Int. J. New. Chem., 2021, Vol. 8, Issue 3, pp 345-355.

International Journal of New Chemistry

Published online 2021 in http://www.ijnc.ir/.

Open Access

Print ISSN: 2645-7237

Online ISSN: 2383-188x

Original Research Article

Computational Review of Conformers 2- Choroacetaldehyd

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Received: 2020-06-11 *Accepted: 2020-12-05* *Published: 2021-07-01*

ABSTRACT

Abstract In studies performed on 2- chloroacetalidehyde by abinitio beginning with the LC-WPBE, B3LYP and m06-2x functionals and 6-311++G (d, p) basis set. Also, by checking the total energy, HOMO-LUMO gaps and dipole moment, it was found that the keto form is more stable than the enol form. Theoretical calculations With LC-WPBE/6-311G(d,p) shows the more stability of I- conformer in compared to other conformers . NBO analysis was practical for illustrating the negative hyperconjugative effect on the conformers. In the basis of NBO analysis, the LP(2)O $\rightarrow \sigma^{*}(C-H)$ and LP(2)O $\rightarrow \sigma^{*}(C-C)$ Interactions were responsible of the negative hyperconjugation in the examined compounds. The deletion of all thw donor – acceptor electronic interaction from the fock matrices and off –diagonal elements, values of these interaction were reported.

Keywords: 2- choroacetaldehyd, NBO (natural bond orbital analysis), Negative hyperconjugative effect, Second order the stabilization energies (E_2)

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