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BOOK OF ABSTRACTS

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Synthesis, characterization, crystal structure and antimicrobial activity of *bis*[4-bromo-*N*-(diethylcarbamothioyl)benzamide- κ^2 O,S]palladium(II)

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Bis[4-bromo-*N*-(diethylcarbamothioyl)benzamide- κ^2 O,S]palladium(II) was synthesized and characterized by elemental analyses, FT-IR and NMR techniques. The obtained metal complex was also characterized by single crystal X-ray diffraction study. Crystal data of palladium complex, C₁₂H₁₄BrN₂OPd_{0.5}S (*M* = 367.42 g/mol): Tetragonal, space group I4₁/a (no. 88), *a* = 9.9930(4) Å, *c* = 57.483(3) Å, *V* = 5740.3(4) Å³, *Z* = 16, *D*_{calc} = 1.701 g/cm³, 17151 reflections measured (4.14° ≤ 2θ ≤ 55.5°), 3388 unique (*R*_{int} = 0.0331, *R*_{sigma} = 0.0306) which were used in all calculations. The final *R*₁ was 0.0382 (*I* > 2σ(*I*)) and *wR*₂ was 0.0960 (all data). A tetrahedron coordination geometry is formed around the Pd atom by two S atoms and two O atoms of 4-bromo-*N*-(diethylcarbamothioyl)benzamide ligand. The bond distance Pd1-O1 and Pd1-S1 are 2.029(2) and 2.2420(10) Å, and bond angles O1-Pd1-S1 and O1-Pd1-O1 are 93.81(7)° and 85.28(13)°, respectively.

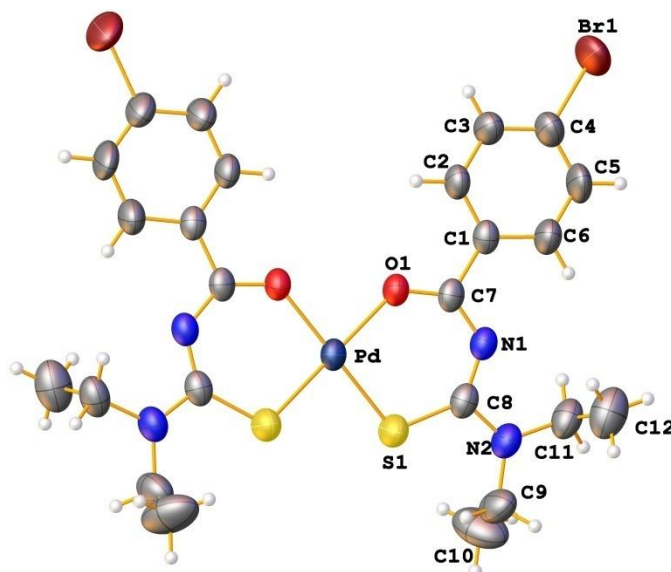


Figure 1. Molecular structure of title compound.

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

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Reference

[1] Solmaz, U. *Synthesis and characterization of palladium complexes of thiourea derivatives*, MSc. Thesis, Mersin University, Mersin, Turkey, 2014.