Kinetic Energy Dependence and Potential Energy Surface of the Spin-forbidden Reaction Sm^+ (^8F) + N_2O ($^1\Sigma^+$) → SmO^+ ($^6\Delta$) + N_2 ($^1\Sigma_g^+$)

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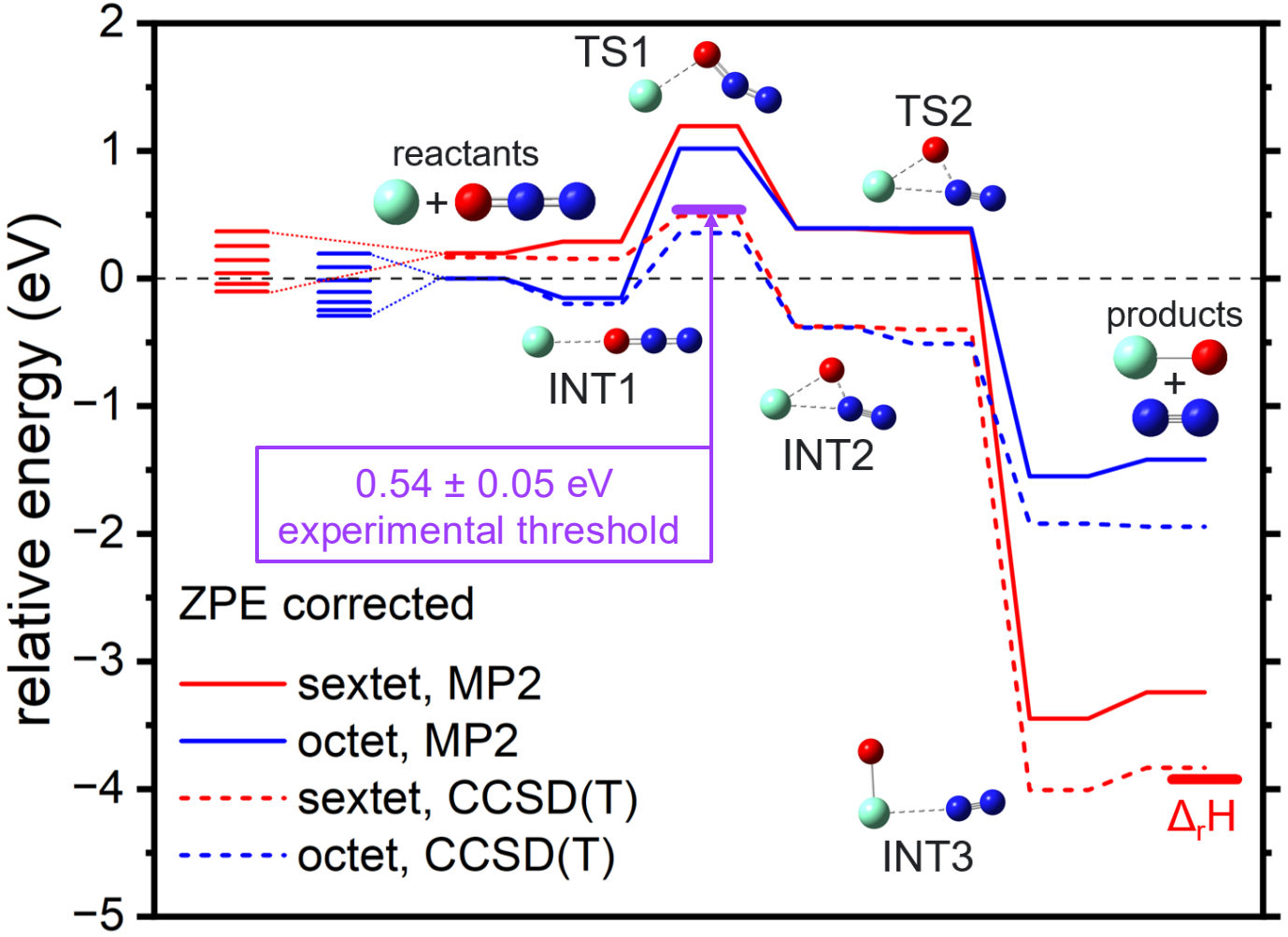
Chemical reactions that require a change in electron spin have slow reaction rates and reduced efficiency. The gas-phase oxidation reaction between samarium ions (Sm^+) and nitrous oxide (N_2O), which is relevant to atmospheric modification to improve satellite communications, is a spin-forbidden reaction with curious behavior. Guided-Ion beam tandem mass spectrometry experiments shown that the reaction rate and efficiency increase significantly as energy is added to the reactants. This dramatic change occurs only when a threshold energy (0.54 ± 0.05 eV) is reached. To investigate the origins of this behavior, we used the CHPC's resources to calculate potential energy surfaces as maps for the reaction (shown at right). These surfaces show that the threshold energy we observed most likely corresponds to the initial transition state (TS1) of the reaction, as shown by the agreement between CCSD(T) surfaces and the magnitude of the threshold (purple line).



Funding for this work was provided by the Air Force Office of Scientific Research (AFOSR) under award no. FA9550-20-1-0329.