Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-{[(1,3-Benzothiazolium-2-yl)-hydrazono](phenyl)methyl}-3-methyl-1-phenyl-1*H*-pyrazol-5-olate monohydrate

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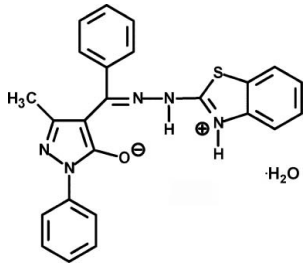
Received 24 February 2008; accepted 6 March 2008

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.052; wR factor = 0.140; data-to-parameter ratio = 13.3.

The title compound, $C_{24}H_{19}N_5OS\cdot H_2O$, was synthesized by the reaction of 4-benzoyl-3-methyl-1-phenylpyrazol-5-one and 2-hydrazino-1,3-benzothiazole. Proton transfer leads to the formation of a zwitterionic structure and the molecule exists in the enolate form. The pyrazolone ring makes dihedral angles of 35.4 (3), 69.7 (3) and 40.1 (3)° with the 1-phenyl, indirectly bound phenyl and benzothiazole ring systems, respectively. The molecules are linked into one-dimensional chains by a combination of N—H···O, O—H···N and O—H···O hydrogen bonds.

Related literature

For related literature, see: Akama & Tong (1996); Eller & Holzer (2004); Morakot *et al.* (2008); Rana *et al.* (2007); Sieroń (2007); Kim *et al.* (2005); Costa *et al.* (2006); Usman *et al.* (2003). Two related compounds we have previously reported exist in the enamine–keto tautomeric form (Sun *et al.*, 2006, 2007).



Experimental

Crystal data

$C_{24}H_{19}N_5OS\cdot H_2O$
M_r = 443.52
Triclinic, $P\overline{1}$
a = 7.1059 (16) Å
b = 12.906 (3) Å
c = 13.439 (3) Å
α = 67.173 (4)°
β = 85.597 (4)°
γ = 76.226 (4)°
V = 1103.1 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 273 (2) K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.974, T_{max} = 0.982
5750 measured reflections
3850 independent reflections
3210 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.139
S = 1.09
3850 reflections
290 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H25···N5^{i}	0.85	1.97	2.815 (3)	178
O2—H26···O1^{ii}	0.85	2.00	2.829 (3)	166
N1—H1···O2	0.86	1.81	2.662 (3)	173
N2—H2···O1	0.86	1.78	2.541 (3)	146

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This project was supported by the Jiangsu Planned Projects for Postdoctoral Research Funds (No. 0701001B).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2599).

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supplementary materials

Acta Cryst. (2008). E**64**, o690 [**doi:10.1107/S1600536808006193**]

4-{[(1,3-Benzothiazolium-2-yl)hydrazono](phenyl)methyl}-3-methyl-1-phenyl-1*H*-pyrazol-5-olate monohydrate

Y.-F. Sun and Y.-P. Cui

Comment

Pyrazolone derivatives play an important role as substructures of numerous pharmaceuticals, agrochemicals, dyes and pigments, as well as chelating and extracting agents. Moreover, they are capable of prototropic tautomerism (Akama & Tong, 1996; Eller & Holzer, 2004). Furthermore, interest in the study of compounds containing the benzothiazole moiety has increased on account of their broad spectrum of biological activities (Rana *et al.*, 2007), and also their potential applications in the areas of sensor (Morakot *et al.*, 2008; Kim *et al.*, 2005), non-linear optics, laser dyes, electroluminescent devices (Costa *et al.*, 2006) and also as chelating agents (Usman *et al.*, 2003; Sieroń, 2007). In continuation of our studies on pyrazolone derivatives, we report here the synthesis and crystal structure of the title compound, (I).

