

Supporting Information

Impact of Ambient Gases on the Mechanism of the [Cs₈Nb₆O₁₉]-Promoted Nerve-Agent Decomposition

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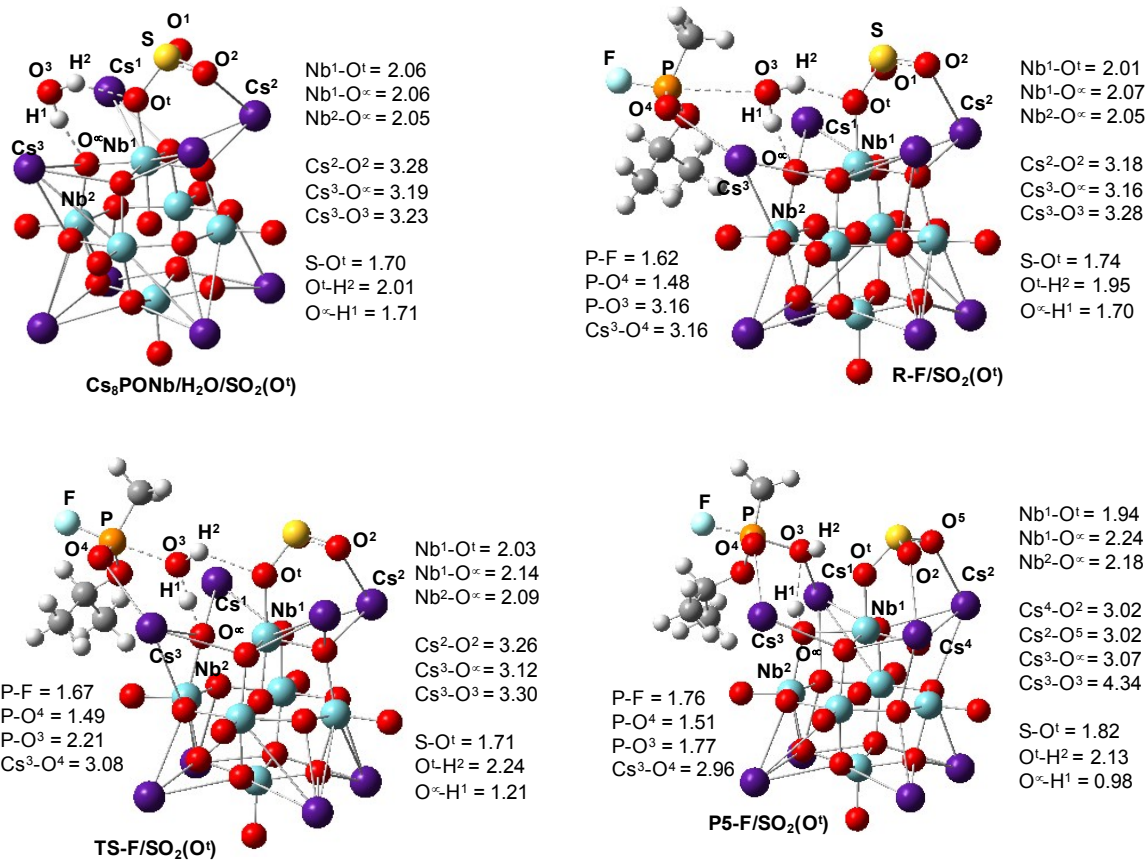


Figure S1. Calculated pre-reaction complexes, transition state and product of the GB hydrolysis by Cs₈Nb₆O₁₉/SO₂ (i.e. reaction Cs₈Nb₆O₁₉/SO₂ + H₂O + GB → R-F_SO₂ → TS-F_SO₂ → P5-F_SO₂) and their important geometry parameters (in Å).

