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Crystallographic study of self-organization in the solid state including quasi-aromatic pseudo-ring stacking interactions in 1-benzoyl-3-(3,4-dimethoxyphenyl)thiourea and 1-benzoyl-3-(2-hydroxypropyl)thiourea

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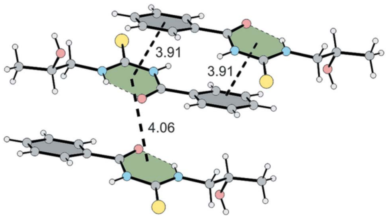
1-Benzoylthioureas contain both carbonyl and thiocarbonyl functional groups and are of interest for their biological activity, metal coordination ability and involvement in hydrogen-bond formation. Two novel 1-benzoylthiourea derivatives, namely 1-benzoyl-3-(3,4-dimethoxyphenyl)thiourea, $C_{16}H_{16}N_2O_3S$, (I), and 1-benzoyl-3-(2-hydroxypropyl)thiourea, $C_{11}H_{14}N_2O_2S$, (II), have been synthesized and characterized. Compound (I) crystallizes in the space group $P\overline{1}$, while (II) crystallizes in the space group $P2_1/c$. In both structures, intramolecular $N—H\cdots O$ hydrogen bonding is present. The resulting six-membered pseudo-rings are quasi-aromatic and, in each case, interact with phenyl rings *via* stacking-type interactions. $C—H\cdots O$, $C—H\cdots S$ and $C—H\cdots\pi$ interactions are also present. In (I), there is one molecule in the asymmetric unit. Pairs of molecules are connected *via* two intermolecular $N—H\cdots S$ hydrogen bonds, forming centrosymmetric dimers. In (II), there are two symmetry-independent molecules that differ mainly in the relative orientations of the phenyl rings with respect to the thiourea cores. Additional strong hydrogen-bond donor and acceptor –OH groups participate in the formation of intermolecular $N—H\cdots O$ and $O—H\cdots S$ hydrogen bonds that join molecules into chains extending in the [001] direction.



1. Introduction

A few years ago, we became interested in the properties and crystal structures of thioureas (Okuniewski *et al.*, 2011*a*,*b*; Mietlarek-Kropidłowska *et al.*, 2012). Recently, we have focused our attention on especially interesting 1-benzoylthioureas as they simultaneously contain carbonyl and thiocarbonyl functions (Okuniewski *et al.*, 2012). Because of their biological activity, metal coordination ability and involvement in hydrogen-bond formation (Aly *et al.*, 2007; Saeed *et al.*, 2013, 2016), they are the subject of extensive research, with several hundred structures deposited to the Cambridge Structural Database (CSD; Groom *et al.*, 2016).

In most structures of 3-monosubstituted 1-benzoylthioureas, intramolecular $N—H\cdots O$ hydrogen bonds are present and form six-membered pseudo-rings. These rings exhibit some aromatic properties and, for this reason, are called quasi-aromatic (Karabıyık *et al.*, 2012). For some time, we have been searching for novel examples of such quasi-aromatic ring interactions. For this reason, we have prepared two 1-benzoylthiourea derivatives that contain such rings. The first compound contains an aromatic substituent, while the second contains an aliphatic substituent, both with additional O atoms

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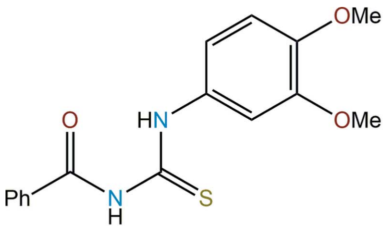
Table 1
Experimental details.

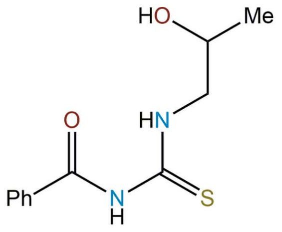
	(I)	(II)
Crystal data		
Chemical formula	$C_{16}H_{16}N_2O_3S$	$C_{11}H_{14}N_2O_2S$
M_r	316.37	238.3
Crystal system, space group	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/c$
Temperature (K)	293	293
a, b, c (Å)	6.5450 (4), 9.3526 (6), 12.7820 (8)	22.4150 (17), 8.1479 (5), 13.4592 (9)
α, β, γ (°)	94.047 (5), 93.143 (5), 95.735 (5)	90, 102.618 (7), 90
V (Å^3)	775.05 (8)	2398.8 (3)
Z	2	8
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.22	0.26
Crystal size (mm)	0.73 × 0.41 × 0.27	0.52 × 0.46 × 0.14
Data collection		
Diffractometer	Agilent Xcalibur (Sapphire2, large Be window)	Agilent Xcalibur (Sapphire2, large Be window)
Absorption correction	Analytical [*CrysAlis PRO* (Agilent, 2013), based on expressions derived by Clark & Reid (1995)]	Analytical [*CrysAlis PRO* (Agilent, 2013), based on expressions derived by Clark & Reid (1995)]
T_{min}, T_{max}	0.923, 0.959	0.911, 0.971
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4858, 3039, 1883	8922, 4710, 2847
R_{int}	0.026	0.038
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617	0.617
Refinement		
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.071, 0.209, 1.04	0.066, 0.220, 1.04
No. of reflections	3039	4710
No. of parameters	201	293
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.59, −0.25	0.71, −0.30

Computer programs: *CrysAlis PRO* (Agilent, 2013), *SHELXS2013* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

that can participate in hydrogen bonding. The compounds are 1-benzoyl-3-(3,4-dimethoxyphenyl)thiourea, (I), and 1-benzoyl-3-(2-hydroxypropyl)thiourea, (II), and the crystal structures were determined by single-crystal X-ray diffraction.



(I)



(II)

2. Experimental

2.1. Synthesis and crystallization

Both title compounds were synthesized according to a procedure proposed by Douglass & Dains (1934). Ammonium thiocyanate (46 mmol, 3.50 g) and dry acetone (30 ml) were placed in a two-necked flask. Through a dropping funnel, benzoyl chloride (40 mmol, 4.64 ml) in acetone (20 ml) was added with stirring. When addition was complete, the mixture was refluxed for an additional 15 min and then amine [40 mmol; 6.13 g of 3,4-dimethoxyaniline for (I) and 3.09 ml of 1-aminopropan-2-ol for (II)] in acetone (20 ml) was added through the dropping funnel. The mixture was poured carefully into cold water (500 ml) with stirring. In the case of (I), the resulting precipitate was filtered on a Büchner funnel. The crude product was recrystallized from acetone. In the case of (II), the resulting oil was extracted with toluene, dried with anhydrous magnesium sulfate and left to evaporate slowly. In both cases, colourless single crystals suitable for X-ray diffraction analysis were isolated.