The title compound (Fig. 1) is a prototropic isomer, in which proton transfer leads to the formation of a zwitterionic structure. The molecule exists in the enolate form, in contrast to the enamine–keto tautomeric form which is exhibited by related pyrazolone analogues reported previously by us (Sun *et al.*, 2006, 2007). In the title molecule the central pyrazolone (C15—C17/N4/N5) ring is essentially planar, with an r.m.s. deviation of 0.0033 Å for the fitted atoms. This ring makes dihedral angles of 35.4 (3), 69.7 (3) and 40.1 (3) ° with the 1-phenyl, methylene-bound phenyl and benzothiazole rings, respectively. In addition, the molecule features an intramolecular hydrogen bond between the N2 and O1 atoms (Table 1) arising from the fact that atoms O1 and N2 are on the same side of the N3—C8 bond. In the crystal structure, molecules are linked into a one-dimensional chains by a combination of N—H···O, O—H···N and O—H···O hydrogen bonds (Table 1 and Fig. 2).

Experimental

A mixture of 1-phenyl-3-methyl-4-benzoyl-pyrazolone-5 (1 mmol) and 2-hydrazino-1,3-benzothiazole (1 mmol) in anhydrous ethanol (20 ml) was refluxed for 3 hr, and then cooled to room temperature. The precipitate was filtered and dried. The crude product was recrystallized from ethanol. Yellow crystals were thus obtained in 65% yield. m.p. 447–449 K. Spectroscopic analysis:^{1}H NMR (600 MHz, MSO-d$_6$, δ, p.p.m.): 1.70(s, 3H), 7.13–7.61(m, 11H), 7.76(d, 1H, J = 7.8 Hz), 7.87(d, 2H, J = 7.8 Hz). A single-crystal suitable for an X-ray structural analysis was obtained by slowly evaporating a ethanolic solution of the title compound at room temperature.

Refinement

All H atoms were initially located in a difference Fourier map and were subsequebtly treated as riding atoms, with C—H = 0.93 Å (aromatic), 0.96 Å(methyl), N—H = 0.86 Å and O—H = 0.85 Å, and with U_{iso}(H) = kU_{eq}(C,*N*,*O*), where k = 1.5 for the methyl group or 1.2 for all other H atoms.

Figures

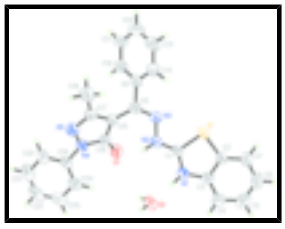

Fig. 1. The molecular structure showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii.

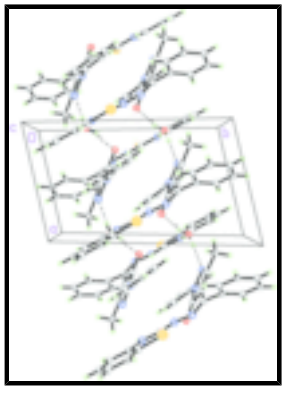

Fig. 2. The chain structure formed *via* hydrogen bonds, indicated by dashed lines.

4-{[(1,3-Benzothiazolium-2-yl)hydrazono](phenyl)methyl}-3-methyl-1- phenyl-1*H*-pyrazol-5-olate monohydrate

Crystal data

$C_{24}H_{19}N_5OS·H_2O$	$Z = 2$
$M_r = 443.52$	$F_{000} = 464$
Triclinic, $P\overline{1}$	$D_x = 1.335$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.1059$ (16) Å	Cell parameters from 2939 reflections
$b = 12.906$ (3) Å	$\theta = 3.0$–27.6º
$c = 13.439$ (3) Å	$\mu = 0.18$ mm^{-1}
$\alpha = 67.173$ (4)º	$T = 273$ (2) K
$\beta = 85.597$ (4)º	Block, yellow
$\gamma = 76.226$ (4)º	0.15 × 0.12 × 0.10 mm
$V = 1103.1$ (4) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3850 independent reflections
Radiation source: fine-focus sealed tube	3210 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.018$
$T = 273(2)$ K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.6$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 8$

T_{min} = 0.974, T_{max} = 0.982	k = −11→15
5750 measured reflections	l = −15→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H-atom parameters constrained
$wR(F^2)$ = 0.139	$w = 1/[\sigma^2(F_o^2) + (0.0377P)^2 + 1.1858P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.09	$(\Delta/\sigma)_{max} < 0.001$
3850 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
290 parameters	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
3 restraints	Extinction correction: SHELXL97 (Sheldrick, 2008)
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0158 (18)

