Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-(3-Methyl-5-phenoxy-1-phenylpyrazol-4-yl)-1,3,4-thiadiazol-2-amine

Yan-Rong Sun,[a] Gang Liu,[a] Chen-Jiang Liu[a,b]* and Ji-De Wang[a,b]

[a]Key Laboratory of Oil and Gas Fine Chemicals, Ministry of Education, School of Chemistry and Chemical Engineering, Xinjiang University, Urumqi 830046, People's Republic of China, and [b]School of Sciences, Xi'an Jiaotong University, Xian 710049, People's Republic of China
Correspondence e-mail: pxylcj@126.com

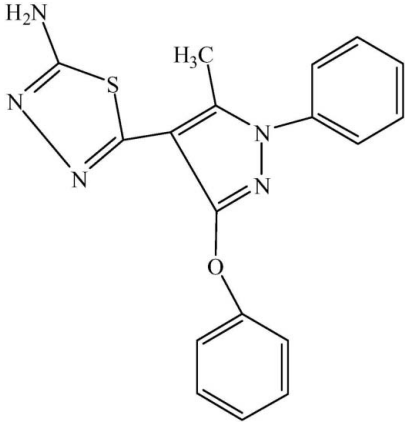
Received 16 June 2007; accepted 12 July 2007

Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.101; data-to-parameter ratio = 17.2.

There are two molecules in the asymmetric unit of the title compound, $C_{18}H_{15}N_5OS$. The two molecules differ by less than 3° in the dihedral angles between corresponding planar units. Hydrogen bonding between the two molecules creates a one-dimensional chain along the c direction.

Related literature

For related literature, see: Akbas *et al.* (2005); Daidone *et al.* (2004); Foroumadi *et al.* (2002); Park *et al.* (2005); Supuran & Scozzafava (2000); Thomasco *et al.* (2003).



Experimental

Crystal data

$C_{18}H_{15}N_5OS$
M_r = 349.41
Monoclinic, $P2_1/c$
a = 20.2987 (5) Å
b = 9.6934 (3) Å
c = 19.0726 (6) Å
β = 114.846 (1)°
V = 3405.43 (17) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 153 (2) K
0.66 × 0.43 × 0.31 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.876, T_{max} = 0.939
32693 measured reflections
7772 independent reflections
6769 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
S = 1.05
7772 reflections
453 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 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···N7	0.88	2.19	3.0266 (16)	158
N1—H1B···N4^{i}	0.88	2.21	3.0113 (15)	150
N6—H6A···N2	0.88	2.11	2.9467 (15)	159
N6—H6B···N9^{ii}	0.88	2.23	2.9915 (16)	145

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

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors gratefully acknowledge support from the National Natural Science Foundation of China (grant No. 20662009), the Program for Century Excellent Talents in Universities (grant No. NCET-04-0987) and the Specialized Research Fund for the Doctoral Program of Higher Education (grant No. 20050755003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2139).

References

Akbas, E., Berber, I., Sener, A. & Hasanov, B. (2005). *Farmaco*, **60**, 23–26.
Daidone, G., Maggio, B., Raffa, D., Plescia, S., Schillaci, D. & Raimondi, M. V. (2004). *Farmaco*, **59**, 413–417.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Foroumadi, A., Asadipour, A., Mirzaei, M., Karimi, J. & Emami, S. (2002). *Farmaco*, **57**, 765–769.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Park, H.-J., Lee, K., Park, S.-J., Ahn, B., Lee, J.-C., Cho, H. Y. & Lee, K.-I. (2005). *Bioorg. Med. Chem. Lett.* **15**, 3307–3312.
Rigaku (2004). *RAPID-AUTO*. Version 3.0. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Supuran, C. T. & Scozzafava, A. (2000). *Eur. J. Med. Chem.* **35**, 867–874.
Thomasco, L. M., Gadwood, R. C., Weaver, E. A., Ochoada, J. M., Ford, C. W., Zurenko, G. E., Hamel, J. C., Stapert, D., Moerman, J. K., Schaadt, R. D. & Yagi, B. H. (2003). *Bioorg. Med. Chem. Lett.* **13**, 4193–4196.

 doi:10.1107/S1600536807034009

supplementary materials

Acta Cryst. (2007). E**63**, o3509 [**doi:10.1107/S1600536807034009**]

5-(3-Methyl-5-phenoxy-1-phenylpyrazol-4-yl)-1,3,4-thiadiazol-2-amine

Y.-R. Sun, G. Liu, C.-J. Liu and J.-D. Wang

Comment

Compounds including 1,3,4-thiadiazole ring are known to possess several biological properties, such as antibacterial, antitubercular, antineoplastic activities (Thomasco *et al.*, 2003; Foroumadi *et al.*, 2002; Supuran & Scozzafava, 2000). Pyrazoles also have widespread biological activity, such as antisepsis, antileukosis, antitumor (Akbas *et al.*, 2005; Daidone *et al.*, 2004; Park *et al.*, 2005). In an attempt to achieve new compounds with possible biological activities, we designed and synthesized 2-amino-5-(1-phenyl-3-methyl-5-phenoxylpyrazole-4-yl)-1,3,4-thiadiazole(1). The asymmetric unit has two molecules, and structures of the two molecules are nearly identical.