2.2. Analytic and spectroscopic data

2.2.1. 1-Benzoyl-3-(3,4-dimethoxyphenyl)thiourea, (I). For (I), yield 79%; m.p. 403 (1) K; ^{1}H NMR (500 MHz, COMe$_2$-d_6): δ 12.71 (*s*, 1H), 10.22 (*s*, 1H), 8.10–6.95 (*m*, 8H), 3.85 (*s*, 6H); ^{1}H NMR (400 MHz, CDCl$_3$): δ 12.52 (*s*, 1H), 9.15 (*s*, 1H), 7.94–6.89 (*m*, 8H), 3.91 (*s*, 3H), 3.90 (*s*, 3H); ^{13}C NMR (101 MHz, CDCl$_3$): δ 178.09, 167.01, 148.84, 147.70, 133.73, 131.64, 130.80, 129.21 (2C), 127.51 (2C), 116.35, 110.90, 108.18, 56.06 (2C).

2.2.2. 1-Benzoyl-3-(2-hydroxypropyl)thiourea, (II). For (II), yield 66%; m.p. 408 (1) K; ^{1}H NMR (500 MHz, COMe$_2$-d_6): δ 11.10 (*s*, 1H), 10.05 (*s*, 1H), 8.10–7.50 (*m*, 5H), 4.23 (*d*, J = 4.8 Hz, 1H), 4.16–4.05 (*m*, 1H), 3.92–3.84 (*m*, 1H), 3.55–3.46 (*m*, 1H), 1.24 (*d*, J = 6.3 Hz, 3H); ^{1}H NMR (400 MHz, CDCl$_3$): δ 11.03 (*t*, J = 5.4 Hz, 1H), 9.30 (*s*, 1H), 7.88–7.25 (*m*, 5H), 4.25–4.12 (*m*, 1H), 3.91 (*ddd*, J = 13.8, 6.0, 3.5 Hz, 1H), 3.57 (*ddd*, J = 13.8, 7.9, 5.0 Hz, 1H), 2.89 (*s*, 1H), 1.28 (*d*, J = 6.3 Hz, 3H); ^{13}C

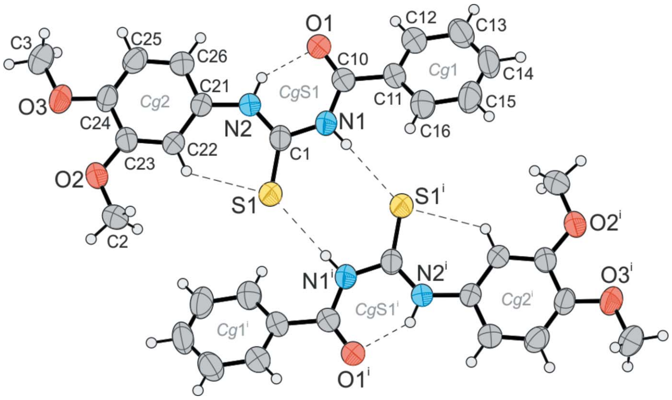


Figure 1
The structure of the centrosymmetric dimer found in (I). Displacement ellipsoids are drawn at the 50% probability level. Selected hydrogen bonds are marked with dashed lines. [Symmetry code: (i) $-x+1, -y+1, -z$.]

NMR (101 MHz, $CDCl_3$): δ 180.44, 167.02, 133.51, 131.71, 129.02 (2C), 127.61 (2C), 66.10, 52.65, 21.16.

2.3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were placed at calculated positions (C—H = 0.93–0.98 Å, N—H = 0.86 Å and O—H = 0.82 Å) and were treated as riding on their parent atoms, with $U_{\rm iso}$(H) values set at 1.2–1.5$U_{\rm eq}$(C), 1.2$U_{\rm eq}$(N) or 1.5$U_{\rm eq}$(O).

3. Results and discussion

The molecules of compounds (I) and (II) (Figs. 1 and 2) both adopt an S-type conformation (Woldu & Dillen, 2008), with intramolecular N—H···O hydrogen bonds (for their parameters, see Tables 2 and 3) forming an *S*(6) motif (Etter, 1990) that is common among 3-monosubstituted 1-acylthioureas (Okuniewski *et al.*, 2012). The resulting six-membered pseudo-rings are quasi-aromatic (Karabıyık *et al.*, 2012). The HOMA indices of aromaticity (Krygowski, 1993) are equal to 0.80 [(I), *Cg*S1], 0.74 [(II), *Cg*S1] and 0.78 [(II), *Cg*S3], indicating that such motifs are rather aromatic. The mean HOMA value for O/C/N/C/N/H hydrogen-bridged chelate rings that interact with phenyl groups in the 153 compounds deposited to the CSD (Groom *et al.*, 2016) is equal to 0.78 (5) (Okuniewski *et al.*, 2015).

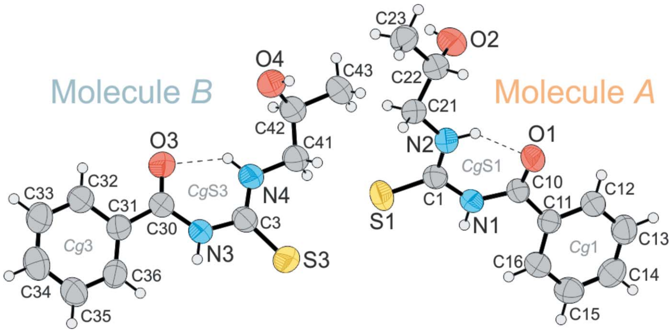


Figure 2
The structure of the two symmetry-independent molecules found in (II). Displacement ellipsoids are drawn at the 50% probability level. Selected hydrogen bonds are marked with dashed lines.

Table 2
Hydrogen-bond geometry (Å, °) for (I).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1	0.86	1.9	2.633 (3)	143
N1—H1···S1$^{\rm i}$	0.86	2.79	3.485 (3)	139
C14—H14···O2$^{\rm ii}$	0.93	2.52	3.453 (4)	178
C22—H22···S1	0.93	2.54	3.203 (3)	129

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

Compound (I) is a derivative of 1-benzoyl-3-phenylthiourea (Yamin & Yusof, 2003) substituted with two methoxy groups (Fig. 1). It crystallizes in the space group $P\overline{1}$ with one molecule in the asymmetric unit. The $(MeO)_2C_6H_3NHC(S)NHC(O)$ fragment is almost flat (the maximum distances from the mean plane *d* are 0.26 Å for atoms S1 and C3). The planarity of this fragment is reinforced by intramolecular a C22—H22···S1 interaction [motif *S*(6)]. The phenyl ring of the benzoyl group is twisted; it forms a dihedral angle of 31° with the mean plane of the thiourea core, *i.e.* the NC(S)N fragment.

