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1-Acetyl-3-[4-(methylsulfanyl)phenyl]-5-(4-nitrophenyl)-4,5-dihydro-1*H*-pyrazole

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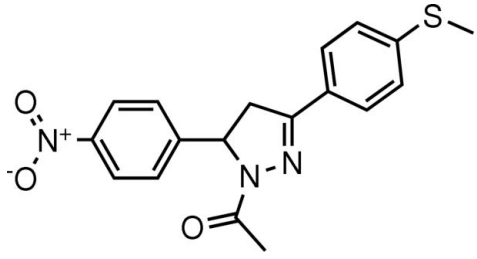
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.003 Å; R factor = 0.071; wR factor = 0.141; data-to-parameter ratio = 24.7.

In the title molecule, $C_{18}H_{17}N_3O_3S$, the dihedral angle between the two benzene rings is 72.8 (1)°. C—H···O and C—H···N hydrogen bonds are found in the crystal structure.

Related literature

For the uses of pyrazolines, see Bilgin *et al.* (1993); Chen *et al.* (1995); Hiroshi *et al.* (1970); Korgaokar *et al.* (1996); Kumar *et al.* (2003); Mancera *et al.*, (1991); Nauduri & Reddy, (1998); Nugent *et al.* (1993); Udupi *et al.* (1998);



Experimental

Crystal data

$C_{18}H_{17}N_3O_3S$
M_r = 355.42
Monoclinic, $P2_1/c$
a = 5.2630 (2) Å
b = 35.631 (2) Å
c = 9.0145 (3) Å
β = 91.651 (4)°
V = 1689.76 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 200 (2) K
0.41 × 0.33 × 0.28 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.822, T_{max} = 1.000 (expected range = 0.774–0.942)
16654 measured reflections
5637 independent reflections
3490 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.141
S = 1.07
5637 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23···O1^{i}	0.95	2.45	3.382 (3)	165
C26—H26···O1^{ii}	0.95	2.41	3.149 (3)	134
C26—H26···N1	0.95	2.53	2.853 (3)	100

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

RJB acknowledges the NSF–MRI program for funding to purchase the X-ray CCD diffractometer. AT thanks the UGC, India, for the award of a Minor Research Project [File No. MRP-2355/06(UGC-SERO), Link No. 2355, 10/01/2007].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2044).

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supplementary materials

Acta Cryst. (2007). E**63**, o4770 [**doi:10.1107/S1600536807058205**]

1-Acetyl-3-[4-(methylsulfanyl)phenyl]-5-(4-nitrophenyl)-4,5-dihydro-1*H*-pyrazole

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Comment

Pyrazolines have been reported to exhibit a broad spectrum of biological activities including antibacterial, antifungal, anti-inflammatory, anti-depressant, antiviral agents (Nauduri & Reddy, 1998; Korgaokar *et al.*, 1996; Udupi *et al.*, 1998 & Bilgin *et al.*, 1993). Some of these compounds have also shown ulcerogenic, anaesthetic and analgesic properties(Mancera *et al.*, 1991; Kumar *et al.*, 2003 & Nugent *et al.*, 1993). For instance, 1-thiocarbonyl-3,5-diphenyl-2-pyrazolines exhibit antidepressant activity(Hiroshi *et al.*, 1970), while (5-benzoyl-2,4-dihydro-3*H*-pyrazol-3-ylidene) bis phosphonic acid tetraethyl ester has been reported to possess novel anti-inflammatory activity. It also inhibits chronic arthritis and inflammation in animals. 3-Amino-1-[*m*-(trifluoromethyl)phenyl]-2-pyrazoline, besides acting as dual lipoxygenase/cycloxygenase inhibitor, attenuates postischemic brain hypoperfusion and repercussion injury(Bilgin *et al.*, 1993). Many pyrazolines also find utility as polymer intermediates in industry(Chen *et al.*, 1995).

