

Supporting information

-for-

The effect of $(\text{H}_2\text{O})_n$ ($n=1-3$) clusters on the reaction of HONO with HCl: mechanistic and kinetic study

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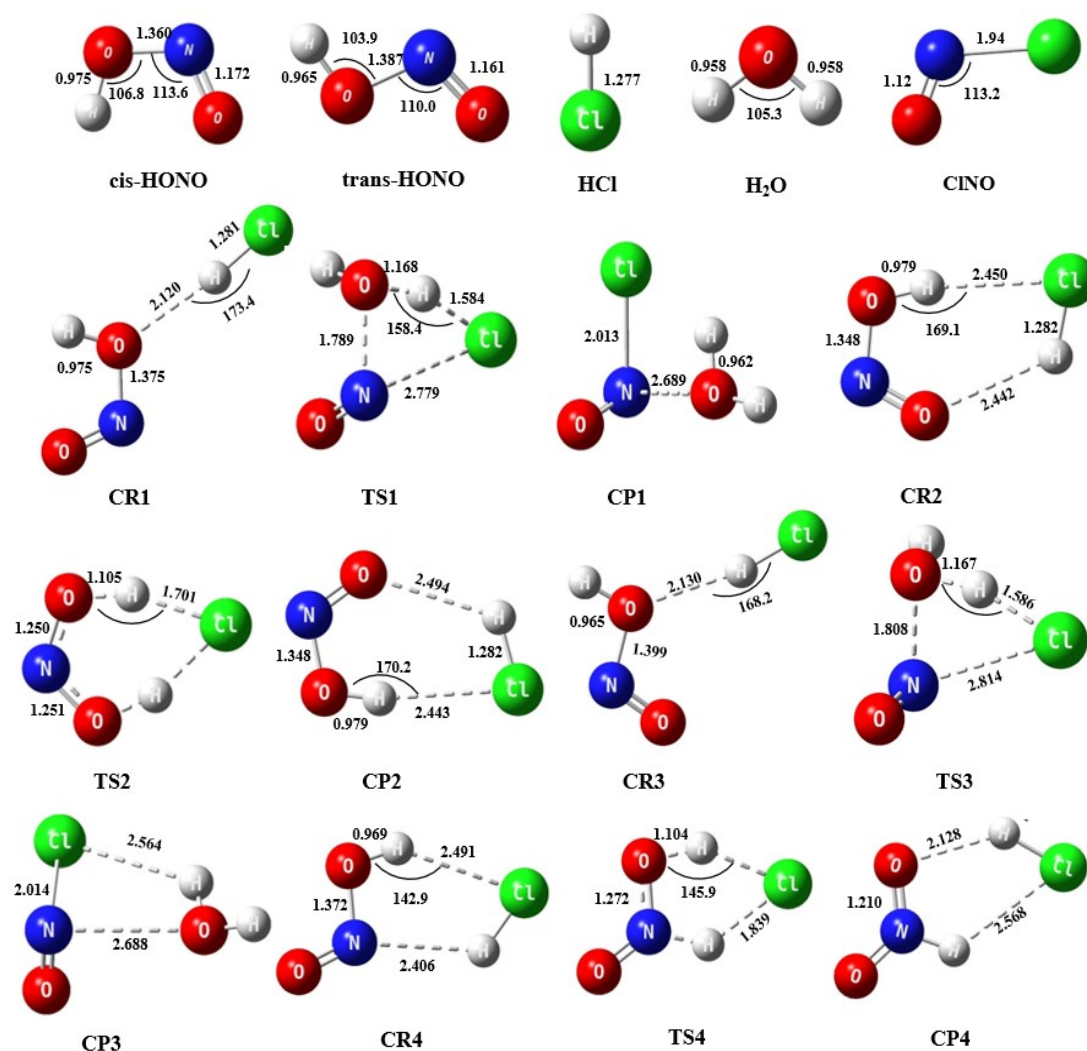


Fig. S 1 Optimized geometries calculated at the M06-2X/6-311+G (2df, 2p) level of theory for the reaction between HONO and HCl

