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1-Benzoyl-3-(5-quinolyl)thiourea

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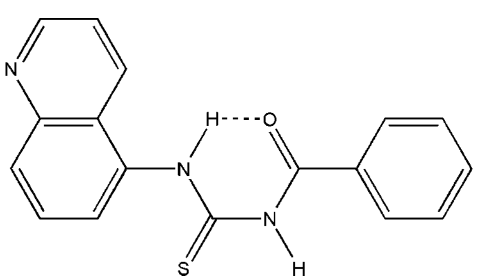
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.129; data-to-parameter ratio = 16.5.

The title compound, $C_{17}H_{13}N_3OS$, was obtained by the reaction of benzoyl chloride, ammonium thiocyanate and 5-aminoquinoline in the presence of polyethyleneglycol-400 (PEG-400) as a phase-transfer catalyst. The compound crystallized as discrete molecules linked by N—H···N and C—H···N hydrogen bonds involving all the potential donors, generating sheets parallel to (100). An intramolecular N—H···O bond is also present.

Related literature

For the biological activity of acyl thioureas, see: Hackmann (1960); Sarkis & Faisal (1985). For their application in the synthesis of supramolecular complexes, see: Pluta & Sadlej (2001); Kaminsky *et al.* (2002). For a related structure, see: Xue *et al.* (2004).



Experimental

Crystal data

$C_{17}H_{13}N_3OS$
M_r = 307.36
Monoclinic, $P2_1/n$
a = 5.0875 (1) Å
b = 16.1718 (4) Å
c = 18.2847 (4) Å
β = 95.892 (2)°
V = 1496.41 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 296 (2) K
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.939, T_{max} = 0.969
13322 measured reflections
3411 independent reflections
2184 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
3 standard reflections every 97 reflections intensity decay: 2.1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.129
S = 1.04
3411 reflections
207 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H6···N3^{i}	0.825 (17)	2.283 (17)	3.100 (3)	170.5 (18)
N2—H7···O1	0.91 (3)	1.84 (3)	2.619 (3)	143 (3)
C6—H5···N3^{i}	0.93	2.46	3.252 (3)	143

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

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: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2453).

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supplementary materials

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1-Benzoyl-3-(5-quinolyl)thiourea

W.-H. Du, C.-M. Wei and W.-F. Wang

Comment

Acyl thioureas have extensive biological activities such as bacteriostasis, weeding (Hackmann, 1960) and plant growth regulating (Sarkis & Faisal, 1985). In addition, acyl thioureas are excellent ligands, and have been widely applied in synthesis of supramolecular complexes (Pluta & Sadlej, 2001; Kaminsky *et al.*, 2002). The title compound, (I) crystallizes as discrete molecules (Fig. 1). The full molecule is a big conjugated system because the bond lengths of C1—C7, C7—N1, C8—N1, C8—N2 and C9—N2 become shorter than standard values, and the bond lengths of C7—O1 and C8—S1 become longer than standard values. In (I) the torsion angle for C17—C9—N2—C8 of -78.2 (3)° indicates the quinoline ring is approximately orthogonal to the rest of the molecule. The molecules in (I) are linked by N1—H6···N3, N2—H7···O1 and C6—H5···N3 hydrogen bonds involving all the potential donors, generating sheets parallel to (100), as shown in Fig. 2. In addition, the bond lengths of S—C (1.655 (2)Å) and O—C(1.223 (2)Å) in (I) are longer than the bond lengths of S—C(1.6503Å) and O—C(1.201Å) in *N*-(4,6-dimethylpyrimidin-2-ylcarbamothioyl)benzamide (Xue *et al.*, 2004)

Experimental

The title compound was synthesized as following. A mixture of benzoyl chloride (1400 mg, 10 mmol), ammonium thiocyanate (1140 mg, 15 mmol), 5-aminoquinoline (1300 mg, 9 mmol) and dichloromethane (50 ml) in the presence of PEG-400 (1200 mg, 3 mmol) as phase transfer catalyst at room temperature for 8h with stirring. The reaction mixture was evaporated to give a residue. Singles crystals suitable for X-ray analysis were obtained by slow evaporation of a mixture solution of dichloromethane and ethanol.

