



Synthesis, Characterization And Crystal Structures of Two N-(Arylsulfonyl)-Arylamides

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ABSTRACT

Two N-(arylsulfonyl)-arylamides, namely N-(4-methylphenylsulfonyl)-3-methylbenzamide(**1**) and N-(2-methylphenylsulfonyl)-2-chlorobenzamide(**2**), are synthesized by the reaction of the 4-methylbenzenesulfonamide/2-methylbenzenesulfonamide, 3-methylbenzoic acid / 2-chlorobenzoic acid and phosphorous oxy chloride. The synthesized compounds are characterized by IR, LCMS, ¹H-NMR and ¹³C-NMR studies. The structures are further confirmed by determining their single crystal XRD data. Compound **1** crystallizes in the monoclinic space group P2₁/c, with a = 9.895(3) Å, b = 11.022(4) Å, c = 13.639(4) Å, β = 97.78(3)°, V = 1473.8(8) Å³, Z = 4, R[F² > 2σ(F²)] = 0.0810 and wR(F²) = 0.2383, while compound **2** crystallizes in tetragonal, non-centrosymmetric space group I4₁cd, with a = 20.047(1) Å, b = 20.047(1) Å, c = 14.634(1) Å, V = 5881.1(7) Å³, Z = 16, R[F² > 2σ(F²)] = 0.1046 and wR(F²) = 0.1422. The dihedral angle between the two benzene rings is 89.6(2)° in compound **1**, while that in compound **2** is 60.7(5)°. In the crystal structure of compound **1**, the crystal packing is stabilized by strong N-H...O(Sulfonyl) hydrogen bonds, forming R₂²(8) rings, and by weak C-H...π interactions, forming C(8) chains. In **2**, the crystal packing is stabilized by strong N-H...O(Carbonyl) hydrogen bonds and weak C-H...O interactions, respectively forming C(4) and zigzag C(7) chains running along [001].

Keywords: N-(Arylsulfonyl)-arylamides, Non-centrosymmetric, Hydrogen bonds, C-H...O interactions, C-H...π interactions.