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ABSTRACT BOOK

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Synthesis, characterization and crystal structure of *cis-bis*[4-chloro-*N*-(dibutylcarbamothioyl) benzamido- κ^2 O,S]palladium(II)

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cis-Bis[4-chloro-*N*-(dibutylcarbamothioyl)benzamido- κ^2 O,S]palladium(II) has been synthesized and characterized by elemental analyses, FT-IR and NMR methods [1]. The obtained metal complex was also characterized by a single crystal X-ray diffraction study. Molecule formula of the title compound, C₆₄H₈₈O₄S₄Cl₄Pd₂N₈: orthorhombic, space group P2₁2₁2₁ (no. 19), $a = 8.5141(9)$ Å, $b = 16.5890(17)$ Å, $c = 51.924(6)$ Å, $V = 7333.8(13)$ Å³, $Z = 4$, $\mu(\text{MoK}\alpha) = 0.798$ mm⁻¹, $D_{\text{calc}} = 1.373$ g/mm³, 26461 reflections measured ($2.578 \leq 2\theta \leq 66.352$), 13708 unique ($R_{\text{int}} = 0.0755$) which were used in all calculations. The final R_1 was 0.0604 ($I > 2\sigma(I)$) and wR_2 was 0.1350 (all data). Title compound shows the palladium ion is four-coordinated by two O and two S atoms (S(1)-Pd-O(2) 179.1(3)°, O(1)-Pd-S(2) 178.7(2)°). In the title complex, the Pd atom has a *cis*-square-planar geometry defined by two 4-chloro-*N*-(dibutylcarbamothioyl)benzamide ligands (The dihedral angle between the S(1)PdO(1) and S(2)PdO(2) planes: 0.08(1)°).

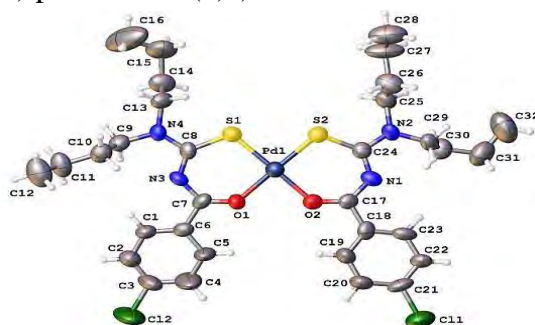


Figure 1. Molecular structure of title compound.

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**.