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CHEMISTRY
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APRIL 22-25, 2015

V. ULUSAL
**ANORGANİK
KİMYA
KONGRESİ**
ÖZET KİTABI
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Synthesis, Characterization and Crystal Structure of Dichloro bis[4-flouro-*N*-(diethylcarbamothioyl)benzamide- κ S] palladium(II)

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Cis-dichloro bis[4-flouro-*N*-(diethylcarbamothioyl)benzamide- κ S] palladium(II), *cis*-[PdCl₂(HL-S)₂], 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 (Figure 1). Molecule formula of the title compound, C₉₆H₁₁₂C₁₈F₈N₁₆O₈Pd₈S₈; Monoclinic, Space group C2/c (no. 15), *a* = 10.8397(3) Å, *b* = 21.5837(5) Å, *c* = 13.3820(3) Å, β = 107.6313(12)°, *V* = 2983.79(13) Å³, *Z* = 1, *D*_{calc} = 1.7593 g/cm³, 24642 reflections measured (3.78° ≤ 2 θ ≤ 69.68°), 6471 unique (*R*_{int} = 0.0248, *R*_{sigma} = 0.0237) which were used in all calculations. The final *R*₁ was 0.1573 (*I* ≥ 2 σ (*I*)) and *wR*₂ was 0.4447 (All data). Title compound shows the palladium ion is four-coordinated by two S and two Cl atoms. The palladium atom in *cis*-[PdCl₂(HL-S)₂] is located on a center of inversion so that the *cis*-Cl₂S₂ donor set is planar. The observed molecular conformation is stabilized by an intramolecular N-H...Cl interaction.

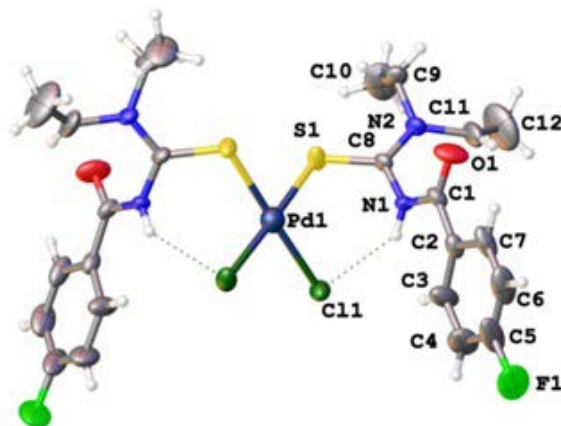


Figure 1. Molecular structure of title compound.

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

Reference

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