Malaysian Journal of Science **21A**: 1-5 (2002)

X-ray crystal structures of ortho isomers of chlorophenylbenzoylthiourea and nitrophenylbenzoylthiourea

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ABSTRACT Both ortho isomers of chlorophenylbenzoylthiourea (I) and nitrophenylthiourea (II) has *trans-cis* configuration. The carbonyl-thiourea moiety, O1/C7/N1/C8/S1/N1/C9 of molecule (II) is essentially planar but is less planar in (I) with C7 and O1 atoms deviated by 0.198(2) and 0.284(1) Å respectively. However the dihedral angle between the aryl and the benzoyl planes in (II) is larger, 78.29(9)° compared with 38.67(10)° in (I). Three six-membered rings are formed in each molecule by three intramolecular hydrogen bondings. In the lattice, the molecules in both compounds are arranged as dimers along the two dimensional axes.

(Chlorophenylbenzoylthiourea (I), Nitrophenylthiourea (II))

INTRODUCTION

Current studies on thiourea derivatives are driven not only from the synthesis and structural point of view but also by their potential as biological active agents and material applications. Several thiourea derivatives and their complexes have been reported to have antifungal activity against the major plant pathogens responsible for important plant desease [1]. N-[1-(1-furoylmethyl)]-N'-[2-(thiazoyl)] thiourea was reported to be a promising compound against two NNRTI-resistant HIV-1 isolates (A17 and A17 variant) at nanomolar concentration [2]. Chelation of the tiourea derivatives with metals such as copper, gold and uranium enable it to be used for the separation of metal in a solvent extraction process [3-4]. Despite the vast potential of studies on thiourea the number of structurally known thiourea derivatives are still scarce. The main difficulty is to obtain good crystals suitable for x-ray investigation. In the course of our work on the synthesis of new thiourea derivatives and their complexation with metals, good crystals of the ortho isomers of chlorophenylbenzoylthiourea and nitrophenylbwenzoylthiourea were obtained and subjected to x-ray crystallographic investigation. This paper presents the structure of the two ortho isomers representing the common feature of benzoylthiourea derivatives with regard to hydrogen bondings and molecular interactions in the lattice.

EXPERIMENTAL

Materials

The chemicals used in this work were reagent or Analar grade. Ethanol was distilled before being used as solvents.

Preparation of ortho-cloro- and -nitrophenylbenzoylthiourea

Equimolar mixture of benzoylisothiocynate and ortho-chloroanaline or ortho-nitroanaline in dried ethanol was refluxed for one hour. The mixture was then poured into a beaker containing some ice. The white precipitate was filtered and washed with distilled water and followed by cold ethanol. The product was recrystallized from DMF.

X-ray crystallographic experiment

A selected crystal was mounted on a SMART APEX CCD diffractometer. Reflection data were measured at 20 °C using graphite monochromated Mo-K_α (λ=0.71073 Å) radiation with a detector