The molecules are connected *via* N1—H1···S1$^{\rm i}$ hydrogen bonds (Fig. 3 and Table 2) into centrosymmetric dimers with

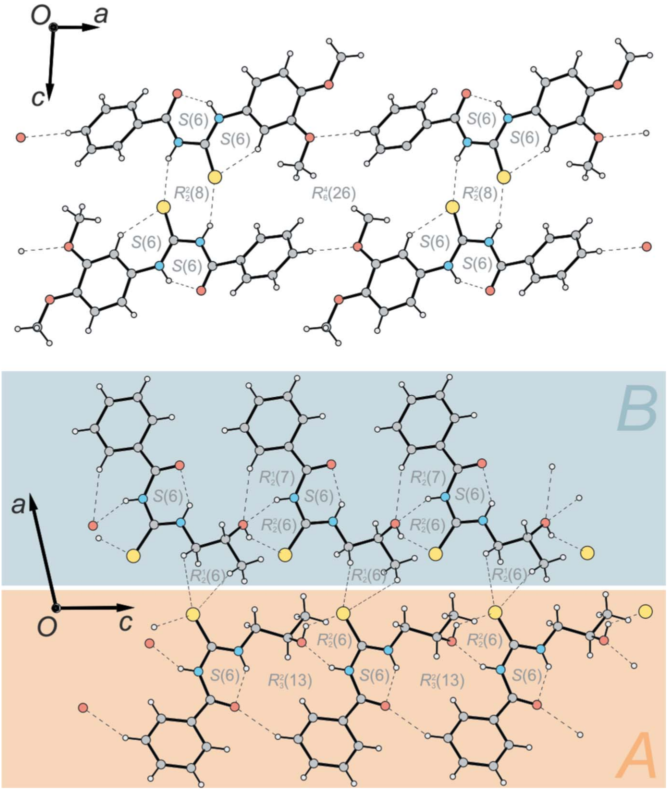


Figure 3
Hydrogen bonds, C—H···(O,S) interactions and selected motifs present in the structures of (I) (top) and (II) (bottom), viewed in the [0$\overline{1}$0] direction. In the case of (II), the background colours correspond to the colour codes of symmetrically independent molecules (for designations, see Fig. 2).

an $R_2^2(8)$ motif. Additionally, quite strong C14—H14···O2$^{\rm ii}$ interactions connect molecules into chains with a $C(13)$ motif extending in the [210] direction.

The quasi-aromatic pseudo-rings form interactions with phenyl groups [CgS1···$Cg1^{\rm iii}$ (d = 4.10 Å and α = 30°) and CgS1···$Cg2^{\rm iv}$ (d = 3.83 Å and α = 8°); symmetry codes: (iii) $x - 1, y, z$; (iv) $x + 1, y, z$], so molecules are stacked one over another. These interactions are depicted in Fig. 4.

Compound (II) is a hydroxy derivative of 1-benzoyl-3-propylthiourea (Dago *et al.*, 1989). Its molecules are chiral, but the crystal is formed out of a racemic mixture that crystallizes in the centrosymmetric space group $P2_1/c$. In the asymmetric unit, there are two similar molecules (molecule A refers to the molecule containing atom S1, while the second molecule, containing atom S3, will be referred to as B; see: Fig. 2). The planes of the phenyl rings in both molecules are at different dihedral angles in relation to the mean plane of the thiourea core, *viz. ca* 19° for molecule A and *ca* 5° for molecule B. If these two molecules are superimposed with respect to the NC(S)NC(O) group (r.m.s. deviation = 0.033 Å), then it is revealed that the conformations of the $CH_2CH(OH)CH_3$ groups are also slightly different.

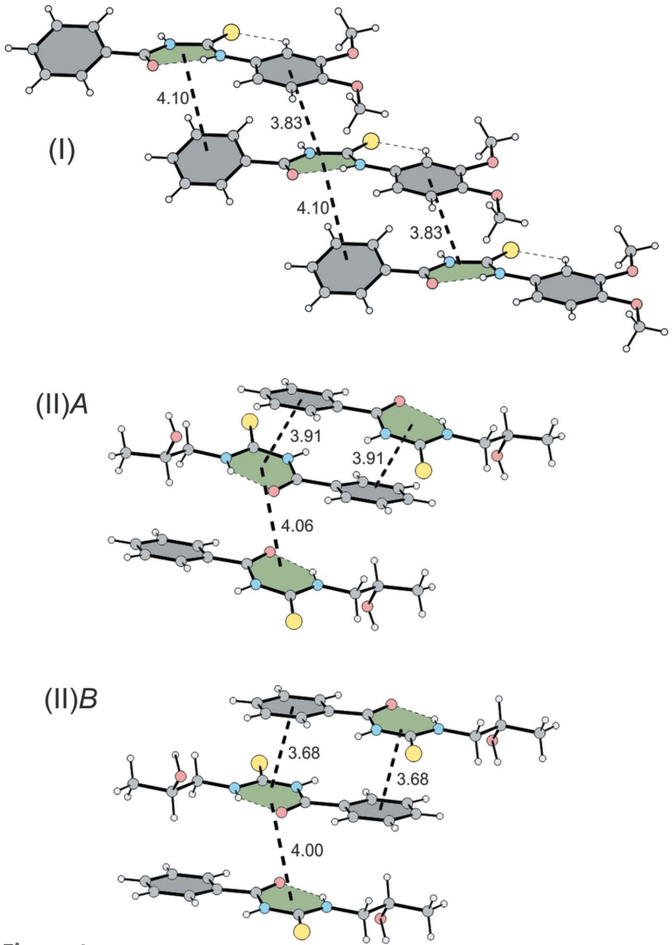


Figure 4
Stacking-type interactions found in (I) and (II). Ordinary aromatic rings are drawn as gray planes, while quasiaromatic pseudo-rings are coloured green. Centroid–centroid distances are marked with bold dashed lines and their values are provided in Å.

Table 3
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2$^{\rm i}$	0.86	2.2	2.977 (3)	151
N2—H2···O1	0.86	1.94	2.632 (3)	137
O2—H2A···S1$^{\rm ii}$	0.82	2.66	3.242 (3)	130
N3—H3···O4$^{\rm i}$	0.86	2.21	2.999 (4)	153
N4—H4···O3	0.86	1.96	2.640 (4)	135
O4—H4A···S3$^{\rm ii}$	0.82	2.41	3.161 (3)	152
C15—H15···O1$^{\rm i}$	0.93	2.53	3.265 (4)	136
C36—H36···O4$^{\rm i}$	0.93	2.57	3.412 (5)	150
C21—H21B···S3$^{\rm ii}$	0.97	2.98	3.844 (4)	149
C23—H23C···S3$^{\rm ii}$	0.96	2.98	3.842 (4)	150

Symmetry codes: (i) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (ii) $x, -y + \frac{3}{2}, z + \frac{1}{2}$.

