×10^{-21}	2.9×10^{-21}	2.3×10^{-21}	1.9×10^{-21}	1.8×10^{-21}	1.4×10^{-21}	1.2×10^{-21}
			K_{eq}^{2}-Path2	1.5×10^{-22}	1.2×10^{-22}	1.0×10^{-22}	7.7×10^{-23}	5.6×10^{-23}	4.4×10^{-23}	2.2×10^{-23}	1.5×10^{-23}	7.2×10^{-24}	5.2×10^{-24}	4.1×10^{-24}	3.9×10^{-24}	3.0×10^{-24}	2.3×10^{-24}
			k_{uni}-Path2	3.3×10^{-11}	6.6×10^{-11}	1.3×10^{-10}	3.9×10^{-10}	1.4×10^{-9}	3.7×10^{-9}	5.8×10^{-8}	2.6×10^{-7}	5.8×10^{-6}	2.2×10^{-5}	5.8×10^{-5}	7.4×10^{-5}	2.3×10^{-4}	6.8×10^{-4}
			k_r-Path2	1.6×10^{-52}	2.4×10^{-52}	3.4×10^{-52}	6.2×10^{-52}	1.2×10^{-51}	2.1×10^{-51}	9.5×10^{-51}	2.2×10^{-50}	1.2×10^{-49}	2.5×10^{-49}	4.4×10^{-49}	5.1×10^{-49}	9.8×10^{-49}	1.8×10^{-48}
		K	K_{eq}^{1}-Path3	4.9×10^{-22}	4.4×10^{-22}	4.0×10^{-22}	3.4×10^{-22}	2.8×10^{-22}	2.4×10^{-22}	1.6×10^{-22}	1.3×10^{-22}	8.5×10^{-23}	7.1×10^{-23}	6.2×10^{-23}	6.0×10^{-23}	5.2×10^{-23}	4.5×10^{-23}
			K_{eq}^{2}-Path3	1.0×10^{-20}	8.1×10^{-21}	6.6×10^{-21}	4.7×10^{-21}	3.2×10^{-21}	2.3×10^{-21}	1.0×10^{-21}	6.4×10^{-22}	2.5×10^{-22}	1.7×10^{-22}	1.2×10^{-22}	1.2×10^{-22}	8.2×10^{-23}	5.9×10^{-23}
			k_{uni}-Path3	3.3×10^{-11}	6.6×10^{-11}	1.3×10^{-10}	3.9×10^{-10}	1.4×10^{-9}	3.7×10^{-9}	5.8×10^{-8}	2.6×10^{-7}	5.8×10^{-6}	2.2×10^{-5}	5.8×10^{-5}	7.4×10^{-5}	2.3×10^{-4}	6.8×10^{-4}
			k_r-Path3	1.6×10^{-52}	2.4×10^{-52}	3.4×10^{-52}	6.2×10^{-52}	1.2×10^{-51}	2.1×10^{-51}	9.5×10^{-51}	2.2×10^{-50}	1.2×10^{-49}	2.5×10^{-49}	4.4×10^{-49}	5.1×10^{-49}	9.8×10^{-49}	1.8×10^{-48}
Ammonolysis	Uncat	B	$K_{eq}^{N_2O_5-NH_3}$	4.9×10^{-22}	4.4×10^{-22}	4.0×10^{-22}	3.4×10^{-22}	2.8×10^{-22}	2.4×10^{-22}	1.6×10^{-22}	1.3×10^{-22}	8.5×10^{-23}	7.1×10^{-23}	6.2×10^{-23}	6.0×10^{-23}	5.2×10^{-23}	4.5×10^{-23}
			$k_{uni}^{N_2O_5-NH_3}$	4.3×10^{-7}	7.4×10^{-7}	1.3×10^{-6}	2.9×10^{-6}	7.6×10^{-6}	1.6×10^{-5}	1.4×10^{-4}	4.3×10^{-4}	4.7×10^{-3}	1.3×10^{-2}	2.8×10^{-2}	3.3×10^{-2}	8.1×10^{-2}	1.8×10^{-1}