Experimental

To the mixture of 1-phenyl-3-methyl-5-phenoxylpyrazole-4-formylic acid(4 mmol) and aminothiourea(4 mmol), phosphorus oxychloride(10 mL) was slowly added with stirring in ice bath. The reaction mixture was slowly heated to reflux 2 h at about 358 K, then cooled, and cold water (30 mL) added. The solution was slowly heated to reflux 6 h at about 393 K, then filtered. To neutralize the filtrate, 25% KOH was added to reach pH = 8–9. The product was isolated by filtration, washed with water, and dried at room temperature for a yield 65.2% (0.912 g), m.p. 497–498 K. Block-like single-crystal of the title compound were grown from a solution of ethanol by slow evaporation.

Refinement

The H atoms attached to the parent C or N atoms were geometrically fixed, and were treated as riding atoms, whereas the methyl H atoms were refined as rigid groups, coupled with rotation of the group to best fit the electron density map. The distances were N—H = 0.88 Å, C—H = 0.95–0.98 Å, with U_{iso}(H) = 1.2Ueq(C or N), U(iso(methylH) = 1.5Ueq(C).

Figures

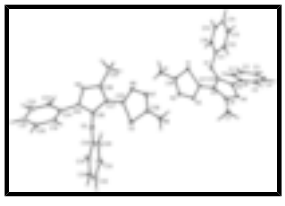


Fig. 1. A view of the moleculer structure of the two molecules of the aymmetric unit, showing the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level, and H atoms are shown as small spheres of arbitrary radii.

5-(3-Methyl-5-phenoxy-1-phenylpyrazol-4-yl)-1,3,4-thiadiazol-2-amine

Crystal data

$C_{18}H_{15}N_5OS$	D_x = 1.363 Mg m^{-3}
M_r = 349.41	Melting point: 498 K

Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 20.2987$ (5) Å	Cell parameters from 26663 reflections
$b = 9.6934$ (3) Å	$\theta = 3.0–27.5^\circ$
$c = 19.0726$ (6) Å	$\mu = 0.21$ mm^{-1}
$\beta = 114.846$ (1)°	$T = 153$ (2) K
$V = 3405.43$ (17) Å^3	Block, colorless
$Z = 8$	0.66 × 0.43 × 0.31 mm
$F_{000} = 1456$	

Data collection

Rigaku R-AXIS SPIDER diffractometer	7772 independent reflections
Radiation source: fine-focus sealed tube	6769 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 153$(2) K	$\theta_{max} = 27.5^\circ$
ω scans	$\theta_{min} = 3.0^\circ$
Absorption correction: empirical (using intensity measurements) (ABSCOR; Higashi, 1995)	$h = -24\rightarrow26$
$T_{min} = 0.876$, $T_{max} = 0.939$	$k = -12\rightarrow12$
32693 measured reflections	$l = -24\rightarrow23$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H-atom parameters constrained
$wR(F^2) = 0.101$	$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.8824P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
7772 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
453 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 calculat-