Refinement

The atom H6 attached to N1 and the atom H7 attached to N2 was located in a difference Fourier map and refined with N—H distance restrained to 0.87 (2)Å, and with U_{iso}(H) = 0.85U_{eq}(N) and U_{iso}(H) = 1.91U_{eq}(N) All H atoms bound to carbon were refined using riding models with d(C—H) = 0.93Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

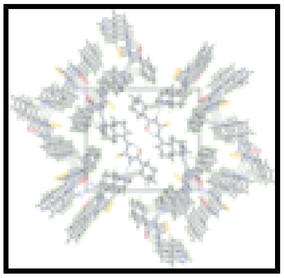

Fig. 2. The packing of (I), viewed down the *a* axis, showing two layers of molecules connected by van der waals.

1-Benzoyl-3-(5-quinolyl)thiourea

Crystal data

$C_{17}H_{13}N_3OS$	F_{000} = 640
M_r = 307.36	D_x = 1.364 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point = 446.2–446.7 K
Hall symbol: -P 2yn	Mo *K*α radiation λ = 0.71073 Å
a = 5.0875 (1) Å	Cell parameters from 3090 reflections
b = 16.1718 (4) Å	θ = 2.2–22.4º
c = 18.2847 (4) Å	μ = 0.22 mm^{-1}
β = 95.892 (2)º	*T* = 296 (2) K
V = 1496.41 (6) Å^3	Rod, yellow
Z = 4	0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.032
Radiation source: fine-focus sealed tube	θ_{max} = 27.4º
Monochromator: graphite	θ_{min} = 1.7º
T = 296(2) K	*h* = −6→6
ω/2θ scans	*k* = −20→18
Absorption correction: ψ scan (North *et al.*, 1968)	*l* = −23→23
T_{min} = 0.939, T_{max} = 0.969	3 standard reflections
13322 measured reflections	every 97 reflections
3411 independent reflections	intensity decay: 2.1%
2184 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.129	$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 0.4696P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
3411 reflections	$\Delta\rho_{max} = 0.30$ e Å^{-3}
207 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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	−0.00333 (14)	0.14855 (4)	0.20925 (4)	0.0704 (2)
O1	0.5088 (4)	0.09876 (10)	0.02568 (9)	0.0724 (5)
N1	0.2883 (4)	0.17950 (11)	0.10117 (10)	0.0503 (4)
N2	0.2175 (4)	0.04129 (12)	0.12428 (10)	0.0602 (5)
C17	0.2711 (4)	−0.05169 (12)	0.23117 (11)	0.0442 (5)
C13	0.1919 (4)	−0.12237 (12)	0.26802 (11)	0.0482 (5)
C7	0.4431 (5)	0.16753 (13)	0.04478 (11)	0.0524 (5)
N3	0.3173 (4)	−0.14846 (11)	0.33306 (10)	0.0579 (5)
C1	0.5204 (4)	0.24240 (13)	0.00465 (10)	0.0470 (5)
C16	0.4940 (4)	−0.00801 (14)	0.26304 (13)	0.0558 (6)
H13	0.5538	0.0389	0.2404	0.067*
C8	0.1748 (4)	0.11985 (13)	0.14277 (11)	0.0511 (5)
C12	−0.0297 (5)	−0.16872 (13)	0.23615 (14)	0.0582 (6)
H10	−0.0850	−0.2156	0.2597	0.070*
C9	0.1265 (4)	−0.02866 (13)	0.16352 (12)	0.0520 (5)
C11	−0.1587 (5)	−0.14385 (14)	0.17142 (14)	0.0607 (6)
H9	−0.3023	−0.1745	0.1508	0.073*
C2	0.7141 (5)	0.23490 (16)	−0.04248 (13)	0.0650 (6)
H1	0.8019	0.1848	−0.0458	0.078*
C15	0.6203 (5)	−0.03616 (15)	0.32799 (13)	0.0621 (6)
H12	0.7686	−0.0090	0.3502	0.075*
C14	0.5228 (5)	−0.10613 (16)	0.36003 (13)	0.0637 (6)
H11	0.6111	−0.1242	0.4042	0.076*
C6	0.3941 (5)	0.31702 (15)	0.00781 (13)	0.0658 (7)
H5	0.2610	0.3232	0.0386	0.079*

