Available online at **www.joac.info**

ISSN: 2278-1862

Journal of Applicable Chemistry

2014, 3 (5): 2102-2122

(International Peer Reviewed Journal)

DFT and MP2 Study of Pd(II) and Ni(II) PhCN, DMSO and Dithiooxamide Complexes- Part II: Theoretical

Lubna S. Mohammed[1], Isam S. Hamza[2], Falah R Muhi AL-Deen[3] and Bahjat R. J. Muhyedeen[4]

1. College of Science, Al-Nahrain University, Baghdad, **IRAQ**
2. Ministry of Science and Technology, **IRAQ**
3. Faidh AL-Rafidyen for Industrial Fertilizers, **IRAQ**
4. College of Science, Baghdad University, Baghdad, **IRAQ**

Email: bahjatrj@mass-energy-e-mbc.com

Accepted on 14th September 2014

ABSTRACT

The DFT and MP2 method at high level were used for calculating the relative energies of the 24 conformers of the prepared compounds $PdCl_2(PhCN)_2$, $PdCl_2(DMSO)_2$, $PdCl_2(DTO)$, $NiCl_2(DTO)$. The DFT, MP2, PM7 and PM3 energy calculations help to predict the most stable structure among the other probable structures.Both quantum method showed that PD1-trans isomer was the most stable for $PdCl_2(PhCN)_2$. For $PdC1_2(DMSO)_2$, the PD9-DMSO-trans(S,S) was more stable than the other three isomers.The relative energy calculations for the six $PdCl_2(DTO)$ isomers, showed that, among the three amide isomers, the PD5-trans-A(N,S) was the most stable, and among the three imide isomers the PD6-cis-I-(N,N) was the most stable, among the total six amide and imide isomers, the PD5-trans-A(N,S) was more stable than PD6-cis-I(N,N).For Ni complexes, the results of relative energies calculated showed that, among amide and imide complexes, Ni5-trans-A(N,S) was the most stable complexes, while among the three imide isomers the Ni6-cis-I(N,N) was the most stable. The TD-DFT and Semi-empirical PM7 method were used for calculating the UV and IR spectra. The results of the vibrational calculations were in good agreement with those obtained from the energy calculations and the experimental UV and IR study came in accordance with the theoretical calculation.

Keywords: Palladium DTO, DMSO complexes, Nickel DTO, DMSO complexes, IR, UV Spectra of Pd and Ni complexes, Theoretical DFT-IR and TD-UV.