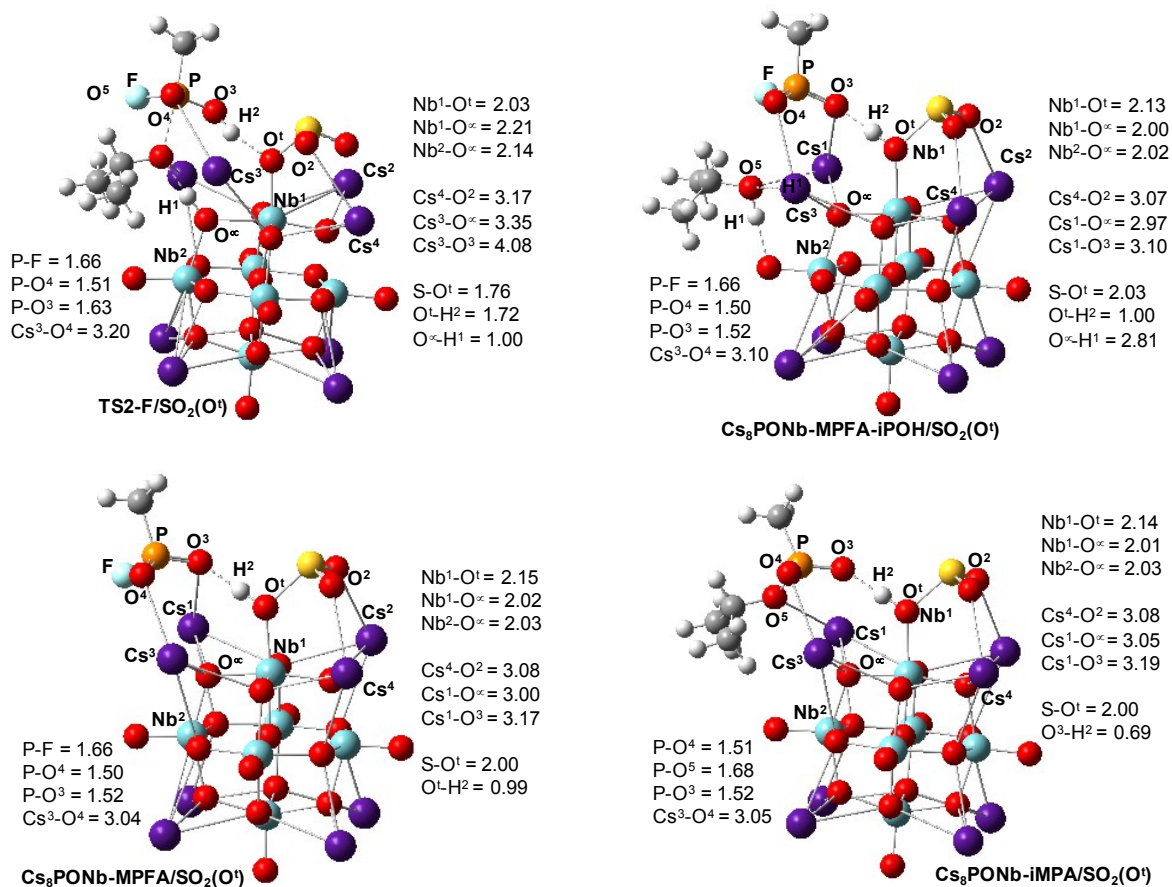


Figure S2. The calculated transition states, intermediates and products of the pentacoordinated P5-F₂SO₂ dissociation (i.e. reactions: P5-F₂SO₂ → Cs₈Nb₆O₁₉/SO₂-(MPFA)-(i-POH) → Cs₈Nb₆O₁₉/SO₂ + MPFAH + (i-POH) and P5-F₂X → Cs₈Nb₆O₁₉/SO₂-(MPA)-HF → Cs₈Nb₆O₁₉/SO₂ + MPAH + HF) with their important geometry parameters (in Å).

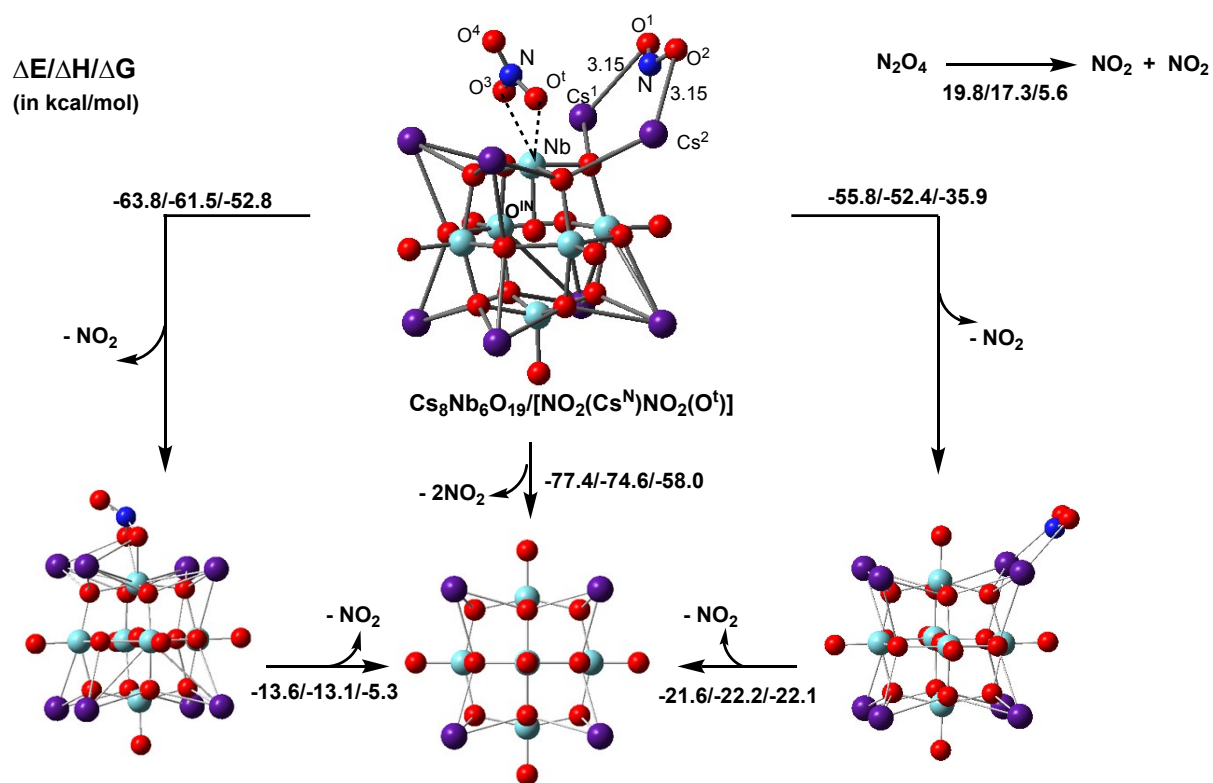


Figure S3. The calculated adsorption energies (in kcal/mol) of NO₂ radicals to Cs₈Nb₆O₁₉