

Supplementary Material for

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

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Figure S1. DMol³ optimized geometries for H₂O, ClONO₂ and N₂O₅. Distances are in angstrom, and angles are in degree. The values in parentheses are experimental data.

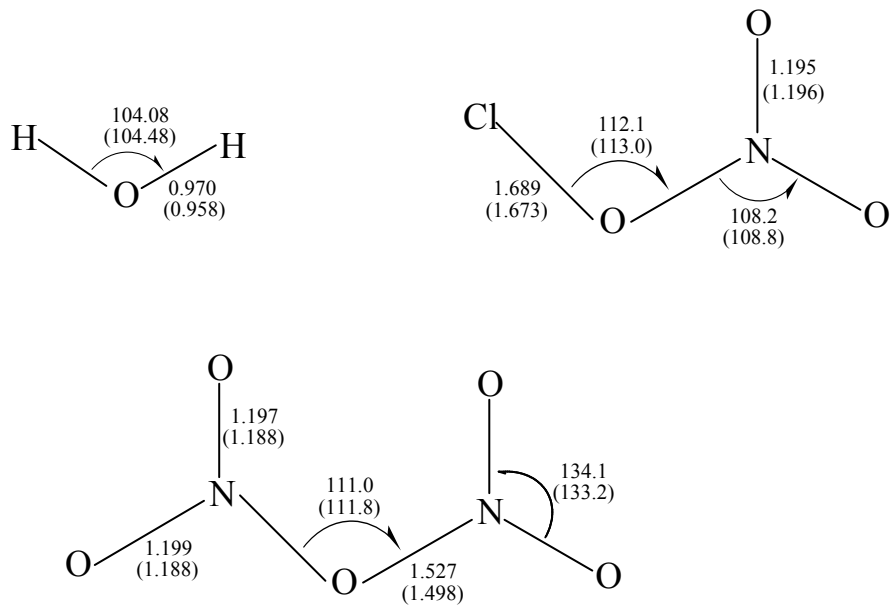
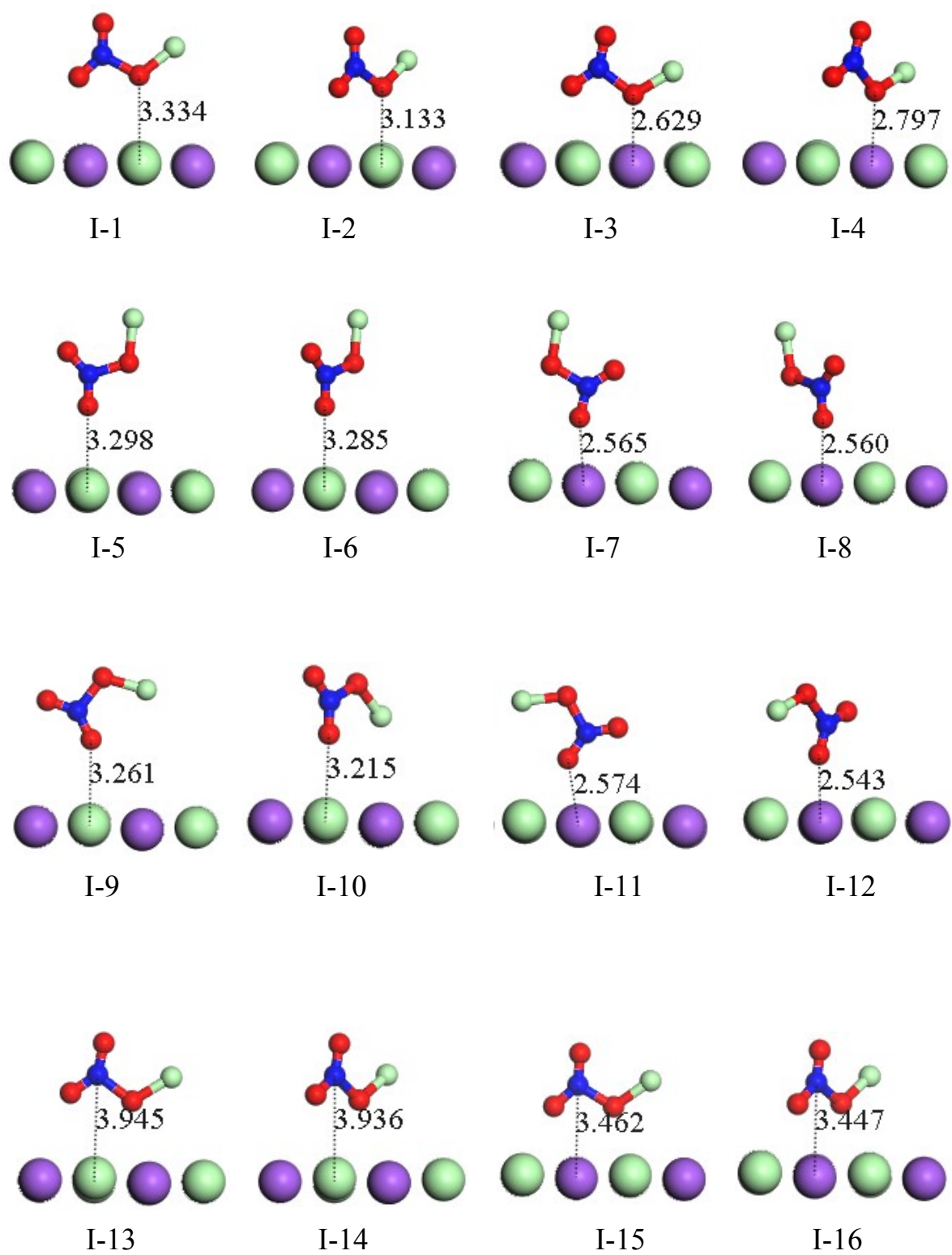


