22nd Iranian Inorganic Chemistry Conference,
23-25 August, 2023
University of Kurdistan

The First Row Transitional Metals Effects on Stabilization of Biliverdin Complexes, Theortical Study

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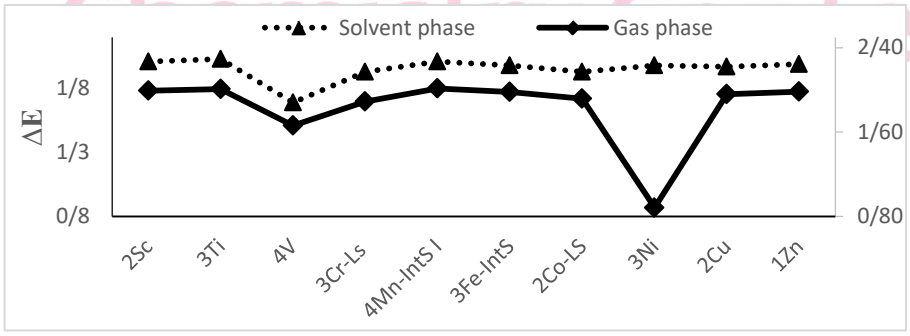
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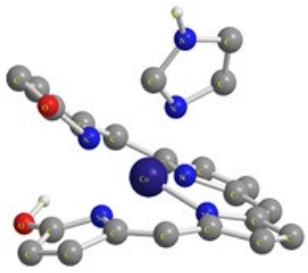
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Biliverdin is a product of heme catabolism. It is the pigment responsible for a greenish color sometimes seen in bruises. Biliverdin has been found in excess in the blood of humans suffering from hepatic diseases. Structure of biliverdin from catabolism process of heme is one of the cases that has been less discussed. In this research characterization of biliverdin analogues in the presence of hydroxide as a nucleophile and imidazole as axial ligands was investigated using the B3LYP method and the 6-31G basis set both in gas and solvent phases. Theoretical studies have shown that the absolute energy of the metal biliverdins increase with atomic mass both in gas and solvent phases. By changing the central metal in the structure of billiverdin, some features such as gap energy, hardness and softness, electrophilicity index and exact polarizability were studied and copmared with iron. the nickel and vanadium biliverdin have the least stability in gas and solvent phases respectively and the titanium biliverdin has the most one in both gas and solvent phases. Calculation of hardness (η) of these complexes confirms these stabilities in which the titanium is the hardest among the other metals. Electrophilicity calculation shows the nickel biliverdin in gas phase and copper in solvent phase are the most electrophile.

Keywords: hemeoxygenase, b3lyp, first row transitional metal biliverdin,heme degradation





Cobalt Biliverdin

References:

[1] A. Taghizadeh, P.R.Jmaat, and M. Daghighi Asli, *Russian Journal of inorganic chemistry*, **2021**, 66, 516.