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 $F^2 > 2$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	0.85393 (12)	0.44604 (7)	0.44483 (6)	0.0482 (2)
O1	0.8025 (3)	0.58715 (19)	0.03090 (16)	0.0513 (5)
O2	0.9942 (3)	0.28493 (19)	0.14541 (16)	0.0551 (6)
H25	0.8965	0.2751	0.1203	0.066*
H26	1.0389	0.3328	0.0912	0.066*
N1	0.9422 (3)	0.3293 (2)	0.32447 (18)	0.0416 (5)
H1	0.9531	0.3109	0.2689	0.050*
N2	0.7798 (3)	0.5218 (2)	0.23487 (19)	0.0448 (6)
H2	0.7755	0.5181	0.1726	0.054*
N3	0.7050 (4)	0.6224 (2)	0.25456 (19)	0.0475 (6)
N4	0.5118 (3)	0.6743 (2)	−0.06729 (18)	0.0425 (6)
N5	0.3329 (4)	0.7428 (2)	−0.0612 (2)	0.0483 (6)
C1	0.8564 (4)	0.4347 (2)	0.3203 (2)	0.0379 (6)
C2	0.9815 (4)	0.3026 (3)	0.5016 (2)	0.0458 (7)
C3	1.0124 (4)	0.2522 (2)	0.4260 (2)	0.0424 (6)
C4	1.1057 (5)	0.1373 (3)	0.4546 (3)	0.0580 (8)

H4	1.1238	0.1024	0.4046	0.070*
C5	1.1705 (6)	0.0766 (3)	0.5594 (3)	0.0730 (11)
H5	1.2329	−0.0009	0.5805	0.088*
C6	1.1459 (6)	0.1268 (3)	0.6336 (3)	0.0743 (11)
H6	1.1942	0.0836	0.7036	0.089*
C7	1.0508 (5)	0.2401 (3)	0.6061 (3)	0.0618 (9)
H7	1.0334	0.2741	0.6567	0.074*
C8	0.5842 (4)	0.7029 (2)	0.1837 (2)	0.0424 (6)
C9	0.5070 (4)	0.8052 (2)	0.2121 (2)	0.0450 (7)
C10	0.5184 (6)	0.9135 (3)	0.1387 (3)	0.0637 (10)
H10	0.5788	0.9211	0.0732	0.076*
C11	0.4416 (7)	1.0104 (3)	0.1612 (3)	0.0761 (12)
H11	0.4489	1.0829	0.1106	0.091*
C12	0.3545 (6)	0.9999 (3)	0.2576 (3)	0.0722 (11)
H12	0.2995	1.0654	0.2723	0.087*
C13	0.3485 (6)	0.8927 (3)	0.3327 (3)	0.0683 (10)
H13	0.2921	0.8854	0.3991	0.082*
C14	0.4252 (5)	0.7953 (3)	0.3107 (2)	0.0544 (8)
H14	0.4217	0.7228	0.3626	0.065*
C15	0.5207 (4)	0.7042 (2)	0.0832 (2)	0.0400 (6)
C16	0.6280 (4)	0.6487 (2)	0.0189 (2)	0.0412 (6)
C17	0.3392 (4)	0.7598 (3)	0.0289 (2)	0.0462 (7)
C18	0.1601 (5)	0.8263 (3)	0.0615 (3)	0.0729 (11)
H18A	0.1789	0.9005	0.0529	0.109*
H18B	0.1335	0.7847	0.1357	0.109*
H18C	0.0528	0.8363	0.0168	0.109*
C19	0.5566 (4)	0.6468 (3)	−0.1605 (2)	0.0432 (7)
C20	0.4799 (5)	0.7263 (3)	−0.2587 (2)	0.0567 (8)
H20	0.4028	0.7975	−0.2639	0.068*
C21	0.5176 (6)	0.7001 (4)	−0.3495 (3)	0.0697 (10)
H21	0.4660	0.7539	−0.4161	0.084*
C22	0.6305 (6)	0.5954 (4)	−0.3418 (3)	0.0713 (11)
H22	0.6546	0.5776	−0.4030	0.086*
C23	0.7080 (5)	0.5169 (3)	−0.2440 (3)	0.0656 (10)
H23	0.7860	0.4461	−0.2391	0.079*
C24	0.6718 (5)	0.5417 (3)	−0.1523 (3)	0.0533 (8)
H24	0.7245	0.4881	−0.0859	0.064*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0615 (5)	0.0509 (5)	0.0402 (4)	−0.0127 (4)	−0.0018 (3)	−0.0254 (3)
O1	0.0423 (12)	0.0656 (14)	0.0433 (11)	−0.0049 (10)	0.0022 (9)	−0.0223 (10)
O2	0.0562 (13)	0.0765 (15)	0.0451 (12)	−0.0244 (11)	0.0044 (10)	−0.0317 (11)
N1	0.0471 (13)	0.0462 (13)	0.0386 (12)	−0.0140 (11)	0.0022 (10)	−0.0219 (11)
N2	0.0536 (15)	0.0465 (14)	0.0398 (13)	−0.0094 (11)	−0.0044 (11)	−0.0225 (11)
N3	0.0593 (16)	0.0439 (14)	0.0441 (14)	−0.0107 (12)	−0.0025 (12)	−0.0217 (12)
N4	0.0437 (13)	0.0494 (14)	0.0378 (12)	−0.0101 (11)	0.0015 (10)	−0.0207 (11)