Figure S2. Possible configurations of adsorbed ClONO₂ on the NaCl (100) surface.



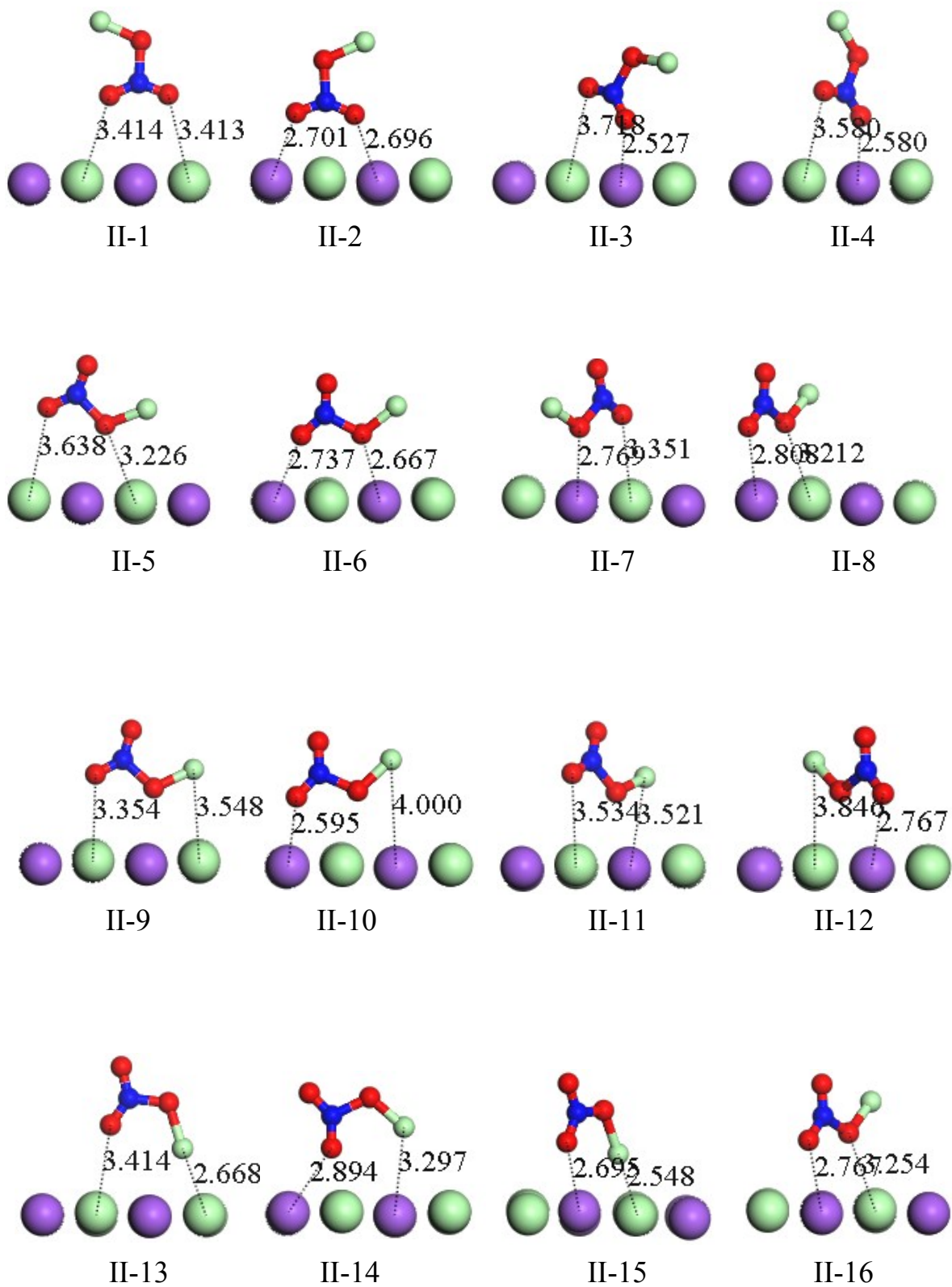


Figure S2 (Continued)

