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ABSTRACT BOOK

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Single crystal structure of *bis*(2-methyl-*N*-(diethylcarbamothioyl) benzamido)copper(II) complex

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Bis(2-methyl-*N*-(diethylcarbamothioyl)benzamido)copper(II) complex has been synthesized and characterized by elemental analyses, FT-IR and NMR methods [1,2]. The obtained metal complex was also characterized by a single crystal X-ray diffraction study. Molecule formula of the title compound, $C_{26}H_{34}CuN_4O_2S_2$: monoclinic, space group $P2_1/c$ (no. 14), a = 11.7617(14) Å, b = 9.1338(11) Å, c = 26.558(3) Å, β = 109.822(5)°, V = 2684.1(5) Å^3, Z = 4, μ(MoKα) = 1.000 mm^{-1}, *Dcalc* = 1.391 g/mm^3, 22933 reflections measured ($3.68 \leq 2\Theta \leq 55.76$), 6392 unique ($R_{int}$ = 0.0400, R_{sigma} = 0.0415) which were used in all calculations. The final R_1 was 0.0447 (>2sigma(I)) and wR_2 was 0.1168 (all data). In this compound, the copper atom is coordinated by two sulphur and two oxygen atoms from two 2-methyl-*N*-(diethylcarbamothioyl)benzamide molecules forming an distorted square-planar geometry (S(1)-Cu-O(1) 94.59(6)°, O(2)-Cu-S(2) 93.84(6)°). The dihedral angle between the S(1)-Cu-O(1) and S(2)-Cu-O(2) planes of 19.91° confirms distortion from square planar towards tetrahedral geometry.

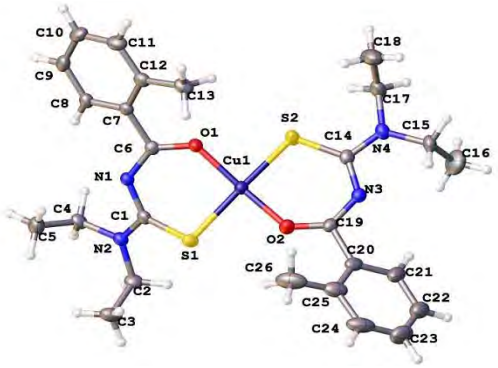

Figure 1. Molecular structure of title compound.

***Keywords*:** Copper complex, Thiourea, Benzoyl thiourea X-ray single crystal diffraction, Synthesis.

[1] G. Kavak, S. Ozbey, G. Binzet, N. Kulcu, *Turk. J. Chem.* **2009**, *33(6)*, 857-868.
[2] G. Binzet, U. Flörke, N. Külcü, H. Arslan, *Eur. J. Chem.* **2012**, *3(1)*, 37-39.