

Supporting Information for

Mechanisms and Kinetic Parameters for the Gas-phase Reactions of Anthracene and Pyrene with Cl Atoms in the Presence of NO_x

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Six pages

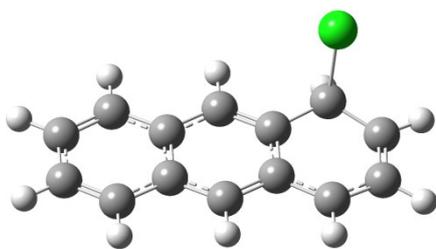
Contains four figures

Figure S1. Configuration of the Cl-Ant adducts and Cl-Pyr adducts (IM1-IM5).

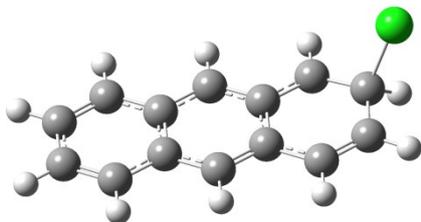
Figure S2. The O₂ addition reaction schemes of Ant and Pyr embedded with the potential barrier ΔE (kcal/mol) and reaction heat ΔH (kcal/mol).

Figure S3. Configuration of the transition states for the elimination of water and HCl from the Cl-NO₂-Ant adducts. TS1: Cl-NO₂-Ant→nitro-Ant+HCl, TS2: Cl-NO₂-Ant+H₂O→nitro-Ant+HCl+H₂O, TS3: Cl-NO₂-Ant+2H₂O→nitro-Ant+HCl+2H₂O.

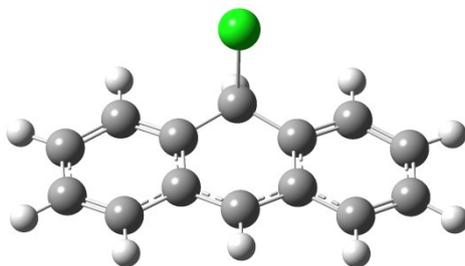
Figure S4. Resonance structures of the Cl-Ant adduct.