			$k_{bi}^{N_2O_5+NH_3}$	2.1×10^{-28}	3.3×10^{-28}	5.0×10^{-28}	9.8×10^{-28}	2.1×10^{-27}	4.0×10^{-27}	2.2×10^{-26}	5.6×10^{-26}	4.0×10^{-25}	9.1×10^{-25}	1.7×10^{-24}	2.0×10^{-24}	4.2×10^{-24}	8.3×10^{-24}
	H_2O-cat	E	K_{eq}^{1}-Path1	4.9×10^{-22}	4.4×10^{-22}	4.0×10^{-22}	3.4×10^{-22}	2.8×10^{-22}	2.4×10^{-22}	1.6×10^{-22}	1.3×10^{-22}	8.5×10^{-23}	7.1×10^{-23}	6.2×10^{-23}	6.0×10^{-23}	5.2×10^{-23}	4.5×10^{-23}
			K_{eq}^{2}-Path1	2.1×10^{-24}	1.9×10^{-24}	1.8×10^{-24}	1.5×10^{-24}	1.3×10^{-24}	1.1×10^{-24}	7.9×10^{-25}	6.5×10^{-25}	4.4×10^{-25}	3.8×10^{-25}	3.3×10^{-25}	3.2×10^{-25}	2.8×10^{-25}	2.5×10^{-25}
			k_{uni}-Path1	2.3×10^{-2}	3.5×10^{-2}	5.3×10^{-2}	1.0×10^{-1}	2.1×10^{-1}	3.9×10^{-1}	2.0	4.9	$3.1\times10^{+1}$	$6.8\times10^{+1}$	$1.2\times10^{+2}$	$1.4\times10^{+2}$	$2.8\times10^{+2}$	$5.3\times10^{+2}$
			k_r-Path1	2.4×10^{-47}	3.0×10^{-47}	3.7×10^{-47}	5.2×10^{-47}	7.8×10^{-47}	1.1×10^{-46}	2.6×10^{-46}	4.2×10^{-46}	1.2×10^{-45}	1.8×10^{-45}	2.5×10^{-45}	2.7×10^{-45}	4.1×10^{-45}	5.9×10^{-45}
		L	K_{eq}^{1}-Path3	7.9×10^{-23}	7.2×10^{-23}	6.6×10^{-23}	5.7×10^{-23}	4.9×10^{-23}	4.3×10^{-23}	3.0×10^{-23}	2.5×10^{-23}	1.7×10^{-23}	1.5×10^{-23}	1.3×10^{-23}	1.3×10^{-23}	1.1×10^{-23}	1.0×10^{-23}
			K_{eq}^{2}-Path3	1.5×10^{-22}	1.2×10^{-22}	1.0×10^{-22}	7.7×10^{-23}	5.6×10^{-23}	4.4×10^{-23}	2.2×10^{-23}	1.5×10^{-23}	7.2×10^{-24}	5.2×10^{-24}	4.1×10^{-24}	3.9×10^{-24}	3.0×10^{-24}	2.3×10^{-24}
			k_{uni}-Path3	2.1×10^{-24}	1.9×10^{-24}	1.8×10^{-24}	1.5×10^{-24}	1.3×10^{-24}	1.1×10^{-24}	7.9×10^{-25}	6.5×10^{-25}	4.4×10^{-25}	3.8×10^{-25}	3.3×10^{-25}	3.2×10^{-25}	2.8×10^{-25}	2.5×10^{-25}
			k_r-Path3	1.3×10^{-23}	1.2×10^{-23}	1.1×10^{-23}	9.0×10^{-24}	7.4×10^{-24}	6.4×10^{-24}	4.2×10^{-24}	3.4×10^{-24}	2.1×10^{-24}	1.8×10^{-24}	1.5×10^{-24}	1.5×10^{-24}	1.3×10^{-24}	1.1×10^{-24}

