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4-[(1,3-Dioxo-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-2-yl)methyl]-*N*′-[(*E*)-4-nitrobenzylidene]benzenesulfonohydrazide dimethyl sulfoxide monosolvate

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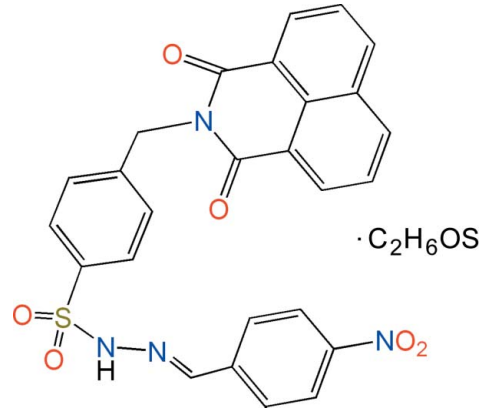
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.052; wR factor = 0.163; data-to-parameter ratio = 12.8.

The molecular structure of the title compound, $C_{26}H_{18}N_4O_6S\cdot C_2H_6OS$, shows an E conformation of the hydrazone double bond. The presence of a methylene group between the benzo[*de*]isoquinoline and benzenesulfonyl moieties allows the 4-nitrophenyl ring and the benzo[*de*]isoquinoline system to be parallel with respect to each other, so that the molecule adopts a U-shaped spatial conformation. The dihedral angle between mean planes of these aromatic groups is 4.4 (1)°. This special arrangement enables neighboring molecules to be intercalated, forming slipped π–π interactions [centroid–centroid distance = 3.535 (2) Å] between the 4-nitrophenyl and benzo[*de*]isoquinoline groups and point-to-face C—H$\cdots\pi$ interactions between the benzo[*de*]isoquinoline and benzenesulfonyl aromatic systems. In addition, the crystal packing also features an intermolecular N—H$\cdots$O interaction involving the amine group and the dimethyl sulfoxide solvent molecule.

Related literature

For the therapeutic properties of sulfonylhydrazones, see: Rollas *et al.* (2002); Frlan *et al.* (2008); Lima *et al.* (1999); Sondhi *et al.* (2006) and for their biological activity, see: Kendall *et al.* (2007); Sadek *et al.* (2008). For the anticancer activity of naphthalimides, see: Braña & Ramos (2001); Braña *et al.* (2001); Suárez & Sánchez (1992); Ingrassia *et al.* (2009); Wu *et al.* (2009); Norton *et al.* (2008). For the therapeutic properties of cyclic imides, see: Cechinel Filho *et al.* (2003); Walter *et al.* (2002). For background to this study, see: Silva *et al.* (2006); Oliveira & Nunes (2006).



Experimental

Crystal data

$C_{26}H_{18}N_4O_6S\cdot C_2H_6OS$
M_r = 592.63
Triclinic, $P\overline{1}$
a = 9.152 (1) Å
b = 11.971 (1) Å
c = 13.910 (1) Å
α = 107.268 (7)°
β = 101.789 (7)°
γ = 96.319 (8)°
V = 1400.6 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 293 K
0.50 × 0.16 × 0.13 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
5055 measured reflections
4737 independent reflections
3075 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.163
S = 1.04
4737 reflections
371 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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

Cg is the centroid of the *p*-nitrophenyl (C22–C27) ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2*N*$\cdots$O1*S*	0.80	1.99	2.764 (4)	163
C8—H8$\cdots Cg^{i}$	0.93	2.90	3.799 (6)	162

Symmetry code: (i) $-x+2, -y+2, -z+2$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *HELENA* (Spek, 1996); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2001).

