Poster

Crystal structure of a copper(I) complex with the Schiff base of 2-(diphenylphosphino)benzaldehyde and aminoguanidine

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The refluxing ethanolic solution of 2-(diphenylphosphino)benzaldehyde and aminoguanidine in the molar ratio 1:1 gave pale yellow single crystals of the Schiff base derivative, (HL)Cl. The composition and purity of the Schiff base were confirmed by the IR and NMR spectra and elemental analysis, while its structure was proved by SC-XRD. Fig. 1. shows the molecular and crystal structure of the obtained Schiff base. *Crystallographic data:* monoclinic crystal system, $P2_1/c$, a = 13.4402(4), b = 15.2095(3), c = 10.8606(3) Å, β = 113.794(3)°, V = 2031.40(10) Å^3, Z = 9. Refinement based on F^2 (252 parameters): R_1 = 0.0457, wR_2 = 0.0998, S = 1.034, for all data, and R_1 = 0.0353 for 4144 reflections with $I \geq 2\sigma(I)$.

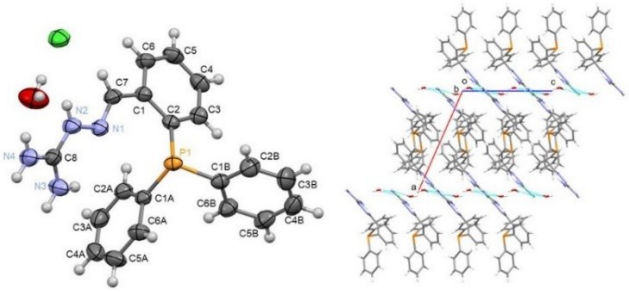

Figure 1. The molecular (left) and crystal structure along the *b*-axis of the Schiff base (right).

The coordination properties of this Schiff base were examined by the reaction with different metal salts. In the reaction of the methanolic solution of the obtained ligand and copper(II)-bromide, yellow single crystals of the copper(I) complex of the formula [{Cu(HL)(μ-Br/Cl)Br}$_2$] (Fig. 2) were obtained. The aminoguanidine residue is not coordinated, and the Schiff base in its monoprotonated form acts as a monodentate P-donor ligand. Both chloride and bromide ions present lead to a substitutional disorder. Namely, two copper(I) centers are bridged through two halide anions, while an additional bromide ligand is coordinated to both metal centers, which makes copper(I) situated in tetrahedral surroundings (τ_4 = 0.83) [1]. *Crystallographic data:* triclinic crystal system, $P\bar{1}$, a = 8.5408(3), b = 9.8790(3), c = 13.1853(4) Å, α = 94.725(2), β = 107.616(3), γ = 100.599(2)°, V = 1030.87(5) Å^3, Z = 2. Refinement
based on F^2 (253 parameters): R_1 = 0.0630, wR_2 = 0.2323, S = 0.992, for all data, and R_1 = 0.0532 for 4899 reflections with $I \geq 2\sigma(I)$.

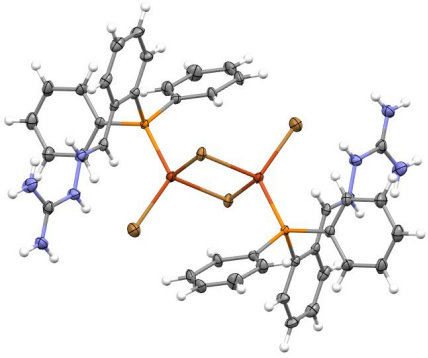

Figure 2. The molecular structure of the complex [{Cu(HL)(μ-Br/Cl)Br}$_2$].

[1] Yang, L., Powell, D. R. & Houser, R. P. (2007). *Dalton Trans.* (9), 955.

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