ing *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	0.430303 (16)	0.79622 (3)	0.268570 (16)	0.02420 (8)
S2	0.053694 (17)	0.72302 (4)	0.263009 (18)	0.03485 (10)
O1	0.52710 (4)	0.88205 (9)	0.18168 (5)	0.02343 (18)
O2	−0.04172 (5)	0.82952 (9)	0.34655 (5)	0.02735 (19)
N1	0.33984 (6)	0.79945 (13)	0.34137 (6)	0.0323 (3)
H1A	0.2967	0.7916	0.3416	0.039*
H1B	0.3779	0.8193	0.3844	0.039*
N2	0.29285 (6)	0.75129 (12)	0.20940 (6)	0.0250 (2)
N3	0.31332 (5)	0.73761 (11)	0.14935 (6)	0.0236 (2)
N4	0.43532 (5)	0.68631 (11)	0.01202 (6)	0.0234 (2)
N5	0.49192 (5)	0.76583 (11)	0.06123 (6)	0.0225 (2)
N6	0.14095 (6)	0.71887 (15)	0.18704 (7)	0.0384 (3)
H6A	0.1835	0.7101	0.1857	0.046*
H6B	0.1017	0.7308	0.1439	0.046*
N7	0.19232 (6)	0.69641 (13)	0.32166 (6)	0.0295 (2)
N8	0.17298 (6)	0.68692 (12)	0.38289 (6)	0.0285 (2)
N9	0.05654 (5)	0.67127 (12)	0.52749 (6)	0.0269 (2)
N10	−0.00125 (5)	0.74338 (12)	0.47454 (6)	0.0249 (2)
C1	0.58095 (6)	0.93578 (13)	0.06074 (7)	0.0267 (3)
H1C	0.5691	0.9941	0.0938	0.032*
C2	0.63228 (7)	0.97676 (15)	0.03447 (8)	0.0316 (3)
H2B	0.6565	1.0627	0.0506	0.038*
C3	0.64825 (8)	0.89297 (16)	−0.01502 (9)	0.0380 (3)
H3B	0.6829	0.9219	−0.0333	0.046*
C4	0.61364 (9)	0.76660 (17)	−0.03796 (10)	0.0414 (3)
H4B	0.6242	0.7099	−0.0726	0.050*
C5	0.56374 (8)	0.72254 (15)	−0.01070 (8)	0.0334 (3)
H5A	0.5412	0.6348	−0.0251	0.040*
C6	0.54718 (6)	0.80857 (13)	0.03806 (7)	0.0235 (2)
C7	0.32015 (7)	0.59679 (14)	0.00612 (7)	0.0283 (3)
H7B	0.3224	0.5393	−0.0351	0.042*
H7C	0.2798	0.6622	−0.0161	0.042*
H7D	0.3126	0.5380	0.0439	0.042*
C8	0.38972 (6)	0.67421 (12)	0.04516 (6)	0.0218 (2)
C9	0.41636 (6)	0.74462 (12)	0.11713 (6)	0.0212 (2)
C10	0.48134 (6)	0.80017 (12)	0.12464 (6)	0.0209 (2)
C11	0.59244 (6)	0.82460 (12)	0.23525 (6)	0.0206 (2)
C12	0.60255 (7)	0.68515 (13)	0.25028 (8)	0.0289 (3)
H12A	0.5653	0.6208	0.2227	0.035*
C13	0.66881 (8)	0.64136 (15)	0.30706 (8)	0.0342 (3)
H13A	0.6770	0.5457	0.3182	0.041*
C14	0.72283 (7)	0.73517 (15)	0.34745 (8)	0.0324 (3)

H14A	0.7677	0.7042	0.3864	0.039*
C15	0.71116 (7)	0.87414 (15)	0.33085 (8)	0.0334 (3)
H15A	0.7482	0.9389	0.3583	0.040*
C16	0.64566 (7)	0.91945 (13)	0.27442 (7)	0.0288 (3)
H16A	0.6376	1.0150	0.2629	0.035*
C17	0.38236 (6)	0.75766 (12)	0.17010 (6)	0.0208 (2)
C18	0.34753 (7)	0.78104 (12)	0.27530 (7)	0.0236 (2)
C19	−0.08683 (7)	0.92639 (14)	0.46842 (8)	0.0306 (3)
H19A	−0.0778	0.9722	0.4293	0.037*
C20	−0.13382 (7)	0.98335 (16)	0.49647 (8)	0.0371 (3)
H20A	−0.1574	1.0683	0.4760	0.044*
C21	−0.14653 (8)	0.9176 (2)	0.55371 (9)	0.0460 (4)
H21A	−0.1782	0.9578	0.5731	0.055*
C22	−0.11300 (8)	0.7928 (2)	0.58291 (9)	0.0484 (4)
H22A	−0.1219	0.7475	0.6223	0.058*
C23	−0.06649 (7)	0.73330 (17)	0.55515 (8)	0.0360 (3)
H23A	−0.0440	0.6471	0.5747	0.043*
C24	−0.05322 (6)	0.80151 (14)	0.49835 (7)	0.0261 (3)
C25	0.16923 (7)	0.56799 (15)	0.53478 (8)	0.0318 (3)
H25A	0.1701	0.5290	0.5826	0.048*
H25B	0.2101	0.6317	0.5473	0.048*
H25C	0.1731	0.4934	0.5020	0.048*
C26	0.09973 (6)	0.64382 (13)	0.49282 (7)	0.0248 (2)
C27	0.07052 (6)	0.69711 (13)	0.41642 (7)	0.0238 (2)
C28	0.00615 (6)	0.75820 (13)	0.40755 (7)	0.0238 (2)
C29	−0.10629 (6)	0.76360 (14)	0.29741 (7)	0.0249 (2)
C30	−0.11821 (7)	0.62435 (15)	0.29970 (9)	0.0356 (3)
H30A	−0.0826	0.5666	0.3365	0.043*
C31	−0.18401 (9)	0.57004 (19)	0.24642 (10)	0.0491 (4)
H31A	−0.1932	0.4741	0.2471	0.059*
C32	−0.23534 (8)	0.6529 (2)	0.19326 (9)	0.0497 (4)
H32A	−0.2797	0.6145	0.1571	0.060*
C33	−0.22249 (8)	0.7914 (2)	0.19243 (9)	0.0504 (5)
H33A	−0.2583	0.8489	0.1557	0.061*
C34	−0.15764 (8)	0.84882 (17)	0.24470 (8)	0.0378 (3)
H34A	−0.1489	0.9450	0.2441	0.045*
C35	0.10357 (6)	0.69930 (13)	0.36219 (7)	0.0242 (2)
C36	0.13585 (7)	0.71394 (14)	0.25529 (7)	0.0280 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02217 (15)	0.03248 (17)	0.01766 (15)	−0.00192 (11)	0.00807 (12)	−0.00262 (11)
S2	0.02132 (15)	0.0625 (2)	0.01953 (16)	0.00335 (14)	0.00740 (13)	0.00420 (14)
O1	0.0210 (4)	0.0248 (4)	0.0194 (4)	0.0012 (3)	0.0036 (3)	−0.0025 (3)
O2	0.0248 (4)	0.0307 (5)	0.0223 (4)	0.0007 (3)	0.0059 (4)	0.0038 (3)
N1	0.0266 (5)	0.0531 (7)	0.0187 (5)	0.0006 (5)	0.0112 (4)	−0.0021 (5)
N2	0.0228 (5)	0.0347 (6)	0.0186 (5)	0.0040 (4)	0.0098 (4)	0.0025 (4)