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supplementary materials

Acta Cryst. (2011). E**67**, o627-o628 [**doi:10.1107/S1600536811004697**]

4-[(1,3-Dioxo-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-2-yl)methyl]-*N*'-[(*E*)-4-nitrobenzylidene]benzenesulfonohydrazide dimethyl sulfoxide monosolvate

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Comment

Sulfonyl-hydrazones are known for their therapeutic properties, such as, antimicrobial (Rollas *et al.* 2002, Frlan *et al.* 2008), analgesic (Lima *et al.* 1999, Sondhi *et al.* 2006), *etc*. Sulfonyl-hydrazones was selective inhibitor of p110α, a phosphoinositide-3-kinase that is over-expressed in 30% of tumors (Kendall *et al.* 2007). In innovative study, the sulfonyl-hydrazones were reported by enhance myocardial repair by stem cells by activating cardiac differentiation in human mobilized peripheral blood mononuclear cells (*M*-PBMCs) (Sadek *et al.* 2008).

Cyclic imides have also many therapeutic properties including antibacterial, antitumor, diuretic and antiviral (Cechinel Filho *et al.* 2003). In a previous publication, we reported the synthesis of imidobenzenesulfonyl compounds that showed promising analgesic profiles in the acetic acid- induced mice writhing test. The mechanism of action occurred possibly due to additional non-covalent interactions with the COX active site (Walter *et al.* 2002). The naphthalimides, in special, are known of their high DNA-binding ability and consequently many of them have anticancer property (Braña & Ramos, 2001); Braña *et al.* 2001). Mitonafide and Amonafide are classical examples of naphthalimides derivatives with antitumoral activity (Suárez *et al.* 1992). Recently, many similar compounds have been showed activity against different cancer cell lines (Ingrassia *et al.* 2009, Wu *et al.* 2009, Norton *et al.* 2008).

The title compound (I) (Scheme 1) was synthesized as a part of our work to investigate the antitumoral activity of the sulfonyl-hydrazones cyclic imides derivatives (Oliveira *et al.* 2006, Silva *et al.* 2006).

The molecular structure of the title compound (Fig. 1) shows **E** conformation on the hydrazone double bond, which is evidenced by the torsion angle S1–N2–N3–C21 of 165.8 (2)°. The presence of a methylene group among benzo[*de*]isoquinoline and benzenesulfonyl moieties allows *p*-nitrophenyl ring and benzo[*de*]isoquinoline system to be parallel with respect to each other, so that the molecule adopts an U-shaped spatial conformation. The dihedral angle between mean planes of these planar groups is 4.4 (1)°. This special arrangement enables the neighboring molecule be intercalated by a center of symmetry, forming pairs of molecules in a centrosymmetric structure (Fig. 2). Slipped π–π interaction between *p*-nitrophenyl and benzo[*de*]isoquinoline, with centroid–C12 distance of 3.589 Å, and point-to-face C–H···π interaction between benzenesulfonyl and benzo[*de*]isoquinoline aromatic systems, with centroid-H8 distance of 2.903 Å, are observed. In addition, crystal packing also shows an intermolecular N2–H···O1S interaction involving amine group and DMSO solvate.

Experimental

4-nitrobenzaldehyde (79 mg, 0.52 mmol) was added in a mixture of 4-[(1,3-dioxo-1*H*-benzo[*de*]isoquinolin-2(3*H*)-yl)methyl] benzenesulfonohydrazide (200 mg, 0.52 mmol) in ethanol (10 ml), with a drop of hydrochloric acid as catalyst, as described for similar compounds (Silva *et al.* 2006, Oliveira *et al.* 2006). The reaction was carried out by stirring at room temperature for one hour. The solid was filtered off with suction. The crystal used for data collection was obtained by dissolving 30 mg of (I) in 10 ml of dimethylsulfoxide and by slow evaporation of the solvent.

Refinement

All non-H atoms were refined with anisotropic displacement parameters. H atoms were placed at their idealized positions with distances of 0.93 and 0.97 Å and U_{eq} fixed at 1.2 times U_{iso} of the preceding atom for C–H_{Ar} and C–H_2, respectively and at 1.5 times U_{iso} of the preceding atom for C–H_3. The H atom of the amino group was found from Fourier map and treated with riding model and its U_{eq} was refined freely.