In the title molecule, $C_{18}H_{17}N_3O_3S$, Fig.1., the dihedral angle between the two phenyl rings is 72.8 (1)°. The pyrazole ring makes a dihedral angle of 16.0 (1)° and 78.1 (1)°, with that of the methylthiophenyl and nitrophenyl rings respectively. The acetyl group is coplanar with the attached pyrazole ring, except the methyl H atoms. C—H···O, and C—H···N hydrogen bonds are found in the crystal structure; see hydrogen bond table.

Experimental

A mixture of 1-[4-(methylthio)phenyl]-3-(4-nitrophenyl)prop-2-en-1-one (5 g, 0.016 mol) and a molar equivalent of hydrazine hydrate (80%) in glacial acetic acid (25 ml) was heated on water bath at 363–5 K for 5–6 hr. The reaction mass was then poured into ice-cold water. The solid obtained was filtered, washed with water, dried and crystallized from methanol to yield the title compound. Yield 5.2 g (88%),

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95–1.00Å and U_{iso}=1.2–1.5 times U_{eq}(C).

Figures

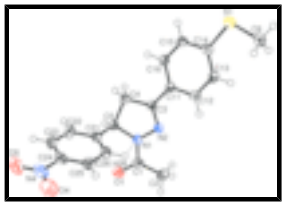

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. Dashed line indicate hydrogen bond.

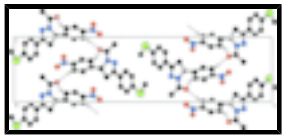

Fig. 2. The packing of the title compound, viewed down the *c* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

1-Acetyl-3-[4-(methylsulfanyl)phenyl]-5-(4-nitrophenyl)-4,5-dihydro-1*H*-pyrazole

Crystal data

$C_{18}H_{17}N_3O_3S$	F_{000} = 744
M_r = 355.42	D_x = 1.397 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 396(1) K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 5.2630 (2) Å	Cell parameters from 4988 reflections
b = 35.631 (2) Å	θ = 4.6–32.4º
c = 9.0145 (3) Å	μ = 0.21 mm^{-1}
β = 91.651 (4)º	T = 200 (2) K
V = 1689.76 (13) Å^3	Prism, colourless
Z = 4	0.41 × 0.33 × 0.28 mm

Data collection

Oxford Diffraction Gemini diffractometer	5637 independent reflections
Radiation source: fine-focus sealed tube	3490 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.038
T = 200(2) K	θ_{max} = 32.5º
φ and ω scans	θ_{min} = 4.6º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	h = −7→5
T_{min} = 0.822, T_{max} = 1.000	k = −43→53
16654 measured reflections	l = −11→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.071	H-atom parameters constrained
$wR(F^2)$ = 0.141	$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.9398P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = <0.001
5637 reflections	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
228 parameters	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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	1.27204 (11)	0.00962 (2)	0.63858 (6)	0.0396 (2)
O1	0.1107 (3)	0.16677 (5)	1.30061 (16)	0.0396 (5)
O4	0.9584 (5)	0.30750 (6)	1.1909 (3)	0.0774 (9)
O5	0.6845 (4)	0.33244 (5)	1.0406 (2)	0.0635 (7)
N1	0.3441 (3)	0.13614 (5)	1.13728 (17)	0.0283 (5)
N2	0.5244 (3)	0.10911 (4)	1.10260 (17)	0.0268 (5)
N4	0.7752 (4)	0.30532 (6)	1.1052 (2)	0.0486 (7)
C1	0.2485 (4)	0.14011 (6)	1.2751 (2)	0.0306 (6)
C2	0.3161 (5)	0.11025 (7)	1.3860 (2)	0.0473 (8)
C3	0.5669 (3)	0.11213 (5)	0.9637 (2)	0.0247 (5)
C4	0.4033 (4)	0.14086 (6)	0.8842 (2)	0.0298 (6)
C5	0.2927 (4)	0.16276 (6)	1.0149 (2)	0.0276 (6)
C6	1.4986 (4)	−0.00883 (6)	0.7715 (3)	0.0365 (7)
C11	0.7510 (3)	0.08801 (5)	0.8899 (2)	0.0237 (5)
C12	0.9297 (3)	0.06650 (6)	0.9694 (2)	0.0262 (5)
C13	1.0945 (4)	0.04292 (6)	0.8973 (2)	0.0286 (6)
C14	1.0853 (3)	0.04011 (5)	0.7425 (2)	0.0269 (6)
C15	0.9118 (4)	0.06228 (6)	0.6628 (2)	0.0288 (6)
C16	0.7480 (4)	0.08588 (6)	0.7351 (2)	0.0285 (6)
C21	0.4226 (4)	0.20011 (6)	1.0414 (2)	0.0269 (5)
C22	0.3251 (4)	0.23200 (6)	0.9717 (2)	0.0366 (7)
C23	0.4400 (4)	0.26651 (6)	0.9913 (3)	0.0393 (7)
C24	0.6563 (4)	0.26848 (6)	1.0810 (2)	0.0358 (7)
C25	0.7595 (4)	0.23736 (6)	1.1511 (2)	0.0377 (7)
C26	0.6407 (4)	0.20312 (6)	1.1311 (2)	0.0319 (6)
H2A	0.25307	0.11740	1.48332	0.0710*
H2B	0.50120	0.10735	1.39278	0.0710*
H2C	0.23819	0.08645	1.35470	0.0710*
H4A	0.26750	0.12880	0.82265	0.0357*
H4B	0.50570	0.15734	0.82069	0.0357*
H5	0.10549	0.16637	0.99905	0.0331*
H6A	1.62916	−0.02295	0.71986	0.0547*
H6B	1.41215	−0.02551	0.84020	0.0547*
H6C	1.57844	0.01188	0.82709	0.0547*

