Int. J. New. Chem., 2021, Vol. 8, Issue 2, pp 198-221.

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

Theoretical Study of M_2X_4 (M=C, X=H, F and Cl) Structures by using HOMO, LUMO, NBO and NMR analysis

Golrokh Mahmoudzadeh

Chemistry Department, Arak Branch, Islamic Azad University, Arak, Iran

Received: 2020-03-06 *Accepted: 2020-11-23* *Published: 2021-06-01*

ABSTRACT

All calculations were performed within the MP2 / 6-311 G (d, p) method to evaluate the effects of substituent groups which affect the structural stability and molecular energy. A natural bond orbital (NBO) analysis and isotopic, and anisotropic NMR chemistry, were used also for a better understanding of the C_2X_4 electronic structure and its derivatives. The NBO analysis shows that the occupancy of lone pair electrons of halogen atoms in all compounds decreases with increasing p character of the lone pair of halogen atoms. Furthermore, NBO analysis demonstrated the effects of donates substituent groups including (CH3, NH2, and OH) that donates some of its electron density into a π system via resonance or inductive effects, thus making the π system more nucleophilic on electron density. The obtained values from NMR tensors parameters shows electronegativity in excellent agreement with the expected chemical shielding values. Therefore, we suggest that is correlations between donates substituent groups with electronegativity along with the total stability energy of the studied molecules. The energies gap of frontier molecular orbital (ε_{LUMO}- ε_{HOMO}) is recorded in order to find the suitability correlation between this energy with chemical hardness (η) of the studied molecules.

Keywords: MP2 method, NBO analysis, NMR shielding, HOMO-LUMO

*Corresponding Author: Tel.: +98 (00) 000000000
E-mail: gmahmoudzadeh@yahoo.com