N3	0.0222 (5)	0.0309 (5)	0.0181 (5)	0.0034 (4)	0.0090 (4)	0.0021 (4)
N4	0.0203 (5)	0.0300 (5)	0.0181 (5)	−0.0027 (4)	0.0064 (4)	−0.0027 (4)
N5	0.0190 (5)	0.0291 (5)	0.0184 (5)	−0.0018 (4)	0.0070 (4)	−0.0017 (4)
N6	0.0264 (6)	0.0677 (9)	0.0219 (6)	0.0031 (5)	0.0110 (5)	0.0056 (5)
N7	0.0234 (5)	0.0446 (7)	0.0214 (5)	0.0003 (4)	0.0102 (4)	0.0019 (4)
N8	0.0228 (5)	0.0421 (6)	0.0203 (5)	−0.0014 (4)	0.0088 (4)	0.0003 (4)
N9	0.0213 (5)	0.0372 (6)	0.0192 (5)	0.0019 (4)	0.0058 (4)	0.0016 (4)
N10	0.0194 (5)	0.0349 (6)	0.0189 (5)	0.0014 (4)	0.0065 (4)	0.0007 (4)
C1	0.0248 (6)	0.0296 (6)	0.0249 (6)	0.0019 (5)	0.0094 (5)	0.0029 (5)
C2	0.0276 (6)	0.0338 (7)	0.0319 (7)	−0.0019 (5)	0.0111 (5)	0.0075 (5)
C3	0.0332 (7)	0.0480 (9)	0.0409 (8)	−0.0021 (6)	0.0235 (6)	0.0069 (6)
C4	0.0443 (8)	0.0474 (9)	0.0465 (9)	−0.0021 (7)	0.0328 (8)	−0.0055 (7)
C5	0.0348 (7)	0.0354 (7)	0.0379 (7)	−0.0032 (5)	0.0230 (6)	−0.0048 (6)
C6	0.0190 (5)	0.0310 (6)	0.0209 (6)	0.0022 (4)	0.0088 (5)	0.0045 (5)
C7	0.0250 (6)	0.0360 (7)	0.0230 (6)	−0.0064 (5)	0.0094 (5)	−0.0040 (5)
C8	0.0215 (5)	0.0261 (6)	0.0166 (5)	0.0001 (4)	0.0066 (4)	0.0007 (4)
C9	0.0213 (5)	0.0251 (6)	0.0165 (5)	0.0014 (4)	0.0071 (4)	0.0016 (4)
C10	0.0205 (5)	0.0236 (5)	0.0167 (5)	0.0020 (4)	0.0059 (4)	0.0006 (4)
C11	0.0196 (5)	0.0254 (6)	0.0165 (5)	0.0011 (4)	0.0073 (4)	−0.0005 (4)
C12	0.0289 (6)	0.0244 (6)	0.0284 (6)	−0.0028 (5)	0.0070 (5)	0.0001 (5)
C13	0.0364 (7)	0.0276 (6)	0.0333 (7)	0.0070 (5)	0.0096 (6)	0.0044 (5)
C14	0.0245 (6)	0.0436 (8)	0.0243 (6)	0.0088 (5)	0.0055 (5)	0.0011 (5)
C15	0.0241 (6)	0.0394 (8)	0.0292 (7)	−0.0045 (5)	0.0038 (5)	−0.0072 (6)
C16	0.0283 (6)	0.0247 (6)	0.0285 (6)	−0.0015 (5)	0.0070 (5)	−0.0028 (5)
C17	0.0220 (5)	0.0232 (5)	0.0161 (5)	0.0021 (4)	0.0070 (4)	0.0017 (4)
C18	0.0246 (6)	0.0260 (6)	0.0214 (6)	0.0039 (4)	0.0110 (5)	0.0031 (4)
C19	0.0246 (6)	0.0352 (7)	0.0295 (7)	−0.0037 (5)	0.0089 (5)	−0.0052 (5)
C20	0.0254 (6)	0.0434 (8)	0.0360 (8)	0.0026 (6)	0.0066 (6)	−0.0123 (6)
C21	0.0279 (7)	0.0770 (12)	0.0327 (8)	0.0111 (7)	0.0124 (6)	−0.0084 (7)
C22	0.0328 (7)	0.0861 (13)	0.0318 (8)	0.0097 (8)	0.0191 (7)	0.0092 (8)
C23	0.0266 (6)	0.0548 (9)	0.0276 (7)	0.0049 (6)	0.0123 (6)	0.0064 (6)
C24	0.0180 (5)	0.0374 (7)	0.0216 (6)	−0.0028 (5)	0.0070 (5)	−0.0061 (5)
C25	0.0244 (6)	0.0430 (8)	0.0245 (6)	0.0050 (5)	0.0068 (5)	0.0028 (5)
C26	0.0212 (5)	0.0312 (6)	0.0196 (5)	−0.0021 (5)	0.0063 (5)	−0.0018 (5)
C27	0.0213 (5)	0.0296 (6)	0.0189 (6)	−0.0020 (4)	0.0070 (5)	−0.0017 (4)
C28	0.0211 (5)	0.0293 (6)	0.0189 (6)	−0.0021 (4)	0.0063 (5)	−0.0004 (4)
C29	0.0214 (5)	0.0349 (7)	0.0181 (5)	0.0048 (5)	0.0081 (5)	−0.0011 (5)
C30	0.0286 (6)	0.0337 (7)	0.0373 (7)	0.0028 (5)	0.0069 (6)	−0.0039 (6)
C31	0.0389 (8)	0.0492 (10)	0.0530 (10)	−0.0079 (7)	0.0133 (8)	−0.0193 (8)
C32	0.0275 (7)	0.0824 (13)	0.0322 (8)	−0.0039 (8)	0.0056 (6)	−0.0215 (8)
C33	0.0302 (7)	0.0860 (14)	0.0261 (7)	0.0194 (8)	0.0031 (6)	0.0071 (8)
C34	0.0354 (7)	0.0438 (8)	0.0304 (7)	0.0124 (6)	0.0102 (6)	0.0085 (6)
C35	0.0228 (5)	0.0294 (6)	0.0184 (5)	−0.0013 (4)	0.0066 (5)	−0.0016 (4)
C36	0.0244 (6)	0.0373 (7)	0.0230 (6)	0.0000 (5)	0.0106 (5)	0.0010 (5)