N5	0.0455 (14)	0.0536 (15)	0.0499 (14)	−0.0085 (12)	−0.0035 (11)	−0.0251 (12)
C1	0.0398 (15)	0.0432 (15)	0.0370 (14)	−0.0147 (12)	0.0009 (11)	−0.0189 (12)
C2	0.0505 (17)	0.0499 (17)	0.0410 (15)	−0.0163 (14)	−0.0009 (13)	−0.0183 (13)
C3	0.0420 (15)	0.0445 (16)	0.0437 (15)	−0.0146 (13)	0.0014 (12)	−0.0174 (13)
C4	0.063 (2)	0.0499 (19)	0.061 (2)	−0.0114 (16)	0.0041 (16)	−0.0227 (16)
C5	0.074 (2)	0.052 (2)	0.077 (3)	−0.0050 (18)	−0.012 (2)	−0.0091 (19)
C6	0.081 (3)	0.072 (3)	0.055 (2)	−0.014 (2)	−0.0184 (19)	−0.0072 (19)
C7	0.074 (2)	0.066 (2)	0.0454 (18)	−0.0179 (18)	−0.0098 (16)	−0.0188 (16)
C8	0.0502 (17)	0.0423 (16)	0.0381 (15)	−0.0157 (13)	0.0042 (13)	−0.0165 (13)
C9	0.0537 (17)	0.0456 (16)	0.0399 (15)	−0.0136 (14)	−0.0020 (13)	−0.0190 (13)
C10	0.105 (3)	0.0468 (18)	0.0417 (17)	−0.0216 (18)	0.0103 (17)	−0.0185 (14)
C11	0.130 (4)	0.0421 (18)	0.057 (2)	−0.024 (2)	0.013 (2)	−0.0198 (16)
C12	0.097 (3)	0.054 (2)	0.072 (2)	−0.009 (2)	0.013 (2)	−0.0373 (19)
C13	0.078 (2)	0.072 (2)	0.060 (2)	−0.0152 (19)	0.0226 (18)	−0.0352 (19)
C14	0.065 (2)	0.0505 (18)	0.0456 (17)	−0.0155 (16)	0.0107 (15)	−0.0167 (14)
C15	0.0466 (16)	0.0393 (15)	0.0368 (14)	−0.0130 (12)	0.0011 (12)	−0.0154 (12)
C16	0.0446 (16)	0.0427 (15)	0.0362 (14)	−0.0158 (13)	0.0031 (12)	−0.0121 (12)
C17	0.0479 (17)	0.0460 (16)	0.0473 (16)	−0.0101 (13)	0.0000 (13)	−0.0208 (14)
C18	0.060 (2)	0.085 (3)	0.077 (3)	0.0082 (19)	−0.0081 (19)	−0.047 (2)
C19	0.0476 (16)	0.0533 (17)	0.0388 (15)	−0.0244 (14)	0.0074 (12)	−0.0221 (13)
C20	0.060 (2)	0.069 (2)	0.0448 (17)	−0.0205 (17)	−0.0010 (15)	−0.0217 (16)
C21	0.068 (2)	0.107 (3)	0.0412 (18)	−0.035 (2)	0.0035 (16)	−0.028 (2)
C22	0.071 (2)	0.116 (3)	0.061 (2)	−0.052 (2)	0.0242 (19)	−0.057 (2)
C23	0.065 (2)	0.078 (2)	0.081 (3)	−0.0356 (19)	0.0250 (19)	−0.053 (2)
C24	0.0599 (19)	0.0571 (19)	0.0522 (18)	−0.0248 (16)	0.0109 (15)	−0.0259 (15)

