Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,3-Bis(4-bromophenyl)thiourea

Niaz Muhammed,[a] Zia-ur-Rehman,[a] Saqib Ali[a] and Auke Meetsma[b]*

[a]Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and [b]Crystal Structure Center, Chemical Physics, Materials Science Center, University of Groningen, Nijenborgh 4, NL-9747 AG Groningen, The Netherlands

Correspondence e-mail: A.Meetsma@rug.nl

Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.028
wR factor = 0.072
Data-to-parameter ratio = 16.3

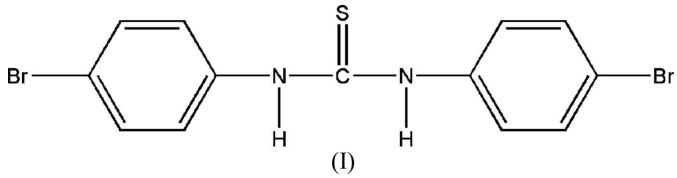
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 6 December 2006
Accepted 28 December 2006

The two bromophenyl rings in the title compound, $C_{13}H_{10}Br_2N_2S$, adopt a *cis–cis* configuration to S with respect to the C—N thiourea bonds. The crystal packing is characterized by N—H···S hydrogen bonds.

Comment

N,*N*-disubstituted thiourea derivatives have attracted attention due to their coordination behavior with transition metals (Schuster *et al.*, 1990). Complexes with thiourea derivatives have also been investigated for their biological activities, such as antibacterial, antifungal, antitubercular, antithyroid and insecticidal activities (Madan & Taneja, 1991; Frech *et al.*, 1970).



(I)

The molecular structure of (I) is illustrated in Fig. 1. The short C—S distance [1.688 (2) Å] clearly shows its double-bond character. The two bromophenyl rings adopt a *cis–cis* configuration to S with respect to the C—N thiourea bonds, as observed in a homologous compound, (dichlorophenyl)thiourea (Soriano-Garcia *et al.*, 2001). The dihedral angles between the planes of the thiourea and the two bromophenyl rings (C1–C6, C8–C13) are 47.55 (10) and 52.78 (10)°, respectively. A search of the distances yielded intermolecular contacts shorter than the sum of the van der Waals radii for N and S; the units are linked by hydrogen bonds (Steiner, 1996), forming an infinite one-dimensional chain along [010] (Table 1).

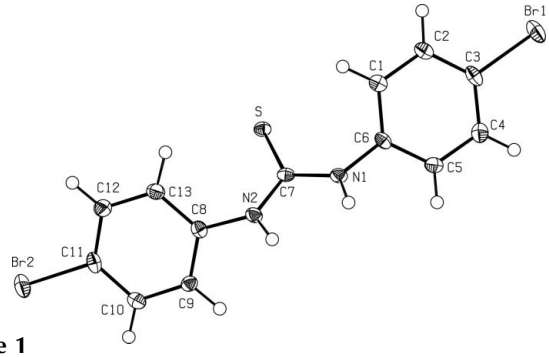


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

A solution of 4-bromoaniline (1.72 g, 10 mmol) in acetone (20 ml) was added dropwise to a solution of CS_2 (0.90 ml, 10 mmol) and NH_3 (0.60 ml, 15 mmol) in acetone (20 ml). The mixture was stirred for about 4 h at room temperature. The solution was rotary-evaporated under vacuum. The crude product was then added to 10% HCl (200 ml) and stirred well. The solid product was separated off and recrystallized from dry acetone (yield 80%).

Crystal data

$C_{13}H_{10}Br_2N_2S$
M_r = 386.11
Monoclinic, $P2_1/c$
a = 14.077 (1) Å
b = 7.0804 (6) Å
c = 14.054 (1) Å
β = 104.026 (1)°
V = 1359.01 (18) Å^3
Z = 4
D_x = 1.887 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 6.10 mm^{-1}
T = 100 (1) K
Block, colorless
0.46 × 0.42 × 0.37 mm

Data collection

Bruker SMART APEX diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.073, T_{max} = 0.106
10894 measured reflections
3318 independent reflections
2769 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 28.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.072
S = 1.04
3318 reflections
203 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.2476P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H21···S^{i}	0.79 (2)	2.61 (2)	3.355 (2)	158 (2)
N2—H22···S^{i}	0.79 (3)	2.53 (3)	3.316 (2)	168 (3)

Symmetry code: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$.

All the H atoms were located in a difference map, and all coordinates and isotropic displacement parameters were refined.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2001); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

NM and Zia-ur-Rehman are grateful to the Higher Education Commission of Pakistan for financial support.

References

Bruker, (2001). *SMART* (Version 5.62), *SAINT-Plus* (Version 6.02A) and *XPREP* (Version 5.1/NT). Bruker AXS Inc., Madison, Wisconsin, USA.
Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.
Frech, F. A., Blanz, E. J., Amaral, J. R. D. & French, D. A. (1970). *J. Med. Chem.* **13**, 1117–1124.
Madan, V. K. & Taneja, A. D. (1991). *J. Indian Chem. Soc.* **68**, 471–472.
Schuster, M., Kugler, B. & Konig, K. H. (1990). *J. Anal. Chem.* **338**, 717–720.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SADABS*. University of Göttingen, Germany.
Soriano-Garcia, M. S., Chavez, G. T., Cedillo, F. D., Perez, A. E. D. & Hernandez, G. A. (2001). *Anal. Sciences*, **17**, 799–800.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Steiner, Th. (1996). *Cryst. Rev.* **6**, 1–57.