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1-(2-Nitrophenyl)-3-phenylthiourea

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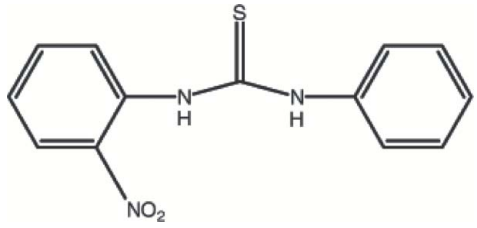
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.045; wR factor = 0.132; data-to-parameter ratio = 16.0.

The title compound, $C_{13}H_{11}N_3O_2S$, was prepared by reaction of 2-nitrobenzenamine, KOH and 1-isothiocyanatobenzene in an ethanol solution at room temperature. The dihedral angles formed between the thiourea plane and the phenyl rings are 61.9 and 31.0°. The dihedral angle between the two phenyl rings is 78.1°. In the crystal structure, there are weak intermolecular N—H···S and C—H···S hydrogen-bonding interactions.

Related literature

For related literature, see: Reinbold & Morar (1984); Xue *et al.* (2004); Madan & Taneja (1991).



Experimental

Crystal data

$C_{13}H_{11}N_3O_2S$
M_r = 273.31
Monoclinic, $P2_1/c$
a = 7.3110 (15) Å
b = 24.113 (5) Å
c = 7.4320 (15) Å
β = 90.22 (3)°
V = 1310.2 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 293 (2) K
0.25 × 0.20 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
2964 measured reflections
2764 independent reflections
2022 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
3 standard reflections every 100 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.132
S = 1.09
2764 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···S1^{i}	0.86	2.56	3.3744 (19)	158
C3—H3A···S1^{ii}	0.93	2.84	3.725 (3)	159

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2515).

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supporting information

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1-(2-Nitrophenyl)-3-phenylthiourea

Yongqi Qin, Fangfang Jian, Mingna Jiang and Xiangyan Yang

S1. Comment

Thioureas have been studied for many years because of their broad antibiosis and sterilization properties Recent years study shows that thioureas not only can be used to kill insects and adjust plant growth but also have anti-viral activities (Madan *et al.*, 1991; Reinbold *et al.*,1984). From our early quantum study on these compounds, we find that they have several active centers and can form polyligand complexes with metals easily (Xue *et al.*, 2004).These complexes are widely used as anticancer medicines Therefore study on thioureas has important impact on the future. In order to search for new compounds with higher bioactivity, the title compound was synthesized and we herein report its crystal structure.

In the title compound, bond lengths and angles are generally normal. The C7—S1 bond length of 1.686 (2)Å is indicative of considerable double-bond character. The dihedral angle between the plane (C6—C8/N1/N2/S1) and the plane (C8—C13/N2) is 31.01°. The torsion angles of S1—C7—N2—C8 and N1—C7—N2—C8 are -1.31 and -179.19°, respectively.

In the crystal structure, there are weak intermolecular C—H···S and N—H···S hydrogen bonding interactions. These interactions stabilize the title structure.

S2. Experimental

The title compound was prepared by reaction of 2-nitrobenzenamine (0.05 mol), KOH (0.15 mol) and 1-isothiocyanato-benzene (0.05 mol) in the ethanol solution (40 ml) at room temperature. Single crystals of the title compound suitable for X-ray measurements was obtained by recrystallization from ethanol/acetone (*v*/*v*=1:1) at room temperature.

S3. Refinement

The H atoms were fixed geometrically and were treated as riding on the parent C atoms, with C—H = 0.93 Å and N—H = 0.86 Å, and U_{iso}=1.2 times U_{eq} of the parent atoms.