Figures

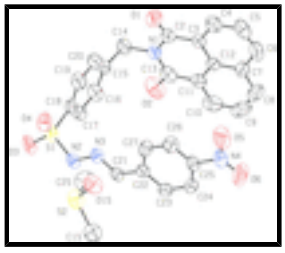

Fig. 1. The molecular structure of the title compound with the labelling scheme. Displacement ellipsoids are shown at the 40% probability level.

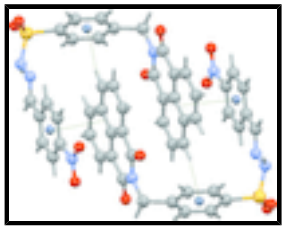

Fig. 2. Intermolecular interactions observed in (I).

4-[(1,3-Dioxo-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-2-yl)methyl]- *N*'-[(*E*)-4-nitrobenzylidene]benzenesulfonohydrazide dimethyl sulfoxide monosolvate

Crystal data

$C_{26}H_{18}N_4O_6S·C_2H_6OS$	$Z = 2$
$M_r = 592.63$	$F(000) = 616$
Triclinic, $P\overline{1}$	$D_x = 1.405$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.152$ (1) Å	Cell parameters from 25 reflections
$b = 11.971$ (1) Å	$\theta = 8.5$–$13.4°$
$c = 13.910$ (1) Å	$\mu = 0.24$ mm^{-1}
$\alpha = 107.268$ (7)°	$T = 293$ K
$\beta = 101.789$ (7)°	Prismatic, colourless
$\gamma = 96.319$ (8)°	0.50 × 0.16 × 0.13 mm
$V = 1400.6$ (2) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.017$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.1°$, $\theta_{min} = 2.3°$

graphite
ω–2θ scans
5055 measured reflections
4737 independent reflections
3075 reflections with $I > 2\sigma(I)$

$h = 0 \rightarrow 10$
$k = -14 \rightarrow 14$
$l = -16 \rightarrow 16$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.163$
$S = 1.04$
4737 reflections
371 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0792P)^2 + 0.613P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.34031 (11)	0.73620 (8)	0.53120 (6)	0.0597 (3)
N1	0.8354 (3)	1.1992 (2)	0.8805 (2)	0.0571 (7)
N2	0.4477 (3)	0.6426 (2)	0.55446 (19)	0.0540 (7)
H2N	0.5170	0.6398	0.5273	0.058 (12)*
N3	0.4776 (3)	0.6399 (2)	0.65605 (19)	0.0501 (6)
O1	0.6771 (4)	1.2526 (3)	0.9840 (2)	0.1026 (11)
O2	0.9903 (3)	1.1379 (3)	0.7756 (2)	0.0987 (10)
O3	0.3260 (3)	0.7192 (2)	0.42331 (18)	0.0797 (8)
O4	0.2088 (3)	0.7188 (2)	0.5685 (2)	0.0766 (8)
C2	0.7994 (4)	1.2237 (3)	0.9760 (3)	0.0626 (9)
C3	0.9105 (4)	1.2127 (3)	1.0630 (2)	0.0547 (8)
C4	0.8859 (5)	1.2441 (4)	1.1612 (3)	0.0767 (11)
H4	0.7994	1.2747	1.1724	0.092*
C5	0.9881 (6)	1.2309 (4)	1.2432 (3)	0.0864 (13)
H5	0.9706	1.2547	1.3092	0.104*
C6	1.1117 (6)	1.1846 (4)	1.2296 (3)	0.0803 (13)
H6	1.1779	1.1753	1.2858	0.096*
C7	1.1429 (4)	1.1495 (3)	1.1304 (3)	0.0645 (10)
C8	1.2697 (5)	1.1010 (4)	1.1103 (5)	0.0918 (15)
H8	1.3383	1.0895	1.1643	0.110*
C9	1.2953 (5)	1.0705 (4)	1.0149 (6)	0.1053 (19)
H9	1.3799	1.0370	1.0038	0.126*
C10	1.1970 (5)	1.0884 (4)	0.9325 (4)	0.0845 (13)
H10	1.2170	1.0683	0.8672	0.101*
C11	1.0701 (4)	1.1359 (3)	0.9479 (3)	0.0547 (8)

