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ABSTRACT BOOK

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Synthesis, characterization and crystal structure of *N*-((4-chlorophenyl)carbamothioyl)pivalamide

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We report the synthesis of *N*-((4-chlorophenyl)carbamothioyl)pivalamide of an benzoylthiourea derivative formulated as $C_{12}H_{15}ClN_2OS$. The structure of compound has been characterized by single-crystal X-ray diffraction analysis. It crystallizes in the triclinic, space group P-1 (no. 2), with unit cell dimensions of a = 5.8690(19) Å, b = 11.110(4) Å, c =20.564(7) Å, α =89.551(5)°, β =88.197(5)°, γ =80.962(5)°, V = 1323.6(7) Å^3, Z = 4, μ(MoKα) = 0.432 mm^{-1}, *Dcalc* = 1.359 g/mm^3, 26983 reflections measured ($3.72 \leq 2\Theta \leq 61.24$), 8047 unique ($R_{int}$ = 0.0472) which were used in all calculations. The final R_1 was 0.0420 (>2sigma(I)) and wR_2 was 0.1088 (all data). The bond lengths and angles in the thiourea moiety are typical for thiourea derivatives; the C2-S1 and C1-O1 bonds both show a typical double-bond character with 1.6675(16) and 1.220(2) Å, respectively. Similar shortening for the C-N bonds C1-N2 1.384(2) Å, C2-N2 1.3904(19) Å, C2-N1 1.333(2) Å, and C7-N1 1.4311(19) Å also indicates a partial double-bond character. The intramolecular hydrogen bond N1-H1···O1 (1.972(3) Å) forms a 6-membered ring with C1, N2 and C2.

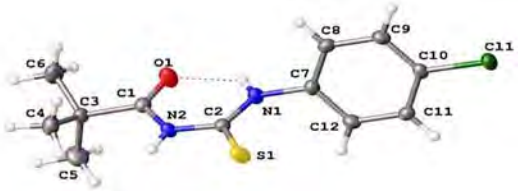

Figure 1. Molecular structure of *N*-((4-chlorophenyl)carbamothioyl)pivalamide.

***Keywords*:** Thiourea, Pivaloyl thiourea, X-ray single crystal diffraction, Synthesis, Pivalamide derivatives.

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[1] H. Gedik, *Synthesis and characterization of the various urea compounds*, MSc. Thesis, Mersin University, Mersin, Turkey, **2012**.