Theme: Chemical Sciences

Synthesis, characterisation and crystal structure of a novel compound derived from 3-formylchromone and 3-amino-5-methylthio-1*H*-1,2,4-triazole

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Abstract

A new compound (2-hydroxyphenyl)(2-(methylthio)-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone was synthesised from 3-formylchromone and 3-amino-5-methylthio-1*H*-1,2,4-triazole. The compound structure was characterised by ^{1}H NMR, ^{13}C NMR, Mass, FTIR and X-Ray Single Crystal Diffraction studies. Yellow coloured single crystals were formed in methanol at room temperature. The crystals were monoclinic, with space group $P2_1/n$ and the unit cell dimensions were a = 7.6043(4) Å, b = 13.2004(8) Å, c = 12.9589(6) Å; α = 90°, β = 105.543(5)°, γ = 90°. From all the characterisation techniques the structure of the compound was confirmed. Further, this ligand used for the preparation of metal complexes.

***Keywords**: 3-formylchromone, 3-amino-5-methylthio-1H-1,2,4-triazole, crystal structure.*

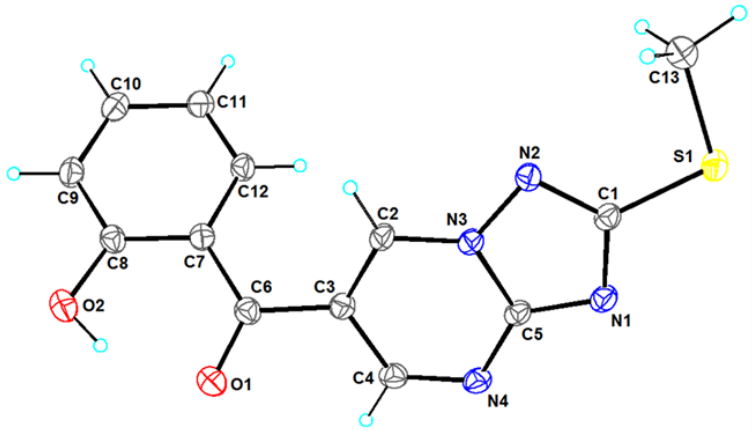

Figure 1. ORTEP representation of the compound. The thermal ellipsoids are drawn at 30% probability level