H12	0.93834	0.06808	1.07463	0.0314*
H13	1.21493	0.02850	0.95339	0.0343*
H15	0.90594	0.06116	0.55746	0.0344*
H16	0.63156	0.10090	0.67875	0.0342*
H22	0.17677	0.23001	0.90960	0.0439*
H23	0.37202	0.28832	0.94423	0.0472*
H25	0.90938	0.23945	1.21179	0.0453*
H26	0.70853	0.18145	1.17909	0.0383*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0357 (3)	0.0470 (3)	0.0358 (3)	0.0106 (3)	−0.0015 (2)	−0.0129 (3)
O1	0.0377 (8)	0.0484 (10)	0.0328 (8)	0.0106 (7)	0.0047 (6)	−0.0037 (7)
O4	0.0953 (17)	0.0550 (13)	0.0806 (15)	−0.0236 (12)	−0.0203 (13)	−0.0130 (11)
O5	0.0779 (14)	0.0311 (10)	0.0826 (14)	−0.0010 (9)	0.0200 (11)	−0.0011 (10)
N1	0.0312 (8)	0.0272 (9)	0.0266 (8)	0.0052 (7)	0.0039 (7)	0.0035 (7)
N2	0.0294 (8)	0.0238 (8)	0.0272 (8)	0.0014 (7)	0.0025 (6)	0.0006 (7)
N4	0.0621 (14)	0.0361 (12)	0.0487 (12)	−0.0054 (10)	0.0188 (11)	−0.0128 (10)
C1	0.0326 (10)	0.0350 (11)	0.0242 (10)	−0.0022 (9)	0.0024 (8)	−0.0012 (8)
C2	0.0686 (16)	0.0472 (15)	0.0267 (11)	0.0060 (12)	0.0098 (10)	0.0068 (10)
C3	0.0259 (9)	0.0228 (9)	0.0254 (9)	−0.0027 (8)	−0.0007 (7)	0.0009 (8)
C4	0.0338 (10)	0.0313 (11)	0.0243 (9)	0.0041 (9)	0.0008 (8)	0.0016 (8)
C5	0.0277 (9)	0.0299 (11)	0.0251 (9)	0.0048 (8)	0.0008 (7)	0.0040 (8)
C6	0.0331 (11)	0.0314 (11)	0.0450 (12)	0.0044 (9)	0.0038 (9)	0.0012 (10)
C11	0.0255 (9)	0.0223 (9)	0.0232 (9)	−0.0028 (7)	0.0015 (7)	0.0001 (7)
C12	0.0280 (9)	0.0309 (10)	0.0195 (9)	−0.0020 (8)	−0.0003 (7)	0.0004 (8)
C13	0.0252 (9)	0.0307 (11)	0.0298 (10)	0.0019 (8)	−0.0030 (8)	0.0029 (8)
C14	0.0237 (9)	0.0270 (10)	0.0300 (10)	−0.0027 (8)	0.0025 (7)	−0.0035 (8)
C15	0.0342 (10)	0.0317 (11)	0.0204 (9)	−0.0011 (8)	0.0019 (7)	−0.0004 (8)
C16	0.0302 (10)	0.0272 (10)	0.0280 (10)	0.0014 (8)	−0.0023 (8)	0.0027 (8)
C21	0.0277 (9)	0.0281 (10)	0.0251 (9)	0.0048 (8)	0.0053 (7)	0.0014 (8)
C22	0.0352 (11)	0.0351 (12)	0.0391 (12)	0.0036 (9)	−0.0045 (9)	0.0093 (10)
C23	0.0453 (13)	0.0312 (12)	0.0418 (12)	0.0056 (10)	0.0060 (10)	0.0095 (10)
C24	0.0441 (13)	0.0288 (11)	0.0351 (11)	−0.0019 (9)	0.0138 (9)	−0.0062 (9)
C25	0.0361 (11)	0.0400 (13)	0.0369 (12)	−0.0001 (10)	−0.0015 (9)	−0.0048 (10)
C26	0.0308 (10)	0.0311 (11)	0.0337 (11)	0.0060 (8)	−0.0016 (8)	0.0021 (9)