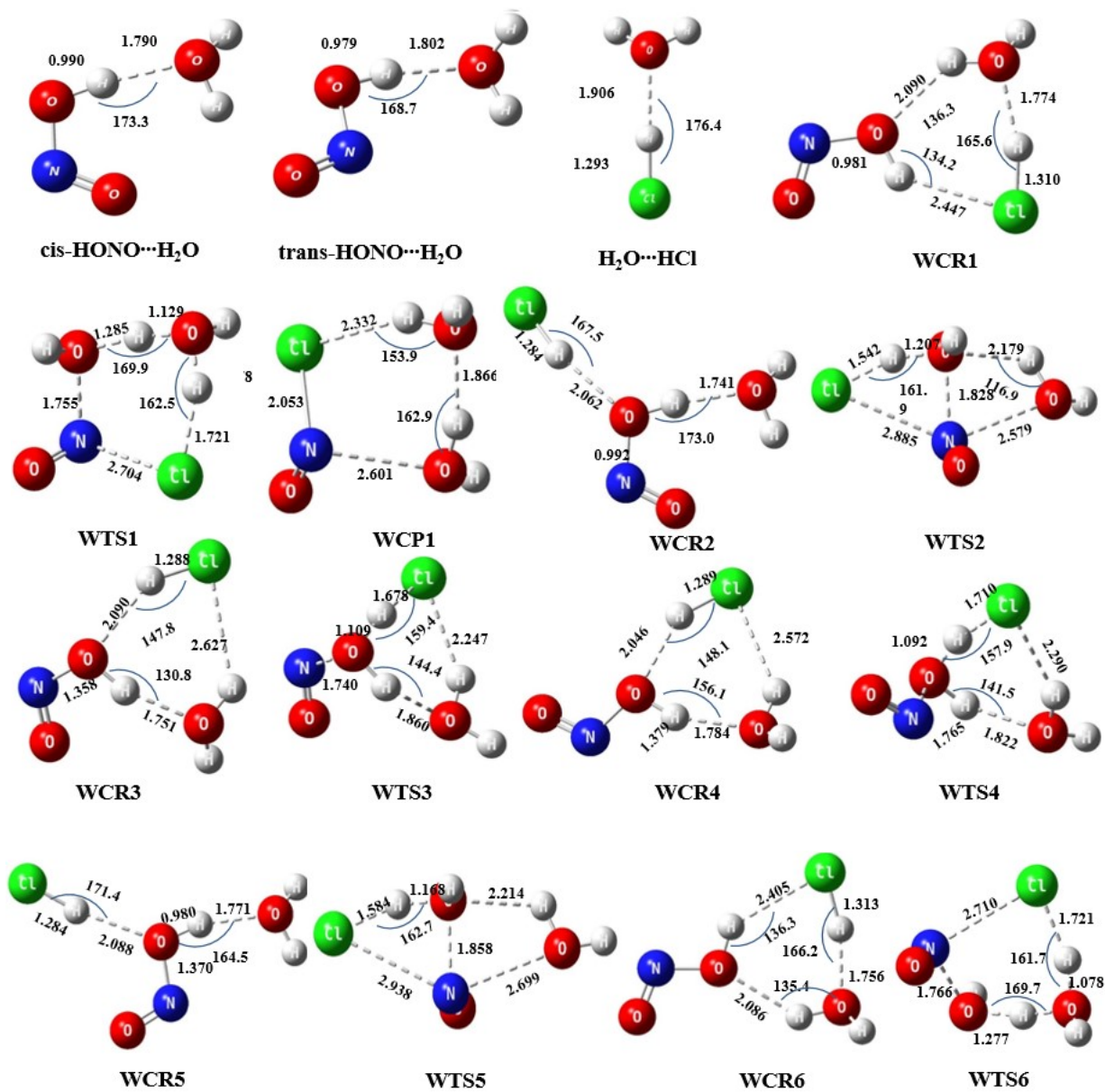


Fig. S 2 Optimized geometries calculated at the M06-2X/6-311+G (2df, 2p) level of theory for the reaction between HONO and HCl in the presence of a water molecule

