Accepted Manuscript

Hal(oh)₂ molecular structures and reaction paths. post-hartree-fock, dft calculations and infrared spectroscopic

Rafael Añez, Paola Alejos, Anibal Sierraalta

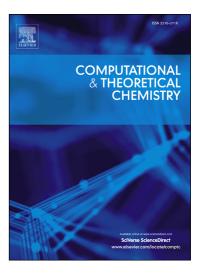
PII: S2210-271X(15)00079-1

DOI: http://dx.doi.org/10.1016/j.comptc.2015.02.008

Reference: COMPTC 1743

To appear in: Computational & Theoretical Chemistry

Received Date: 1 October 2014
Revised Date: 13 January 2015
Accepted Date: 16 February 2015



Please cite this article as: R. Añez, P. Alejos, A. Sierraalta, Hal(oh)₂ molecular structures and reaction paths. post-hartree-fock, dft calculations and infrared spectroscopic, *Computational & Theoretical Chemistry* (2015), doi: http://dx.doi.org/10.1016/j.comptc.2015.02.008

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

ACCEPTED MANUSCRIPT

HAI(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 $HAI(OH)_2$ 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 $HAI(OH)_2$ 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 $H_2 + O_2$.

Download English Version:

https://daneshyari.com/en/article/5393143

Download Persian Version:

https://daneshyari.com/article/5393143

<u>Daneshyari.com</u>