Geometric parameters (Å, °)

S1—C18	1.7442 (12)	C8—C9	1.4207 (16)
S1—C17	1.7545 (12)	C9—C10	1.3755 (16)

S2—C36	1.7370 (13)	C9—C17	1.4488 (15)
S2—C35	1.7454 (12)	C11—C16	1.3757 (17)
O1—C10	1.3517 (14)	C11—C12	1.3791 (17)
O1—C11	1.4050 (14)	C12—C13	1.3922 (18)
O2—C28	1.3512 (15)	C12—H12A	0.9500
O2—C29	1.4043 (15)	C13—C14	1.383 (2)
N1—C18	1.3452 (15)	C13—H13A	0.9500
N1—H1A	0.8800	C14—C15	1.381 (2)
N1—H1B	0.8800	C14—H14A	0.9500
N2—C18	1.3124 (16)	C15—C16	1.3844 (18)
N2—N3	1.3791 (13)	C15—H15A	0.9500
N3—C17	1.3007 (15)	C16—H16A	0.9500
N4—C8	1.3272 (15)	C19—C20	1.3892 (18)
N4—N5	1.3743 (14)	C19—C24	1.3891 (19)
N5—C10	1.3556 (15)	C19—H19A	0.9500
N5—C6	1.4288 (15)	C20—C21	1.379 (2)
N6—C36	1.3493 (17)	C20—H20A	0.9500
N6—H6A	0.8800	C21—C22	1.385 (3)
N6—H6B	0.8800	C21—H21A	0.9500
N7—C36	1.3136 (17)	C22—C23	1.387 (2)
N7—N8	1.3826 (14)	C22—H22A	0.9500
N8—C35	1.2991 (16)	C23—C24	1.3888 (19)
N9—C26	1.3279 (16)	C23—H23A	0.9500
N9—N10	1.3744 (14)	C25—C26	1.4908 (17)
N10—C28	1.3555 (15)	C25—H25A	0.9800
N10—C24	1.4279 (15)	C25—H25B	0.9800
C1—C6	1.3887 (18)	C25—H25C	0.9800
C1—C2	1.3904 (17)	C26—C27	1.4198 (17)
C1—H1C	0.9500	C27—C28	1.3787 (17)
C2—C3	1.383 (2)	C27—C35	1.4503 (16)
C2—H2B	0.9500	C29—C30	1.375 (2)
C3—C4	1.388 (2)	C29—C34	1.3781 (18)
C3—H3B	0.9500	C30—C31	1.398 (2)
C4—C5	1.3859 (19)	C30—H30A	0.9500
C4—H4B	0.9500	C31—C32	1.368 (3)
C5—C6	1.3915 (18)	C31—H31A	0.9500
C5—H5A	0.9500	C32—C33	1.369 (3)
C7—C8	1.4927 (16)	C32—H32A	0.9500
C7—H7B	0.9800	C33—C34	1.391 (2)
C7—H7C	0.9800	C33—H33A	0.9500
C7—H7D	0.9800	C34—H34A	0.9500
C18—S1—C17	86.71 (5)	C14—C15—H15A	119.9
C36—S2—C35	86.84 (6)	C16—C15—H15A	119.9
C10—O1—C11	118.17 (9)	C11—C16—C15	119.26 (12)
C28—O2—C29	118.28 (10)	C11—C16—H16A	120.4
C18—N1—H1A	120.0	C15—C16—H16A	120.4
C18—N1—H1B	120.0	N3—C17—C9	122.87 (10)
H1A—N1—H1B	120.0	N3—C17—S1	113.56 (8)
C18—N2—N3	112.82 (10)	C9—C17—S1	123.54 (9)