C12	1.0410 (4)	1.1663 (3)	1.0464 (3)	0.0492 (8)
C13	0.9662 (4)	1.1572 (3)	0.8612 (3)	0.0636 (10)
C14	0.7269 (5)	1.2149 (3)	0.7930 (3)	0.0737 (11)
H14A	0.7827	1.2462	0.7515	0.088*
H14B	0.6660	1.2723	0.8202	0.088*
C15	0.6233 (4)	1.0984 (3)	0.7248 (3)	0.0602 (9)
C16	0.6623 (5)	1.0275 (3)	0.6388 (3)	0.0680 (10)
H16	0.7496	1.0539	0.6214	0.082*
C17	0.5738 (4)	0.9184 (3)	0.5784 (3)	0.0636 (9)
H17	0.6009	0.8715	0.5208	0.076*
C18	0.4443 (4)	0.8797 (3)	0.6049 (2)	0.0535 (8)
C19	0.4011 (4)	0.9501 (4)	0.6880 (3)	0.0714 (10)
H19	0.3127	0.9246	0.7045	0.086*
C20	0.4909 (5)	1.0596 (4)	0.7469 (3)	0.0765 (11)
H20	0.4611	1.1079	0.8027	0.092*
C21	0.5844 (4)	0.5873 (3)	0.6806 (2)	0.0500 (8)
H21	0.6372	0.5541	0.6320	0.060*
C22	0.6255 (4)	0.5781 (3)	0.7849 (2)	0.0475 (7)
C23	0.7517 (4)	0.5304 (3)	0.8140 (3)	0.0580 (9)
H23	0.8057	0.4994	0.7655	0.070*
C24	0.7984 (4)	0.5285 (3)	0.9143 (3)	0.0613 (9)
H24	0.8839	0.4973	0.9341	0.074*
C25	0.7162 (4)	0.5734 (3)	0.9838 (2)	0.0550 (8)
C26	0.5894 (4)	0.6196 (3)	0.9578 (3)	0.0638 (9)
H26	0.5356	0.6495	1.0067	0.077*
C27	0.5431 (4)	0.6209 (3)	0.8576 (3)	0.0615 (9)
H27	0.4561	0.6507	0.8382	0.074*
N4	0.7691 (4)	0.5767 (3)	1.0923 (3)	0.0733 (9)
O5	0.6974 (4)	0.6209 (4)	1.1535 (2)	0.1111 (12)
O6	0.8819 (4)	0.5387 (4)	1.1166 (2)	0.1188 (13)
S2	0.74498 (12)	0.64956 (10)	0.39415 (8)	0.0747 (3)
O1S	0.7208 (3)	0.6673 (3)	0.5003 (2)	0.0830 (8)
C1S	0.8748 (5)	0.5522 (4)	0.3777 (3)	0.0833 (12)
H1S1	0.8257	0.4734	0.3689	0.125*
H1S2	0.9591	0.5784	0.4379	0.125*
H1S3	0.9105	0.5515	0.3173	0.125*
C2S	0.8693 (6)	0.7814 (4)	0.4070 (4)	0.1081 (17)
H2S1	0.8157	0.8468	0.4170	0.162*
H2S2	0.9049	0.7705	0.3451	0.162*
H2S3	0.9542	0.7979	0.4657	0.162*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0667 (6)	0.0595 (5)	0.0449 (5)	−0.0013 (4)	−0.0036 (4)	0.0219 (4)
N1	0.0665 (19)	0.0523 (16)	0.0478 (16)	0.0087 (14)	0.0064 (14)	0.0155 (13)
N2	0.0696 (19)	0.0552 (16)	0.0371 (14)	0.0016 (14)	0.0122 (14)	0.0193 (12)
N3	0.0566 (16)	0.0536 (15)	0.0412 (14)	0.0033 (13)	0.0094 (12)	0.0217 (12)