Geometric parameters (Å, °)

S1—C6	1.791 (2)	C21—C26	1.389 (3)
S1—C14	1.7541 (18)	C22—C23	1.379 (3)
O1—C1	1.221 (3)	C23—C24	1.379 (3)
O4—N4	1.221 (3)	C24—C25	1.380 (3)
O5—N4	1.219 (3)	C25—C26	1.380 (3)
N1—N2	1.394 (2)	C2—H2A	0.9800
N1—C1	1.361 (2)	C2—H2B	0.9800
N1—C5	1.474 (3)	C2—H2C	0.9800
N2—C3	1.283 (2)	C4—H4A	0.9900

N4—C24	1.468 (3)	C4—H4B	0.9900
C1—C2	1.496 (3)	C5—H5	1.0000
C3—C4	1.506 (3)	C6—H6A	0.9800
C3—C11	1.469 (2)	C6—H6B	0.9800
C4—C5	1.541 (3)	C6—H6C	0.9800
C5—C21	1.512 (3)	C12—H12	0.9500
C11—C12	1.395 (2)	C13—H13	0.9500
C11—C16	1.397 (3)	C15—H15	0.9500
C12—C13	1.383 (3)	C16—H16	0.9500
C13—C14	1.399 (3)	C22—H22	0.9500
C14—C15	1.392 (3)	C23—H23	0.9500
C15—C16	1.381 (3)	C25—H25	0.9500
C21—C22	1.390 (3)	C26—H26	0.9500
S1···S1^{i}	3.5799 (8)	C13···H6B	3.0100
O1···C21	3.128 (2)	C13···H6C^{ii}	2.9800
O1···C25^{ii}	3.379 (3)	C13···H6C	2.8600
O1···C26^{ii}	3.149 (3)	C14···H6C^{ii}	2.9700
O1···O5^{iii}	3.161 (2)	C15···H6C^{ii}	2.9400
O1···C23^{iv}	3.382 (3)	C16···H4B	2.9600
O4···C4^{v}	3.416 (3)	C16···H6C^{ii}	2.9100
O5···C2^{vi}	3.117 (3)	C16···H4A	3.0800
O5···O1^{vii}	3.161 (2)	C26···H5^{ix}	3.0500
O5···C1^{vi}	3.411 (3)	H2B···N2	2.6200
O5···C16^{iv}	3.409 (3)	H2B···O5^{iv}	2.6900
O1···H25^{ii}	2.9000	H2C···N2	2.8800
O1···H26^{ii}	2.4100	H2C···H6A^{xii}	2.4700
O1···H23^{iv}	2.4500	H4A···C16	3.0800
O1···H5	2.7200	H4A···H16	2.5500
O4···H22^{v}	2.6200	H4B···C16	2.9600
O4···H25	2.4500	H4B···H16	2.4800
O5···H23	2.4200	H4B···O5^{vi}	2.7400
O5···H2B^{vi}	2.6900	H4B···N4^{vi}	2.7800
O5···H4B^{iv}	2.7400	H5···O1	2.7200
O5···H16^{iv}	2.7000	H5···C26^{ii}	3.0500
N2···C26	3.414 (3)	H5···H22	2.4400
N1···H26	2.5300	H6A···H2C^{xii}	2.4700
N2···H2B	2.6200	H6B···C13	3.0100
N2···H2C	2.8800	H6B···H13	2.4300
N2···H12	2.6400	H6B···C12^{xii}	2.9100
N2···H26	2.8300	H6B···H12^{xii}	2.5200
N4···H4B^{iv}	2.7800	H6C···C11^{ix}	2.9100
C1···C26	3.338 (3)	H6C···C12^{ix}	2.9500
C1···O5^{iv}	3.411 (3)	H6C···C13	2.8600