C17—N3—N2	113.26 (10)	N2—C18—N1	122.82 (11)
C8—N4—N5	105.94 (9)	N2—C18—S1	113.65 (9)
C10—N5—N4	110.28 (9)	N1—C18—S1	123.52 (10)
C10—N5—C6	130.08 (10)	C20—C19—C24	119.10 (13)
N4—N5—C6	119.42 (9)	C20—C19—H19A	120.4
C36—N6—H6A	120.0	C24—C19—H19A	120.4
C36—N6—H6B	120.0	C21—C20—C19	120.55 (14)
H6A—N6—H6B	120.0	C21—C20—H20A	119.7
C36—N7—N8	112.34 (10)	C19—C20—H20A	119.7
C35—N8—N7	113.19 (10)	C20—C21—C22	119.89 (13)
C26—N9—N10	105.92 (10)	C20—C21—H21A	120.1
C28—N10—N9	110.37 (10)	C22—C21—H21A	120.1
C28—N10—C24	130.33 (11)	C21—C22—C23	120.51 (15)
N9—N10—C24	118.92 (10)	C21—C22—H22A	119.7
C6—C1—C2	119.22 (12)	C23—C22—H22A	119.7
C6—C1—H1C	120.4	C22—C23—C24	119.09 (15)
C2—C1—H1C	120.4	C22—C23—H23A	120.5
C3—C2—C1	120.27 (13)	C24—C23—H23A	120.5
C3—C2—H2B	119.9	C23—C24—C19	120.84 (12)
C1—C2—H2B	119.9	C23—C24—N10	118.13 (12)
C2—C3—C4	120.04 (12)	C19—C24—N10	120.95 (11)
C2—C3—H3B	120.0	C26—C25—H25A	109.5
C4—C3—H3B	120.0	C26—C25—H25B	109.5
C5—C4—C3	120.43 (14)	H25A—C25—H25B	109.5
C5—C4—H4B	119.8	C26—C25—H25C	109.5
C3—C4—H4B	119.8	H25A—C25—H25C	109.5
C4—C5—C6	119.08 (13)	H25B—C25—H25C	109.5
C4—C5—H5A	120.5	N9—C26—C27	111.09 (11)
C6—C5—H5A	120.5	N9—C26—C25	120.35 (11)
C1—C6—C5	120.93 (11)	C27—C26—C25	128.55 (11)
C1—C6—N5	120.67 (11)	C28—C27—C26	104.34 (10)
C5—C6—N5	118.33 (11)	C28—C27—C35	127.21 (11)
C8—C7—H7B	109.5	C26—C27—C35	128.21 (11)
C8—C7—H7C	109.5	O2—C28—N10	122.78 (11)
H7B—C7—H7C	109.5	O2—C28—C27	128.84 (11)
C8—C7—H7D	109.5	N10—C28—C27	108.27 (11)
H7B—C7—H7D	109.5	C30—C29—C34	121.48 (13)
H7C—C7—H7D	109.5	C30—C29—O2	123.56 (11)
N4—C8—C9	111.05 (10)	C34—C29—O2	114.95 (12)
N4—C8—C7	120.65 (10)	C29—C30—C31	118.28 (14)
C9—C8—C7	128.29 (10)	C29—C30—H30A	120.9
C10—C9—C8	104.34 (10)	C31—C30—H30A	120.9
C10—C9—C17	127.61 (11)	C32—C31—C30	121.03 (17)
C8—C9—C17	128.04 (11)	C32—C31—H31A	119.5
O1—C10—N5	123.32 (10)	C30—C31—H31A	119.5
O1—C10—C9	128.20 (10)	C31—C32—C33	119.66 (15)
N5—C10—C9	108.38 (10)	C31—C32—H32A	120.2
C16—C11—C12	121.86 (11)	C33—C32—H32A	120.2
C16—C11—O1	114.58 (10)	C32—C33—C34	120.81 (15)

