Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3,3′-Bis(2,4-dichlorophenoxyacetyl)-1,1′-(2,2′-dimethylbiphenyl-4,4′-diyl)dithiourea *N*,*N*-dimethylformamide disolvate

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Received 9 August 2006
Accepted 18 August 2006

In the title compound, $C_{32}H_{26}Cl_4N_4O_4S_2\cdot 2C_3H_7NO$, the molecule of 3,3′-bis(2,4-dichlorophenoxyacetyl)-1,1′-(2,2′-dimethylbiphenyl-4,4′-diyl)dithiourea (BT) possesses a crystallographically imposed centre of symmetry at the mid-point of the central C—C bond. Intramolecular N—H···O and C—H···S hydrogen bonds contribute to the essential planarity of the BT skeleton, with a maximum deviation from the mean plane of 0.196 (2) Å for the S atoms.

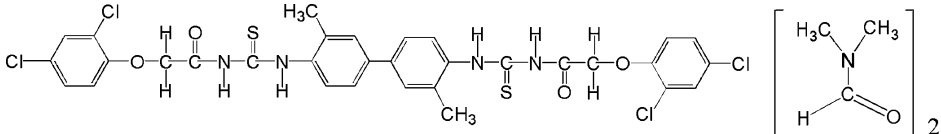
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
Disorder in solvent or counterion
R factor = 0.076
wR factor = 0.161
Data-to-parameter ratio = 13.7

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

Comment

The title compound, (I), belongs to the family of aroylthiourea compounds, which exhibit various biological properties such as antiviral, herbicidal, pesticidal, and plant-growth regulating activities (Xu *et al.*, 2003; Sun *et al.*, 2006; Du & Ye, 2002). We present here its crystal structure.



(I)

The triclinic unit cell of (I) contains one molecule of 3,3′-bis(2,4-dichlorophenoxyacetyl)-1,1′-(2,2′-dimethylbiphenyl-4,4′-diyl)dithiourea (BT) and two molecules of *N*,*N*-dimethylformamide (DMF). All bond lengths and angles are normal (Allen *et al.*, 1987). The BT molecule possesses a crystallographically imposed centre of symmetry at the mid-point of the central C—C bond (Fig. 1).

Intramolecular N—H···O and C—H···S hydrogen bonds (Table 1) contribute to the essential planarity of the BT skeleton, with a maximum deviation from the mean plane of 0.196 (2) Å for the S atoms.

Experimental

BT was prepared according to the method of Zhang & Lin (1992). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a DMF solution at 293 K.

Crystal data

$C_{32}H_{26}Cl_4N_4O_4S_2\cdot 2C_3H_7NO$
M_r = 882.70
Triclinic, $P\overline{1}$
a = 10.012 (2) Å
b = 10.488 (2) Å
c = 11.124 (2) Å
α = 67.78 (3)°
β = 77.92 (3)°
γ = 78.07 (3)°
V = 1046.8 (4) Å^3
Z = 1
D_x = 1.400 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.44 mm^{-1}
T = 293 (2) K
Prism, yellow
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.881, T_{max} = 0.958
4104 measured reflections
4104 independent reflections
1798 reflections with $I > 2\sigma(I)$
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.161
S = 1.00
4104 reflections
300 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.047P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.86	2.09	2.558 (5)	114
N2—H2A···O2	0.86	1.93	2.669 (5)	143
C15—H15A···S1	0.93	2.49	3.182 (5)	131

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å and N—H = 0.86 Å) and refined as riding, with U_{iso}(H) = 1.2–1.5U_{eq}(C) of the parent atom. The DMF solvent molecule was treated as disordered over two positions, with refined occupancies of 0.552 (10) and 0.448 (10).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

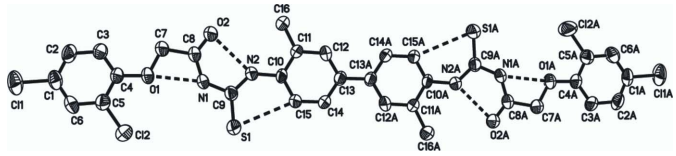


Figure 1
View of the BT molecular structure in (I) showing the atom-labelling scheme [symmetry code: (A) −1 − x, 1 − y, 1 − z]. Displacement ellipsoids are drawn at the 50% probability level. The dashed lines denote intramolecular hydrogen bonds. H atoms have been omitted.

We are grateful to H. Q. Wang for the X-ray data collection.

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