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Crystal Structure of Two Biologically Active Biphenyl Derivatives. Nancy Naguib[a], Ibrahim Farag [b], Zein K. Heiba[a], Karimat El-Sayed[a]. [a]*Physics Department, Faculty of Science, Ain Shams University, Cairo, Egypt*. [b]*National Research Center, Cairo, Egypt.*
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The structure of two biphenyl derivatives was investigated by X- ray single crystal diffraction technique. The first compound is 6-(2-biphenyl-4-ylethyl)-4,5-dihydropyridazin -3(2H)-one, $C_{18}H_{18}N_2O$, with molecular weight: 278.355 , monoclinic, $P2_1/c$, a=7.2564 (3)Å, b=8.8986 (3)Å, c=23.2598 (11)Å, β = 100.00(18)°,V = 1471.00(11)Å^3, Z = 4,Dcal = 1.523Mgm^{-3}, μ = 0.08 mm^{-1}, with 1022 observed reflections (R (int) = 0.032), λ (MoK_α) = 0.71073Å, final R and wR are 0.044 and 0.081, respectively. While the other compound is (5Z)-6-biphenyl-4-yl-4-oxohex-5-enoic acid, $C_{18}H_{16}O_3$,with molecular weight: 280.323, monoclinic, $P2_1/c$, a=15.2407 (13)Å, b=7.9037 (6)Å, c=12.9131 (8)Å, β = 110.116 (3)°, V = 1460.6 (2)Å^3, Z = 4,Dcal = 1.275Mgm^{-3}, μ = 0.09 mm-1, with 882 observed reflections (R(int) = 0.049), λ (MoK_α) = 0.71073Å, final R1 and wR2 are 0.058 and 0.115, respectively. There are four crystallographically independent molecules in the asymmetric unit of the two compounds. The molecules are stabilized by C-H…N, C-H…O and C-H…N types of intermolecular hydrogen bonds in the unit cell in addition to van der Waals forces.

Key words: **crystal structure; conformation; COX**

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Molecular and Crystalline Structure of Two New Nitrogen-Sulphur Pro-Ligands from Single Crystal Diffraction Data and Solid-State DFTB Calculations. Edward E. Ávila[a], Asiloé J. Mora[a], Gerzon E. Delgado[a], Ricardo R. Contreras[a], William Mendéz[a], Alexander Briceño[b]. [a]*Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, Mérida, Venezuela.* [b]*Instituto Venezolano de Investigaciones Científicas, Centro de Química, Altos de Pipe, Venezuela.*
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The complexity of problems dealt by bioinorganic chemistry begins with the development of model compounds of low molecular weight. These models mimic the properties of active metal sites in metabiomolecules of interest, which allow the understanding of the role played by metal ions in biological processes. In particular, efforts [1] have been made to reproduce the pseudo-tetrahedrical coordination spheres of metal ions linked with pro-ligands containing two nitrogen atoms and two sulphur atoms as donor groups, since Nature has used this type of surroundings in the coordination of metal ions such as, for example, Cu(II) in plastocyanin or azurin [2]. Contreras *et al*., [3-4] have recently designed and synthesized a series of bidentated nitrogen-sulfur pro-ligands shown in Fig. 1. These compounds have been made available as single crystals.

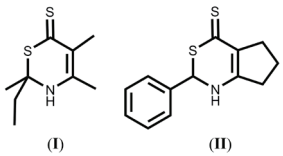

Figure 1

Diffraction data for the compounds: 2-ethyl-2,4,5-trimethyl-2H-1,3-thiazine-6(3H)-thione (**I**) and 2-phenyl-1,2,6,7-tetra hydrocyclopenta[d][1,3]thiazine-4(5H)-thione (**II**) were collected on a Rigaku AFC7S diffractometer using the programs *CrystalClear* [5] for the data collection and cell refinement, *CrystalStructure* [6] for the data reduction, and *SHELX97* [7] for the structure solution and refinement. The solution of their crystal structures found 1 fragment (12 non-hydrogen atoms) for compound (**I**) and 2 fragments (32 non-hydrogen atoms) for compound (**II**). The molecular packings consist of zig-zag chains with hydrogen bonds of the type N-H···S with gaph symbols $[C(6)]_S$ for (**I**), $[C^2_2(12)]_{S1}$ and $[C^2_2(12)]_{S3}$ for (**II**). Finally, the molecular structures obtained by X-ray single diffraction are compared with the ones optimized by solid state DFTB calculations [8].

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Keywords: bioinorganic compounds; solid-state DFTB calculations

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A Thermodynamic Comparison of Hydrophobic vs. Hydrophilic Ligand-Protein Interactions. Caitriona Dennis[a], Neil Syme[a], Agnieszka Bronowska[a], Steve Homans[a]. [a]*Institute of Molecular and Cellular Biology, University of Leeds, Leeds LS2 9JT, U.K.*
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Highly specific molecular recognition is the driving force behind every biological process. Carefully tuned affinities govern the intricate recognition event but despite the universal nature of these interactions, our understanding of their molecular basis is limited. This limited knowledge, in turn, compromises the structure-based drug design of small molecules that modulate these interactions. The limited ability to predict ligand affinity is largely due to the complexity of all the contributions from the ligand, the protein and solvent rearrangement. In order to gain a better understanding of ligand binding, the global thermodynamics of ligand binding within two classical systems has been