Strong hydrogen-bond donor and acceptor –OH groups participate in the formation of intermolecular hydrogen bonds that join the molecules of (II) into chains extending in the [001] direction with a $C(7)R_2^2(6)$ motif: N1—H1···O2$^{\rm i}$ and O2—H2A···S1$^{\rm ii}$ for molecule A and N3—H3···O4$^{\rm i}$ and O4—H4A···S3$^{\rm ii}$ for molecule B (Table 3). Hydrogen bonds are formed only within the symmetry equivalents of molecules, so that two types of chains can be distinguished, *i.e.* ···A—A—A··· and ···B—B—B··· (Fig. 3), both of $\not{p}c11$ (R5) rod group symmetry (*International Tables for Crystallography*, 2010).

Chains of B molecules are additionally stabilized by a C36—H36···O4$^{\rm i}$ interaction, while a greater twist of the phenyl ring in molecule A causes the corresponding interaction to be insignificant. On the other hand, in the chains of A molecules, the C15—H15···O1$^{\rm i}$ interaction is stronger than the corresponding interaction in molecule B (Fig. 3). Overall, molecules B form stronger interactions with each other (-23.7 kJ mol^{-1}) than do molecules A (-22.5 kJ mol^{-1}). The energies were estimated as counterpoise BSSE-corrected (Boys & Bernardi, 1970) differences of half of the energy of the dimer and the energy of isolated molecules, with normalized C—H (1.089 Å), N—H (1.015 Å) and O—H (0.993 Å) bond lengths, in *GAUSSIAN09* (Frisch *et al.*, 2009) at the MP2/6-31+G(d,p) level of theory. Chains A and B are interconnected by weak acceptor-bifurcated interactions, *i.e.* C21—H21B···S3$^{\rm ii}$ and C23—H23C···S3$^{\rm ii}$ (Fig. 3 and Table 3).

In (II), like in (I), quasi-aromatic pseudo-rings are involved in all parallel-displaced stacking-type interactions with phenyl rings [CgS1···$Cg1^{\rm iii}$ (d = 3.91 Å and α = 18°) and CgS3···$Cg3^{\rm iv}$ (d = 3.68 Å and α = 8°); symmetry codes: (iii) $-x, -y + 1, -z + 1$; (iv) $-x + 1, -y + 2, -z + 1$;], but also with each other [CgS1···CgS1$^{\rm iv}$ (d = 4.06 Å, α = 0° and slippage = 2.52 Å), CgS3···CgS3$^{\rm v}$ (d = 4.00 Å, α = 0° and slippage = 2.14 Å); symmetry code: (v) $-x + 1, -y + 1, -z + 1$]. In the latter two interactions, the mid-points of the centroid–centroid distances are the centres of inversion. Stacking interactions for (II) are depicted in Fig. 4.

4. Conclusions

Both achiral (I) and racemic (II) crystallize in centrosymmetric space groups. Intramolecular N—H···O hydrogen bonds allow the formation of quasi-aromatic pseudo-rings. In both (I) and (II), all the stacking interactions involve such rings (they interact with phenyl rings or with each other). Weak C—H···(O,S) interactions also play an important role in the formation of the three-dimensional structures of the crystals. Our results are further confirmation that hydrogen-bridged chelate rings are formed readily within 3-mono-substituted 1-benzoylthioureas and that such quasi-aromatic rings have a significant contribution to the stabilization of the crystal structures.

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supporting information

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Crystallographic study of self-organization in the solid state including quasi-aromatic pseudo-ring stacking interactions in 1-benzoyl-3-(3,4-dimethoxyphenyl)thiourea and 1-benzoyl-3-(2-hydroxypropyl)thiourea

Andrzej Okuniewski, Damian Rosiak, Jarosław Chojnacki and Barbara Becker

Computing details

For both compounds, data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO* (Agilent, 2013); data reduction: *CrysAlis PRO* (Agilent, 2013); program(s) used to solve structure: *SHELXS2016* (Sheldrick, 2015); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

(I) *N*-[(3,4-Dimethoxyphenyl)carbamothioyl]benzamide

Crystal data

$C_{16}H_{16}N_2O_3S$
$M_r = 316.37$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.5450\ (4)$ Å
$b = 9.3526\ (6)$ Å
$c = 12.7820\ (8)$ Å
$\alpha = 94.047\ (5)°$
$\beta = 93.143\ (5)°$
$\gamma = 95.735\ (5)°$
$V = 775.05\ (8)$ Å^3

$Z = 2$
$F(000) = 332$
$D_x = 1.356$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1629 reflections
$\theta = 2.7–26.2°$
$\mu = 0.22$ mm^{-1}
$T = 293$ K
Prism, colourless
0.73 × 0.41 × 0.27 mm

Data collection

Agilent Xcalibur (Sapphire2, large Be window) diffractometer
Graphite monochromator
Detector resolution: 8.1883 pixels mm^{-1}
ω scans
Absorption correction: analytical [CrysAlis PRO (Agilent, 2013), based on expressions derived by Clark & Reid (1995)]
$T_{min} = 0.923$, $T_{max} = 0.959$

4858 measured reflections
3039 independent reflections
1883 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.6°$
$h = -6 \rightarrow 8$
$k = -11 \rightarrow 10$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.071$
$wR(F^2) = 0.209$
$S = 1.04$

