each other. Compound **1** forms a 1D ladder chain from centrosymmetric dimmers that are produced by intermolecular P=O…H-N hydrogen bonds. The ^{1}H NMR and ^{13}C NMR spectra show $^{3}J(H,F)$ and $^{1-3}J(C,F)$. The ^{13}C NMR spectrum of compound **1**, containing six-membered ring diamine group, shows that $^{3}J(P,C_{aliphatic}) >^{2}J(P,C_{aliphatic})$.

Synthesis, spectroscopic characterization and crystal structure of 3-$FC_6H_4C(O)N(H)P(O)X$, X=$N(CH_3)$-CH_2-C_6H_5

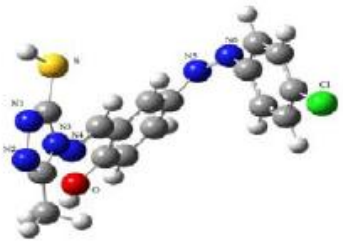
Samad ShoSghpour, Mehrdad Pourayoubi*, Mojtaba Keikha, Hassan Fadaei
Department of Chemistry, Ferdowsi University of Mashhad, P.O. Box 91779-1436, Mashhad, Iran
mehrdad_pourayoubi@yahoo.com, s.zhoghpour@gmail.com

A new phosphoric triamide compound with formula 3-$FC_6H_4C(O)N(H)P(O)X_2$, X=$N(CH_3)$-CH_2-C_6H_5 (**1**) was synthesized and characterized by ^{1}H, ^{13}C, ^{19}F, $^{31}P\{^{1}H\}$ NMR, IR spectroscopy, CHN elemental analysis and X-ray crystallography. In the crystal structure of **1**, pairs of intermolecular $N_{C(O)NHP(O)}$-H…O(P) hydrogen bonds form centrosymmetric dimers. These centrosymmetric dimmers 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 $^{2}J(P,CH_2) >^{2}J(P,CH_3)$.

Newazo-azomethine dye and its copper complex: NMR and TD-DFT studies

MaliheErfantalab, Hamid. Khanmohammadi
Faculty of science, Department of chemistry, Arak University, Arak, 38156-8-8349, Iran
h-khanmohammadi@araku.ac.ir

Density functional theory (DFT) has gained a great deal of popularity as a tool for quantum chemistry in the last years. 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/inorganic compounds and their metal complexes in solution [3]. This study deals with the investigation of the solvatochromic properties of new azo-azomethineligandand its copper complex by TD-DFT inB3LYP/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.



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Theoretical study of some recently synthesized mercury complexes with a Schiff base ligand

M. Montazerozohori*, H. Tavakol, S. A. Musavi and S. Yadegari
Department of Chemistry, Yasouj University, Yasouj, 7591874831 Iran
E-mail: mmzohori@mail.yu.ac.ir

Metal complexes with nitrogen donor Schiff base ligands have been isolated and described in a huge 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[1] with azomethine group (RC=N-) are usually formed by the condensation of a primary amine with an active carbonyl compound[2-4]. Schiff base ligands are chosen for their versatility in transition metal chemistry[5]. Schiff bases are widely used as biologically active substances, liquid crystals, antitomor, antiphlogistic, dyes, luminophores and polymer stabilizers[6-8]. Schiff bases can be used to obtain optical materials and conducting polymers[9]. 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 $HgLX_2$ have been subjected to theoretical calculation. Molecular structures of the complexes have been optimized at the UB3LYP/LANL2MBlevel of theory. In final some theoretical parameters such as HF-energy, Gibbs free energy, entalpy, selected bond distances, bond angles and torsion angles of optimized structures are presented.

Keywords: Schiff base ligand, MetalComplex, Bidentate, Spectra, Azomethine.

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