Geometric parameters (Å, °)

S1—C1	1.735 (3)	C9—C14	1.377 (4)
S1—C2	1.744 (3)	C9—C10	1.379 (4)
O1—C16	1.287 (3)	C10—C11	1.377 (5)
O2—H25	0.8500	C10—H10	0.9300
O2—H26	0.8500	C11—C12	1.365 (5)
N1—C1	1.332 (3)	C11—H11	0.9300
N1—C3	1.384 (4)	C12—C13	1.369 (5)
N1—H1	0.8600	C12—H12	0.9300
N2—C1	1.297 (3)	C13—C14	1.379 (5)
N2—N3	1.397 (3)	C13—H13	0.9300
N2—H2	0.8600	C14—H14	0.9300
N3—C8	1.288 (4)	C15—C16	1.400 (4)
N4—C16	1.361 (3)	C15—C17	1.418 (4)
N4—N5	1.382 (3)	C17—C18	1.495 (4)
N4—C19	1.424 (3)	C18—H18A	0.9600
N5—C17	1.317 (4)	C18—H18B	0.9600
C2—C7	1.380 (4)	C18—H18C	0.9600
C2—C3	1.384 (4)	C19—C20	1.373 (4)
C3—C4	1.384 (4)	C19—C24	1.375 (4)
C4—C5	1.372 (5)	C20—C21	1.379 (5)
C4—H4	0.9300	C20—H20	0.9300

C5—C6	1.365 (5)	C21—C22	1.367 (6)
C5—H5	0.9300	C21—H21	0.9300
C6—C7	1.371 (5)	C22—C23	1.368 (5)
C6—H6	0.9300	C22—H22	0.9300
C7—H7	0.9300	C23—C24	1.379 (4)
C8—C15	1.449 (4)	C23—H23	0.9300
C8—C9	1.484 (4)	C24—H24	0.9300
C1—S1—C2	89.71 (13)	C12—C11—H11	120.0
H25—O2—H26	104.4	C10—C11—H11	120.0
C1—N1—C3	114.1 (2)	C11—C12—C13	119.7 (3)
C1—N1—H1	122.9	C11—C12—H12	120.2
C3—N1—H1	122.9	C13—C12—H12	120.2
C1—N2—N3	113.0 (2)	C12—C13—C14	120.6 (3)
C1—N2—H2	123.5	C12—C13—H13	119.7
N3—N2—H2	123.5	C14—C13—H13	119.7
C8—N3—N2	116.6 (2)	C9—C14—C13	120.1 (3)
C16—N4—N5	111.7 (2)	C9—C14—H14	119.9
C16—N4—C19	128.9 (2)	C13—C14—H14	119.9
N5—N4—C19	119.3 (2)	C16—C15—C17	104.9 (2)
C17—N5—N4	105.4 (2)	C16—C15—C8	126.7 (3)
N2—C1—N1	125.9 (2)	C17—C15—C8	128.4 (3)
N2—C1—S1	121.5 (2)	O1—C16—N4	123.3 (3)
N1—C1—S1	112.7 (2)	O1—C16—C15	130.4 (3)
C7—C2—C3	120.3 (3)	N4—C16—C15	106.3 (2)
C7—C2—S1	128.5 (3)	N5—C17—C15	111.8 (3)
C3—C2—S1	111.2 (2)	N5—C17—C18	118.1 (3)
C4—C3—N1	126.9 (3)	C15—C17—C18	130.1 (3)
C4—C3—C2	120.8 (3)	C17—C18—H18A	109.5
N1—C3—C2	112.2 (3)	C17—C18—H18B	109.5
C5—C4—C3	117.7 (3)	H18A—C18—H18B	109.5
C5—C4—H4	121.2	C17—C18—H18C	109.5
C3—C4—H4	121.2	H18A—C18—H18C	109.5
C6—C5—C4	121.8 (4)	H18B—C18—H18C	109.5
C6—C5—H5	119.1	C20—C19—C24	120.5 (3)
C4—C5—H5	119.1	C20—C19—N4	118.8 (3)
C5—C6—C7	120.7 (3)	C24—C19—N4	120.7 (3)
C5—C6—H6	119.6	C19—C20—C21	119.7 (3)
C7—C6—H6	119.6	C19—C20—H20	120.2
C6—C7—C2	118.6 (3)	C21—C20—H20	120.2
C6—C7—H7	120.7	C22—C21—C20	120.2 (4)
C2—C7—H7	120.7	C22—C21—H21	119.9
N3—C8—C15	127.9 (3)	C20—C21—H21	119.9
N3—C8—C9	113.3 (2)	C21—C22—C23	119.8 (3)
C15—C8—C9	118.8 (2)	C21—C22—H22	120.1
C14—C9—C10	118.6 (3)	C23—C22—H22	120.1
C14—C9—C8	121.8 (3)	C22—C23—C24	120.7 (4)
C10—C9—C8	119.7 (3)	C22—C23—H23	119.6
C11—C10—C9	121.0 (3)	C24—C23—H23	119.6
C11—C10—H10	119.5	C19—C24—C23	119.1 (3)