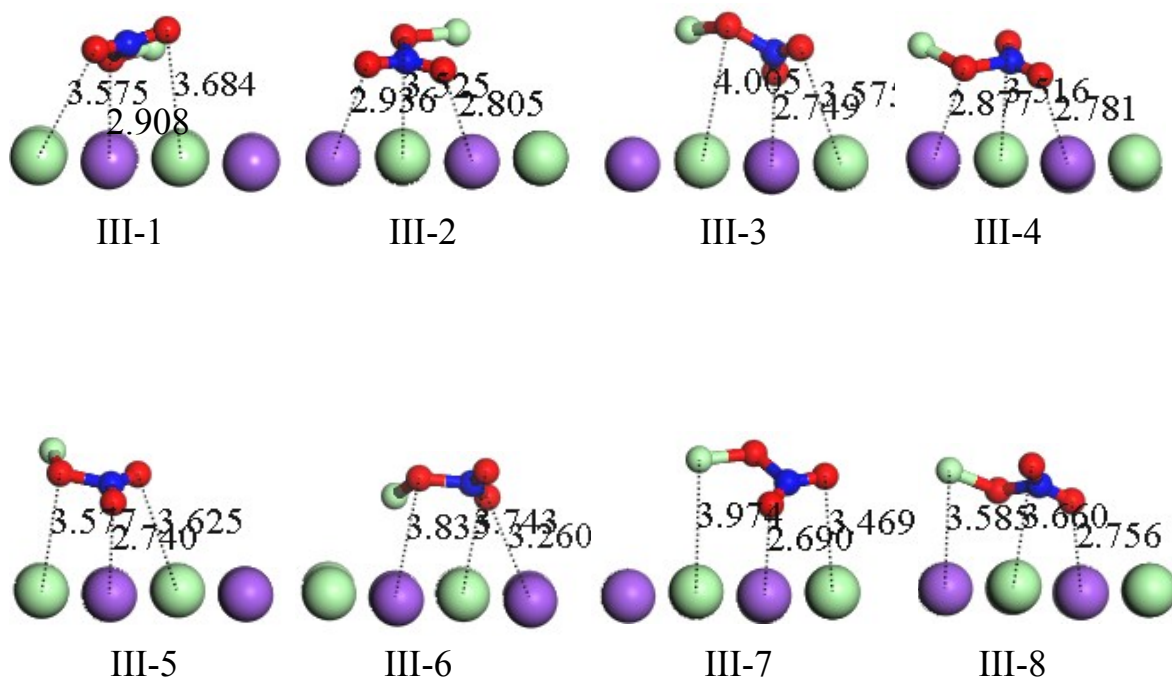
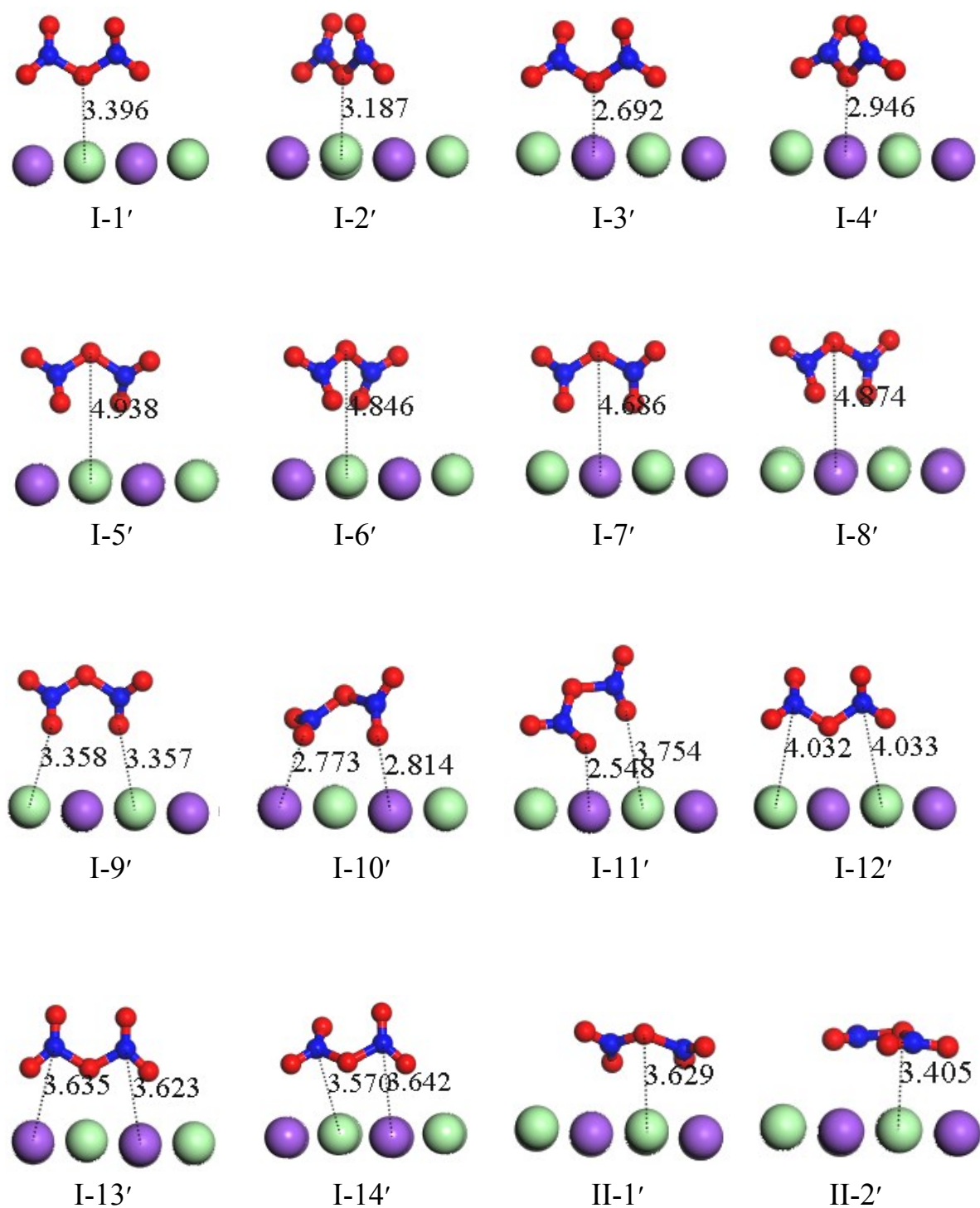


Figure S2 (Continued)

Figure S3. Possible configurations of adsorbed N_2O_5 on the NaCl (100) surface.