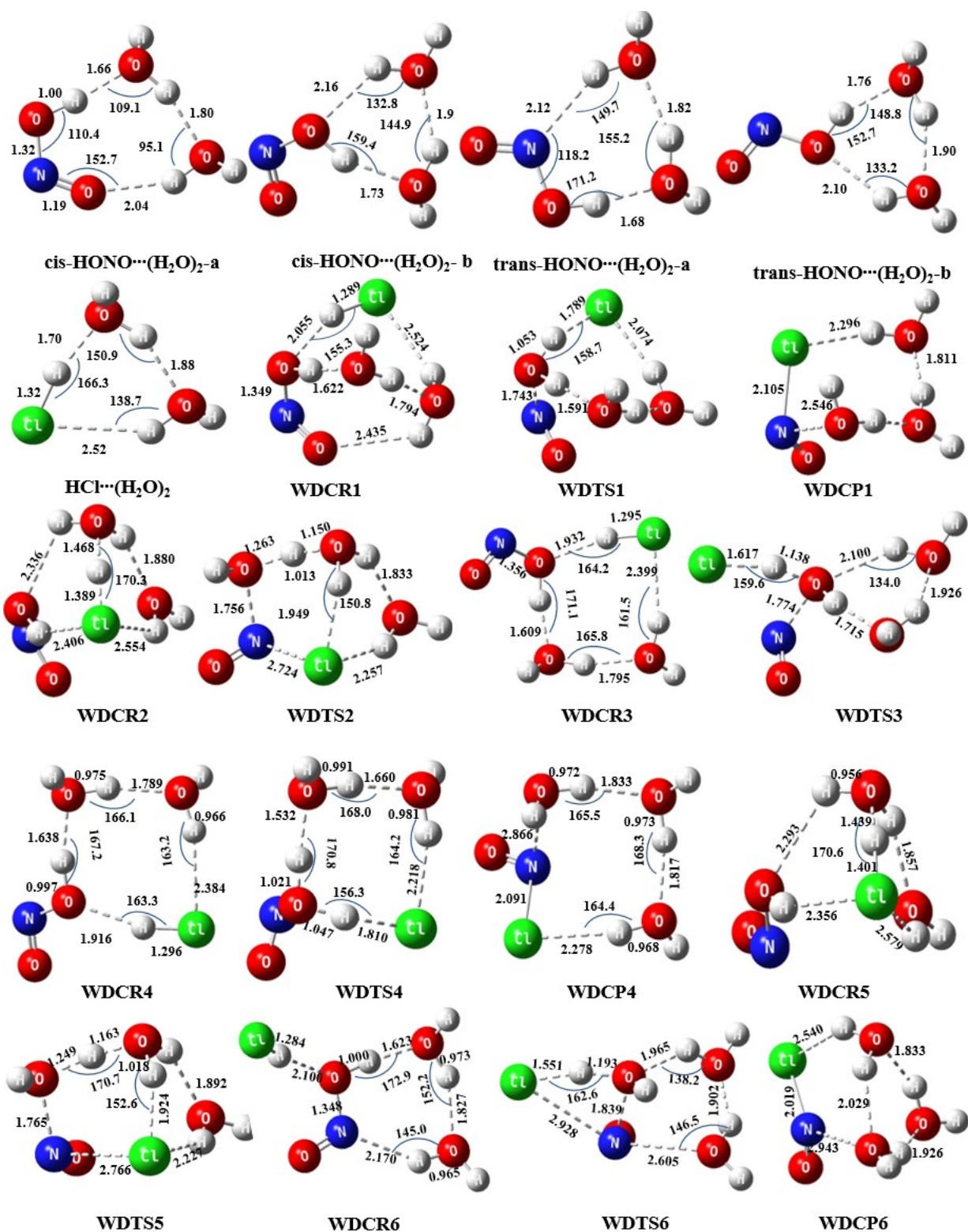


Fig. S 3 Optimized geometries calculated at the M06-2X/6-311+G (2df, 2p) level of theory for the reaction between HONO and HCl in the presence of water dimer

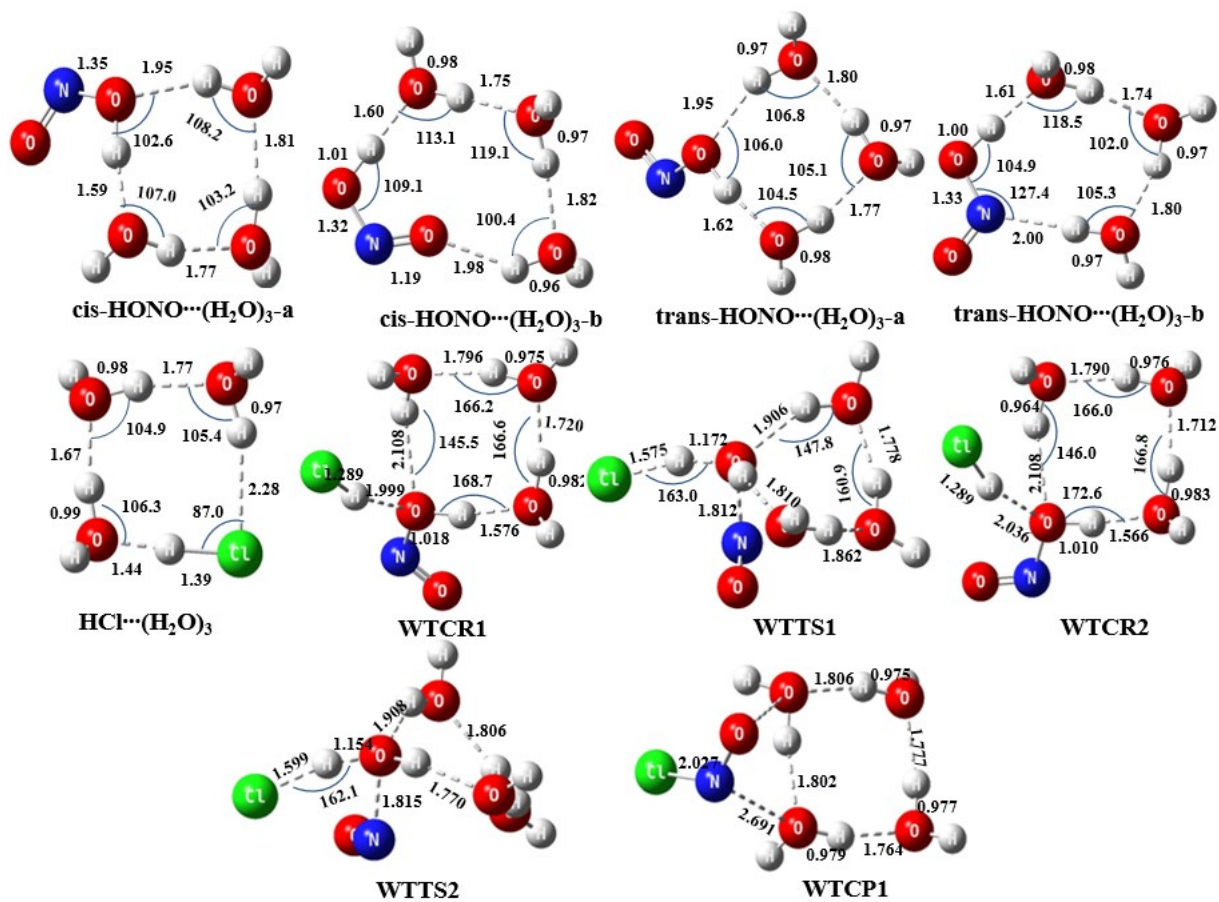


Fig. S 4 Optimized geometries calculated at the M06-2X/6-311+G (2df, 2p) level of theory for the reaction between HONO and HCl in the presence of water trimer