C2···O5^{iv}	3.117 (3)	H6C···C13^{ix}	2.9800
C3···C26	3.592 (3)	H6C···C14^{ix}	2.9700
C3···C13^{ii}	3.541 (3)	H6C···C15^{ix}	2.9400
C4···O4^{viii}	3.416 (3)	H6C···C16^{ix}	2.9100
C6···C15^{ix}	3.497 (3)	H6C···H13	2.3300
C6···C14^{ix}	3.562 (3)	H12···N2	2.6400
C13···C3^{ix}	3.541 (3)	H12···H6B^{xii}	2.5200
C14···C6^{ii}	3.562 (3)	H13···C6	2.6100
C15···C6^{ii}	3.497 (3)	H13···H6B	2.4300
C16···O5^{vi}	3.409 (3)	H13···H6C	2.3300
C21···O1	3.128 (2)	H13···C6^{xi}	2.9500
C22···C25^{ii}	3.434 (3)	H16···C2^{xiii}	3.1000
C23···C25^{vi}	3.542 (3)	H16···C4	2.6500
C23···O1^{vi}	3.382 (3)	H16···H4A	2.5500
C25···C23^{iv}	3.542 (3)	H16···H4B	2.4800
C25···C22^{ix}	3.434 (3)	H16···O5^{vi}	2.7000
C25···O1^{ix}	3.379 (3)	H22···H5	2.4400
C26···N2	3.414 (3)	H22···O4^{viii}	2.6200
C26···C3	3.592 (3)	H22···H25^{viii}	2.4900
C26···C1	3.338 (3)	H23···O5	2.4200
C26···O1^{ix}	3.149 (3)	H23···O1^{vi}	2.4500
C1···H26	2.9800	H23···C1^{vi}	3.0300
C1···H23^{iv}	3.0300	H25···O1^{ix}	2.9000
C2···H16^{x}	3.1000	H25···O4	2.4500
C4···H16	2.6500	H25···H22^{v}	2.4900
C6···H13	2.6100	H26···O1^{ix}	2.4100
C6···H13^{xi}	2.9500	H26···N1	2.5300
C11···H6C^{ii}	2.9100	H26···N2	2.8300
C12···H6B^{xii}	2.9100	H26···C1	2.9800
C12···H6C^{ii}	2.9500		
C6—S1—C14	104.04 (10)	C21—C26—C25	120.52 (19)
N2—N1—C1	123.26 (16)	C1—C2—H2A	109.00
N2—N1—C5	112.84 (14)	C1—C2—H2B	109.00
C1—N1—C5	123.48 (17)	C1—C2—H2C	109.00
N1—N2—C3	107.45 (14)	H2A—C2—H2B	109.00
O4—N4—O5	122.9 (2)	H2A—C2—H2C	109.00
O4—N4—C24	118.5 (2)	H2B—C2—H2C	109.00
O5—N4—C24	118.60 (19)	C3—C4—H4A	111.00
O1—C1—N1	119.34 (18)	C3—C4—H4B	111.00
O1—C1—C2	123.96 (18)	C5—C4—H4A	111.00
N1—C1—C2	116.68 (18)	C5—C4—H4B	111.00
N2—C3—C4	114.09 (15)	H4A—C4—H4B	109.00
N2—C3—C11	121.93 (16)	N1—C5—H5	110.00