O1	0.084 (2)	0.137 (3)	0.079 (2)	0.060 (2)	0.0151 (16)	0.0140 (19)
O2	0.103 (2)	0.127 (3)	0.0623 (18)	−0.0099 (19)	0.0389 (17)	0.0240 (17)
O3	0.113 (2)	0.0723 (17)	0.0391 (13)	−0.0025 (15)	−0.0086 (13)	0.0230 (12)
O4	0.0539 (15)	0.0878 (19)	0.0830 (19)	0.0021 (13)	0.0062 (13)	0.0319 (15)
C2	0.064 (2)	0.062 (2)	0.055 (2)	0.0181 (18)	0.0125 (18)	0.0088 (17)
C3	0.059 (2)	0.055 (2)	0.0449 (19)	0.0089 (16)	0.0094 (16)	0.0111 (15)
C4	0.077 (3)	0.085 (3)	0.059 (2)	0.014 (2)	0.019 (2)	0.010 (2)
C5	0.103 (4)	0.097 (3)	0.046 (2)	−0.003 (3)	0.011 (2)	0.019 (2)
C6	0.094 (3)	0.068 (3)	0.062 (3)	−0.011 (2)	−0.012 (2)	0.028 (2)
C7	0.058 (2)	0.0424 (18)	0.079 (3)	−0.0036 (16)	−0.0068 (19)	0.0200 (17)
C8	0.062 (3)	0.057 (2)	0.136 (5)	0.007 (2)	−0.012 (3)	0.028 (3)
C9	0.053 (3)	0.075 (3)	0.170 (6)	0.020 (2)	0.022 (3)	0.015 (3)
C10	0.062 (3)	0.068 (3)	0.111 (4)	0.003 (2)	0.038 (3)	0.004 (2)
C11	0.0454 (19)	0.0446 (17)	0.066 (2)	−0.0026 (15)	0.0159 (17)	0.0083 (16)
C12	0.0477 (19)	0.0370 (16)	0.057 (2)	−0.0010 (14)	0.0091 (15)	0.0119 (14)
C13	0.073 (3)	0.054 (2)	0.058 (2)	−0.0128 (18)	0.0226 (19)	0.0129 (17)
C14	0.099 (3)	0.054 (2)	0.058 (2)	0.008 (2)	−0.003 (2)	0.0214 (17)
C15	0.083 (3)	0.0477 (19)	0.0437 (19)	0.0127 (18)	−0.0020 (18)	0.0186 (15)
C16	0.082 (3)	0.060 (2)	0.059 (2)	−0.0055 (19)	0.014 (2)	0.0247 (18)
C17	0.080 (3)	0.056 (2)	0.051 (2)	0.0032 (19)	0.0152 (19)	0.0167 (16)
C18	0.062 (2)	0.0540 (19)	0.0415 (18)	0.0084 (16)	0.0002 (15)	0.0211 (15)
C19	0.067 (2)	0.080 (3)	0.061 (2)	0.007 (2)	0.0146 (19)	0.017 (2)
C20	0.080 (3)	0.072 (3)	0.060 (2)	0.009 (2)	0.012 (2)	0.004 (2)
C21	0.061 (2)	0.0471 (17)	0.0396 (17)	0.0028 (16)	0.0122 (15)	0.0141 (14)
C22	0.0561 (19)	0.0409 (16)	0.0446 (17)	0.0047 (14)	0.0108 (15)	0.0152 (13)
C23	0.073 (2)	0.053 (2)	0.051 (2)	0.0212 (17)	0.0210 (17)	0.0152 (16)
C24	0.069 (2)	0.062 (2)	0.055 (2)	0.0231 (18)	0.0075 (18)	0.0227 (17)
C25	0.064 (2)	0.055 (2)	0.0431 (18)	0.0007 (17)	0.0074 (16)	0.0192 (15)
C26	0.068 (2)	0.081 (3)	0.053 (2)	0.017 (2)	0.0235 (18)	0.0292 (19)
C27	0.057 (2)	0.083 (3)	0.057 (2)	0.0212 (19)	0.0184 (17)	0.0352 (19)
N4	0.080 (2)	0.087 (2)	0.052 (2)	0.0088 (19)	0.0094 (18)	0.0279 (17)
O5	0.115 (3)	0.171 (3)	0.0557 (18)	0.032 (2)	0.0289 (19)	0.043 (2)
O6	0.121 (3)	0.182 (4)	0.072 (2)	0.070 (3)	0.0121 (19)	0.062 (2)
S2	0.0732 (7)	0.1007 (8)	0.0565 (6)	0.0068 (6)	0.0234 (5)	0.0332 (5)
O1S	0.103 (2)	0.095 (2)	0.0608 (16)	0.0099 (16)	0.0414 (15)	0.0291 (14)
C1S	0.080 (3)	0.094 (3)	0.077 (3)	0.010 (2)	0.028 (2)	0.025 (2)
C2S	0.130 (4)	0.101 (4)	0.115 (4)	0.005 (3)	0.060 (3)	0.053 (3)

