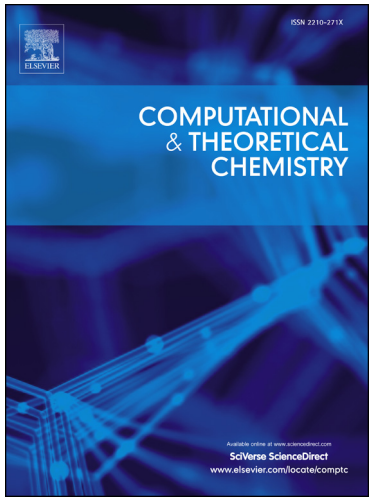

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$HAl(OH)_2$ MOLECULAR STRUCTURES AND REACTION PATHS. POST-HARTREE-FOCK, DFT CALCULATIONS AND INFRARED SPECTROSCOPIC.

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ABSTRACT

Quantum chemical calculations were performed to determine the structures and formation path for the $HAl(OH)_2$ molecule. The analyses of the anharmonic frequencies as well the potential energy surface (PES) using coupled cluster, Møller-Plesset and density functional calculations, support the idea that the *Syn* structure proposed in the literature for $HAl(OH)_2$ is not right. Unlike the *Syn* conformer, the *Endo-Exo* structure is consistent with the PES, the statistical thermodynamic results and infrared spectra. Different reaction channels for the reaction of laser-ablated Al atoms with a $H_2 + O_2$ mixture in gas phase were analyzed. The results show that there are three possible reaction channels that involve two possible intermediates for the reaction of Al with $H_2 + O_2$.