C9—C10—H10	119.5	C19—C24—H24	120.5
C12—C11—C10	119.9 (3)	C23—C24—H24	120.5
C1—N2—N3—C8	−162.4 (3)	C11—C12—C13—C14	−1.6 (6)
C16—N4—N5—C17	0.3 (3)	C10—C9—C14—C13	3.1 (5)
C19—N4—N5—C17	−175.6 (2)	C8—C9—C14—C13	−177.5 (3)
N3—N2—C1—N1	−178.3 (2)	C12—C13—C14—C9	−0.7 (6)
N3—N2—C1—S1	2.1 (3)	N3—C8—C15—C16	−30.2 (5)
C3—N1—C1—N2	179.8 (3)	C9—C8—C15—C16	149.0 (3)
C3—N1—C1—S1	−0.6 (3)	N3—C8—C15—C17	149.2 (3)
C2—S1—C1—N2	−178.6 (2)	C9—C8—C15—C17	−31.6 (4)
C2—S1—C1—N1	1.7 (2)	N5—N4—C16—O1	−179.2 (2)
C1—S1—C2—C7	176.8 (3)	C19—N4—C16—O1	−3.8 (4)
C1—S1—C2—C3	−2.5 (2)	N5—N4—C16—C15	−0.8 (3)
C1—N1—C3—C4	179.2 (3)	C19—N4—C16—C15	174.6 (3)
C1—N1—C3—C2	−1.4 (3)	C17—C15—C16—O1	179.2 (3)
C7—C2—C3—C4	2.8 (5)	C8—C15—C16—O1	−1.2 (5)
S1—C2—C3—C4	−177.9 (2)	C17—C15—C16—N4	0.9 (3)
C7—C2—C3—N1	−176.7 (3)	C8—C15—C16—N4	−179.5 (3)
S1—C2—C3—N1	2.6 (3)	N4—N5—C17—C15	0.4 (3)
N1—C3—C4—C5	177.6 (3)	N4—N5—C17—C18	−176.6 (3)
C2—C3—C4—C5	−1.7 (5)	C16—C15—C17—N5	−0.8 (3)
C3—C4—C5—C6	−0.4 (6)	C8—C15—C17—N5	179.7 (3)
C4—C5—C6—C7	1.5 (6)	C16—C15—C17—C18	175.6 (3)
C5—C6—C7—C2	−0.4 (6)	C8—C15—C17—C18	−3.9 (5)
C3—C2—C7—C6	−1.7 (5)	C16—N4—C19—C20	−142.4 (3)
S1—C2—C7—C6	179.2 (3)	N5—N4—C19—C20	32.7 (4)
N2—N3—C8—C15	−2.5 (4)	C16—N4—C19—C24	38.7 (4)
N2—N3—C8—C9	178.3 (2)	N5—N4—C19—C24	−146.2 (3)
N3—C8—C9—C14	−52.3 (4)	C24—C19—C20—C21	0.5 (5)
C15—C8—C9—C14	128.3 (3)	N4—C19—C20—C21	−178.4 (3)
N3—C8—C9—C10	127.0 (3)	C19—C20—C21—C22	0.1 (5)
C15—C8—C9—C10	−52.3 (4)	C20—C21—C22—C23	−0.7 (5)
C14—C9—C10—C11	−3.1 (6)	C21—C22—C23—C24	0.7 (5)
C8—C9—C10—C11	177.5 (3)	C20—C19—C24—C23	−0.5 (4)
C9—C10—C11—C12	0.7 (7)	N4—C19—C24—C23	178.4 (3)
C10—C11—C12—C13	1.6 (7)	C22—C23—C24—C19	−0.1 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H25···N5^{i}	0.85	1.97	2.815 (3)	178
O2—H26···O1^{ii}	0.85	2.00	2.829 (3)	166
N1—H1···O2	0.86	1.81	2.662 (3)	173
N2—H2···O1	0.86	1.78	2.541 (3)	146

