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Rafael Añez, Paola Alejos, Anibal Sierraalta

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HA_l(OH)₂ MOLECULAR STRUCTURES AND REACTION PATHS. POST-HARTREE-FOCK, DFT CALCULATIONS AND INFRARED SPECTROSCOPIC.

Rafael Añez, Paola Alejos and Anibal Sierraalta*

Laboratorio de Química-Física y Catálisis Computacional, Centro de Química, Instituto Venezolano de Investigaciones Científicas, Apartado 21827, Caracas 1020-A, Venezuela.

*E-mail: asierral@ivic.ve.

ABSTRACT

Quantum chemical calculations were performed to determine the structures and formation path for the HA_l(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 HA_l(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 H₂ + O₂ 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 H₂ + O₂.

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