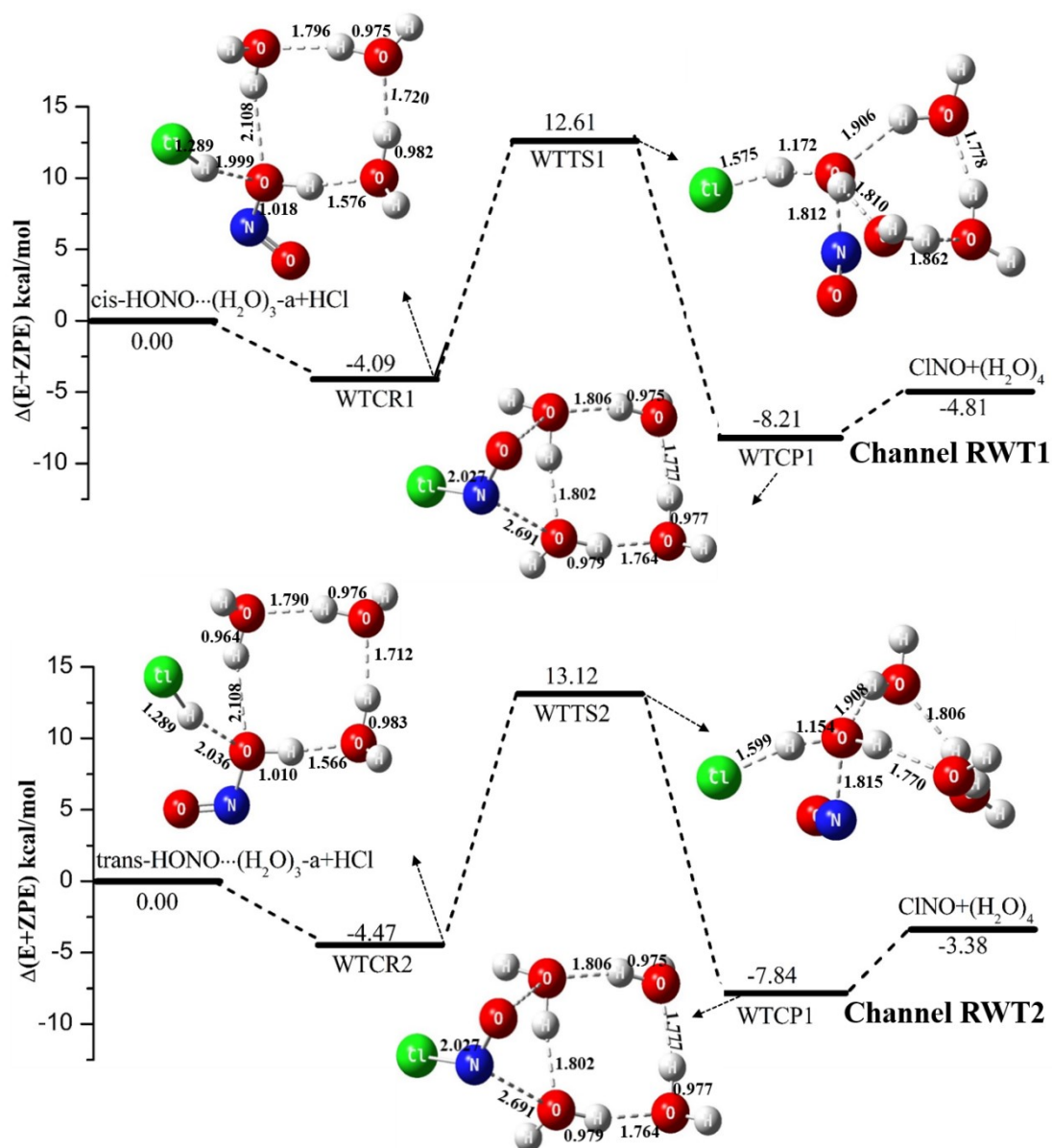


Fig. S5 Potential energy surface for the reaction HONO+HCl with water trimer at the CCSD(T)/aug-cc-pVTZ// M06-2X/6-311+G (2df,2p) level

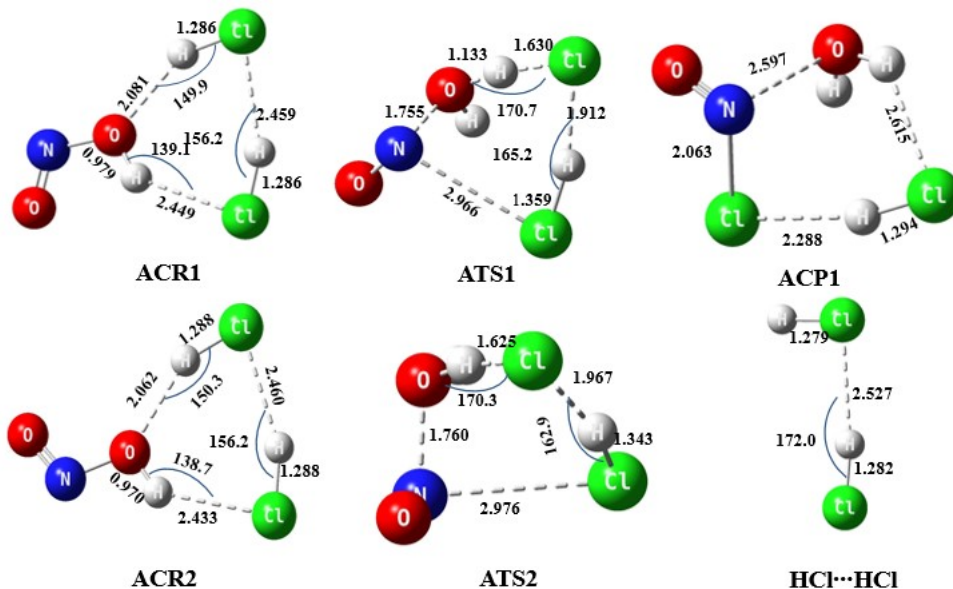


Fig. S 6 Optimized geometries calculated at the M06-2X/6-311+G (2df, 2p) level of theory for the HONO+2HCl reaction