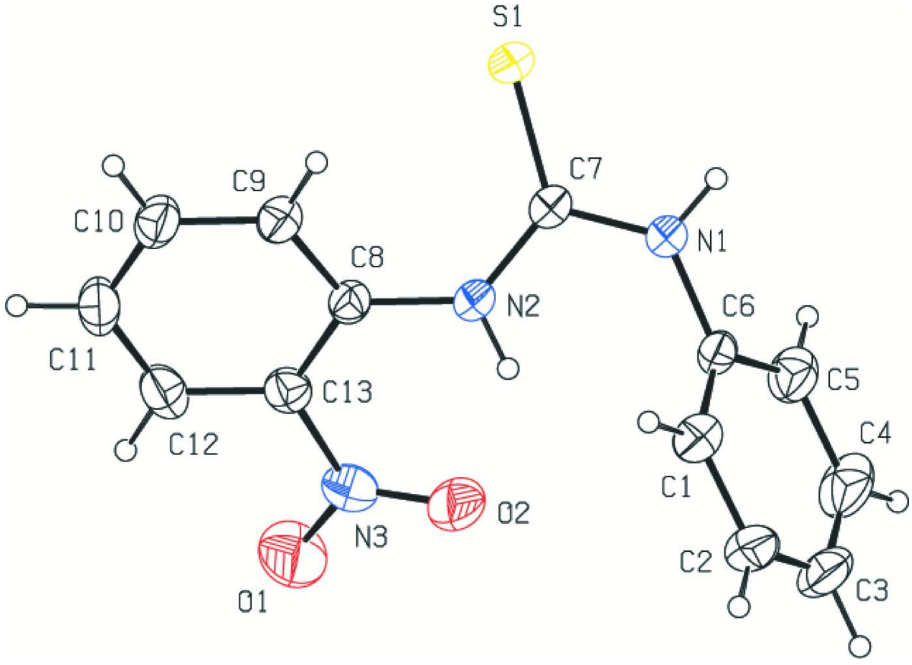

Figure 1

The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

1-(2-Nitrophenyl)-3-phenylthiourea

Crystal data

$C_{13}H_{11}N_3O_2S$
$M_r = 273.31$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.3110\ (15)$ Å
$b = 24.113\ (5)$ Å
$c = 7.4320\ (15)$ Å
$\beta = 90.22\ (3)°$
$V = 1310.2\ (5)$ Å^3
$Z = 4$
$F(000) = 568$
$D_x = 1.386$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 1.7–27.0°$
$\mu = 0.25$ mm^{-1}
$T = 293$ K
Block, yellow
0.25 × 0.20 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
2964 measured reflections
2764 independent reflections
2022 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.7°$
$h = 0\rightarrow8$
$k = 0\rightarrow28$
$l = -8\rightarrow8$
3 standard reflections every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.132$
$S = 1.09$
2764 reflections
173 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 0.4395P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.115 (6)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.20879 (9)	0.56603 (3)	0.96789 (9)	0.0669 (3)
O1	−0.0828 (3)	0.79863 (8)	1.3139 (4)	0.1026 (8)
O2	−0.1250 (3)	0.71304 (8)	1.3693 (3)	0.0785 (6)
N1	−0.0460 (3)	0.55266 (7)	1.2122 (3)	0.0556 (5)
H1A	−0.0549	0.5206	1.1619	0.067*
N2	0.0901 (2)	0.63776 (7)	1.2248 (2)	0.0482 (4)
H2A	0.0145	0.6425	1.3119	0.058*
N3	−0.0333 (3)	0.75057 (8)	1.3045 (3)	0.0577 (5)
C1	−0.1032 (4)	0.57222 (10)	1.5305 (3)	0.0622 (6)
H1B	0.0220	0.5731	1.5528	0.075*
C2	−0.2268 (5)	0.58020 (11)	1.6701 (4)	0.0767 (8)
H2B	−0.1840	0.5866	1.7863	0.092*
C3	−0.4120 (5)	0.57870 (12)	1.6372 (5)	0.0844 (10)
H3A	−0.4939	0.5848	1.7305	0.101*
C4	−0.4759 (4)	0.56819 (12)	1.4666 (5)	0.0853 (10)
H4A	−0.6013	0.5663	1.4458	0.102*
C5	−0.3554 (3)	0.56029 (10)	1.3246 (4)	0.0635 (6)
H5A	−0.3990	0.5533	1.2091	0.076*
C6	−0.1685 (3)	0.56302 (8)	1.3585 (3)	0.0477 (5)
C7	0.0815 (3)	0.58703 (9)	1.1440 (3)	0.0462 (5)
C8	0.2032 (3)	0.68340 (8)	1.1878 (2)	0.0423 (5)
C9	0.3819 (3)	0.67718 (9)	1.1219 (3)	0.0509 (5)
H9A	0.4277	0.6417	1.1030	0.061*
C10	0.4912 (3)	0.72225 (11)	1.0846 (3)	0.0601 (6)
H10A	0.6086	0.7167	1.0403	0.072*
C11	0.4284 (4)	0.77548 (10)	1.1125 (3)	0.0649 (7)
H11A	0.5015	0.8057	1.0836	0.078*
C12	0.2561 (4)	0.78358 (9)	1.1834 (3)	0.0599 (6)