Geometric parameters (Å, °)

S1—O4	1.423 (3)	C15—C20	1.375 (5)
S1—O3	1.429 (2)	C15—C16	1.384 (5)
S1—N2	1.630 (3)	C16—C17	1.381 (5)
S1—C18	1.762 (3)	C16—H16	0.9300
N1—C2	1.388 (4)	C17—C18	1.383 (5)
N1—C13	1.394 (5)	C17—H17	0.9300
N1—C14	1.478 (4)	C18—C19	1.373 (5)
N2—N3	1.394 (3)	C19—C20	1.383 (5)
N2—H2N	0.8006	C19—H19	0.9300

N3—C21	1.263 (4)	C20—H20	0.9300
O1—C2	1.224 (4)	C21—C22	1.462 (4)
O2—C13	1.214 (4)	C21—H21	0.9300
C2—C3	1.461 (5)	C22—C23	1.383 (4)
C3—C4	1.377 (5)	C22—C27	1.394 (4)
C3—C12	1.404 (5)	C23—C24	1.381 (5)
C4—C5	1.380 (6)	C23—H23	0.9300
C4—H4	0.9300	C24—C25	1.367 (5)
C5—C6	1.336 (6)	C24—H24	0.9300
C5—H5	0.9300	C25—C26	1.369 (5)
C6—C7	1.415 (6)	C25—N4	1.474 (4)
C6—H6	0.9300	C26—C27	1.377 (5)
C7—C8	1.395 (6)	C26—H26	0.9300
C7—C12	1.418 (5)	C27—H27	0.9300
C8—C9	1.344 (7)	N4—O6	1.200 (4)
C8—H8	0.9300	N4—O5	1.213 (4)
C9—C10	1.391 (7)	S2—O1S	1.494 (3)
C9—H9	0.9300	S2—C1S	1.755 (4)
C10—C11	1.375 (5)	S2—C2S	1.781 (5)
C10—H10	0.9300	C1S—H1S1	0.9600
C11—C12	1.399 (5)	C1S—H1S2	0.9600
C11—C13	1.481 (5)	C1S—H1S3	0.9600
C14—C15	1.517 (5)	C2S—H2S1	0.9600
C14—H14A	0.9700	C2S—H2S2	0.9600
C14—H14B	0.9700	C2S—H2S3	0.9600
O4—S1—O3	120.25 (16)	C20—C15—C14	121.5 (4)
O4—S1—N2	108.61 (16)	C16—C15—C14	120.0 (4)
O3—S1—N2	103.64 (16)	C17—C16—C15	121.1 (4)
O4—S1—C18	107.94 (17)	C17—C16—H16	119.5
O3—S1—C18	109.03 (15)	C15—C16—H16	119.5
N2—S1—C18	106.58 (15)	C16—C17—C18	119.1 (4)
C2—N1—C13	123.8 (3)	C16—C17—H17	120.4
C2—N1—C14	118.4 (3)	C18—C17—H17	120.4
C13—N1—C14	117.7 (3)	C19—C18—C17	120.7 (3)
N3—N2—S1	115.3 (2)	C19—C18—S1	121.3 (3)
N3—N2—H2N	117.1	C17—C18—S1	118.0 (3)
S1—N2—H2N	114.1	C18—C19—C20	119.2 (4)
C21—N3—N2	115.5 (3)	C18—C19—H19	120.4
O1—C2—N1	119.3 (3)	C20—C19—H19	120.4
O1—C2—C3	122.8 (3)	C15—C20—C19	121.4 (4)
N1—C2—C3	117.9 (3)	C15—C20—H20	119.3
C4—C3—C12	119.4 (3)	C19—C20—H20	119.3
C4—C3—C2	120.4 (3)	N3—C21—C22	120.5 (3)
C12—C3—C2	120.1 (3)	N3—C21—H21	119.7
C3—C4—C5	120.8 (4)	C22—C21—H21	119.7
C3—C4—H4	119.6	C23—C22—C27	118.9 (3)
C5—C4—H4	119.6	C23—C22—C21	119.9 (3)
C6—C5—C4	121.3 (4)	C27—C22—C21	121.1 (3)
C6—C5—H5	119.4	C24—C23—C22	120.7 (3)