cis-HONO+trans-HONO+HCl

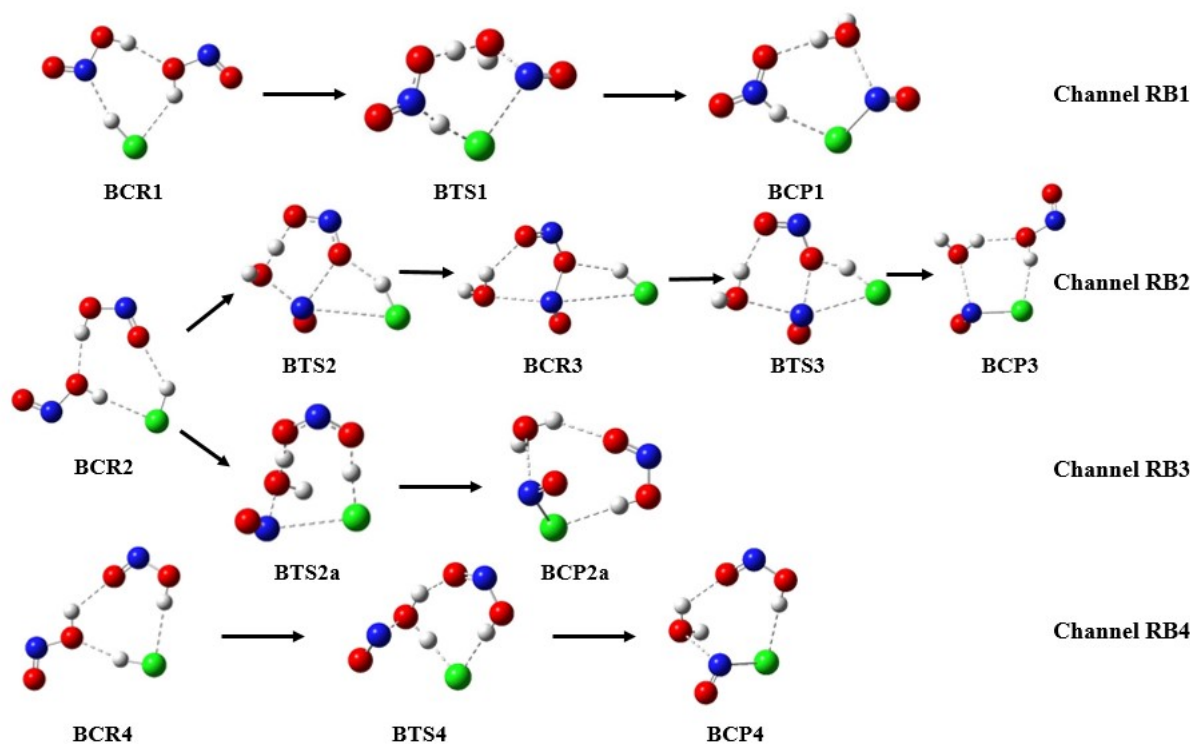


Fig. S 7 Optimized geometries calculated at the M06-2X/6-311+G (2df, 2p) level of theory for the cis-HONO+trans-HONO+HCl reaction

Table S1 The imaginary frequencies (cm^{-1}) of transition states calculated at the M06-2X/6-311+G (2df, 2p) level of theory for HONO+HCl reactions without and with catalyst

Species	Imaginary frequency	Species	Imaginary frequency
TS1	796.06i	WDTS4	174.98i
TS2	549.32i	WDTS5	517.96i

TS3	734.53i	WDTS6	528.79i
TS4	689.87i	WTTS1	553.96i
WTS1	548.63i	WTTS2	439.90i
WTS2	751.27i	ATS1	239.55i
WTS3	234.28i	ATS2	267.38i
WTS4	314.89i	BTS1	892.61i
WTS5	621.63i	BTS2	512.72i
WTS6	601.91i	BTS2a	1010.09i
WDTS1	116.33i	BTS3	363.66i
WDTS2	465.85i	BTS4	208.50i
WDTS3	498.54i		

Table S2 Values of relative energies (ΔE with and without out ZPE/(kcal·mol⁻¹)), enthalpy (ΔH (298K)/(kcal·mol⁻¹)), and Gibbs free energy (ΔG (298K)/(kcal·mol⁻¹)) for the HONO+HCl reaction

System	ΔE	$\Delta(E+ZPE)$	ΔH	ΔG
cis-HONO+HCl	0.46	0.39	0.35	0.39
CR1	-2.43	-1.45	-1.53	5.01
TS1	16.79	16.73	15.70	25.11
CP1	-8.91	-6.87	-6.70	0.18
CR2	-2.77	-1.41	-1.68	5.75
TS2	13.43	13.91	12.26	23.34
CP2	-2.76	-1.35	-1.67	5.91
trans-HONO+HCl	0.00	0.00	0.00	0.00
CR3	-3.20	-2.22	-2.29	4.20
TS3	14.27	14.24	13.22	22.63
CP3	-8.92	-6.96	-6.74	0.01
CR4	-3.44	-2.12	-2.34	4.97
TS4	18.26	19.63	18.06	28.60
CP4	3.26	5.47	5.08	12.88
CINO+H ₂ O	-4.23	-3.95	-3.54	-4.65
HNO ₂ +HCl	8.25	9.25	9.11	9.76

Table S3 Values of relative energies (ΔE with and without out ZPE/(kcal·mol⁻¹)), enthalpy (ΔH (298K)/(kcal·mol⁻¹)), and Gibbs free energy (ΔG (298K)/(kcal·mol⁻¹)) for the HONO+HCl+H₂O reaction

