2ND TURKISH CRYSTALLOGRAPHIC MEETING

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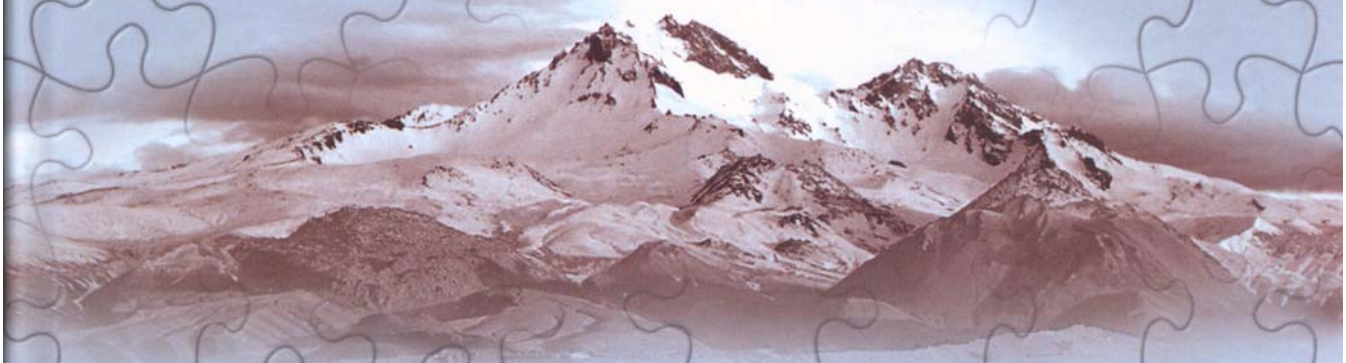
Erciyes University,
Faculty of Arts and Sciences, Department of Physics
KAYSERI, TURKEY



ABSTRACT BOOK

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N,N-DIMETHYL-N'-(2-CHLOROBENZOYL)THIOUREA

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Benzoylthiourea ligands containing S and N as donor atoms are know to possess antibacterial activities. These ligands are also used as gravimetric reagents for the estimation of semi-noble metals such as Cu, Co,Ni, Pd, [1].

The title compound is another example of our newly synthesised thiourea derivatives [2-3]. The bond lenghts and angles in the thiourea moiety are typical for thiourea derivatives; the S(1)-C(8)=1.669(3) Å and C(7)-O(1)= 1.199(3) bonds both show typical double- bound character. However, the C-N bond lenghts N(1)-C(7)= 1.383(3), N(1)-C(8)= 1.398(3) and C(8)-N(2)= 1.314(3) are shorter than the normal C-N single bound lenght of about 1,48 Å . The shortening of these C-N boundts reveals the effects of rezonance in this part of the molecule. All other bond lenghts fall within the expected ranges; the teminal C(1)-Cl(1) bond lenght 1.716(3) Å.

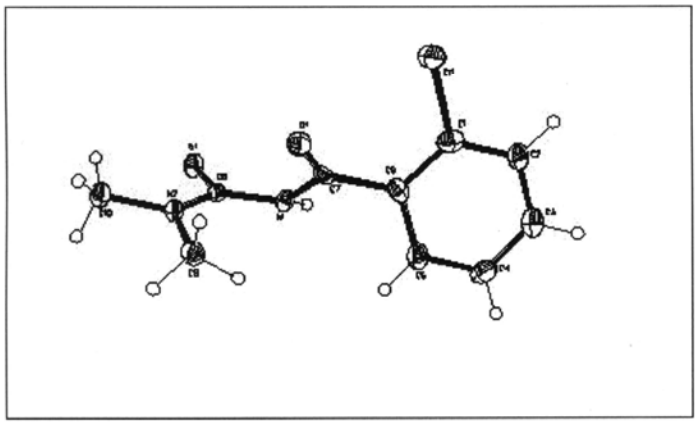

Fig 1. The molecular structure of *N,N*-Dimethyl-*N'*-(2-Chlorobenzoyl)Thiourea. Displacement elipsoids are drawn at the %50 probability

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] Fatih Mehmet Emen, Ulrich Flörke, Nevzat Külcü and Hakan Arslan, cisBis(N,N-Dimethyl-N'-(2-chlorobenzoyl)thioureato]nickel(II), Acta Cryst. (2003) E59, m582-m583.

[3] G. Binzet, U. Flörke, N. Külcü and H. Arslan, Crystal structure of 3-(2-chlorobenzoyl) 1,1-diphenyl-thiourea., Z. Kristallogr. NCS 219 (2004) 395-397.