C4—C3—C11	123.91 (16)	C4—C5—H5	110.00
C3—C4—C5	101.76 (15)	C21—C5—H5	110.00
N1—C5—C4	100.44 (16)	S1—C6—H6A	109.00
N1—C5—C21	112.07 (16)	S1—C6—H6B	109.00
C4—C5—C21	112.79 (17)	S1—C6—H6C	109.00
C3—C11—C12	122.17 (16)	H6A—C6—H6B	109.00
C3—C11—C16	119.71 (16)	H6A—C6—H6C	109.00
C12—C11—C16	118.11 (17)	H6B—C6—H6C	109.00
C11—C12—C13	120.99 (17)	C11—C12—H12	120.00
C12—C13—C14	120.55 (18)	C13—C12—H12	120.00
S1—C14—C13	124.99 (14)	C12—C13—H13	120.00
S1—C14—C15	116.44 (14)	C14—C13—H13	120.00
C13—C14—C15	118.55 (17)	C14—C15—H15	120.00
C14—C15—C16	120.75 (17)	C16—C15—H15	120.00
C11—C16—C15	121.01 (18)	C11—C16—H16	119.00
C5—C21—C22	119.27 (18)	C15—C16—H16	120.00
C5—C21—C26	121.48 (18)	C21—C22—H22	119.00
C22—C21—C26	119.23 (19)	C23—C22—H22	119.00
C21—C22—C23	121.08 (19)	C22—C23—H23	121.00
C22—C23—C24	118.2 (2)	C24—C23—H23	121.00
N4—C24—C23	118.29 (19)	C24—C25—H25	121.00
N4—C24—C25	119.35 (18)	C26—C25—H25	121.00
C23—C24—C25	122.4 (2)	C21—C26—H26	120.00
C24—C25—C26	118.66 (19)	C25—C26—H26	120.00
C6—S1—C14—C13	−9.62 (19)	C3—C4—C5—C21	102.45 (18)
C6—S1—C14—C15	172.01 (15)	N1—C5—C21—C22	−155.98 (17)
C1—N1—N2—C3	177.91 (18)	N1—C5—C21—C26	25.6 (3)
C5—N1—N2—C3	−9.3 (2)	C4—C5—C21—C22	91.5 (2)
N2—N1—C1—O1	172.68 (18)	C4—C5—C21—C26	−86.9 (2)
N2—N1—C1—C2	−8.9 (3)	C3—C11—C12—C13	177.49 (18)
C5—N1—C1—O1	0.7 (3)	C16—C11—C12—C13	−1.8 (3)
C5—N1—C1—C2	179.12 (19)	C3—C11—C16—C15	−177.32 (18)
N2—N1—C5—C4	17.1 (2)	C12—C11—C16—C15	2.0 (3)
N2—N1—C5—C21	−102.86 (18)	C11—C12—C13—C14	−0.1 (3)
C1—N1—C5—C4	−170.11 (18)	C12—C13—C14—S1	−176.62 (15)
C1—N1—C5—C21	69.9 (2)	C12—C13—C14—C15	1.7 (3)
N1—N2—C3—C4	−3.7 (2)	S1—C14—C15—C16	176.95 (16)
N1—N2—C3—C11	179.23 (15)	C13—C14—C15—C16	−1.5 (3)
O4—N4—C24—C23	176.1 (2)	C14—C15—C16—C11	−0.3 (3)
O4—N4—C24—C25	−2.3 (3)	C5—C21—C22—C23	−179.09 (19)
O5—N4—C24—C23	−2.9 (3)	C26—C21—C22—C23	−0.6 (3)
O5—N4—C24—C25	178.8 (2)	C5—C21—C26—C25	178.53 (18)
N2—C3—C4—C5	14.0 (2)	C22—C21—C26—C25	0.1 (3)
C11—C3—C4—C5	−168.96 (16)	C21—C22—C23—C24	0.6 (3)
N2—C3—C11—C12	−14.6 (3)	C22—C23—C24—N4	−178.43 (19)
N2—C3—C11—C16	164.69 (18)	C22—C23—C24—C25	−0.2 (3)
C4—C3—C11—C12	168.59 (18)	N4—C24—C25—C26	177.90 (18)
C4—C3—C11—C16	−12.1 (3)	C23—C24—C25—C26	−0.4 (3)
C3—C4—C5—N1	−17.02 (18)	C24—C25—C26—C21	0.4 (3)