System	ΔE	$\Delta(E+ZPE)$	ΔH	ΔG
H ₂ O···HCl+cis-HONO	0.00	0.00	0.00	0.00
WCR1	-6.28	-4.91	-5.03	4.50
WTS1	11.91	12.71	11.27	24.30
WCP1	-12.18	-9.59	-9.24	-0.28
CINO+(H ₂ O) ₂	-4.40	-3.54	0.31	-4.30
HCl+cis-HONO···H ₂ O	0.00	0.00	0.00	0.00
WCR2	-3.88	-2.44	-2.75	4.66
WTS2	16.94	16.56	15.70	25.26
WCP1	-10.16	-7.93	-7.79	-0.55
WCR3	-4.55	-3.56	-3.74	3.34
WTS3	9.55	10.92	9.61	20.30
WCP1	-9.35	-6.89	-6.90	0.83
CINO+(H ₂ O) ₂	-2.20	-1.59	2.00	-4.31
trans-HONO···H ₂ O+HCl	0.00	0.00	0.00	0.00
WCR4	-5.35	-4.44	-4.60	2.84
WTS4	8.40	9.64	8.40	18.83
WCR5	-4.20	-3.27	-3.33	3.32
WTS5	15.66	15.06	14.34	23.39
WCP1	-9.64	-7.61	-7.50	-0.32
CINO+(H ₂ O) ₂	-1.79	-1.44	2.15	-4.17

H ₂ O⋯HCl+trans-HONO	0.00	0.00	0.00	0.00
WCR6	-6.92	-5.35	-5.59	4.36
WTS6	10.94	11.70	10.20	23.38
WCP1	-11.83	-9.18	-8.96	0.47
CINO+(H ₂ O) ₂	-3.94	-3.16	0.66	-3.90

Table S4 Values of relative energies (ΔE with and without out ZPE/(kcal·mol⁻¹)), enthalpy (ΔH (298K)/(kcal·mol⁻¹)), and Gibbs free energy (ΔG (298K)/(kcal·mol⁻¹)) for the HONO+HCl+(H₂O)₂ reaction

System	ΔE	$\Delta(E+ZPE)$	ΔH	ΔG
cis-HONO⋯(H ₂ O) ₂ -a+HCl	0.00	0.00	0.00	0.00
WDCR1	-4.25	-3.34	-3.49	4.12
WDTS1	4.80	6.66	5.30	16.42
WDCP1	-8.23	-5.92	-5.73	1.71
CINO+(H ₂ O) ₃	-3.78	-2.44	-2.60	-4.79
cis-HONO+HCl⋯(H ₂ O) ₂	0.00	0.00	0.00	0.00
WDCR2	-4.23	-3.12	-3.10	7.38
WDTS2	6.78	8.18	7.19	19.96
WDCP1	-11.14	-8.72	-7.92	0.47
CINO+(H ₂ O) ₃	-6.83	-5.30	-5.02	-5.44
cis-HONO⋯(H ₂ O) ₂ -b+HCl	0.00	0.00	0.00	0.00
WDCR3	-7.40	-6.17	-6.64	1.60
WDTS3	13.06	13.19	12.39	21.34
WDCP1	-10.90	-8.03	-8.20	0.41
CINO+(H ₂ O) ₃	-5.55	-3.99	-4.36	-5.90
trans-HONO⋯(H ₂ O) ₂ -b+HCl	0.00	0.00	0.00	0.00
WDCR4	-5.93	-4.81	-5.08	3.03
WDTS4	2.90	5.24	3.56	15.08
WDCP4	-9.51	-6.84	-6.94	0.73
CINO+(H ₂ O) ₃	-4.32	-2.75	-3.20	-4.60
trans-HONO+HCl⋯(H ₂ O) ₂	0.00	0.00	0.00	0.00
WDCR5	-4.69	-3.17	-3.27	7.30
WDTS5	5.70	7.32	6.12	19.69
WDCP1	-10.79	-8.52	-7.76	1.00
CINO+(H ₂ O) ₃	-6.37	-4.91	-4.66	-5.06
trans-HONO⋯(H ₂ O) ₂ -a+HCl	0.00	0.00	0.00	0.00
WDCR6	-3.72	-2.92	-2.90	3.64
WDTS6	15.64	15.22	14.47	23.95
WDCP6	-7.95	-5.78	-5.62	1.53
CINO+(H ₂ O) ₃	-2.42	-1.42	-1.55	-3.94

Table S5 Values of relative energies (ΔE with and without out ZPE/(kcal·mol⁻¹)), enthalpy (ΔH (298K)/(kcal·mol⁻¹)), and Gibbs free energy (ΔG (298K)/(kcal·mol⁻¹)) for the HONO+HCl+(H₂O)₃ reaction

System	ΔE	$\Delta(E+ZPE)$	ΔH	ΔG
cis-HONO⋯(H ₂ O) ₃ -a+HCl	0.00	0.00	0.00	0.00
WTCR1	-5.03	-4.09	-4.26	3.63
WTTS1	12.57	12.61	11.87	22.06
WTCP1	-11.21	-8.21	-8.32	0.08
CINO+(H ₂ O) ₄	-6.55	-4.81	-5.20	-6.85
trans-HONO⋯(H ₂ O) ₃ -a+HCl	0.00	0.00	0.00	0.00
WTCR2	-5.45	-4.47	-4.69	3.44
WTTS2	12.96	13.12	12.30	22.47
WTCP1	-10.57	-7.84	-8.02	0.91
CINO+(H ₂ O) ₄	-5.05	-3.38	-3.87	-5.29