Table S4: Absolute electronic energies, ZPE corrections and thermal corrections to Gibbs free energies at 298 K of all the studied species calculated at M062-X/aug-cc-pVTZ level and absolute electronic energies calculated at the CCSD(T)-F12/cc-pVTZ-F12 level (All values are in Hartree)

species	M06-2X/ aug-cc-PVTZ	CCSD(T)-F12/ cc-pVTZ-F12	ZPE correction	Thermal Correction to Gibbs free energy
N_2O_5	-485.3410391	-484.8924455678	0.028614	-0.003024
H_2O	-76.4301065	-76.3690686602	0.021568	0.003281
N_2O_5–H_2O	-561.7793733	-561.2684322232	0.052323	0.016059
$TS_{N_2O_5-H_2O}$	-561.7483301	-561.2350520671	0.052924	0.020086
$PC_{N_2O_5-H_2O}$	-561.8055096	-561.2890183317	0.056015	0.020095
NH_3	-56.5529773	-56.4992333118	0.034461	0.016437
N_2O_5–NH_3	-541.90271	-541.399327781	0.065077	0.027841
$TS_{N_2O_5-NH_3}$	-541.8785328	-541.3730895231	0.066196	0.033004
$pc_{N_2O_5-NH_3}$	-541.9487638	-541.4407112814	0.069158	0.033235
H_2O–H_2O	-152.8684533	-152.7461785266	0.046246	0.019462
N_2O_5–H_2O–H_2O	-638.2229489	-637.6491426847	0.077668	0.038771
$TS_{N_2O_5-H_2O-H_2O}$	-638.1922511	-637.6155447186	0.078035	0.041492
$pc_{N_2O_5-H_2O-H_2O}$	-638.2541885	-637.6759595381	0.080282	0.037876
H_2O–NH_3	-132.9934913	-132.8786032747	0.05975	0.033588
N_2O_5–H_2O–NH_3	-618.347734	-617.7819992844	0.090291	0.050857
$TS_{N_2O_5-H_2O-NH_3}$	-618.3158826	-617.7469605518	0.090341	0.053045
$PC_{N_2O_5-H_2O-NH_3}$	-618.3865156	-617.8132294929	0.091856	0.051932
N_2O_5–NH_3–H_2O	-618.3420052	-617.7757611199	0.089792	0.050203
$TS_{N_2O_5-NH_3-H_2O}$	-618.3232332	-617.7557038079	0.090962	0.05359
$PC_{N_2O_5-NH_3-H_2O}$	-618.397504	-617.8264789812	0.093433	0.052516
HNO_3	-280.897309	-280.6397316791	0.027324	0.001649
H_2NNO_2	-261.0437181	-260.7922358664	0.040176	0.014415

Table S5: Optimized geometries in Cartesian coordinates and normal mode frequencies of all species calculated at M06-2X/aug-cc-pVTZ level of theory

Compound name	Cartesian Coordinate ($\AA$)	Frequencies (cm^{-1})
N_2O_5	N 1.18199200 0.08759300 -0.00054000 O 0.10751900 -0.86124400 0.00428100 N -1.18689600 -0.14072200 0.00076700 O -1.60364400 0.05902000 -1.08217000 O -1.60284900 0.07087700 1.08182700 O 2.22804500 -0.45583200 0.00229600 O 0.87522000 1.23366700 -0.00643400	28.2799 92.8072 220.7528 417.0931 585.3173 592.4012 743.2918 781.4948 788.2113 876.5777 952.2245 1346.2875 1452.6455 1825.1394 1857.4647
H_2O	H 0.76224900 -0.46549300 0.00000000 H -0.76224900 -0.46550800 0.00000000 O 0.00000000 0.11637500 0.00000000	1619.0379 3872.6446 3975.5558
N_2O_5–H_2O	N 0.79094700 -0.84056200 0.07446500 O -0.19988300 -0.32637600 -0.86943000 N -1.35685200 0.15678900 -0.14662000 O -1.36087400 1.33241400 0.01744900 O -2.14436200 -0.67695500 0.13091000 O 1.72099200 -1.26217200 -0.50118200 O 0.50281100 -0.76421800 1.21732200 H 0.76551200 2.19303500 -0.05055100 H 2.15439500 2.25821300 0.59653000 O 1.61149500 1.73920300 -0.00018100	36.9832 73.1319 98.8233 111.6285 123.5872 158.1398 192.1961 227.6224 282.4412 440.7437 543.6416 610.2360 750.4199 772.4144 787.6280 882.8424 954.3818 1350.0244 1455.8566 1614.5989 1822.5384 1864.3172 3854.4214 3958.7233
$TS_{N_2O_5-H_2O}$	N 1.42183500 -0.37571200 0.22208600 O -0.53748400 -0.80438600 -0.50904500 N -1.50383800 -0.10524500 -0.06415700 O -1.24318600 1.07045600 0.31678700 O -2.61415400 -0.55277300 -0.01551700 O 1.98547400 -0.89932700 -0.61250100 O 1.22563300 -0.22316800 1.32761700 O 1.10437100 1.46898100 -0.44943100 H 1.09545900 1.45179400 -1.41378800 H 0.11332600 1.43663700 -0.15500100	-398.5305 68.7299 92.2251 187.7550 237.3158 256.0706 357.7494 367.0496 505.4401 549.8486 626.2006 729.2212 738.0877 767.8946 867.3935 1109.4532 1210.1045 1305.5483 1405.0638 1634.2111 1654.5685 2184.0223 2523.9832 3853.0210
$PC_{N_2O_5-H_2O}$	N -1.76034700 0.09069700 0.05024000 O 0.88780200 -0.88539500 0.44533900 N 1.79332200 -0.16896600 0.09317600 O 1.48332000 1.13917600 -0.13654000 O 2.93350300 -0.44844600 -0.08448500 O -1.31394400 1.11839300 0.47760600 O -2.46137700 -0.70673400 0.58906900 H 0.52521700 1.21119700 0.05115800 H -1.75042300 -1.05897800 -1.41597900 O -1.40500700 -0.16753600 -1.24587500	32.5549 47.6681 66.7683 118.5113 144.0617 153.0002 469.4354 618.6037 640.5070 658.6997 714.3825 716.0993 826.1575 831.2193 1001.2081 1007.5428 1357.2843 1395.9291 1420.3430 1432.0370 1790.9796 1798.0606 3581.1986 3765.4100
NH_3	H 0.00000000 0.94022800 -0.26212800 H 0.81426100 -0.47011400 -0.26212800 N 0.00000000 0.00000000 0.11234100 H -0.81426100 -0.47011400 -0.26212800	1037.1992 1661.5762 1661.6067 3505.0582 3630.4754 3630.5023

