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1-{2-[(4-Nitrobenzylidene)amino]phenyl}-3-phenylthiourea

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.004 Å
R factor = 0.056
wR factor = 0.154
Data-to-parameter ratio = 17.4

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

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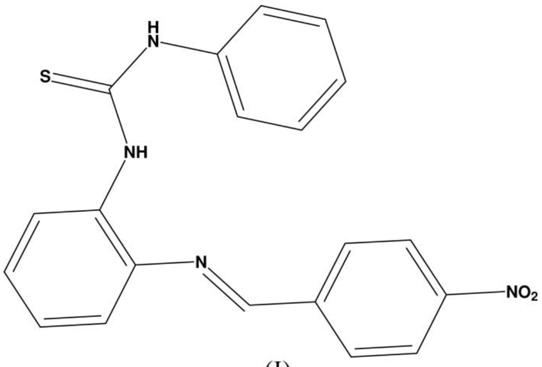
The molecular structure of the title compound, $C_{20}H_{16}N_4O_2S$, is stabilized by N—H···N and weak C—H···S intramolecular interactions. The crystal packing is stabilized by N—H···S and C—H···O intermolecular interactions.

Comment

Considerable attention has been focused on the design of host molecules that recognize and sense anion species selectively through visible, electrochemical and optical responses (Martinez-Manez & Sancenon, 2003). The development of colorimetric anion sensing is very important and increasingly appreciated since naked eye detection can offer qualitative and quantitative information (Gale, 2001). Color changes, as signaling an event detected by the naked eye, are widely used owing to the low cost or lack of equipment required.

The bond lengths and bond angles of the title compound, (I), are comparable to the literature values (Allen *et al.*, 1987). The C2—C1—N1—O1 [−4.7 (4)°] and C2—C1—N1—O2 [173.2 (3)°] torsion angles indicate a slight deviation of the nitro group from the plane of the benzene ring. The dihedral angles made by the benzene rings C1–C6 and C8–C13 with C15–C20 are 41.7 (1) and 69.9 (1)°, respectively, and that between C1–C6 and C8–C13 is 28.4 (1)°.



(I)

The molecular geometry is stabilized by an N—H···N hydrogen bond and a weak C—H···S interaction. The crystal packing is stabilized by N—H···S and C—H···O intermolecular interactions.

Experimental

1-{2-[4-Nitrobenzylidene)amino}phenyl}-3-phenylthiourea was synthesized by Schiff base condensation between 1-(2-aminophenyl)thiourea and 4-nitrobenzaldehyde. To a solution of 1-(2-aminophenyl)thiourea (0.3 g, 1.2 mmol) in methanol (25 ml), 4-

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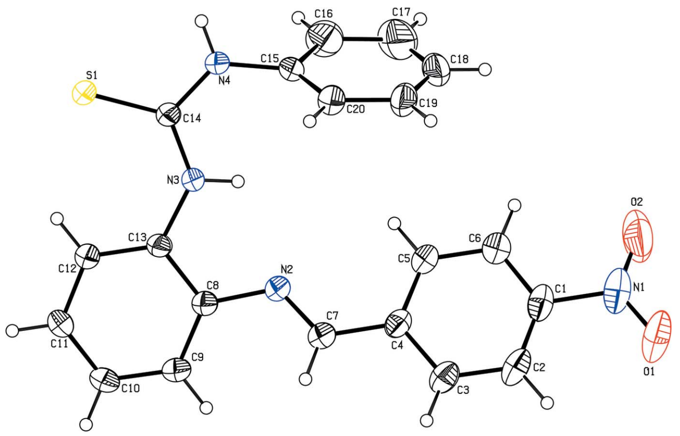

Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

nitrobenzaldehyde (0.206 g, 1.2 mmol) in methanol (25 ml) was added with stirring. The resulting mixture was heated at reflux for 3 h and cooled to room temperature. The solid product was collected by filtration and washed with cold methanol. The microcrystalline compound was recrystallized from hot chloroform; yellow coloured crystals suitable for X-ray diffraction were obtained on slow evaporation. Yield: 71%; m.p. 476 K.

Crystal data

$C_{20}H_{16}N_4O_2S$
$M_r = 376.43$
Triclinic, $P\overline{1}$
$a = 7.2705$ (6) Å
$b = 11.0178$ (9) Å
$c = 12.0137$ (9) Å
$\alpha = 84.776$ (1)°
$\beta = 85.675$ (1)°
$\gamma = 75.405$ (1)°
$V = 926.06$ (13) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.20$ mm^{-1}
$T = 293$ (2) K
0.28 × 0.23 × 0.22 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: none
10737 measured reflections
4234 independent reflections
3312 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.155$
$S = 1.03$
4234 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max} = 0.64$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.42$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N2	0.86	2.18	2.640 (2)	113
C12—H12···S1	0.93	2.51	3.188 (2)	130
N4—H4···S1$^{\rm i}$	0.86	2.46	3.301 (2)	165
C18—H18···O2$^{\rm ii}$	0.93	2.56	3.472 (5)	166

Symmetry codes: (i) $-x+2, -y, -z+1$; (ii) $-x, -y, -z$.

All H atoms were refined using a riding model with C—H = 0.93 Å, N—H = 0.86 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C,N).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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References

Allen, F. H., Kennard, O., Watson, D., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2001). *SMART* (Version 5.625/NT/2000) and *SAINT* (Version 6.28a). Bruker AXS Inc., Madison, Wisconsin, USA.
Gale, P. A. (2001). *Coord. Chem. Rev.* **213**, 79–128.
Martinez-Manez, R. & Sancenon, F. (2003). *Chem. Rev.* **103**, 4419–4476.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.