C5	0.4626 (6)	0.38332 (17)	−0.03438 (14)	0.0784 (8)
H4	0.3787	0.4340	−0.0308	0.094*
C4	0.6519 (6)	0.37434 (18)	−0.08094 (14)	0.0747 (7)
H3	0.6947	0.4184	−0.1102	0.090*
C10	−0.0822 (5)	−0.07367 (14)	0.13504 (13)	0.0599 (6)
H8	−0.1754	−0.0578	0.0909	0.072*
C3	0.7785 (5)	0.30086 (19)	−0.08470 (15)	0.0764 (8)
H2	0.9100	0.2950	−0.1161	0.092*
H6	0.268 (4)	0.2277 (10)	0.1143 (10)	0.043 (6)*
H7	0.324 (5)	0.0371 (19)	0.0876 (14)	0.115 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0932 (5)	0.0458 (4)	0.0790 (4)	0.0004 (3)	0.0421 (4)	0.0001 (3)
O1	0.1085 (14)	0.0473 (10)	0.0671 (10)	0.0049 (9)	0.0359 (10)	−0.0030 (8)
N1	0.0701 (12)	0.0363 (10)	0.0461 (10)	0.0012 (9)	0.0131 (9)	0.0013 (8)
N2	0.0852 (15)	0.0426 (11)	0.0558 (12)	0.0015 (10)	0.0220 (11)	0.0056 (9)
C17	0.0501 (11)	0.0343 (10)	0.0503 (11)	0.0001 (9)	0.0159 (9)	−0.0048 (9)
C13	0.0589 (13)	0.0362 (11)	0.0522 (12)	0.0016 (9)	0.0189 (10)	−0.0032 (9)
C7	0.0653 (14)	0.0480 (13)	0.0443 (11)	0.0010 (10)	0.0080 (10)	−0.0033 (9)
N3	0.0709 (13)	0.0490 (11)	0.0550 (11)	0.0006 (10)	0.0123 (10)	0.0033 (9)
C1	0.0554 (12)	0.0489 (12)	0.0368 (10)	−0.0039 (10)	0.0048 (9)	0.0001 (9)
C16	0.0594 (14)	0.0449 (13)	0.0664 (14)	−0.0077 (10)	0.0227 (12)	−0.0067 (11)
C8	0.0664 (14)	0.0387 (12)	0.0493 (11)	0.0025 (10)	0.0108 (10)	0.0039 (9)
C12	0.0687 (15)	0.0393 (12)	0.0692 (15)	−0.0076 (10)	0.0199 (12)	−0.0077 (10)
C9	0.0642 (14)	0.0401 (12)	0.0536 (12)	0.0027 (10)	0.0154 (11)	−0.0035 (10)
C11	0.0597 (14)	0.0515 (14)	0.0711 (15)	−0.0089 (11)	0.0068 (12)	−0.0150 (12)
C2	0.0682 (15)	0.0633 (16)	0.0668 (15)	0.0042 (12)	0.0220 (13)	0.0018 (12)
C15	0.0542 (14)	0.0669 (16)	0.0655 (15)	−0.0073 (12)	0.0077 (12)	−0.0149 (12)
C14	0.0670 (16)	0.0664 (16)	0.0581 (14)	0.0028 (13)	0.0084 (12)	0.0030 (12)
C6	0.0821 (17)	0.0613 (15)	0.0584 (14)	0.0085 (13)	0.0276 (13)	0.0110 (11)
C5	0.104 (2)	0.0613 (16)	0.0740 (16)	0.0143 (15)	0.0295 (16)	0.0208 (13)
C4	0.0806 (18)	0.0751 (19)	0.0706 (16)	−0.0080 (15)	0.0187 (14)	0.0243 (14)
C10	0.0687 (15)	0.0509 (14)	0.0597 (14)	0.0019 (12)	0.0054 (12)	−0.0091 (11)
C3	0.0728 (17)	0.086 (2)	0.0761 (17)	−0.0040 (15)	0.0362 (14)	0.0121 (15)

