

acid (hypydcH<sub>2</sub>) and acridine (acr). The compound, (acrH)[Zn(hypydc)<sub>2</sub>].10H<sub>2</sub>O, was characterized by elemental analysis, <sup>1</sup>H NMR, <sup>13</sup>C NMR, IR spectroscopy, single crystal X-ray diffraction method. Zn(II) compound crystallized in monoclinic system with 8 molecules per unit cell. The crystallographic analysis revealed that the complex consist of [Zn(hypydc)<sub>2</sub>]<sup>2-</sup> anion, two acrH<sup>+</sup> cations and ten uncoordinated water molecules. Zn(II) atoms in the complex, is coordinated in a distorted octahedral geometry by two nitrogen and four oxygen atoms of 4-hydroxypyridinedicarboxylate ligand. Acridine is known as proton acceptor ligand. In the crystal structures of the complex extensive O–H...O, N–H...O and C–H...O hydrogen bonds as well as electrostatic forces, C–O...π and π–π stacking play important roles in stabilizing structures.

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### Effects of substituents on the conformational diversity of the new *N*-phosphinylureas

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*N*-phosphoniylureas are some important instances of phosphoramidates that little attention has been given to their biological properties [1] and structural studies [2]. These compounds can cause attractive biological activities due to having urea and peptide moieties. Recently, we evaluated anticancer [3] and antibacterial [4] properties of some of these compounds. Further, in our previous studies, we were synthesized and characterized two novel *N*-phosphinylureas with general formula RC<sub>6</sub>H<sub>4</sub>NHC(O)NHP(O)NHCH<sub>2</sub>C(CH<sub>3</sub>)<sub>2</sub>CH<sub>2</sub>NH [4]. The crystal structures of compounds containing (R = H (**1**), NO<sub>2</sub> (**2**)) are composed of two and one conformers, respectively. These molecules showed *anti* and *syn* conformations with respect to the C=O and P=O bonds for (**1**) and (**2**). In order to further investigate, quantum chemical calculations were applied. The results predict a structure with *anti* conformation as the most stable form for **2** due to the packing effect.

In connection with our current work in the field of *N*-phosphinyl ureas chemistry and investigate of effect of substituent, here we synthesized and characterized two novel derivatives with R = CH<sub>3</sub> (**3**) and F (**4**). The 3D structures of these molecules have been determined by X-ray crystallography. The title molecules contain four and two conformers in crystalline lattice, respectively. In molecule **3**, four types of hydrogen bond are established among these conformers, intramolecular P=O...H-NPh, intermolecular C=O...NHP, C=O...NH and P=O...NH hydrogen bonds. These conformers create two types of chains with different arrangements in the crystal lattice of **3**. Linking of these chains by hydrogen bonding leads to form a two-dimensional polymeric chain in the crystal lattice. In molecule **4**, intramolecular P=O...H-NPh, intermolecular C=O...NHP, P=O...NH hydrogen bonds cause to form a two-dimensional polymeric chain. It is noteworthy; the new *N*-phosphinylureas crystallize in the triclinic and monoclinic crystal systems with space groups *P*1̄ and *P*2<sub>1</sub>/*c*, respectively. The symmetry of the unit cell decreases with increase in the multiplicity of conformers that demonstrate our previous study [5]. The mean P=O

distances fall in the range 1.4803-1.4845Å that are slightly longer than the normal P=O bond length (1.45Å). The phosphoryl oxygen atoms (O(2), O(22), O(23), O(24), O(1) and O(1A)) occupy a pseudoaxial position, and the 4-methyl and 4-fluorophenylureido groups adopt a pseudoequatorial orientation.

In all of the compounds, the P-N<sub>amide</sub> bond length is longer than the P-N<sub>amine</sub> bond lengths. All of these bonds are in the range 1.608 (2) - 1.698(18) Å and thus are significantly shorter than a typical P-N single bond (1.77 Å). The phosphorus atoms have slightly distorted tetrahedral configuration.

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### Structural characterization of Mo<sub>3</sub>Fe(NO)S<sub>4</sub> Cubane-type clusters with different electron populations

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Molecule Nitric Oxide plays an important role in biological systems. [1] Many of the important biological functions of NO are iron-mediated, being the synthesis and characterization of new iron nitrosyl complexes a priority target for the understanding of its biological functions. [2] Cubane-type clusters [Mo<sub>3</sub>(FeNO)S<sub>4</sub>(dmpe)<sub>3</sub>Cl<sub>3</sub>]<sup>0/+</sup> (dmpe = 1,2-bis(dimethylphosphine-ethane)) have been isolated (see figure 1). Here we analyze the influence of the different electron population on the molecular structure. A detailed spectroscopic study (NMR, magnetic susceptibility, EPR and IR) is presented to evaluate the effect derived from the non-innocent behaviour of the nitrosyl ligand attached to iron atom on the molecular structure of these clusters.

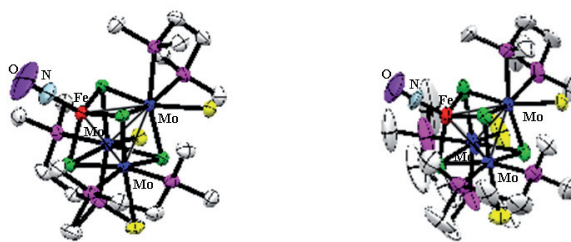


Figure 1: Molecular structure of the molybdenum iron nitrosyl cubane-type clusters [Mo<sub>3</sub>(FeNO)S<sub>4</sub>(dmpe)<sub>3</sub>Cl<sub>3</sub>] (left) and [Mo<sub>3</sub>(FeNO)S<sub>4</sub>(dmpe)<sub>3</sub>Cl<sub>3</sub>]<sup>+</sup> (right)

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