each other. Compound 1 forms a 1D ladder chain from centrosymmetric dimers that are produced by intermolecular N-H...O hydrogen bonds. The $^1$H NMR and $^{13}$C NMR spectra show 3(J(L,F)) and 3(J(C,F)). The $^{15}$C NMR spectrum of compound 1, containing six-membered ring diamine group, shows that $^3$J(P,C$_{pyran}$) $>$ $^3$J(P,C$_{pentane}$).

Synthesis, spectroscopic characterization and crystal structure of 3-FC$_3$H$_7$C(O)(N)(H)(P)(O)X, X=N(CH$_3$)$_2$-CH$_2$-C$_6$H$_5$
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A new phosphonic trimide compound with formula 3-FC$_3$H$_7$C(O)(N)(H)(P)(O)X, X=N(CH$_3$)$_2$-CH$_2$-C$_6$H$_5$ (I) was synthesized and characterized by $^1$H, $^1$C, $^3$P ($^1$H) NMR, IR spectroscopy, CHN elemental analysis and X-ray crystallography. In the crystal structure of I, pairs of intermolecular N$_2$(amino)$\cdots$H...O(P) hydrogen bonds form centrosymmetric dimers. These centrosymmetric dimers are connected to each other via two equal weak C-H...O hydrogen bonds to make $R_2^2$(14) rings in a linear arrangement parallel to [101]. Compound 1, containing carbon atoms with two bond distances from the phosphorus atom, display $^3$J(P, CH$_3$) $>$ $^3$J(P, CH$_2$).

Newazo-azomethine dye and its copper complex: NMR and 1D-DFT studies
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Density functional theory (DFT) has gained a great deal of popularity as a tool for quantum chemistry in the last year. This quantum mechanical approach to solving molecular structure allows the calculation of any molecular property, including geometry, stability and a whole host of spectroscopic properties such as IR/Raman, UV-vis and NMR spectra, to a high level of accuracy [1]. A large number of DFT studies have treated excited state properties based on the time-dependent (TD) propagator method. Most of these studies employ the geometric structure of the electronic ground state, yielding vertical excitation energies and oscillator strength [2]. Because of accuracy and low computational cost, a DFT/TD-DFT method has become the most widely tool for theoretically evaluating excited state energies and simulating the UV–vis spectra of organic/molecular compounds and their metal complexes in solution [3]. This study deals with the investigation of the solvatochromic properties of new azo-azomethine ligand and its copper complex by 1D-DFT HIB3LYP/6-31g(d) basis set. Also, the calculations of NMR chemical shielding for ligand were performed using GIAO/DFT and CSGT/DFT methods at the same basis set.

Reference

Theoretical study of some recently synthesized mercury complexes with a Schiff base ligand
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Metal complexes with nitrogen donor Schiff base ligands have been isolated and described in a large number of publications ranging from the purely synthetic to modern physicochemically to biochemically relevant studies of these complexes. Schiff base compounds that named after Hugo Schiff with azomethine group (RC=N) are usually formed by the condensation of a primary amine with an active carbonyl compound [5]. Schiff base ligands are chosen for their versatility in transition metal chemistry. Schiff bases are widely used as biologically active substances, liquid crystals, antioxidants, antiphlogistic, dyes, lumophores and polymer stabilizers [6]. Schiff bases can be used to obtain optical materials and conducting polymers. Synthesis of new Schiff bases and their metal complexes still the aim of many recent investigations. In this research, some new four coordinated complexes with general formula H$_2$L$_2$X$_2$ have been subjected to theoretical calculation. Molecular structures of the complexes have been optimized at the UB3LYP/LANL2MB level of theory. In final some theoretical parameters such as HF-energy, Gibbs free energy, enthalpy, selected bond distances, bond angles and torsion angles of optimized structures are presented.

Keywords: Schiff base ligand, Metal Complex, Eshentate, Spectra, Azomethine.

Reference