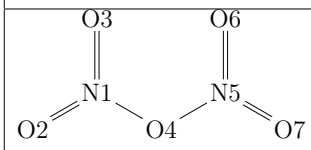
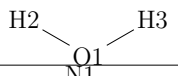
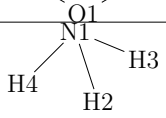
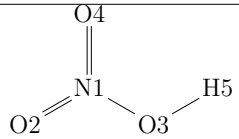
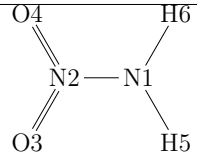
N_2O_5–NH_3	N 0.67630800 -0.91601700 0.05917900 O -0.25898300 -0.30015400 -0.87238500 N -1.37719400 0.27411100 -0.14613800 O -1.32091700 1.45260100 -0.04775300 O -2.19405300 -0.50921600 0.19179900 O 1.55743000 -1.42563900 -0.52653200 O 0.41023600 -0.82078600 1.20502300 H 2.54479400 1.76129500 -0.66198500 H 1.12195000 2.25522800 -0.03734700 N 1.90184300 1.62534600 0.10808000 H 2.37686600 1.92493600 0.95026700	29.2779 50.1409 77.2394 93.2566 114.4233 155.5741 210.9316 224.4227 235.2078 439.8775 539.4015 621.4440 751.3980 764.6252 790.1826 881.7804 955.8520 1060.8639 1352.0798 1458.3358 1654.5852 1661.1976 1829.2720 1866.3828 3499.8639 3620.5914 3627.2143
$TS_{N_2O_5-NH_3}$	N 1.25158700 -0.43021500 0.23772600 O -0.46724900 -0.62028600 -0.63421500 N -1.48786300 -0.02626800 -0.07372800 O -1.28478700 1.05680400 0.47666400 O -2.55824900 -0.56503600 -0.14017700 O 1.89198100 -1.08296700 -0.46911900 O 1.04978300 -0.25576700 1.36144500 H 1.26519400 1.29764000 -1.56019800 H 0.36355800 1.71469800 -0.20743100 N 1.27689000 1.41518500 -0.55483000 H 2.03511900 2.01476900 -0.25333800	-332.9944 56.8431 119.6872 184.8080 195.2344 260.4139 280.9289 294.2622 379.9733 515.1316 631.4012 681.6145 733.4846 752.4389 775.8772 865.2859 1068.9135 1081.0813 1323.6947 1403.9564 1588.1022 1636.5296 1660.7168 1975.8123 3372.8181 3571.4483 3646.0536
$PC_{N_2O_5-NH_3}$	N 1.83123200 -0.11681700 0.00014300 O -0.93988100 -0.93507700 -0.00048100 N -1.86279800 -0.16109000 -0.00006100 O -1.53280500 1.16642000 -0.00002200 O -3.02913400 -0.38612100 0.00025900 O 1.98188600 -0.61610000 -1.08076600 O 1.98124000 -0.61543300 1.08145300 H 1.71582900 1.66146200 -0.84897300 H -0.54915800 1.16926700 -0.00036600 N 1.37832400 1.22043700 -0.00039300 H 1.71557000 1.66205600 0.84798100	28.7709 56.3912 82.9660 99.2710 132.0495 175.8425 423.3716 579.3537 649.4682 693.8788 720.3911 775.4946 809.2225 833.3981 910.7104 1003.2038 1052.0872 1265.9850 1408.0477 1441.8253 1467.1970 1605.7262 1762.9768 1806.7216 3459.5117 3499.7360 3613.4516
H_2O–H_2O	O 1.50451400 0.00135300 -0.12144400 H 0.55692600 -0.00147000 0.06744400 H 1.93822400 -0.00834400 0.73306200 O -1.38712700 -0.00116000 0.11250200 H -1.71579700 0.76942800 -0.35691400 H -1.71844600 -0.76115900 -0.37205700	91.9787 127.6528 136.3411 191.2977 357.1927 605.1494 1619.2227 1635.9396 3771.8085 3859.9575 3943.8452 3959.1887
N_2O_5–H_2O–H_2O	N -0.63352200 -1.24922000 -0.26739200 O -0.24876500 0.00072200 -0.92851700 N -0.62584600 1.25274700 -0.26742300 O 0.20679300 2.06411900 -0.49138800 O -1.64987800 1.29842000 0.30034500 O 0.19434900 -2.06543600 -0.49116600 O -1.65799300 -1.28880900 0.30003100 H 1.57552300 -0.00434600 1.29565600 H 0.77929700 -0.00135700 2.63401600 O 0.68431600 -0.00213400 1.68072500 O 2.69850800 -0.00767200 -0.22435000 H 2.32377900 0.75599300 -0.67571700 H 2.31833500 -0.76866000 -0.67568800	37.8304 65.4595 100.1029 106.9919 119.1838 142.6631 160.3572 190.5239 206.1891 231.1331 251.7611 265.7848 306.8741 380.8034 442.3833 496.2274 667.8648 722.8845 741.3627 776.1475 788.8715 853.2873 934.5402 1352.1554 1442.9757 1609.5701 1630.0238 1813.6645 1885.2004 3680.5670 3829.2817 3913.6915 3945.8149