H12A	0.2143	0.8193	1.2058	0.072*
C13	0.1449 (3)	0.73817 (8)	1.2216 (3)	0.0465 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0690 (4)	0.0677 (4)	0.0644 (4)	−0.0224 (3)	0.0339 (3)	−0.0228 (3)
O1	0.0986 (16)	0.0629 (12)	0.147 (2)	0.0267 (11)	0.0178 (14)	−0.0059 (12)
O2	0.0682 (11)	0.0700 (12)	0.0977 (14)	0.0081 (9)	0.0318 (10)	−0.0063 (10)
N1	0.0613 (12)	0.0468 (10)	0.0589 (11)	−0.0139 (8)	0.0251 (9)	−0.0121 (8)
N2	0.0478 (10)	0.0446 (9)	0.0523 (10)	−0.0057 (7)	0.0190 (8)	−0.0050 (7)
N3	0.0621 (12)	0.0547 (11)	0.0562 (11)	0.0099 (10)	−0.0038 (9)	−0.0074 (9)
C1	0.0589 (14)	0.0683 (15)	0.0595 (15)	−0.0087 (11)	0.0147 (11)	−0.0049 (11)
C2	0.104 (2)	0.0671 (16)	0.0595 (15)	−0.0087 (15)	0.0338 (15)	−0.0044 (12)
C3	0.092 (2)	0.0666 (17)	0.095 (2)	0.0051 (15)	0.0597 (19)	0.0042 (15)
C4	0.0514 (15)	0.0791 (19)	0.126 (3)	0.0074 (13)	0.0338 (16)	0.0107 (18)
C5	0.0527 (14)	0.0594 (14)	0.0787 (17)	0.0021 (11)	0.0120 (12)	0.0061 (12)
C6	0.0504 (12)	0.0376 (10)	0.0552 (12)	−0.0051 (8)	0.0195 (9)	0.0013 (8)
C7	0.0441 (11)	0.0480 (11)	0.0466 (11)	−0.0048 (9)	0.0117 (8)	−0.0016 (9)
C8	0.0460 (11)	0.0449 (10)	0.0362 (10)	−0.0060 (8)	0.0024 (8)	0.0019 (8)
C9	0.0464 (11)	0.0558 (12)	0.0505 (12)	−0.0058 (9)	0.0070 (9)	−0.0018 (9)
C10	0.0529 (13)	0.0753 (17)	0.0522 (13)	−0.0214 (11)	0.0042 (10)	−0.0002 (11)
C11	0.0758 (17)	0.0615 (15)	0.0575 (14)	−0.0303 (13)	−0.0017 (12)	0.0054 (11)
C12	0.0816 (17)	0.0441 (11)	0.0540 (13)	−0.0103 (11)	−0.0096 (12)	0.0012 (9)
C13	0.0517 (12)	0.0484 (11)	0.0394 (10)	−0.0013 (9)	−0.0041 (9)	−0.0005 (8)

Geometric parameters (Å, º)

