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ABSTRACT BOOK

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Synthesis, characterization and crystal structure of *trans*-dichloro bis[4-chloro-*N*-(dibutylcarbamothioyl) benzamido- κ S]palladium(II)

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Trans-[PdCl₂(HL-S)₂] (HL=*N,N*-di-*n*-butyl-*N'*-4-chloro benzoylthiourea) complex was formed from the reaction between PdCl₂ and *N,N*-di-*n*-butyl-*N'*-4-chloro benzoylthiourea in acetonitrile. Pd(II) complex has been characterized by spectral (FT-IR, ¹H NMR and ¹³C NMR, LC-MS/MS) techniques. The molecular structure of the title complex has been confirmed by X-ray crystallography. Molecule formula of the title compound, C₃₂H₄₆Cl₄N₄O₂PdS₂: monoclinic, space group C2/c (no. 15), *a* = 12.282(5) Å, *b* = 18.682(5) Å, *c* = 16.893(5) Å, β = 97.604(5)°, *V* = 3842(2) Å³, *Z* = 4, μ (MoK α) = 0.903 mm⁻¹, *D*_{calc} = 1.437 g/mm³, 29360 reflections measured (4 ≤ 2 θ ≤ 66.62), 7356 unique (*R*_{int} = 0.0233) which were used in all calculations. The final *R*₁ was 0.0443 (>2 σ (*I*)) and *wR*₂ was 0.0993 (all data). Title compound shows the palladium ion is four-coordinated by two S and two Cl atoms. The palladium atom in *trans*-[PdCl₂(HL-S)₂] is located on a center of inversion so that the *trans*-Cl₂S₂ donor set is planar. The observed molecular conformation is stabilized by an intramolecular N-H...Cl interaction [1].

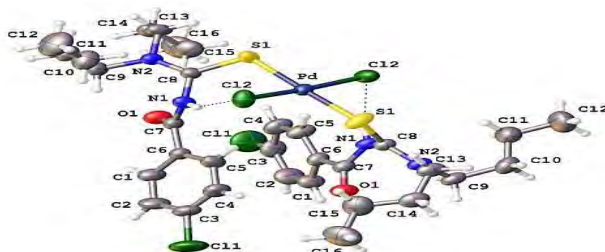


Figure 1. Molecular structure of title compound.

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

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