$TS_{N_2O_5-H_2O-H_2O}$	N 1.45478600 -0.50041800 0.26148800 O -0.37973000 -0.35526400 -0.98504900 N -1.34929300 -0.69825200 -0.23724400 O -2.26361500 0.12557100 -0.05342400 O -1.33690800 -1.78807300 0.30319500 O 2.11669500 -1.02996000 -0.49218100 O 0.98198900 -0.45874900 1.29082100 H 0.64147700 1.75485000 -0.01063800 H 1.52989000 1.30838900 -1.22771600 H -1.01842200 2.73343500 1.00183100 H -1.40872600 1.56608100 0.01832000 O -0.74008200 2.27706800 0.20531200 O 1.56131800 1.35789800 -0.26261300	-257.5737 49.3886 59.1051 107.4274 127.8338 152.8103 218.9554 245.1174 254.9512 279.1569 353.8807 426.1612 452.2510 527.8641 603.3941 652.1150 731.4720 745.5019 805.7757 853.6740 906.1019 1123.6966 1195.1961 1377.6714 1410.9542 1562.0416 1648.2975 1687.2609 2185.5678 2551.4236 3211.5926 3824.9343 3921.7916
$PC_{N_2O_5-H_2O-H_2O}$	N 2.52734300 -0.33866100 -0.02079600 O -1.08554000 -0.83186600 0.08849700 N -2.26823100 -0.55262700 -0.01145700 O -2.59349100 0.74737200 -0.00762500 O -3.17188100 -1.31406600 -0.10737600 O 2.41266600 -1.46804600 0.35513100 O 3.49333800 0.34955600 -0.09429000 H 0.38083200 1.90824900 0.06532000 H 0.63969900 -0.36043700 -0.27872900 H -0.52436800 3.15817700 -0.10359800 H -1.74145600 1.27137400 0.09501400 O -0.49182500 2.27201500 0.26476900 O 1.36567100 0.27774100 -0.44313500	11.7102 29.0999 36.2760 53.5126 73.4677 82.0148 159.9531 172.7508 193.7376 247.5720 381.4936 513.5638 644.6904 650.5776 689.5726 717.6500 733.3747 827.1861 833.1177 901.1293 979.0128 1052.5335 1348.0405 1410.0164 1417.9455 1508.2902 1623.4220 1790.1002 1804.1091 3050.1331 3591.7562 3785.7914 3925.9852
H_2O–NH_3	H 0.58747600 0.04947200 0.00043800 H 1.95085100 0.76407100 0.00086300 N -1.38202900 0.02335000 0.00003800 H -1.63076800 -0.65790800 -0.70666000 H -1.91959500 0.86056600 -0.18564700 H -1.69025400 -0.34296400 0.89221300 O 1.54706200 -0.10458600 -0.00018400	128.5959 169.9395 197.8604 204.4608 449.0967 691.0014 1081.3299 1649.2507 1656.0936 1664.0428 3501.6163 3621.8514 3631.4719 3633.3270 3947.2654
N_2O_5–H_2O–NH_3	N -0.64822600 -1.25675800 -0.26684600 O -0.24175100 -0.00146500 -0.90199700 N -0.66279400 1.25021000 -0.26733000 O 0.14146100 2.08368900 -0.50830200 O -1.68904800 1.27597500 0.29929900 O 0.16480300 -2.08176900 -0.50803600 O -1.67358600 -1.29371800 0.30102900 H 1.54366000 0.00934700 1.23376500 H 0.81473600 0.00147100 2.61958200 O 0.66762700 0.00571700 1.67343900 H 3.75553000 0.01738100 -0.16024900 H 2.45210600 -0.80433500 -0.71817500 N 2.74432100 0.01278400 -0.19393100 H 2.44481500 0.82504800 -0.72162500	55.3570 57.8238 85.2233 101.5799 108.0799 114.2372 129.0893 134.1062 205.4646 241.4800 258.0960 265.0778 271.6945 376.7048 437.2808 525.8963 694.8924 745.6926 771.3609 787.0090 793.1296 849.0096 934.5850 1103.6044 1353.4786 1445.9060 1633.3341 1645.9983 1658.9750 1812.7930 1884.6134 3458.3873 3500.4226 3613.2157 3632.6287 3946.7868