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

Fig. 1

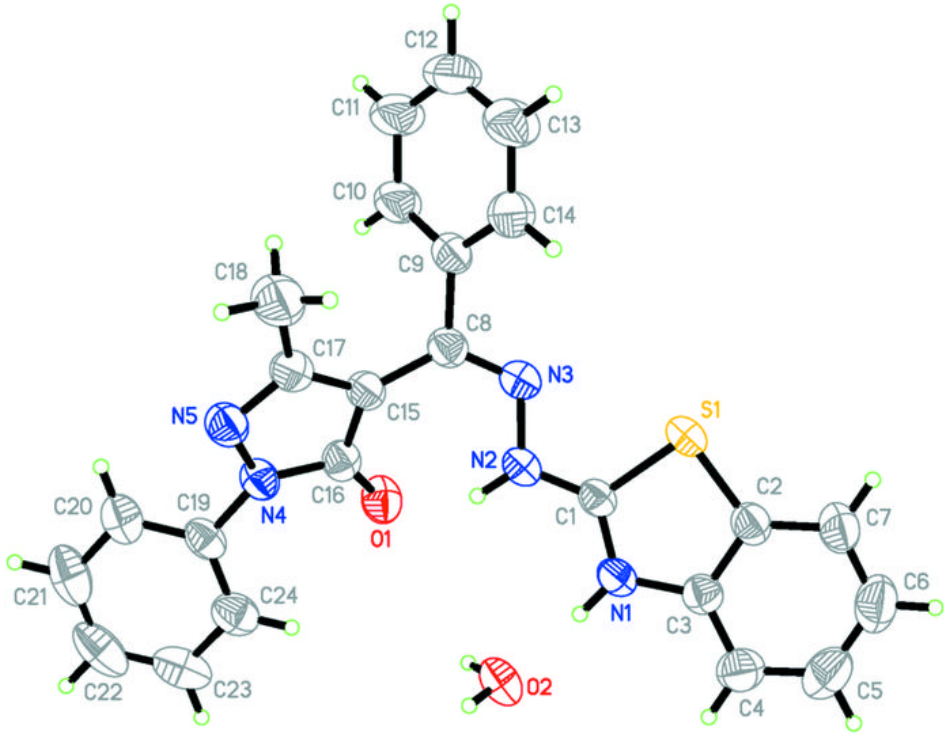
C12
C11
C13
C10
C14
C9
C18
C8
C17
N3
N5
C15
S1
N2
C20
C19
N4
C16
O1
C1
C2
C7
C21
C24
N1
C3
C6
O2
C22
C23
C4
C5

Fig. 2