Geometric parameters (Å, °)

S1—C8	1.655 (2)	C12—C11	1.354 (3)
O1—C7	1.223 (2)	C12—H10	0.9300
N1—C7	1.374 (3)	C9—C10	1.347 (3)
N1—C8	1.390 (3)	C11—C10	1.391 (3)
N1—H6	0.826 (15)	C11—H9	0.9300
N2—C8	1.338 (3)	C2—C3	1.376 (3)
N2—C9	1.441 (3)	C2—H1	0.9300
N2—H7	0.909 (17)	C15—C14	1.389 (3)
C17—C13	1.407 (3)	C15—H12	0.9300
C17—C16	1.410 (3)	C14—H11	0.9300

C17—C9	1.422 (3)	C6—C5	1.386 (3)
C13—N3	1.358 (3)	C6—H5	0.9300
C13—C12	1.427 (3)	C5—C4	1.357 (4)
C7—C1	1.490 (3)	C5—H4	0.9300
N3—C14	1.304 (3)	C4—C3	1.357 (4)
C1—C6	1.371 (3)	C4—H3	0.9300
C1—C2	1.379 (3)	C10—H8	0.9300
C16—C15	1.369 (3)	C3—H2	0.9300
C16—H13	0.9300		

C7—N1—C8	127.96 (19)	C10—C9—N2	120.8 (2)
C7—N1—H6	116.7 (14)	C17—C9—N2	118.35 (19)
C8—N1—H6	115.2 (14)	C12—C11—C10	121.7 (2)
C8—N2—C9	123.42 (19)	C12—C11—H9	119.1
C8—N2—H7	112 (2)	C10—C11—H9	119.1
C9—N2—H7	124 (2)	C3—C2—C1	120.6 (2)
C13—C17—C16	117.8 (2)	C3—C2—H1	119.7
C13—C17—C9	118.79 (19)	C1—C2—H1	119.7
C16—C17—C9	123.39 (19)	C16—C15—C14	118.7 (2)
N3—C13—C17	122.7 (2)	C16—C15—H12	120.6
N3—C13—C12	118.3 (2)	C14—C15—H12	120.6
C17—C13—C12	118.9 (2)	N3—C14—C15	125.1 (2)
O1—C7—N1	122.5 (2)	N3—C14—H11	117.4
O1—C7—C1	120.3 (2)	C15—C14—H11	117.4
N1—C7—C1	117.14 (19)	C1—C6—C5	120.8 (2)
C14—N3—C13	117.0 (2)	C1—C6—H5	119.6
C6—C1—C2	118.1 (2)	C5—C6—H5	119.6
C6—C1—C7	123.1 (2)	C4—C5—C6	120.1 (3)
C2—C1—C7	118.6 (2)	C4—C5—H4	119.9
C15—C16—C17	118.6 (2)	C6—C5—H4	119.9
C15—C16—H13	120.7	C3—C4—C5	119.8 (2)
C17—C16—H13	120.7	C3—C4—H3	120.1
N2—C8—N1	115.68 (19)	C5—C4—H3	120.1
N2—C8—S1	124.54 (17)	C9—C10—C11	120.3 (2)
N1—C8—S1	119.78 (16)	C9—C10—H8	119.9
C11—C12—C13	119.5 (2)	C11—C10—H8	119.9
C11—C12—H10	120.2	C4—C3—C2	120.6 (2)
C13—C12—H10	120.2	C4—C3—H2	119.7
C10—C9—C17	120.8 (2)	C2—C3—H2	119.7

