Supplementary Material for

Adsorption and heterogeneous reactions of
ClONO₂ and N₂O₅ on/with NaCl aerosol

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Figure S2. Possible configurations of adsorbed ClONO$_2$ on the NaCl (100) surface.
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**Figure S5.** Reaction schemes of ClONO$_2$ and N$_2$O$_5$ with HCl or H$_2$O on the NaCl (100) surface. The calculated data without zero-point energy (ZPE) correction are in black and with zero-point energy (ZPE) correction are in red.

**Chemical Equations:**

1. \( \text{III-6} + \text{HCl} \xrightarrow{\Delta E_r = -12.02} \text{IM1} \xrightarrow{\Delta E_r = -11.42} \text{P1} \xrightarrow{\Delta E_r = 8.56} \text{P1-p} \)  
   \( \Delta E_b = 5.42 \)  
   \( \Delta E_r = -21.68 \)  
   \( \Delta E_b = 5.35 \)  
   \( \Delta E_r = -18.98 \)

2. \( \text{III-6} + \text{H}_2\text{O} \xrightarrow{\Delta E_r = -18.22} \text{IM2} \xrightarrow{\Delta E_r = -19.03} \text{P2} \xrightarrow{\Delta E_r = -12.82} \text{P2-p} \)  
   \( \Delta E_b = 7.01 \)  
   \( \Delta E_r = -1.96 \)  
   \( \Delta E_b = 7.13 \)  
   \( \Delta E_r = -1.15 \)

3. \( \text{II-4'} + \text{HCl} \xrightarrow{\Delta E_r = -6.69} \text{IM3} \xrightarrow{\Delta E_r = -5.88} \text{P3} \xrightarrow{\Delta E_r = -5.88} \text{P3-p} \)  
   \( \Delta E_b = 4.80 \)  
   \( \Delta E_r = -15.67 \)  
   \( \Delta E_b = 4.32 \)  
   \( \Delta E_r = -12.99 \)

4. \( \text{II-4'} + \text{H}_2\text{O} \xrightarrow{\Delta E_r = -9.42} \text{IM4} \xrightarrow{\Delta E_r = -7.90} \text{P4} \xrightarrow{\Delta E_r = -0.91} \text{P4-p} \)  
   \( \Delta E_b = 5.75 \)  
   \( \Delta E_r = -19.91 \)  
   \( \Delta E_b = 5.96 \)  
   \( \Delta E_r = -17.82 \)
Figure S6. Reaction schemes of H₂O adsorption and reconstruction on the NaCl (100) surface. The calculated data without zero-point energy (ZPE) correction are in black and with zero-point energy (ZPE) correction are in red.

\[
\text{NaCl} + \text{H}_2\text{O} \xrightarrow{\Delta E_r = -13.99} \text{IM5} \xrightarrow{\Delta E_r = -11.45} \text{TS5} \xrightarrow{\Delta E_r = 10.33} \text{IM6} \\
\Delta E_p = 14.03 \\
\Delta E_r = 14.00 \\
\Delta E_r = 10.71
\]
**Figure S7.** Reaction schemes of ClONO$_2$ and N$_2$O$_5$ with the reconstructed NaCl (100) surface. The calculated data without zero-point energy (ZPE) correction are in black and with zero-point energy (ZPE) correction are in red.

IM6 + ClONO$_2$ $\rightarrow$ IM7 $\rightarrow$ IM8 $\rightarrow$ P5 $\rightarrow$ P5-p

$\Delta E_r = -20.37 \quad \Delta E_r = -19.80 \quad \Delta E_r = 0.24 \quad \Delta E_r = 0.60 \quad \Delta E_r = -5.35 \quad \Delta E_r = -5.35$

TS6 $\rightarrow$ IM9 $\rightarrow$ IM10 $\rightarrow$ P6 $\rightarrow$ P6-p

$\Delta E_r = -20.44 \quad \Delta E_r = -19.80 \quad \Delta E_r = 0.45 \quad \Delta E_r = 0.65 \quad \Delta E_r = -5.35 \quad \Delta E_r = -5.44$

TS7 $\rightarrow$ IM11 $\rightarrow$ IM12 $\rightarrow$ P7 $\rightarrow$ P7-p

IM6 + N$_2$O$_5$ $\rightarrow$ IM11 $\rightarrow$ IM12 $\rightarrow$ P7 $\rightarrow$ P7-p

$\Delta E_r = -14.35 \quad \Delta E_r = -14.11 \quad \Delta E_r = 0.99 \quad \Delta E_r = 1.03 \quad \Delta E_r = -10.63 \quad \Delta E_r = -10.63$

TS8 $\rightarrow$ IM13 $\rightarrow$ IM14 $\rightarrow$ P8 $\rightarrow$ P8-p

IM6 + N$_2$O$_5$ $\rightarrow$ IM13 $\rightarrow$ IM14 $\rightarrow$ P8 $\rightarrow$ P8-p

$\Delta E_r = -14.29 \quad \Delta E_r = -14.04 \quad \Delta E_r = 0.49 \quad \Delta E_r = 0.47 \quad \Delta E_r = -9.91 \quad \Delta E_r = -9.91$

TS9 $\rightarrow$ IM15 $\rightarrow$ IM16 $\rightarrow$ P9 $\rightarrow$ P9-p

IM6 + N$_2$O$_5$ $\rightarrow$ IM15 $\rightarrow$ IM16 $\rightarrow$ P9 $\rightarrow$ P9-p

$\Delta E_r = -14.00 \quad \Delta E_r = -13.86 \quad \Delta E_r = 0.48 \quad \Delta E_r = 0.43 \quad \Delta E_r = -9.96 \quad \Delta E_r = -9.96$