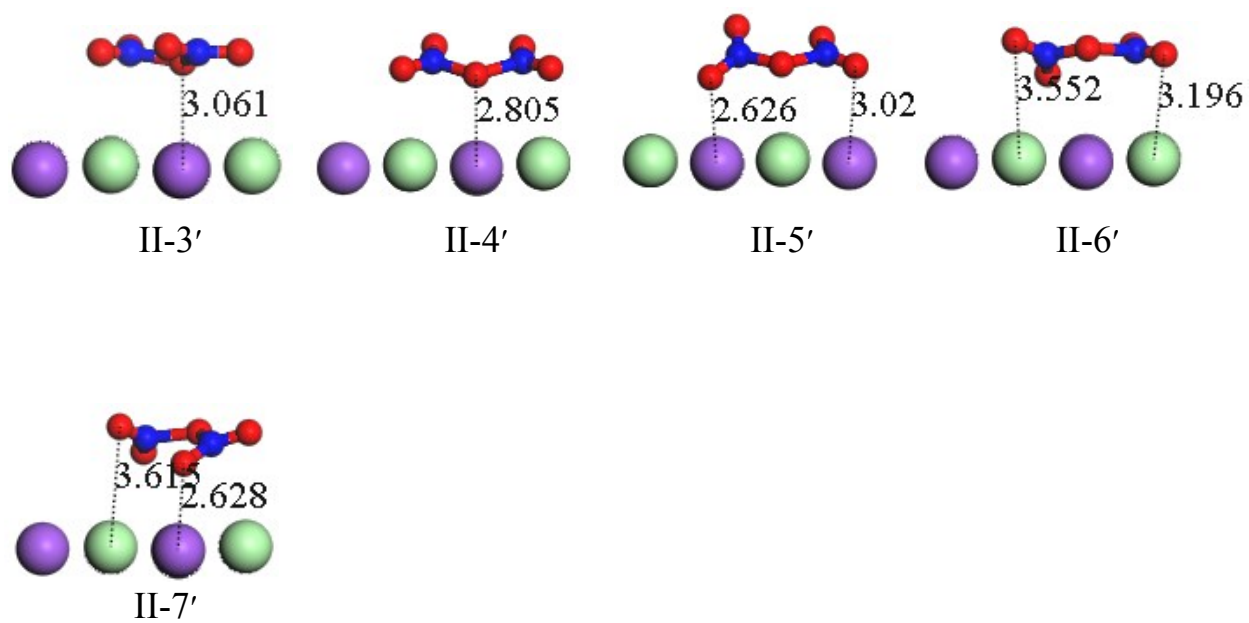
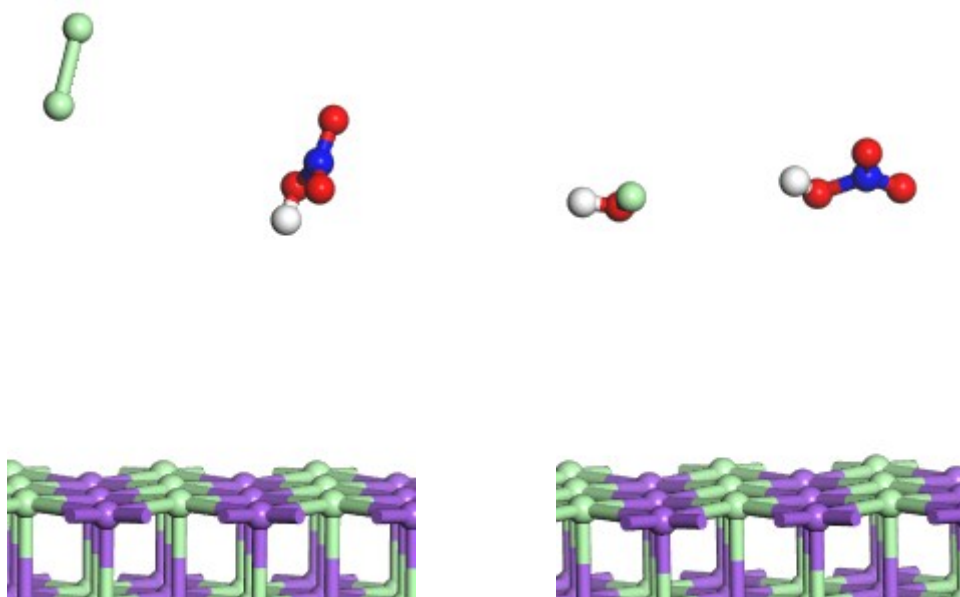