Table S6 Values of relative energies (ΔE with and without out ZPE/(kcal·mol⁻¹)), enthalpy (ΔH (298K)/(kcal·mol⁻¹)), and Gibbs free energy (ΔG (298K)/(kcal·mol⁻¹)) for the HONO+2HCl reaction

System	ΔE	$\Delta(E+ZPE)$	ΔH	ΔG
cis-HONO+HCl \cdots HCl	0.46	0.39	0.35	0.39
ACR1	-5.53	-4.94	-4.72	4.40
ATS1	9.05	8.90	7.95	20.25
ACP1	-11.74	-10.11	-9.54	-0.61
trans-HONO+HCl \cdots HCl	0.00	0.00	0.00	0.00
ACR2	-6.60	-5.84	-5.64	3.27
ATS2	5.68	5.83	4.85	17.30
CINO+HCl+H ₂ O	-2.07	-3.45	-2.37	-9.50

Table S7 Values of relative energies (ΔE with and without out ZPE/(kcal·mol⁻¹), enthalpy ($\Delta H(298K)$ /(kcal·mol⁻¹), and Gibbs free energy ($\Delta G(298K)$ /(kcal·mol⁻¹)) for the 2HONO+HCl reaction

System	ΔE	$\Delta(E+ZPE)$	ΔH	ΔG
cis-HONO+trans-HONO+HCl	0.00	0.00	0.00	0.00
BCR1	-10.48	-8.07	-8.12	8.76
BTS1	10.11	10.67	9.42	30.20
BCP1	-10.78	-6.43	-6.19	10.34
HNO ₂ +CINO+H ₂ O	3.56	4.92	5.22	4.72
BCR2	-10.11	-7.95	-7.79	8.68
BTS2	8.96	8.86	8.11	27.12
BCR3	-3.04	-2.59	-1.88	14.04
BTS3	7.12	7.37	6.88	26.11
BCP3	-16.64	-13.52	-13.02	3.02
trans-HONO+CINO+H ₂ O	-4.69	-4.33	-3.89	-5.05
BTS2a	11.38	10.74	9.63	29.88
BCP2a	-14.20	-11.10	-11.16	6.85
BCR4	-9.54	-7.29	-7.18	8.77
BTS4	1.44	3.76	2.93	21.93
BCP4	-14.20	-11.10	-11.16	6.85
cis-HONO+CINO+H ₂ O	-4.23	-3.95	-3.54	-4.65

Table S8 The equilibrium constants of the relevant complexes HONO \cdots (H₂O)_n(n=1-3) and HCl \cdots (H₂O)_n(n=1-3) at 298K (cm³ molecule⁻¹)

Species	Equilibrium constants	Species	Equilibrium constants
HCl \cdots H ₂ O	1.34×10^{-21}	trans-HONO \cdots (H ₂ O) ₂ -a	1.97×10^{-22}
cis-HONO \cdots H ₂ O	1.27×10^{-21}	trans-HONO \cdots (H ₂ O) ₂ -b	6.53×10^{-23}
trans-HONO \cdots H ₂ O	8.42×10^{-22}	cis-HONO \cdots (H ₂ O) ₃ -a	1.96×10^{-23}
(H ₂ O) ₂	3.83×10^{-22}	cis-HONO \cdots (H ₂ O) ₃ -b	4.65×10^{-24}
cis-HONO \cdots (H ₂ O) ₂ -a	9.06×10^{-23}	HCl \cdots (H ₂ O) ₃	9.10×10^{-24}
cis-HONO \cdots (H ₂ O) ₂ -b	1.39×10^{-23}	trans-HONO \cdots (H ₂ O) ₃ -a	1.42×10^{-22}
HCl \cdots (H ₂ O) ₂	2.95×10^{-23}	trans-HONO \cdots (H ₂ O) ₃ -b	1.78×10^{-23}
(H ₂ O) ₃	5.93×10^{-23}		

1. The proof that k_1 is much larger than k_2 in the calculation formula

In this paper, we used the equilibrium-state model and the steady-state model to obtain the reaction rate constant. The equilibrium-state model can only be applied when the condition of equilibrium-state approximation satisfies, i.e., both the forward reaction and the backward reaction of the first step are fast relative to the second reaction step ($k_1, k_{-1} \gg k_2$). Xiao et al. study^[1] showed that k_1 is less than k_2 at low temperatures and hence the equilibrium-state model is not applicable. With the temperature increasing, the Gibbs free energy of the reaction complex increases, making k_1 increase and $k_1 \gg k_2$ and hence the equilibrium-state model is applicable at high temperatures. In the steady-state model, it is assumed that the

concentration of the reaction complex as an active intermediate remains constant during the reaction and the application condition of the steady-state model is that the consuming process of the reaction complex is much faster than the forming process of the reaction complex. At low temperatures, $k_1 > k_{-1}$ and $k_1 > k_2$; hence, the steady-state model is not applicable at low temperatures, but at high temperatures. Finally, the problem is to determine the temperature at which the equilibrium-state model and the steady-state model satisfy their approximate conditions.