Symmetry codes: (i) −*x*+3, −*y*, −*z*+1; (ii) *x*−1, *y*, *z*; (iii) *x*−1, −*y*+1/2, *z*+1/2; (iv) *x*, −*y*+1/2, *z*+1/2; (v) *x*+1, −*y*+1/2, *z*+1/2; (vi) *x*, −*y*+1/2, *z*−1/2; (vii) *x*+1, −*y*+1/2, *z*−1/2; (viii) *x*−1, −*y*+1/2, *z*−1/2; (ix) *x*+1, *y*, *z*; (x) *x*, *y*, *z*+1; (xi) −*x*+3, −*y*, −*z*+2; (xii) −*x*+2, −*y*, −*z*+2; (xiii) *x*, *y*, *z*−1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C23—H23···O1^{vi}	0.95	2.45	3.382 (3)	165
C26—H26···O1^{ix}	0.95	2.41	3.149 (3)	134
C26—H26···N1	0.95	2.53	2.853 (3)	100

Symmetry codes: (vi) *x*, −*y*+1/2, *z*−1/2; (ix) *x*+1, *y*, *z*.

Fig. 1

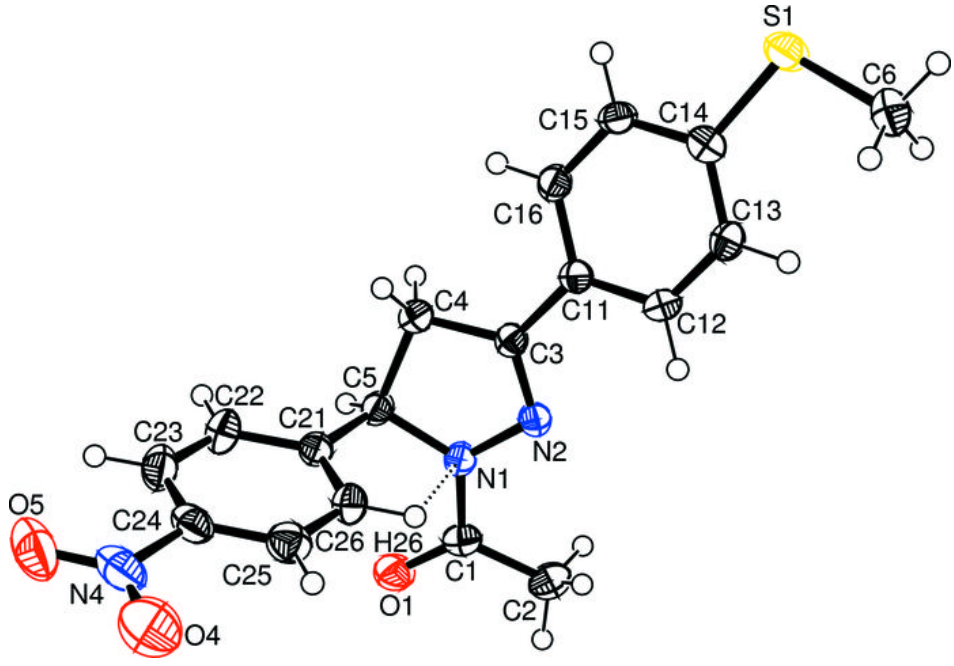
S1
C6
C15
C14
C16
C13
C4
C11
C12
C3
C5
C22
C21
C23
N2
N1
O5
C24
C26
H26
C25
C1
N4
O1
C2
O4

Fig. 2