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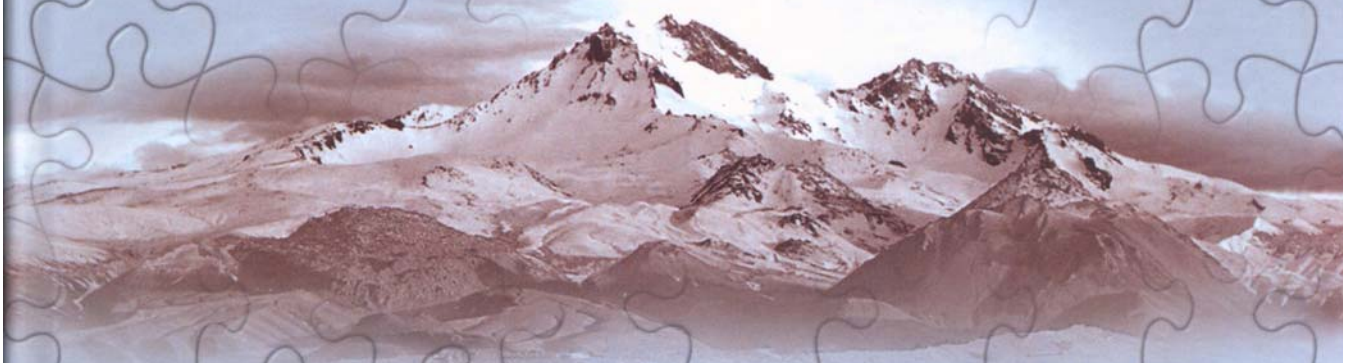

ABSTRACT BOOK

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CRYSTAL STRUCTURE OF 3-(2-CHLOROBENZOYL)-1,1-DIPHENYLTHIOUREA, $(C_2H_5)_2N(CS)(NH)(CO)(C_6H_4Cl)$

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Some thiourea derivatives are selective analytical reagents, espctially for the determination of trasitions metals in complex interfering matrices [1]. In this study 3-(2-chlorobenzoyl)-1,1-diphenylthiourea is synthesised [2,3] and the crystal structure is determined by X-ray diffraction methods.

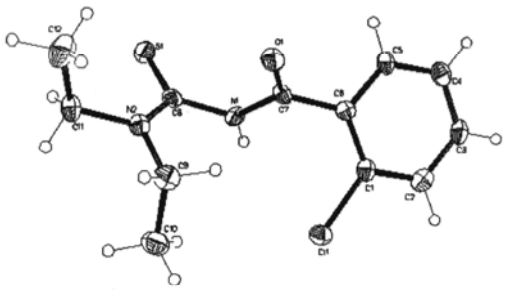

Fig 1. The molecular structure of 3-(2-Chlorobenzoyl)-1,1-Diphenylthiourea. Displacement elipsoids are drawn at the %50 probability level.

It crystallises in the space group Pbca, with a = 9.581(3) Å, b = 9.992(3) Å, c = 26.640(8) Å, $\alpha=\beta=\gamma$ = 90° and D_{cal}=1.410 Mg/m^3 for Z=8. The bond lenghts and angles in the thiourea moiety are typical for thiourea derivatives; S-C and C-O bonds both show typical double-bound character. However, the C-N bond lenghts are shorter than the normal C-N single bound lenght of about 1,48 Å.

Table 1. Selected bond lenghts and angles.

Bond Lenghts (Å)		Bond Angles (°)	
S(1)-C(8)	1.650(5)	N(1)-C(8)-S(1)	119.2(3)
C(7)-O(1)	1.213(5)	N(2)-C(8)-N(1)	115.2(4)
N(1)-C(7)	1.350(5)	O(1)-C(7)-N(1)	121.2(4)
N(1)-C(8)	1.415(5)	C(7)-N(1)-C(8)	122.3(4)
C(8)-N(2)	1.322(5)	C(1)-C(6)-C(7)	124.5(4)

References:

[1] Emen. F.M., Arslan, H., Külcü, N., Flörke, U. And Duran N. Sythesis, charachterization and antimicrobial activities od some metal complexes with N'-(2-chlorobenzoylthiourea ligands: Chrystal structure of *fac*-[CoL_3] and cis-[PdL_2], *Pol J Chem*, 79(10), 1615-1626 (2005).

[2] G. Binzet, H. Arslan, U. Flörke, N. Külcü and Nizam Duran, Synthesis, characterization and antimicrobial activities of transition metal complexes of N,N-dialkyl-N0-(2-chlorobenzoyl)thiourea derivatives, J. of Coordination Chemistry, (2006) baskıda.