3039 reflections
201 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained	$(\Delta/\sigma)_{max} < 0.001$
$w = 1/[\sigma^2(F_o^2) + (0.1069P)^2 + 0.0208P]$ where $P = (F_o^2 + 2F_c^2)/3$	$\Delta\rho_{max} = 0.59$ e Å^{-3} $\Delta\rho_{min} = -0.25$ e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
S1	0.32892 (14)	0.32856 (10)	0.05322 (7)	0.0746 (4)
C1	0.4131 (5)	0.4076 (3)	0.1704 (2)	0.0525 (8)
N1	0.5964 (4)	0.4994 (3)	0.1768 (2)	0.0573 (7)
H1	0.657793	0.504603	0.119202	0.069*
C10	0.6924 (5)	0.5822 (3)	0.2617 (3)	0.0532 (8)
O1	0.6254 (3)	0.5821 (3)	0.34928 (18)	0.0712 (7)
C11	0.8843 (4)	0.6730 (3)	0.2414 (2)	0.0539 (8)
C12	0.9348 (5)	0.7985 (4)	0.3058 (3)	0.0662 (10)
H12	0.847406	0.823665	0.357432	0.079*
C13	1.1126 (6)	0.8867 (4)	0.2942 (3)	0.0781 (11)
H13	1.145054	0.970734	0.337792	0.094*
C14	1.2425 (5)	0.8490 (5)	0.2174 (3)	0.0797 (12)
H14	1.363019	0.907938	0.209513	0.096*
C15	1.1947 (5)	0.7253 (4)	0.1527 (3)	0.0740 (11)
H15	1.282663	0.701004	0.101048	0.089*
C16	1.0151 (5)	0.6361 (4)	0.1640 (3)	0.0635 (9)
H16	0.982791	0.552392	0.120094	0.076*
N2	0.3251 (4)	0.3968 (3)	0.26128 (19)	0.0560 (7)
H2	0.397118	0.442046	0.313960	0.067*
C21	0.1357 (4)	0.3255 (3)	0.2886 (2)	0.0502 (8)
C22	0.0066 (5)	0.2298 (3)	0.2205 (2)	0.0544 (8)
H22	0.043178	0.207574	0.152455	0.065*
C23	−0.1769 (5)	0.1676 (3)	0.2545 (2)	0.0539 (8)
C24	−0.2322 (5)	0.2002 (3)	0.3560 (3)	0.0537 (8)
C25	−0.1021 (5)	0.2949 (4)	0.4232 (3)	0.0621 (9)
H25	−0.138185	0.317599	0.491289	0.075*
C26	0.0820 (5)	0.3560 (4)	0.3894 (3)	0.0597 (9)
H26	0.169978	0.418272	0.435404	0.072*
C2	−0.2492 (6)	0.0273 (4)	0.0926 (3)	0.0800 (12)
H2A	−0.235014	0.109237	0.051399	0.120*
H2B	−0.351384	−0.044283	0.058549	0.120*
H2C	−0.119844	−0.012469	0.099279	0.120*
O2	−0.3101 (3)	0.0704 (3)	0.19344 (18)	0.0705 (7)
C3	−0.4927 (6)	0.1837 (5)	0.4788 (3)	0.0822 (12)
H3A	−0.402770	0.159968	0.535411	0.123*
H3B	−0.628717	0.137493	0.485211	0.123*

H3C	−0.496586	0.286205	0.481580	0.123*
O3	−0.4187 (3)	0.1352 (3)	0.38104 (18)	0.0715 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0804 (7)	0.0811 (7)	0.0543 (6)	−0.0276 (5)	0.0185 (5)	−0.0112 (5)
C1	0.0475 (18)	0.0529 (19)	0.056 (2)	−0.0036 (14)	0.0098 (14)	0.0031 (15)
N1	0.0499 (15)	0.0656 (18)	0.0532 (16)	−0.0093 (13)	0.0125 (12)	−0.0025 (13)
C10	0.0481 (18)	0.059 (2)	0.0511 (19)	−0.0005 (15)	0.0031 (14)	0.0002 (15)
O1	0.0658 (15)	0.0902 (18)	0.0508 (14)	−0.0209 (12)	0.0091 (11)	−0.0049 (12)
C11	0.0447 (18)	0.059 (2)	0.056 (2)	−0.0046 (14)	0.0013 (14)	0.0027 (15)
C12	0.063 (2)	0.071 (2)	0.061 (2)	−0.0083 (18)	0.0038 (16)	−0.0002 (17)
C13	0.073 (3)	0.073 (3)	0.081 (3)	−0.018 (2)	−0.010 (2)	0.009 (2)
C14	0.051 (2)	0.091 (3)	0.093 (3)	−0.021 (2)	−0.002 (2)	0.026 (2)
C15	0.050 (2)	0.091 (3)	0.083 (3)	0.0012 (19)	0.0157 (18)	0.021 (2)
C16	0.052 (2)	0.067 (2)	0.071 (2)	0.0025 (16)	0.0069 (16)	0.0079 (18)
N2	0.0535 (15)	0.0650 (18)	0.0453 (15)	−0.0131 (13)	0.0068 (12)	−0.0015 (12)
C21	0.0500 (18)	0.0528 (19)	0.0462 (18)	−0.0044 (14)	0.0094 (13)	0.0029 (13)
C22	0.0534 (18)	0.063 (2)	0.0443 (17)	−0.0072 (15)	0.0099 (14)	−0.0006 (14)
C23	0.0507 (19)	0.0526 (19)	0.056 (2)	−0.0052 (14)	0.0073 (14)	0.0011 (15)
C24	0.0498 (18)	0.0535 (19)	0.059 (2)	0.0003 (15)	0.0186 (15)	0.0057 (15)
C25	0.071 (2)	0.061 (2)	0.055 (2)	0.0026 (17)	0.0228 (16)	0.0009 (16)
C26	0.062 (2)	0.063 (2)	0.0510 (19)	−0.0061 (16)	0.0082 (15)	−0.0026 (15)
C2	0.075 (2)	0.097 (3)	0.059 (2)	−0.022 (2)	0.0073 (18)	−0.016 (2)
O2	0.0577 (14)	0.0827 (17)	0.0639 (15)	−0.0223 (12)	0.0134 (11)	−0.0108 (12)
C3	0.066 (2)	0.108 (3)	0.074 (3)	0.001 (2)	0.0301 (19)	0.005 (2)
O3	0.0632 (15)	0.0813 (17)	0.0683 (16)	−0.0092 (12)	0.0278 (12)	−0.0020 (12)

Geometric parameters (Å, º)

S1—C1	1.663 (3)	C21—C26	1.372 (4)
C1—N2	1.330 (4)	C21—C22	1.389 (4)
C1—N1	1.399 (4)	C22—C23	1.387 (4)
N1—C10	1.372 (4)	C22—H22	0.9300
N1—H1	0.8600	C23—O2	1.365 (4)
C10—O1	1.224 (4)	C23—C24	1.387 (4)
C10—C11	1.490 (4)	C24—O3	1.373 (3)
C11—C12	1.386 (4)	C24—C25	1.382 (5)
C11—C16	1.391 (4)	C25—C26	1.386 (4)
C12—C13	1.379 (5)	C25—H25	0.9300
C12—H12	0.9300	C26—H26	0.9300
C13—C14	1.384 (6)	C2—O2	1.414 (4)
C13—H13	0.9300	C2—H2A	0.9600
C14—C15	1.373 (5)	C2—H2B	0.9600
C14—H14	0.9300	C2—H2C	0.9600
C15—C16	1.392 (4)	C3—O3	1.426 (4)
C15—H15	0.9300	C3—H3A	0.9600

