Synthesis, Spectroscopic Characterization and Crystal Structure Determination of 3-(*p*-Tolylthio)-3-(4-nitrophenyl)-1-phenylpropan-1-one

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Addition reactions of thiols to α,β-unsaturated carbonyl compounds have received much interest because a number of their derivatives occur in nature and possess a variety of biological activities. [1,2] The title compound (Fig. 1) was prepared from the reaction of *p*-nitrochalcone with *p*-methylthiophenol in the presence of lithium fluoride as nano-catalyst. This β-aryl-β-mercapto ketones characterized by IR, ^{1}HNMR, ^{13}CNMR, elemental analysis, mass spectrometry and single-crystal X-ray determination. The title compound crystallizes in the space group $P2_1/c$, monoclinic, from C_2H_5OH, a = 5.3754(5) Å, b = 15.1897(11) Å, c = 11.8413(9) Å, V = 949.16 (13) Å^3, β = 100.978 (9)°, ρ = 1.321 g/cm^3, Z = 2, μ = 1.70 mm^{-1}, F(000) = 396. In general, all bond distances for the title compound are within the values characteristic according the atom involved, bond distances selected are: C(3)–C(5) 1.524(11), C(5)–C(7) 1.511(11), C(3)–C(4) 1.476(13), C(1)–C(7) 1.484(10), C(3)–S 1.851(9), C(7)–O(1) 1.217(10), C(18)–S 1.771(8), C(14)–C(20) 1.503(13), C(12)–N 1.490(15), N–(O2) 1.187(14), N–(O3) 1.190(11) Å and the angles selected are: C(3)–S–C(18) 99.0(4)°, C(1)–C(7)–O(1) 119.8(7)°, O(3)–N–O(2) 124.5(12)°, O(3)–N–C(12) 118.0(11)° and O(2)–N–C(12) 117.6(9)°. The asymmetric C atom has a slightly distorted tetrahedral configuration with the bond angles in the range of 107.2(6)° [S–C(3)–C(5)] to 114.2 (7)° [C(5)–C(3)–C(4)]. Moreover, the dihedral angles between the phenyl ring relative to the methylphenyl and nitrophenyl rings are 72.05(8)° and 87.58(8)° respectively.

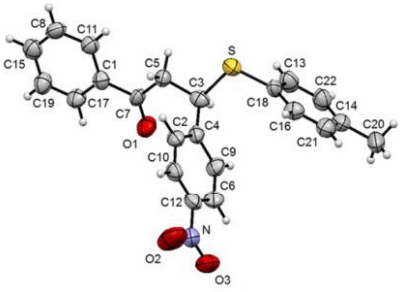

Fig. 1

References
[1] E. Fujita, Y. Nagao, Bioorg. Chem. 6 (1977) 287.
[2] A. L. Fluharty, The Chemistry of the Thiol Group; Patai, S., Ed.; Wiley Interscience: NewYork, NY, 1974.

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