Turkish Journal of Chemistry

Turkish Journal

of

Chemistry

Synthesis and single crystal structure analysis of three novel benzoylthiourea derivatives

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Abstract: N,N-dimethyl-N' -(2-methylbenzoyl)thiourea, $C_{11}H_{14}N_2SO$ (HL^1), N,N-dibutyl-N' -(2-methylben\-zoyl)thiourea, C{17}H{26}N2SO (HL^2), and N,N-dihexyl-N' -(2-methylbenzoyl) thiourea, C{21}H{34}N2SO (HL^3) were synthesized and characterized by elemental analysis, spectroscopic methods (FT-IR, NMR), and single crystal X-ray diffraction. Compound HL^1 crystallizes in the monoclinic system, space group P21/c, Z = 4. Compound HL^3 also crystallizes in the monoclinic system, space group P21/n, Z = 8 with 2 independent molecules in the asymmetric unit. Compound HL^2 crystallizes in the orthorhombic system, space group Pcnn, Z = 8. In all compounds, molecules form dimers through the strong intermolecular N-H...S hydrogen bonds. Moreover, there are different types of intra- and inter-molecular interactions in the crystal structures, and so the molecules of the 3 compounds also pack differently.

Key Words: Thiourea derivatives, benzoylthioureas, single crystal X-ray structures.

Turk. J. Chem., **33**, (2009), 857-868.
Full text: pdf
Other articles published in the same issue: Turk. J. Chem.,vol.33,iss.6.