C16—H16	0.9300	C3—H3B	0.9600
N2—C21	1.421 (3)	C3—H3C	0.9600
N2—H2	0.8600		

N2—C1—N1	114.3 (3)	C26—C21—N2	116.0 (3)
N2—C1—S1	127.9 (2)	C22—C21—N2	124.3 (3)
N1—C1—S1	117.8 (2)	C23—C22—C21	119.7 (3)
C10—N1—C1	129.3 (3)	C23—C22—H22	120.1
C10—N1—H1	115.3	C21—C22—H22	120.1
C1—N1—H1	115.3	O2—C23—C22	123.4 (3)
O1—C10—N1	122.4 (3)	O2—C23—C24	116.1 (3)
O1—C10—C11	121.6 (3)	C22—C23—C24	120.4 (3)
N1—C10—C11	116.1 (3)	O3—C24—C25	124.8 (3)
C12—C11—C16	119.3 (3)	O3—C24—C23	115.8 (3)
C12—C11—C10	117.2 (3)	C25—C24—C23	119.4 (3)
C16—C11—C10	123.5 (3)	C24—C25—C26	120.1 (3)
C13—C12—C11	120.9 (3)	C24—C25—H25	119.9
C13—C12—H12	119.5	C26—C25—H25	119.9
C11—C12—H12	119.5	C21—C26—C25	120.6 (3)
C12—C13—C14	119.5 (4)	C21—C26—H26	119.7
C12—C13—H13	120.3	C25—C26—H26	119.7
C14—C13—H13	120.3	O2—C2—H2A	109.5
C15—C14—C13	120.4 (3)	O2—C2—H2B	109.5
C15—C14—H14	119.8	H2A—C2—H2B	109.5
C13—C14—H14	119.8	O2—C2—H2C	109.5
C14—C15—C16	120.3 (3)	H2A—C2—H2C	109.5
C14—C15—H15	119.9	H2B—C2—H2C	109.5
C16—C15—H15	119.9	C23—O2—C2	117.0 (2)
C11—C16—C15	119.6 (3)	O3—C3—H3A	109.5
C11—C16—H16	120.2	O3—C3—H3B	109.5
C15—C16—H16	120.2	H3A—C3—H3B	109.5
C1—N2—C21	132.8 (3)	O3—C3—H3C	109.5
C1—N2—H2	113.6	H3A—C3—H3C	109.5
C21—N2—H2	113.6	H3B—C3—H3C	109.5
C26—C21—C22	119.7 (3)	C24—O3—C3	116.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1	0.86	1.90	2.633 (3)	143
N1—H1···S1^{i}	0.86	2.79	3.485 (3)	139
C22—H22···S1	0.93	2.54	3.203 (3)	129
C14—H14···O2^{ii}	0.93	2.52	3.453 (4)	178

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

(II) *N*-[(2-Hydroxypropyl)carbamothioyl]benzamide

Crystal data

$C_{11}H_{14}N_2O_2S$
$M_r = 238.3$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 22.4150$ (17) Å
$b = 8.1479$ (5) Å
$c = 13.4592$ (9) Å
$\beta = 102.618$ (7)°
$V = 2398.8$ (3) Å^3
$Z = 8$
$F(000) = 1008$
$D_x = 1.32$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2940 reflections
$\theta = 3.0$–27.0°
$\mu = 0.26$ mm^{-1}
$T = 293$ K
Prism, colourless
0.52 × 0.46 × 0.14 mm

Data collection

Agilent Xcalibur (Sapphire2, large Be window) diffractometer
Graphite monochromator
Detector resolution: 8.1883 pixels mm^{-1}
ω scans
Absorption correction: analytical [CrysAlis PRO (Agilent, 2013), based on expressions derived by Clark & Reid (1995)]
$T_{min} = 0.911$, $T_{max} = 0.971$
8922 measured reflections
4710 independent reflections
2847 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 26°$, $\theta_{min} = 2.7°$
$h = -27 \rightarrow 26$
$k = -10 \rightarrow 5$
$l = -12 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.220$
$S = 1.04$
4710 reflections
293 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1058P)^2 + 0.9789P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.71$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
S1	0.19684 (4)	0.87980 (15)	0.50453 (8)	0.0834 (4)
C1	0.13064 (15)	0.8780 (4)	0.5415 (2)	0.0551 (8)
N1	0.08038 (11)	0.7993 (3)	0.47955 (18)	0.0544 (6)
H1	0.086382	0.757529	0.423876	0.065*
C10	0.02251 (13)	0.7809 (4)	0.4973 (2)	0.0536 (7)
O1	0.00807 (11)	0.8385 (3)	0.57212 (18)	0.0733 (7)
C11	−0.02165 (14)	0.6848 (4)	0.4201 (2)	0.0513 (7)
C12	−0.07310 (15)	0.6253 (4)	0.4510 (3)	0.0628 (9)
H12	−0.078547	0.648068	0.516116	0.075*