$TS_{N_2O_5-H_2O-NH_3}$	N 1.40070300 -0.52944900 0.24263000 O -0.37769900 -0.36557000 -0.95453900 N -1.38287400 -0.69121000 -0.22704900 O -2.35795700 0.06072300 -0.21925300 O -1.31402700 -1.70522800 0.44705700 O 2.04034500 -1.15846500 -0.45988800 O 0.98320100 -0.39697900 1.29494400 H 0.71581600 1.74968400 -0.07711500 H 1.46999100 1.11920400 -1.34812400 O 1.61138100 1.26143800 -0.40243200 H -0.73365500 2.43186600 1.34386600 H -0.74203800 3.30311100 -0.03487900 N -0.59766000 2.37316700 0.34084300 H -1.33325000 1.76122600 -0.02582600	-342.3539 34.6689 55.1938 97.1706 139.9642 149.6044 178.0628 212.1884 238.6308 253.3739 360.9010 380.0445 435.8327 494.2561 534.4772 641.0962 667.8717 731.6867 746.1156 862.5984 880.8737 1112.6033 1240.1434 1320.1527 1373.1732 1406.9899 1567.7204 1644.0786 1668.8957 1719.6289 2003.7889 2132.6433 3380.9627 3553.5229 3613.4214 3822.5846
$PC_{N_2O_5-H_2O-NH_3}$	N 1.93504000 -0.62481300 -0.01682900 O -1.45106100 -1.19195400 0.25604400 N -2.21196600 -0.13897000 -0.06680500 O -1.67213500 0.95391300 -0.08936100 O -3.35383000 -0.37346000 -0.30030900 O 2.01820300 -1.81551700 -0.13412600 O 2.72820800 0.19380800 -0.45917200 H 0.85571000 1.19009200 0.39863800 H -0.51610600 -0.84106300 0.41228400 O 0.89669200 -0.14127800 0.64235700 H 0.93793100 2.93668300 0.86442300 H 1.59979500 2.43144200 -0.57343800 N 0.82826900 2.30710700 0.07689900 H -0.06535000 2.47546800 -0.37822400	25.4632 48.1952 65.0512 81.1307 87.7660 96.8193 137.7130 145.7387 200.9865 368.6779 423.4115 497.6927 666.9439 726.5386 745.8115 754.3619 839.0703 855.3238 969.6899 974.7292 1047.5317 1133.6150 1338.2995 1397.2863 1485.8593 1534.6117 1555.6413 1601.2838 1653.5412 1684.0362 1775.1228 1783.3408 2958.5292 3473.7982 3582.9189 3603.3912
N_2O_5–NH_3–H_2O	N 0.62244200 1.23916200 -0.28876500 O 0.25190700 0.00198100 -0.97369100 N 0.63127100 -1.23338500 -0.29225900 O -0.23291500 -2.03290600 -0.42553800 O 1.69259500 -1.28932000 0.20417200 O -0.24882800 2.03148700 -0.41811900 O 1.68430500 1.30247900 0.20525900 H -2.27980800 0.75507500 -0.69312200 H -2.27974500 -0.76353700 -0.69910600 O -2.76411000 -0.00558300 -0.35801200 N -0.65027000 -0.00931900 1.87706000 H -0.56897700 0.80027600 2.48088300 H -0.56753500 -0.82313800 2.47500100 H -1.59165900 -0.00897800 1.49152700	52.4940 63.5756 91.5899 99.5316 107.9689 132.1145 134.4163 162.5480 166.0824 195.4622 235.2140 254.5906 291.0229 333.7798 400.6456 455.3259 464.8162 694.0314 729.3039 769.6984 785.9151 856.5022 937.3191 1119.4114 1351.7737 1443.5974 1632.6535 1655.1722 1674.2217 1808.2341 1876.4048 3468.9984 3586.0327 3616.6221 3841.3006 3925.6641

