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Structure of the Oxygen-Rich Cluster Cation Al_2O_7^+ and its Reactivity toward Methane and Water

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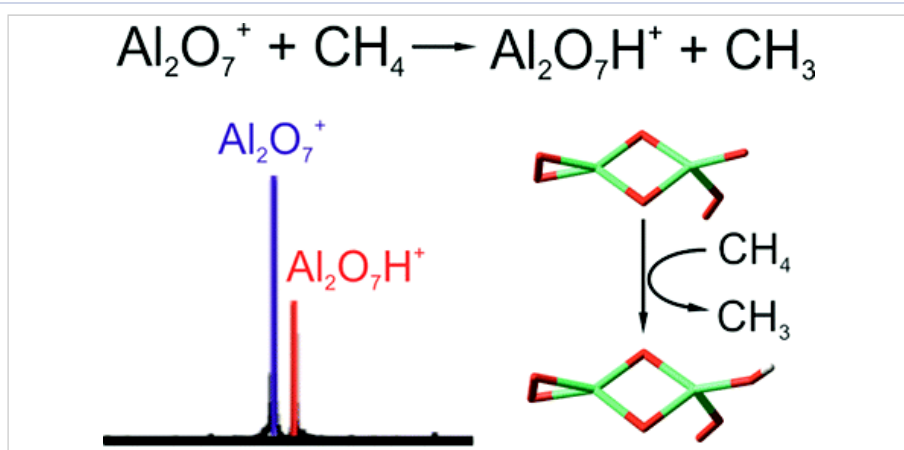
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Abstract



The oxygen-rich cluster Al_2O_7^+ is generated in the gas phase and investigated with respect to both its structure and its reactivity toward small, inert molecules using Fourier-transform ion cyclotron resonance (FT-ICR) mass spectrometry and DFT-based calculations. Al_2O_7^+ reacts with CH_4 under ambient conditions via hydrogen atom transfer (HAT), and with H_2O a ligand exchange occurs which gives rise to the evaporation of two O_2 molecules. The resulting product ion $\text{Al}_2\text{O}_4\text{H}_2^+$ is also capable of abstracting a hydrogen atom from both H_2O and CH_4 . As indicated in the $\text{H}_2\text{O}/2\text{O}_2$ ligand exchange and supported by collision-induced dissociation (CID) experiments, two O_2 units constitute structural elements of Al_2O_7^+ . Further insight is provided by DFT calculations, performed at the unrestricted B3LYP/TZVP level, and reaction mechanisms are suggested on the basis of both the experimental and theoretical results.

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