C13	−0.11598 (17)	0.5328 (4)	0.3850 (3)	0.0715 (10)
H13	−0.150034	0.492347	0.405936	0.086*
C14	−0.10823 (17)	0.5005 (4)	0.2880 (3)	0.0694 (9)
H14	−0.137038	0.437750	0.243800	0.083*
C15	−0.05831 (17)	0.5604 (4)	0.2565 (3)	0.0691 (9)
H15	−0.053570	0.539344	0.190748	0.083*
C16	−0.01498 (16)	0.6522 (4)	0.3224 (2)	0.0601 (8)
H16	0.018903	0.692269	0.300705	0.072*
N2	0.12153 (12)	0.9439 (3)	0.62596 (19)	0.0591 (7)
H2	0.085767	0.934134	0.638807	0.071*
C21	0.16758 (15)	1.0322 (4)	0.6993 (2)	0.0606 (8)
H21A	0.174053	1.139570	0.672334	0.073*
H21B	0.205956	0.972713	0.710785	0.073*
C22	0.14791 (16)	1.0517 (4)	0.7982 (2)	0.0632 (9)
H22	0.108336	1.108048	0.782686	0.076*
C23	0.19148 (17)	1.1614 (5)	0.8704 (3)	0.0723 (10)
H23A	0.179488	1.166057	0.934629	0.108*
H23B	0.190453	1.269822	0.842165	0.108*
H23C	0.232187	1.118107	0.880391	0.108*
O2	0.13845 (13)	0.9014 (3)	0.8418 (2)	0.0840 (8)
H2A	0.171519	0.861159	0.868999	0.126*
S3	0.31682 (5)	0.65289 (16)	0.35460 (8)	0.0899 (4)
C3	0.38036 (16)	0.6539 (4)	0.4467 (2)	0.0604 (8)
N3	0.43299 (12)	0.7287 (3)	0.42895 (19)	0.0606 (7)
H3	0.429205	0.776266	0.370866	0.073*
C30	0.49006 (15)	0.7366 (4)	0.4918 (2)	0.0583 (8)
O3	0.50078 (11)	0.6740 (4)	0.57620 (19)	0.0813 (8)
C31	0.53756 (15)	0.8255 (4)	0.4511 (2)	0.0577 (8)
C32	0.59318 (17)	0.8526 (5)	0.5187 (3)	0.0763 (11)
H32	0.599071	0.815394	0.585456	0.092*
C33	0.63991 (19)	0.9348 (5)	0.4869 (3)	0.0855 (12)
H33	0.676964	0.953283	0.532325	0.103*
C34	0.63133 (18)	0.9883 (5)	0.3887 (3)	0.0778 (11)
H34	0.662525	1.044306	0.367595	0.093*
C35	0.57669 (18)	0.9599 (5)	0.3207 (3)	0.0820 (11)
H35	0.571295	0.995335	0.253641	0.098*
C36	0.53014 (16)	0.8791 (5)	0.3522 (3)	0.0730 (10)
H36	0.493314	0.860439	0.306177	0.088*
N4	0.38426 (13)	0.5899 (3)	0.5372 (2)	0.0658 (8)
H4	0.419002	0.591900	0.579720	0.079*
C41	0.33257 (17)	0.5161 (5)	0.5688 (3)	0.0723 (10)
H41A	0.317194	0.425266	0.523817	0.087*
H41B	0.300098	0.596451	0.563276	0.087*
C42	0.34964 (17)	0.4567 (5)	0.6734 (3)	0.0744 (10)
H42	0.379516	0.368619	0.674185	0.089*
C43	0.29559 (19)	0.3810 (6)	0.7075 (3)	0.0959 (14)
H43A	0.308436	0.342723	0.776353	0.144*
H43B	0.280074	0.290445	0.663856	0.144*

H43C	0.264075	0.461939	0.703996	0.144*
O4	0.37882 (12)	0.5781 (4)	0.7412 (2)	0.0909 (9)
H4A	0.353521	0.645707	0.750645	0.136*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0569 (6)	0.1220 (9)	0.0779 (7)	−0.0110 (5)	0.0288 (5)	−0.0136 (6)
C1	0.0531 (18)	0.0614 (18)	0.0516 (17)	0.0057 (15)	0.0131 (14)	0.0080 (14)
N1	0.0511 (15)	0.0676 (16)	0.0471 (13)	0.0035 (13)	0.0163 (12)	0.0003 (12)
C10	0.0463 (17)	0.0658 (18)	0.0505 (16)	0.0060 (15)	0.0145 (14)	0.0035 (14)
O1	0.0551 (14)	0.1070 (18)	0.0625 (14)	−0.0042 (13)	0.0234 (11)	−0.0203 (13)
C11	0.0478 (17)	0.0562 (17)	0.0502 (16)	0.0087 (14)	0.0115 (13)	0.0036 (13)
C12	0.0552 (19)	0.077 (2)	0.0576 (19)	0.0030 (17)	0.0150 (16)	0.0076 (16)
C13	0.060 (2)	0.074 (2)	0.080 (2)	−0.0027 (18)	0.0150 (19)	0.0137 (19)
C14	0.067 (2)	0.061 (2)	0.074 (2)	−0.0034 (18)	0.0016 (18)	−0.0027 (17)
C15	0.079 (2)	0.071 (2)	0.059 (2)	−0.001 (2)	0.0166 (18)	−0.0064 (17)
C16	0.064 (2)	0.0615 (18)	0.0571 (18)	0.0009 (16)	0.0192 (16)	−0.0009 (15)
N2	0.0488 (15)	0.0744 (17)	0.0548 (15)	−0.0031 (13)	0.0130 (12)	−0.0024 (13)
C21	0.0554 (19)	0.073 (2)	0.0521 (17)	−0.0063 (16)	0.0102 (15)	0.0043 (15)
C22	0.062 (2)	0.069 (2)	0.0584 (19)	−0.0039 (17)	0.0130 (16)	−0.0015 (16)
C23	0.066 (2)	0.085 (2)	0.063 (2)	0.0008 (19)	0.0075 (17)	−0.0092 (18)
O2	0.0850 (18)	0.0949 (19)	0.0745 (17)	−0.0147 (16)	0.0226 (15)	0.0151 (14)
S3	0.0696 (7)	0.1317 (10)	0.0633 (6)	−0.0337 (6)	0.0031 (5)	0.0118 (6)
C3	0.062 (2)	0.0653 (19)	0.0564 (19)	−0.0084 (16)	0.0195 (16)	−0.0024 (15)
N3	0.0547 (16)	0.0760 (18)	0.0521 (15)	−0.0081 (14)	0.0137 (12)	0.0068 (13)
C30	0.0555 (19)	0.0667 (19)	0.0538 (18)	−0.0005 (16)	0.0141 (15)	0.0007 (16)
O3	0.0641 (16)	0.113 (2)	0.0638 (15)	−0.0126 (14)	0.0075 (12)	0.0215 (14)
C31	0.0533 (19)	0.0629 (19)	0.0570 (18)	−0.0002 (15)	0.0122 (15)	−0.0021 (15)
C32	0.068 (2)	0.098 (3)	0.062 (2)	−0.021 (2)	0.0129 (18)	−0.0093 (19)
C33	0.069 (2)	0.106 (3)	0.081 (3)	−0.028 (2)	0.015 (2)	−0.015 (2)
C34	0.069 (2)	0.070 (2)	0.100 (3)	−0.0127 (19)	0.030 (2)	−0.003 (2)
C35	0.069 (2)	0.097 (3)	0.083 (3)	−0.005 (2)	0.022 (2)	0.026 (2)
C36	0.0507 (19)	0.090 (2)	0.076 (2)	−0.0053 (19)	0.0087 (17)	0.0187 (19)
N4	0.0625 (17)	0.0811 (19)	0.0542 (16)	−0.0181 (15)	0.0138 (13)	0.0022 (13)
C41	0.068 (2)	0.091 (2)	0.059 (2)	−0.022 (2)	0.0153 (17)	−0.0016 (18)
C42	0.067 (2)	0.097 (3)	0.061 (2)	−0.018 (2)	0.0192 (17)	−0.003 (2)
C43	0.074 (3)	0.144 (4)	0.072 (3)	−0.028 (3)	0.022 (2)	0.017 (2)
O4	0.0747 (18)	0.133 (3)	0.0643 (16)	−0.0221 (17)	0.0133 (14)	−0.0206 (16)