C12—C11—O1	123.52 (11)	C32—C33—H33A	119.6
C11—C12—C13	118.12 (12)	C34—C33—H33A	119.6
C11—C12—H12A	120.9	C29—C34—C33	118.74 (15)
C13—C12—H12A	120.9	C29—C34—H34A	120.6
C14—C13—C12	120.90 (13)	C33—C34—H34A	120.6
C14—C13—H13A	119.6	N8—C35—C27	123.33 (11)
C12—C13—H13A	119.6	N8—C35—S2	113.75 (9)
C15—C14—C13	119.61 (12)	C27—C35—S2	122.91 (9)
C15—C14—H14A	120.2	N7—C36—N6	123.00 (12)
C13—C14—H14A	120.2	N7—C36—S2	113.89 (9)
C14—C15—C16	120.25 (12)	N6—C36—S2	123.06 (10)
C18—N2—N3—C17	−0.36 (15)	N3—N2—C18—S1	0.46 (14)
C8—N4—N5—C10	0.95 (13)	C17—S1—C18—N2	−0.33 (10)
C8—N4—N5—C6	−174.12 (10)	C17—S1—C18—N1	−179.62 (12)
C36—N7—N8—C35	−0.94 (17)	C24—C19—C20—C21	0.5 (2)
C26—N9—N10—C28	0.83 (14)	C19—C20—C21—C22	−0.9 (2)
C26—N9—N10—C24	−172.83 (11)	C20—C21—C22—C23	0.2 (3)
C6—C1—C2—C3	1.42 (19)	C21—C22—C23—C24	0.8 (2)
C1—C2—C3—C4	−0.8 (2)	C22—C23—C24—C19	−1.1 (2)
C2—C3—C4—C5	−0.9 (2)	C22—C23—C24—N10	175.63 (13)
C3—C4—C5—C6	2.0 (2)	C20—C19—C24—C23	0.46 (19)
C2—C1—C6—C5	−0.36 (19)	C20—C19—C24—N10	−176.23 (11)
C2—C1—C6—N5	−177.25 (11)	C28—N10—C24—C23	156.26 (13)
C4—C5—C6—C1	−1.3 (2)	N9—N10—C24—C23	−31.54 (17)
C4—C5—C6—N5	175.65 (13)	C28—N10—C24—C19	−27.0 (2)
C10—N5—C6—C1	−27.86 (19)	N9—N10—C24—C19	145.24 (12)
N4—N5—C6—C1	146.09 (11)	N10—N9—C26—C27	−0.30 (14)
C10—N5—C6—C5	155.17 (13)	N10—N9—C26—C25	178.83 (11)
N4—N5—C6—C5	−30.88 (17)	N9—C26—C27—C28	−0.31 (14)
N5—N4—C8—C9	−0.65 (13)	C25—C26—C27—C28	−179.36 (13)
N5—N4—C8—C7	178.21 (11)	N9—C26—C27—C35	174.30 (12)
N4—C8—C9—C10	0.12 (14)	C25—C26—C27—C35	−4.7 (2)
C7—C8—C9—C10	−178.63 (12)	C29—O2—C28—N10	−80.86 (15)
N4—C8—C9—C17	179.00 (11)	C29—O2—C28—C27	103.48 (15)
C7—C8—C9—C17	0.3 (2)	N9—N10—C28—O2	−177.49 (11)
C11—O1—C10—N5	−77.24 (14)	C24—N10—C28—O2	−4.8 (2)
C11—O1—C10—C9	106.74 (14)	N9—N10—C28—C27	−1.05 (14)
N4—N5—C10—O1	−177.60 (10)	C24—N10—C28—C27	171.67 (12)
C6—N5—C10—O1	−3.22 (19)	C26—C27—C28—O2	176.96 (12)
N4—N5—C10—C9	−0.90 (13)	C35—C27—C28—O2	2.3 (2)
C6—N5—C10—C9	173.49 (11)	C26—C27—C28—N10	0.81 (14)
C8—C9—C10—O1	176.97 (11)	C35—C27—C28—N10	−173.88 (12)
C17—C9—C10—O1	−1.9 (2)	C28—O2—C29—C30	−11.62 (17)
C8—C9—C10—N5	0.47 (13)	C28—O2—C29—C34	169.42 (11)
C17—C9—C10—N5	−178.42 (11)	C34—C29—C30—C31	0.5 (2)
C10—O1—C11—C16	159.41 (10)	O2—C29—C30—C31	−178.34 (13)
C10—O1—C11—C12	−22.92 (16)	C29—C30—C31—C32	0.0 (2)
C16—C11—C12—C13	0.19 (19)	C30—C31—C32—C33	−0.5 (2)
O1—C11—C12—C13	−177.32 (11)	C31—C32—C33—C34	0.4 (2)