S1—C7	1.686 (2)	C3—H3A	0.9300
O1—N3	1.216 (3)	C4—C5	1.391 (4)
O2—N3	1.226 (3)	C4—H4A	0.9300
N1—C7	1.348 (3)	C5—C6	1.390 (3)
N1—C6	1.433 (3)	C5—H5A	0.9300
N1—H1A	0.8600	C8—C9	1.405 (3)
N2—C7	1.364 (3)	C8—C13	1.411 (3)
N2—C8	1.404 (2)	C9—C10	1.378 (3)
N2—H2A	0.8600	C9—H9A	0.9300
N3—C13	1.474 (3)	C10—C11	1.379 (4)
C1—C6	1.381 (4)	C10—H10A	0.9300
C1—C2	1.392 (3)	C11—C12	1.381 (4)
C1—H1B	0.9300	C11—H11A	0.9300
C2—C3	1.375 (5)	C12—C13	1.394 (3)
C2—H2B	0.9300	C12—H12A	0.9300
C3—C4	1.373 (5)		
C7—N1—C6	127.83 (17)	C1—C6—C5	120.8 (2)
C7—N1—H1A	116.1	C1—C6—N1	121.0 (2)
C6—N1—H1A	116.1	C5—C6—N1	118.1 (2)

C7—N2—C8	129.97 (16)	N1—C7—N2	114.60 (17)
C7—N2—H2A	115.0	N1—C7—S1	119.45 (16)
C8—N2—H2A	115.0	N2—C7—S1	125.92 (15)
O1—N3—O2	121.2 (2)	N2—C8—C9	122.26 (18)
O1—N3—C13	118.8 (2)	N2—C8—C13	121.35 (18)
O2—N3—C13	120.00 (18)	C9—C8—C13	116.35 (18)
C6—C1—C2	119.3 (3)	C10—C9—C8	121.8 (2)
C6—C1—H1B	120.4	C10—C9—H9A	119.1
C2—C1—H1B	120.4	C8—C9—H9A	119.1
C3—C2—C1	120.3 (3)	C9—C10—C11	120.7 (2)
C3—C2—H2B	119.8	C9—C10—H10A	119.7
C1—C2—H2B	119.8	C11—C10—H10A	119.7
C4—C3—C2	120.0 (2)	C10—C11—C12	119.6 (2)
C4—C3—H3A	120.0	C10—C11—H11A	120.2
C2—C3—H3A	120.0	C12—C11—H11A	120.2
C3—C4—C5	120.8 (3)	C11—C12—C13	120.0 (2)
C3—C4—H4A	119.6	C11—C12—H12A	120.0
C5—C4—H4A	119.6	C13—C12—H12A	120.0
C6—C5—C4	118.8 (3)	C12—C13—C8	121.5 (2)
C6—C5—H5A	120.6	C12—C13—N3	116.3 (2)
C4—C5—H5A	120.6	C8—C13—N3	122.17 (18)

C6—C1—C2—C3	0.3 (4)	N2—C8—C9—C10	179.4 (2)
C1—C2—C3—C4	1.3 (4)	C13—C8—C9—C10	−2.8 (3)
C2—C3—C4—C5	−1.6 (4)	C8—C9—C10—C11	0.5 (3)
C3—C4—C5—C6	0.2 (4)	C9—C10—C11—C12	1.9 (4)
C2—C1—C6—C5	−1.6 (3)	C10—C11—C12—C13	−1.9 (4)
C2—C1—C6—N1	−177.8 (2)	C11—C12—C13—C8	−0.6 (3)
C4—C5—C6—C1	1.4 (3)	C11—C12—C13—N3	177.4 (2)
C4—C5—C6—N1	177.6 (2)	N2—C8—C13—C12	−179.37 (19)
C7—N1—C6—C1	−63.3 (3)	C9—C8—C13—C12	2.9 (3)
C7—N1—C6—C5	120.4 (3)	N2—C8—C13—N3	2.8 (3)
C6—N1—C7—N2	−1.0 (3)	C9—C8—C13—N3	−174.95 (18)
C6—N1—C7—S1	−179.05 (19)	O1—N3—C13—C12	9.1 (3)
C8—N2—C7—N1	−179.2 (2)	O2—N3—C13—C12	−167.8 (2)
C8—N2—C7—S1	−1.3 (3)	O1—N3—C13—C8	−172.9 (2)
C7—N2—C8—C9	−31.8 (3)	O2—N3—C13—C8	10.2 (3)
C7—N2—C8—C13	150.6 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···S1^{i}	0.86	2.56	3.3744 (19)	158
C3—H3*A*···S1^{ii}	0.93	2.84	3.725 (3)	159

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