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Synthesis, Spectroscopic Characterization and Crystal Structure Determination of 3-(4-Chlorophenylthio)-1,3-diphenylpropan-1-one

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The conjugate addition of thiols to α,β unsaturated carbonyl compounds leading to the formation of C–S bonds is a key reaction in the synthesis of organosulfur compounds as well as in biosynthesis. Organosulfur compounds have multiple applications in bioorganic chemistry and medicinal areas such as antibiotic, antimicrobial, anti-inflammatory, antitumor, and anti-HIV activities [1,2]. The title compound (Fig. 1) was prepared from the reaction of chalcone with 4-chlorobenzenethiol in the presence of lithium fluoride as nano-catalyst. This thiocarbonyl compound was characterized by elemental analysis, IR, UV-Vis, ^{1}HNMR, ^{13}CNMR and single-crystal X-ray determination. The title compound crystallizes in the space group $P2_1/c$, monoclinic, from $CH_3OH/CHCl_3$, a = 19.638(3) Å, b = 5.3734(11) Å, c = 16.647(4) Å, V = 1702.0(6) Å^3, β = 104.336(19)^o, ρ = 1.377 g/cm^3, Z = 4, μ = 0.35 mm^{-1}, F(000) = 736, R_1 = 0.034, wR_2 = 0.053, GOF = 0.778, largest residual electron density peak/hole in the final difference map: 0.24 / -0.23 e Å^{-3}. In general, all bond distances for the title compound are within the values characteristic according the atom involved, bond distances selected are: C(1)–C(2) 1.527(2), C(2)–C(3) 1.509(3), C(1)–C(10) 1.506(3), C(3)–C(4) 1.490(3), C(1)–S(1) 1.834(2), C(3)–O(1) 1.213(2) and C(16)–S(1) 1.772(2) Å. The asymmetric C atom has a slightly distorted tetrahedral configuration with the bond angles in the range of 106.75(13)^o [S(1)–C(1)–C(2)] to 113.32 (17)^o [C(2)–C(1)–C(10)].

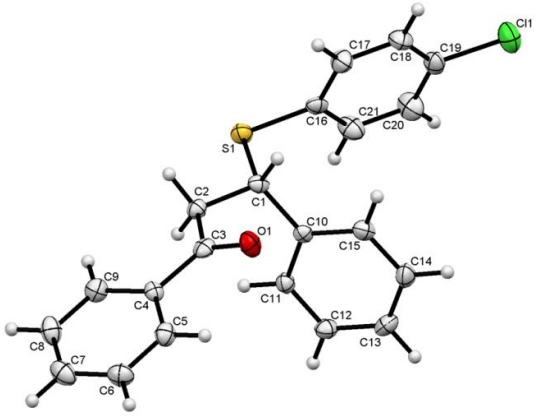

Fig. 1.

References:
[1] M. K. Chaudhuri, S. Hussain, *J. Mol. Catal. A: Chem.* 269 (**2007**) 214.

[2] Z. Xia, X. Lv, W. Wang, X. Wang, *Tetrahedron Lett*. 52 (**2011**) 4906.