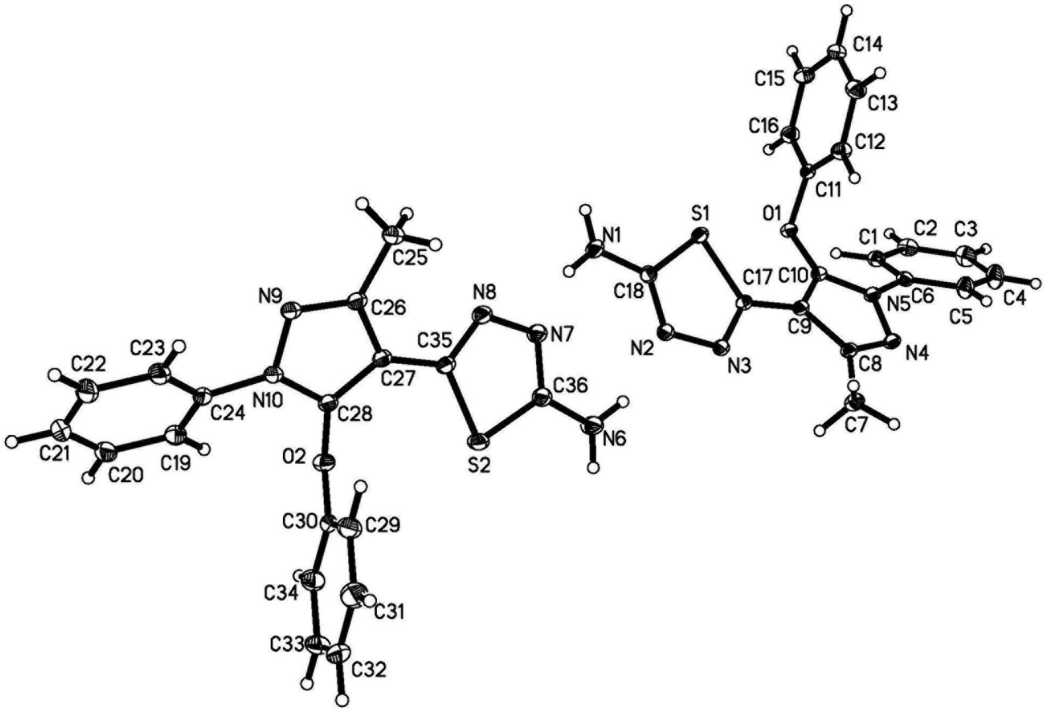
C11—C12—C13—C14	0.3 (2)	C30—C29—C34—C33	−0.6 (2)
C12—C13—C14—C15	−0.5 (2)	O2—C29—C34—C33	178.33 (12)
C13—C14—C15—C16	0.3 (2)	C32—C33—C34—C29	0.2 (2)
C12—C11—C16—C15	−0.36 (19)	N7—N8—C35—C27	−178.05 (11)
O1—C11—C16—C15	177.35 (11)	N7—N8—C35—S2	0.50 (15)
C14—C15—C16—C11	0.1 (2)	C28—C27—C35—N8	153.50 (13)
N2—N3—C17—C9	178.14 (11)	C26—C27—C35—N8	−19.9 (2)
N2—N3—C17—S1	0.10 (13)	C28—C27—C35—S2	−24.92 (18)
C10—C9—C17—N3	159.30 (12)	C26—C27—C35—S2	161.64 (11)
C8—C9—C17—N3	−19.3 (2)	C36—S2—C35—N8	0.03 (11)
C10—C9—C17—S1	−22.85 (18)	C36—S2—C35—C27	178.59 (11)
C8—C9—C17—S1	158.51 (10)	N8—N7—C36—N6	−176.50 (13)
C18—S1—C17—N3	0.12 (10)	N8—N7—C36—S2	0.97 (15)
C18—S1—C17—C9	−177.90 (11)	C35—S2—C36—N7	−0.58 (11)
N3—N2—C18—N1	179.75 (11)	C35—S2—C36—N6	176.89 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···N7	0.88	2.19	3.0266 (16)	158
N1—H1B···N4^{i}	0.88	2.21	3.0113 (15)	150
N6—H6A···N2	0.88	2.11	2.9467 (15)	159
N6—H6B···N9^{ii}	0.88	2.23	2.9915 (16)	145

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

Fig. 1


C14
C15
C13
C16
C12
C11
O1
S1
N1
C1
C2
C3
C25
C17
C10
N9
C26
N8
C18
N5
C6
C4
C5
C9
C23
C35
N7
N2
N3
N4
C22
C27
C8
C24
N10
C28
C36
C7
N6
C21
C20
C19
O2
S2
C30
C29
C34
C31
C33
C32