$TS_{N_2O_5-NH_3-H_2O}$	N 1.40882700 -0.37925500 0.19283100 O -0.23942800 -0.23840700 -0.80657600 N -1.19814400 -0.89425900 -0.20980800 O -2.29710800 -0.35679300 -0.19776800 O -0.94307600 -1.96314300 0.29291500 O 2.14535500 -0.87066600 -0.54759600 O 1.10696500 -0.39456700 1.30667700 H 0.53843200 1.96703000 0.03205400 H 1.48113300 1.63889200 -1.29892200 H -1.88692800 2.71889200 0.88089100 H -1.74635700 1.48351500 -0.03223500 O -1.29610500 2.29519800 0.25596900 N 1.44314200 1.60404600 -0.28728100 H 2.22413200 2.10497800 0.11904200	-293.6234 44.3646 58.4279 101.1800 146.0630 166.7639 177.5418 188.3378 227.5679 269.6067 273.9470 306.5712 374.1266 401.5343 531.6871 605.9715 642.7092 675.1613 730.4639 738.0302 762.5733 871.2172 1075.6719 1150.1101 1331.6904 1415.0806 1606.3304 1630.2595 1640.8663 1658.5398 1982.7090 3332.2401 3558.1492 3637.5104 3681.1306 3933.5002
$PC_{N_2O_5-NH_3-H_2O}$	N -2.03279500 -0.46765900 -0.12392900 O 1.35094200 -1.31336500 0.15993100 N 2.21757200 -0.28769800 -0.02788500 O 1.80615500 0.82091400 0.23571800 O 3.29095600 -0.59604900 -0.42706100 O -2.82633600 -1.34123800 0.11048400 O -1.88963200 0.12564000 -1.16744300 H -0.90285600 0.86816100 0.80025700 H 0.50615600 -0.89302500 0.46077000 H -0.95424100 2.41090600 -0.73212100 H 0.37555800 2.48803200 0.02323300 H -1.55500800 -0.40723600 1.77748900 N -1.14102100 -0.13408600 0.89418800 O -0.57907100 2.52400600 0.14759000	21.0015 33.3145 61.5327 78.8076 89.0028 99.5290 129.1304 162.3536 186.4513 231.8678 396.0910 411.7226 579.8831 617.4022 660.2243 709.2027 718.6611 794.2679 832.3755 861.8671 957.9819 1021.5112 1097.7551 1320.7109 1408.5977 1439.8318 1466.8840 1630.6496 1634.6633 1738.0789 1793.9901 3172.4650 3324.2499 3589.9368 3827.4569 3912.9470
HNO_3	O -0.13761800 1.23667000 -0.00005100 N -0.14091200 0.03554900 0.00015300 O 1.09921400 -0.56803900 0.00000800 O -1.05286200 -0.72221200 -0.00008900 H 1.71651700 0.17980100 -0.00001500	494.9714 622.1574 706.4552 828.6038 980.7984 1354.1493 1418.3041 1813.0459 3775.4210
NH_2NO_2	N 0.14124000 0.00000000 -0.00423700 O 0.67879100 1.08124300 0.00813300 O 0.67879300 -1.08124200 0.00813300 H -1.60492800 0.86125600 0.28071100 N -1.23421500 -0.00000100 -0.09455500 H -1.60492700 -0.86125900 0.28071200	446.7197 592.7632 631.8077 746.0942 839.9629 1063.8739 1257.4458 1455.9779 1613.1144 1735.7592 3558.3747 3693.1584

