World Academy of Science, Engineering and Technology
International Journal of Chemical and Materials Engineering
Vol:9, No:06, 2015

Theoretical Studies on the Formation Constant, Geometry, Vibrational Frequencies and Electronic Properties Dinuclear Molybdenum Complexes

Authors : Mahboobeh Mohadeszadeh, Behzad Padidaran Moghaddam

Abstract : In order to measuring dinuclear molybdenum complexes formation constant First,the reactants and the products were optimized separately and then, their frequencies were measured. In next level , with using Hartree-fock (HF) and density functional theory (DFT) methods ,Theoretical studies on the geometrical parameters, electronic properties and vibrational frequencies of dinuclear molybdenum complexes [C40H44Mo2N2O20] were investigated . These calculations were performed with the B3LYP, BPV86, B3PW91 and HF theoretical method using the LANL2DZ (for Mo's) + 6-311G (for others) basis sets. To estimate the error rate between theoretical data and experimental data, RSquare , SError and RMS values that according with the theoretical and experimental parameters found out DFT methods has more integration with experimental data compare to HF methods. In addition, through electron specification of compounds, the percentage of atomic orbital's attendance in making molecular orbital's, atoms electrical charge, the sustainable energy resulting and also HOMO and LUMO orbital's energy achieved.

Keywords : geometrical parameters, hydrogen bonding, electronic properties, vibrational frequencies
Conference Title : ICCBE 2015 : International Conference on Chemical and Biochemical Engineering
Conference Location : Toronto, Canada
Conference Dates : June 15-16, 2015