

Supramolecular assembly in the solid state of 1-(*o*-Tolyl)thiourea

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Thiourea itself as well as its derivatives are known to be biologically active^[1] Their antimicrobial, cytotoxic and anti-HIV activities have been recently tested. Also, *o*-substituted aromatic thiourea derivatives have received special attention because of their fungicidal activity. In this work we present the supramolecular assembly of *o*-toluidine.

The molecule presents a thioamide form and it is a typical N-monosubstituted thiourea derivative with usual geometric parameters. The C—S bond [1.687 (2) Å] shows the expected double-bond character. The short bond-lengths of the C1—N1 [1.329 (2) Å] and C1—N2 [1.321 (2) Å] indicate partial double bond character, similarly to other thiourea derivatives where electron delocalization in the N—C—S moiety is present^[2]. In addition, the values of the bond angles that are close to 120° also suggest the resonance effect. As might be expected both the central thiourea fragment as well as the *o*-tolyl group are planar.

The *o*-tolyl group is almost perpendicular to the plane formed by the thiourea molecule (82.19 (8)°). Figure 1 shows the assembly of the molecules in the unit cell along to the *b* axis. In the crystal structure, the molecules are linked by N—H···S hydrogen bonds that stabilize the packing. In the previous studies have been reported the N—H···S interactions with the formation of the centrosymmetric dimers^[3]. In this structure, the N—H···S intermolecular interactions form two independent chains parallel to the (110) and (1 $\bar{1}$ 0) planes (Figure 2)^[4].

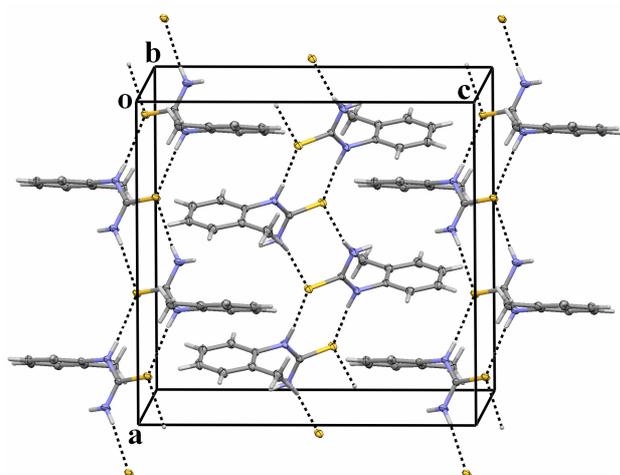


Figure 1: Supramolecular assembly linked by N—H···S hydrogen bonds.

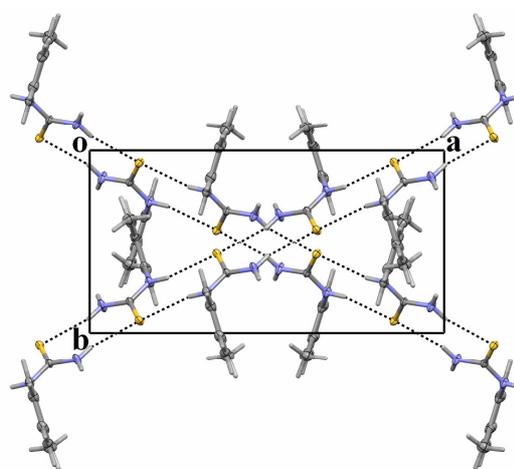


Figure 2: Crystal packing view along *c* axis showing the two independent chains.

References:

- [1] Koketsu, M. & Ishihara, H. *Curr. Org. Synth.*, **3**, 439–455 (2006).
- [2] Corrêa, R. S., Estévez-Hernández, O., Ellena, J. & Duque, J. *Acta Cryst. E*, **64**, 1414 (2008).
- [3] Corrêa, R. S., Santana, S. A., Salloum, R., Silva, R. M. & Doriguetto, A. C. *Acta Cryst. C*, **62**, 115–117 (2006).
- [4] Corrêa, R. S. Ribeiro, L., Ellena, J., Estévez-Hernández, O., Duque, J. *Acta Cryst. E*, **64**, 1670–1671 (2008).

Acknowledges: The authors are grateful for financial support from the Brazilian agencies: CNPq, FAPESP and CAPES. RSC acknowledges the CNPq for a fellowship (Project 134576/2007–1).