According to the thermodynamic theory, the standard molar Gibbs free energy change $\Delta G_{1,m}^\theta$ for the formation reaction of the reaction complex can be expressed as

$$\Delta G_{1,m}^\theta = \Delta H_{1,m}^\theta - T\Delta S_{1,m}^\theta = -RT \ln K_1^\theta \quad (1)$$

where $\Delta H_{1,m}^\theta$ is the standard enthalpy change, $\Delta S_{1,m}^\theta$ is the standard entropy change, and K_1^θ is the standard equilibrium constant between the original reactants and the reaction complex. The standard equilibrium constant K_1^θ can be written as

$$K_1^\theta = K_{c,1} \left(\frac{RT}{P^\theta} \right)^{-1} \quad (2)$$

where P^θ is the standard atmospheric pressure, R is the ideal gas constant, and $K_{c,1}$ is the concentration equilibrium constant between the original reactants and the reaction complex. The expression for the concentration equilibrium constant $K_{c,1}$ can also be written as

$$K_{c,1} = \frac{k_1}{k_{-1}} \quad (3)$$

The enthalpy change and the entropy change are negative in the formation of the reaction complex, and therefore, from eq 7, the entropy term is not dominant if T is low and hence the standard molar Gibbs free energy $\Delta G_{1,m}^\theta$ is less than zero at low temperatures, which leads to a k_1 value that is larger than k_{-1} . With the increase of temperature, $\Delta G_{1,m}^\theta$ is increasing to zero and the corresponding temperature is defined as the conversion temperature T_{C1} in this study

$$\Delta G_{1,m}^\theta = \Delta H_{1,m}^\theta - T_{C,1}\Delta S_{1,m}^\theta = 0 \quad (4)$$

When the temperature is much higher than T_{C1} , $\Delta G_{1,m}^\theta$ is much greater than zero, which leads to that k_{-1} are larger than k_1 and k_1 and k_{-1} are larger than k_2 at higher temperatures, and hence, the steady-state model and the equilibrium-state model are applicable for the radical molecule reactions when the temperature is much higher than T_{C1} .

According to Equation 4, we calculate T_{C1} of the optimal reaction path under different reaction conditions, and the calculation results are shown in Table S1. In our study, the temperature range for calculating the reaction rate constant is 240-425K, which is higher than the temperature in **Table S9**. So we think it's right to assume that k_2 is much less than k_{-1} ,

i.e. $k_{-1} + k_2 \approx k_{-1}$, so that $k = \frac{k_1}{k_{-1} + k_2} k_2$ is approximate to $k = \frac{k_1}{k_{-1}} k_2 = k_{eq} k_2$, the fact that results of our approximate calculation approximates to that of an exact calculation (KiStHeLP) also shows that our approximation is reasonable (see **Table S10**).

. **Table S9** The temperature T_{C1} of the optimal reaction path under different reaction conditions

Reaction conditions	reaction	T_{C1} (K)
No water	cis-HONO+HCl	86

	trans-HONO+HCl	105
One water molecule	cis-HONO...H ₂ O+HCl	157
	trans-HONO...H ₂ O+HCl	184
Water dimer	cis-HONO...(H ₂ O) ₂ -a+HCl	137
	trans-HONO...(H ₂ O) ₂ -b+HCl	187
Water trimer	cis-HONO...(H ₂ O) ₃ -a+HCl	161
	trans-HONO...(H ₂ O) ₃ -a+HCl	172

2. Kinetic computation (KiSThEP)

In order to verify the correctness of the method, we used KiSThEP software to recalculate the reaction rate constant. KiSThEP^[2] includes the theoretical prediction of canonical and microcanonical rate constants for gas-phase chemical reactions. The methods used are conventional TST or variational transition state theory (VTST), or RRKM theory. One-dimensional quantum mechanical tunneling treatments through Wigner correction or an unsymmetrical Eckart potential energy barrier can also be involved. It is not designed to be comprehensive such as for example the PolyRate or MultiWell programs, but it has been successfully applied to the calculation of the rate constant of gas reaction^[3,4].

Based on the potential energy surfaces, the rate constants of the reactions in the aqueous phase were calculated using conventional transition state theory (TST):

$$k^{TST}(T) = \chi(T) \sigma \frac{k_b T}{h} \left(\frac{RT}{P^0} \right)^{\Delta n} e^{-\frac{\Delta G^\ddagger}{k_b T}} \quad (5)$$

$$\Delta G^\ddagger = G_{TS} - G_R \quad (6)$$

$$\chi(T) = 1 + \frac{1}{24} \left| \frac{h\nu^\ddagger}{k_B T} \right|^2 \quad (7)$$

In the formula, k_b , h , and R are the Boltzmann constant, Planck constant, and gas constant, respectively. ΔG^\ddagger is the Gibbs free energy of activation; σ represents the reaction path degeneracy, which accounts for the number of equivalent reaction paths. P^0 and T are pressure and temperature, respectively. Δn corresponds to $n-1$ for an n -molecular reaction, for instance, Δn is 1 for the bimolecular reaction studied herein. $\chi(T)$ is the quantum mechanical tunneling correction.

Table S10 Rate constants (in cm³molecule⁻¹s⁻¹) for the HONO+HCl reaction under different conditions with two methods (298K).

Reaction conditions	Reaction	k (in the article)	k (KiSThEP)
No water	cis-HONO+HCl	2.93×10 ⁻²⁵	6.94×10 ²⁶
	trans-HONO+HCl	9.55×10 ⁻²⁴	2.79×10 ⁻²⁴
One water molecule	cis-HONO...H ₂ O+HCl	3.44×10 ⁻²²	8.21×10 ⁻²³
	trans-HONO...H ₂ O+HCl	4.26×10 ⁻²¹	1.00×10 ⁻²¹
Water dimer	cis-HONO...(H ₂ O) ₂ -a+HCl	2.27×10 ⁻¹⁹	2.31×10 ⁻²⁰
	trans-HONO...(H ₂ O) ₂ -b+HCl	2.24×10 ⁻¹⁸	1.53×10 ⁻¹⁹
Water trimer	cis-HONO...(H ₂ O) ₃ -a+HCl	2.12×10 ⁻²³	7.05×10 ⁻²⁴

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