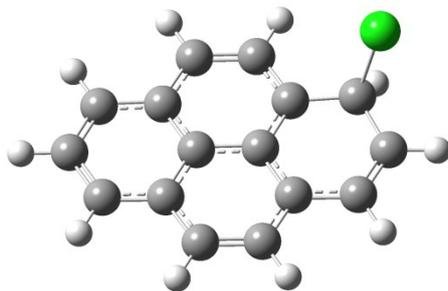
IM1



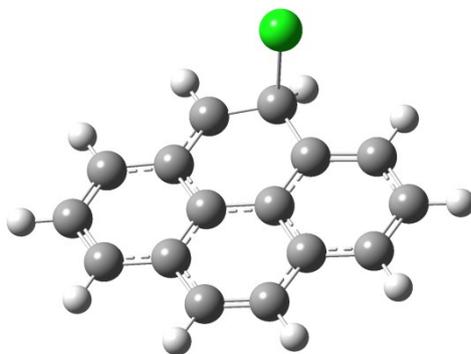
IM2



IM3



IM4



IM5

Figure S1

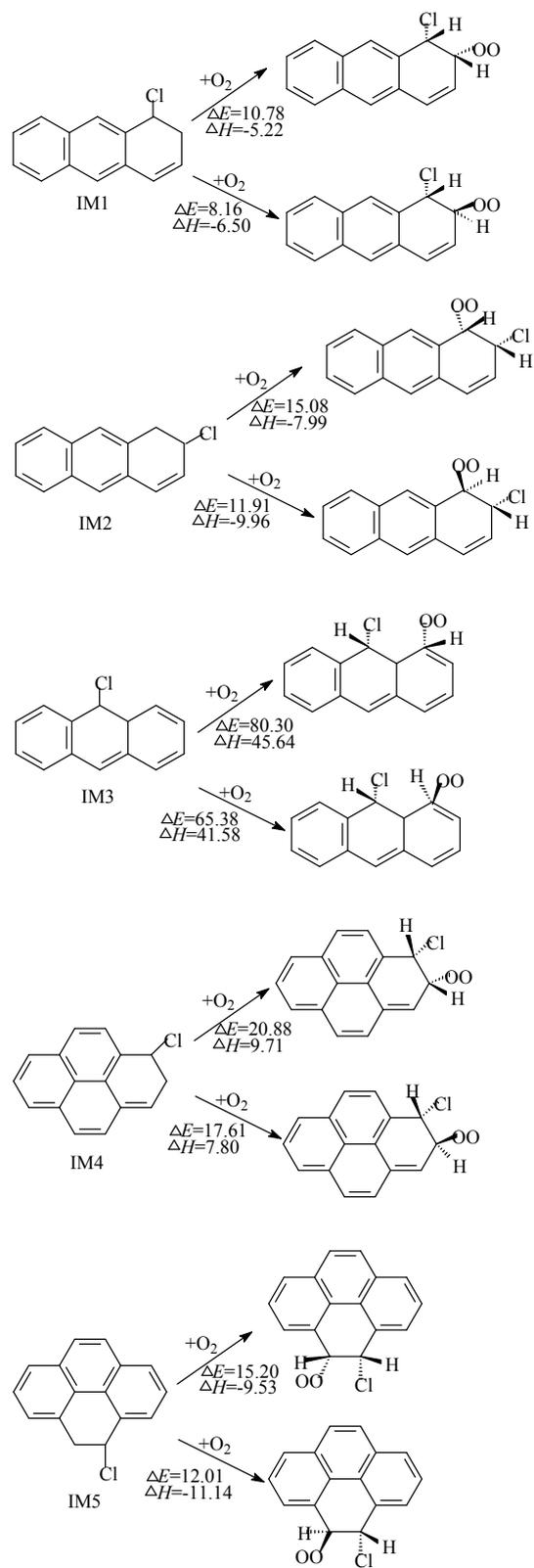
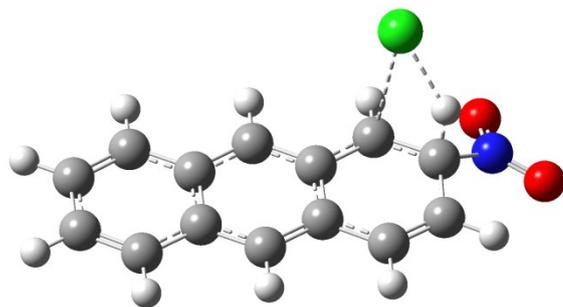
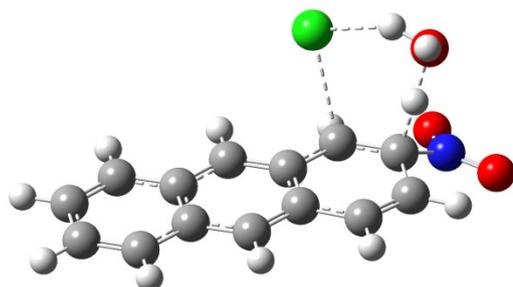


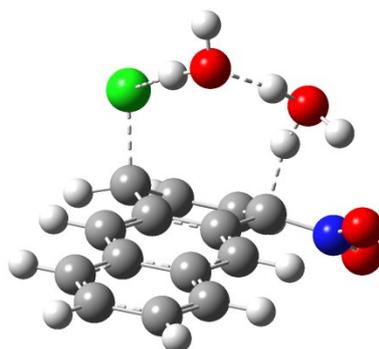
Figure S2



TS1



TS2



TS3

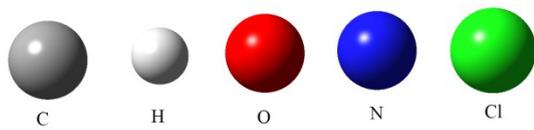


Figure S3

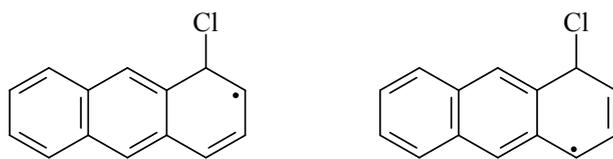


Figure S4