

P-711

Crystal structure, hydrogen bonds and C-X... n

(X = H, F) interactions of a new acetyl phosphorylamidate

A. Tarahhomi^{a,*}, M. Pourayoubi^a

^aDepartment of Chemistry, Ferdowsi University of Mashhad, Mashhad 91779, Iran
e-mail: tarahhomi_at@yahoo.com

Acetyl phosphorylamidates, with the general formula $R^1C(O)NHP(O)R_2$ have been attracted attention due to containing nitrogen-carbonyl and nitrogen-phosphoryl moieties, and special properties resulting from them such as acting as O,O-donor ligands and inhibitory of urease and acetylcholinesterase enzymes. The new compound N-(4-fluorobenzoyl)-N',N''-bis(4-methyl-phenyl) phosphoric triamide was synthesized and characterized by 1H , ^{13}C , $^{31}P\{^1H\}$ -NMR and IR spectroscopies and single crystal X-ray determination. The phosphorus atom has a distorted tetrahedral configuration and the phosphoryl and carbonyl groups are *anti* to each other. Important HBs of this compound is respectively involve the oxygen atoms of P=O and C=O in hydrogen bonding interaction with the $H-N_{C(O)NHP(O)}$ and $H-N_{amide}$ units. Another interesting feature of this structure is the existence of C-X...n (X = H, F) interactions [C(17)-H(17A)...C(20) & C(7)-H(7A)...C(19) and C(5)-F(1)...C(8)]. These non-covalent interactions and additional C(20)-H(20A)...F(1) are extended hydrogen-bonded chains in a 2-D array.

Keywords: Phosphoric triamide, NMR, X-ray crystallography, Hydrogen bonds, C-X...n interactions.

P-712

Synthesis and Characterization of a Fe(III) complex of 1,10-phenanthroline derivatives in two steps; A Raman Studies

S. Tarighi^a, A. Abbasi^{a*}

^aSchool of Chemistry, College of Science, University of Tehran, Tehran, Iran
(e-mail: aabbasi@khayam.ut.ac.ir)

1,10-Phenanthroline-5,6-dione (phendione) is a versatile molecule with applications in inorganic and biological chemistry, and in the synthesis of materials showing interesting properties. A number of researchers have investigated transition metal complexes of phendione because of its application to supramolecular materials with desirable photophysical or magnetic properties. In this work, Synthesis of $[Fe(C_{12}H_8N_2)_2(N,N'-C_{12}H_8N_2O_2)](CF_3SO_3)_3$ is presented in two steps. $[Fe(C_{12}H_8N_2)_2Cl_2]Cl$ was prepared in the first step from an ethanolic solution 1,10-phenanthroline and $FeCl_3 \cdot 6H_2O$. In the second step, substitution of two coordinated chlorine by phendione molecule was done through adding a stoichiometric amount of Ag(trifluoromethanesulfonate) aqueous solution. The Raman spectra was recorded via a Micro-Raman instrument (Renishaw 1000) equipped with several lenses of different magnifying power. Both complexes shows the metal-ligand stretching bands in Raman spectra (Fe-N and Fe-Cl bands at 342 and 379 cm^{-1} , respectively), and also the aromatic part vibrations. A Comparison in the spectra of the two complexes strongly confirms the substitution of the phendione group. Disappearing of the peak related to Fe-Cl bond in the Raman spectra and appearing a sharp peak at 1700 cm^{-1} related to the carbonyl group is in consistent with this claim. The title compound was also characterized by IR, NMR, UV-VIS and Elemental analysis.

Keywords: 1,10-phenanthroline-5,6-dione, Fe(III), complex, Raman spectroscopy