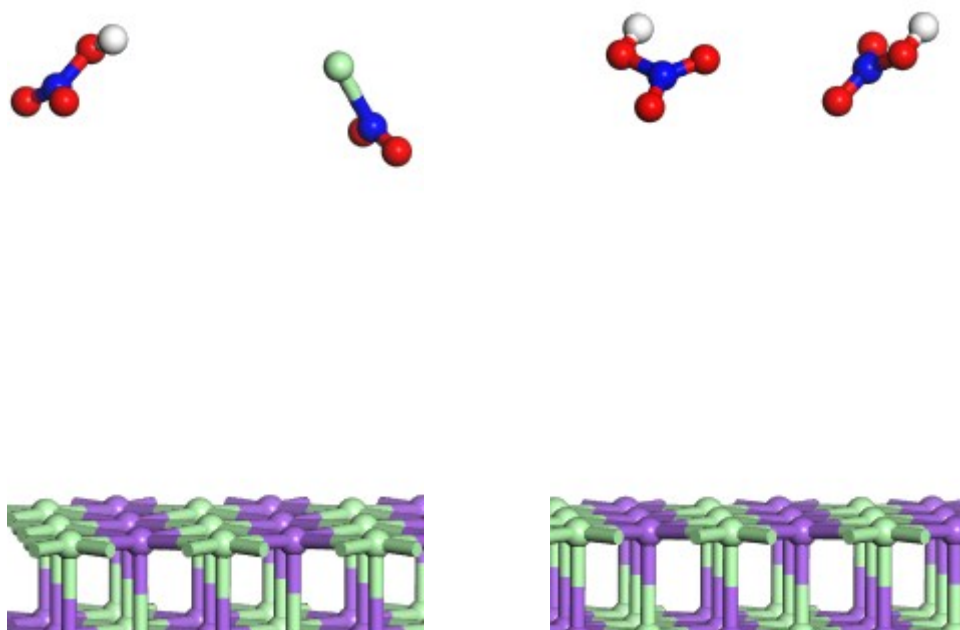
Figure S3 (*Continued*)

Figure S4. Optimized geometries of the “free products” on the NaCl (100) surface.



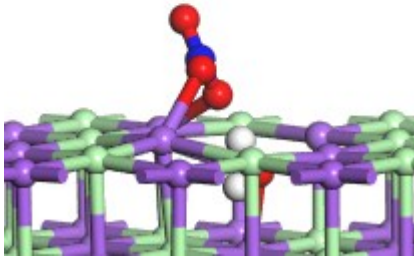
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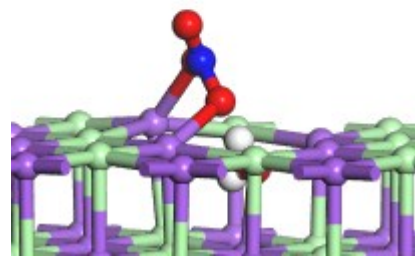


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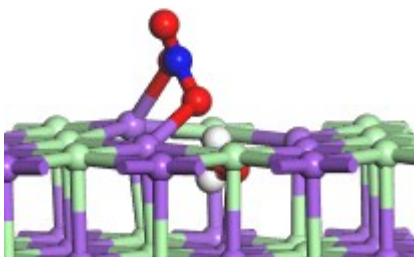
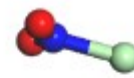
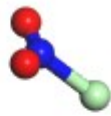
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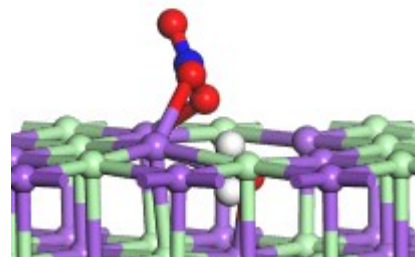
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P6-p



P7-p



P8-p

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.

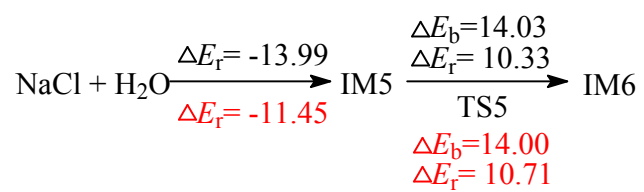


Figure S7. Reaction schemes of ClONO₂ and N₂O₅ with the reconstructed NaCl (100) surface. The calculated data without zero-point energy (ZPE) correction are in black and with zero-point energy (ZPE) correction are in red.