Geometric parameters (Å, º)

S1—C1	1.665 (3)	S3—C3	1.671 (4)
C1—N2	1.313 (4)	C3—N4	1.311 (4)
C1—N1	1.402 (4)	C3—N3	1.394 (4)
N1—C10	1.378 (4)	N3—C30	1.373 (4)
N1—H1	0.8600	N3—H3	0.8600
C10—O1	1.217 (4)	C30—O3	1.220 (4)

C10—C11	1.491 (4)	C30—C31	1.488 (4)
C11—C16	1.382 (4)	C31—C36	1.376 (5)
C11—C12	1.395 (4)	C31—C32	1.391 (5)
C12—C13	1.381 (5)	C32—C33	1.387 (5)
C12—H12	0.9300	C32—H32	0.9300
C13—C14	1.379 (5)	C33—C34	1.364 (6)
C13—H13	0.9300	C33—H33	0.9300
C14—C15	1.370 (5)	C34—C35	1.379 (5)
C14—H14	0.9300	C34—H34	0.9300
C15—C16	1.383 (5)	C35—C36	1.377 (5)
C15—H15	0.9300	C35—H35	0.9300
C16—H16	0.9300	C36—H36	0.9300
N2—C21	1.453 (4)	N4—C41	1.449 (4)
N2—H2	0.8600	N4—H4	0.8600
C21—C22	1.500 (4)	C41—C42	1.459 (5)
C21—H21A	0.9700	C41—H41A	0.9700
C21—H21B	0.9700	C41—H41B	0.9700
C22—O2	1.394 (4)	C42—O4	1.407 (4)
C22—C23	1.511 (5)	C42—C43	1.517 (5)
C22—H22	0.9800	C42—H42	0.9800
C23—H23A	0.9600	C43—H43A	0.9600
C23—H23B	0.9600	C43—H43B	0.9600
C23—H23C	0.9600	C43—H43C	0.9600
O2—H2A	0.8200	O4—H4A	0.8200

N2—C1—N1	116.4 (3)	N4—C3—N3	116.5 (3)
N2—C1—S1	124.9 (3)	N4—C3—S3	124.1 (3)
N1—C1—S1	118.7 (2)	N3—C3—S3	119.4 (2)
C10—N1—C1	127.7 (3)	C30—N3—C3	128.7 (3)
C10—N1—H1	116.1	C30—N3—H3	115.7
C1—N1—H1	116.1	C3—N3—H3	115.7
O1—C10—N1	122.2 (3)	O3—C30—N3	121.5 (3)
O1—C10—C11	121.5 (3)	O3—C30—C31	122.3 (3)
N1—C10—C11	116.3 (3)	N3—C30—C31	116.2 (3)
C16—C11—C12	119.0 (3)	C36—C31—C32	118.9 (3)
C16—C11—C10	124.8 (3)	C36—C31—C30	124.5 (3)
C12—C11—C10	116.2 (3)	C32—C31—C30	116.6 (3)
C13—C12—C11	120.2 (3)	C33—C32—C31	120.3 (4)
C13—C12—H12	119.9	C33—C32—H32	119.9
C11—C12—H12	119.9	C31—C32—H32	119.9
C14—C13—C12	119.9 (3)	C34—C33—C32	119.8 (4)
C14—C13—H13	120.0	C34—C33—H33	120.1
C12—C13—H13	120.0	C32—C33—H33	120.1
C15—C14—C13	120.3 (3)	C33—C34—C35	120.4 (4)
C15—C14—H14	119.8	C33—C34—H34	119.8
C13—C14—H14	119.8	C35—C34—H34	119.8
C14—C15—C16	120.1 (3)	C36—C35—C34	119.9 (4)
C14—C15—H15	120.0	C36—C35—H35	120.0

C16—C15—H15	120.0	C34—C35—H35	120.0
C11—C16—C15	120.5 (3)	C31—C36—C35	120.7 (3)
C11—C16—H16	119.8	C31—C36—H36	119.7
C15—C16—H16	119.8	C35—C36—H36	119.7
C1—N2—C21	124.7 (3)	C3—N4—C41	122.9 (3)
C1—N2—H2	117.7	C3—N4—H4	118.6
C21—N2—H2	117.7	C41—N4—H4	118.6
N2—C21—C22	110.6 (3)	N4—C41—C42	111.3 (3)
N2—C21—H21A	109.5	N4—C41—H41A	109.4
C22—C21—H21A	109.5	C42—C41—H41A	109.4
N2—C21—H21B	109.5	N4—C41—H41B	109.4
C22—C21—H21B	109.5	C42—C41—H41B	109.4
H21A—C21—H21B	108.1	H41A—C41—H41B	108.0
O2—C22—C21	112.4 (3)	O4—C42—C41	112.3 (3)
O2—C22—C23	112.7 (3)	O4—C42—C43	112.2 (3)
C21—C22—C23	111.1 (3)	C41—C42—C43	111.6 (3)
O2—C22—H22	106.7	O4—C42—H42	106.7
C21—C22—H22	106.7	C41—C42—H42	106.7
C23—C22—H22	106.7	C43—C42—H42	106.7
C22—C23—H23A	109.5	C42—C43—H43A	109.5
C22—C23—H23B	109.5	C42—C43—H43B	109.5
H23A—C23—H23B	109.5	H43A—C43—H43B	109.5
C22—C23—H23C	109.5	C42—C43—H43C	109.5
H23A—C23—H23C	109.5	H43A—C43—H43C	109.5
H23B—C23—H23C	109.5	H43B—C43—H43C	109.5
C22—O2—H2A	109.5	C42—O4—H4A	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.20	2.977 (3)	151
N2—H2···O1	0.86	1.94	2.632 (3)	137
O2—H2*A*···S1^{ii}	0.82	2.66	3.242 (3)	130
N3—H3···O4^{i}	0.86	2.21	2.999 (4)	153
N4—H4···O3	0.86	1.96	2.640 (4)	135
O4—H4*A*···S3^{ii}	0.82	2.41	3.161 (3)	152
C15—H15···O1^{i}	0.93	2.53	3.265 (4)	136
C16—H16···O2^{i}	0.93	2.72	3.420 (5)	132
C35—H35···O3^{i}	0.93	2.91	3.531 (5)	126
C36—H36···O4^{i}	0.93	2.57	3.412 (5)	150
C21—H21*B*···S3^{ii}	0.97	2.98	3.844 (3)	149
C23—H23*C*···S3^{ii}	0.96	2.98	3.842 (4)	150

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) *x*, −*y*+3/2, *z*+1/2.