Speaker: PROF. DR. MUSTAFA SERKAN SOYLU

Department of Physics, University of Giresun / TURKEY.

Title: "An example of combined experimental-theoretical characterization of metal (Nickel (II)) complex with neutral ligand"

The term of computational chemistry may be defined as mathematical description and numerical computation of molecular structures. The term computational chemistry is generally used when a mathematical method is sufficiently well developed that it can be automated for implementation on a computer. Computational chemistry has become a useful way to investigate materials that are too difficult to find or too expensive to purchase. It also helps chemists make predictions before running the actual experiments so that they can be better prepared for making observations. It's also useful ways to explain of spectroscopic results of molecular structures.

The mathematical description of the molecular structures based on the Quantum mechanics rules. Because of the Quantum mechanics (QM) is the correct mathematical description of the behaviour of electrons and thus of molecular structures. In theory, QM can predict any property of individual atom or molecule exactly. In practice, the QM equations have only been exactly for one electron systems. A myriad collection of methods has been developed for approximating the solution for multiple electron systems. These approximations can be very useful, but this requires an amount of sophistication on the part the researcher to know when each approximation is valid and how accurate the results are likely to be.

In my presentation, I intend to give you some information about a few examples of our work entitled "Combined experimental–theoretical characterization of chelidamate nickel complex with 4-methylpyrimidine". A new chelidamate complex of nickel (II) ion was synthesized and characterized by single-crystal X-ray diffraction, UV–Vis and FT-IR spectroscopy. Theoretical calculations have been carried out by using Hartree–Fock (HF)/6-31G (d) and Density Functional Theory (DFT)/6-31+G (d). HOMO–LUMO energies, absorption wavelengths and excitation energy were computed by time dependent DFT (TD-DFT) method with polarizable continuum model. The observed FT-IR vibrational frequencies are analysed and compared with theoretically predicted vibrational frequencies.

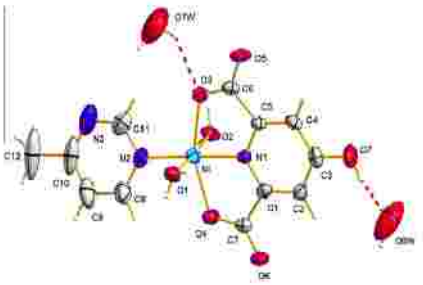

Fig. A view of Ni(II) complex showing the atom-labelling scheme.