Table S6: Comparison of important geometrical parameters (bond length in $\AA$ and bond angle in deg) and frequencies (cm^{-1}) obtained at M06-2X/aug-cc-pVTZ level of theory with experimental results available in literature

Species	Geometrical parameters	Experimental		This Work	
		Geometry	Frequency (cm^{-1})	Geometry	Frequency (cm^{-1})
	N5-O7	1.188[a]	50.0 85.0 353.0[b]	1.179	28.3 92.8 220.8
	N5-O6	1.188	353 614 743	1.186	417.1 585.3 592.4
	N5-O4	1.498	743 860 1247	1.433	743.3 781.5 788.2
	O7-N5-O4	133.2	1338 1728 1728	132.4	876.6 952.2 1346.3
	N5-O4-N1	111.8		109.5	1452.6 1825.1 1857.5
	O1-H3	0.958[c]	1595.0 3657.0 3756.0[d]	0.959	1619.0 3872.6 3975.6
	H2-O1-H3	104.48		105.29	
	N1-H3	1.012[e]	950.0 1627.0 3337.0[f]	1.012	1037.2 1661.6 1661.6
	H3-N1-H2	106.68	3444.0	107.14	3505.1 3630.5 3630.5
	H2-N1-H4	112.15		107.14	
	O3-H5	0.964[g]		0.969	
	O3-N1	1.406		1.379	
	N1-O4	1.211	456.0 579.0 674.0[h]	1.201	495.0 622.2 706.5
	N1-O2	1.199	762.0 879.0 1325.0	1.186	828.6 980.8 1354.1
	H5-O3-N1	102.15	1331.0 1708.0 3550.0	103.59	1418.3 1813.0 3775.4
	O3-N1-O4	115.09		115.80	
	O4-N1-O2	130.27		129.88	
	O2-N1-O3	113.85		114.32	
	N1-H5	0.86[i]		1.009	
	N2-O4	1.237	434.0 484.0 587.0[j]	1.207	446.7 592.8 631.8
	N1-N2	1.321	714.0 776.0 951.0	1.378	746.1 840.0 1063.9
	H5-N1-N2	117.00	1238.0 1968.0 1581.0	109.99	1257.4 1456.0 1613.1
	N1-N1-O4	118.51	1610.0 3361.0 3474.0	116.41	1735.8 3558.4 3693.2
	O4-N2-O3	123.00		127.12	

a-References-9,10

b-References-11 and 12

c-Reference-13

d-Reference-14

e-Reference-15

f-Reference-14

g-Reference-16

h-References-14 and 17

i-Reference-18

j-Reference-19

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