C16—C17—C13—N3	1.5 (3)	C16—C17—C9—C10	178.8 (2)
C9—C17—C13—N3	−179.51 (18)	C13—C17—C9—N2	−176.79 (18)
C16—C17—C13—C12	−178.68 (18)	C16—C17—C9—N2	2.1 (3)
C9—C17—C13—C12	0.3 (3)	C8—N2—C9—C10	105.1 (3)
C8—N1—C7—O1	−2.7 (4)	C8—N2—C9—C17	−78.2 (3)
C8—N1—C7—C1	174.7 (2)	C13—C12—C11—C10	−0.4 (3)
C17—C13—N3—C14	−1.8 (3)	C6—C1—C2—C3	0.3 (3)
C12—C13—N3—C14	178.4 (2)	C7—C1—C2—C3	175.3 (2)
O1—C7—C1—C6	160.1 (2)	C17—C16—C15—C14	−0.4 (3)
N1—C7—C1—C6	−17.3 (3)	C13—N3—C14—C15	1.0 (4)

O1—C7—C1—C2	−14.6 (3)	C16—C15—C14—N3	0.1 (4)
N1—C7—C1—C2	168.0 (2)	C2—C1—C6—C5	−1.0 (4)
C13—C17—C16—C15	−0.4 (3)	C7—C1—C6—C5	−175.7 (2)
C9—C17—C16—C15	−179.3 (2)	C1—C6—C5—C4	1.7 (4)
C9—N2—C8—N1	176.8 (2)	C6—C5—C4—C3	−1.6 (4)
C9—N2—C8—S1	−4.2 (3)	C17—C9—C10—C11	−0.3 (3)
C7—N1—C8—N2	−1.6 (3)	N2—C9—C10—C11	176.3 (2)
C7—N1—C8—S1	179.31 (18)	C12—C11—C10—C9	0.6 (4)
N3—C13—C12—C11	179.8 (2)	C5—C4—C3—C2	0.9 (4)
C17—C13—C12—C11	0.0 (3)	C1—C2—C3—C4	−0.3 (4)
C13—C17—C9—C10	−0.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H6···N3^{i}	0.825 (17)	2.283 (17)	3.100 (3)	170.5 (18)
N2—H7···O1	0.91 (3)	1.84 (3)	2.619 (3)	143 (3)
C6—H5···N3^{i}	0.93	2.46	3.252 (3)	143

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

Fig. 1

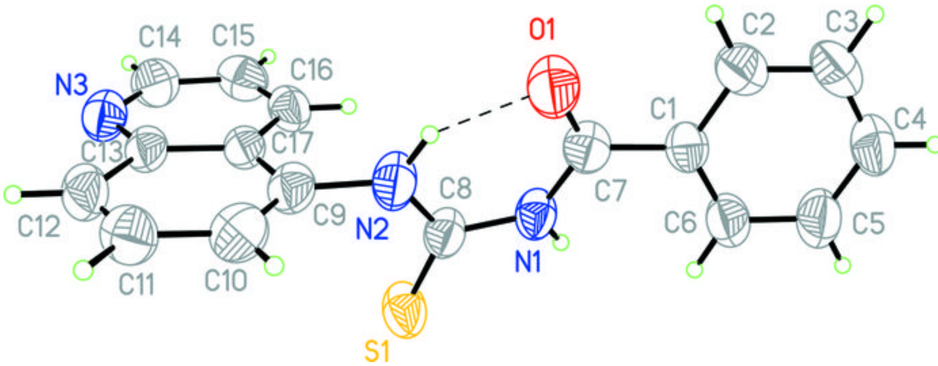
O1
C2
C3
C14
C15
C16
N3
C1
C4
C13
C17
C8
C7
C12
C9
N2
N1
C6
C5
C11
C10
S1

Fig. 2