C4—C5—H5	119.4	C24—C23—H23	119.6
C5—C6—C7	120.7 (4)	C22—C23—H23	119.6
C5—C6—H6	119.6	C25—C24—C23	118.5 (3)
C7—C6—H6	119.6	C25—C24—H24	120.7
C8—C7—C6	124.0 (4)	C23—C24—H24	120.7
C8—C7—C12	117.6 (4)	C24—C25—C26	122.6 (3)
C6—C7—C12	118.3 (4)	C24—C25—N4	118.9 (3)
C9—C8—C7	121.7 (5)	C26—C25—N4	118.5 (3)
C9—C8—H8	119.1	C25—C26—C27	118.6 (3)
C7—C8—H8	119.1	C25—C26—H26	120.7
C8—C9—C10	120.9 (4)	C27—C26—H26	120.7
C8—C9—H9	119.6	C26—C27—C22	120.6 (3)
C10—C9—H9	119.6	C26—C27—H27	119.7
C11—C10—C9	119.9 (5)	C22—C27—H27	119.7
C11—C10—H10	120.1	O6—N4—O5	123.1 (4)
C9—C10—H10	120.1	O6—N4—C25	119.1 (4)
C10—C11—C12	119.8 (4)	O5—N4—C25	117.7 (4)
C10—C11—C13	120.2 (4)	O1S—S2—C1S	106.61 (19)
C12—C11—C13	119.9 (3)	O1S—S2—C2S	104.8 (2)
C11—C12—C3	120.5 (3)	C1S—S2—C2S	97.5 (2)
C11—C12—C7	120.1 (3)	S2—C1S—H1S1	109.5
C3—C12—C7	119.4 (3)	S2—C1S—H1S2	109.5
O2—C13—N1	120.1 (4)	H1S1—C1S—H1S2	109.5
O2—C13—C11	122.6 (4)	S2—C1S—H1S3	109.5
N1—C13—C11	117.3 (3)	H1S1—C1S—H1S3	109.5
N1—C14—C15	111.5 (3)	H1S2—C1S—H1S3	109.5
N1—C14—H14A	109.3	S2—C2S—H2S1	109.5
C15—C14—H14A	109.3	S2—C2S—H2S2	109.5
N1—C14—H14B	109.3	H2S1—C2S—H2S2	109.5
C15—C14—H14B	109.3	S2—C2S—H2S3	109.5
H14A—C14—H14B	108.0	H2S1—C2S—H2S3	109.5
C20—C15—C16	118.5 (3)	H2S2—C2S—H2S3	109.5
O4—S1—N2—N3	−49.9 (3)	C12—C11—C13—O2	176.2 (3)
O3—S1—N2—N3	−178.9 (2)	C10—C11—C13—N1	176.5 (3)
C18—S1—N2—N3	66.1 (3)	C12—C11—C13—N1	−4.8 (4)
S1—N2—N3—C21	−165.8 (2)	C2—N1—C14—C15	−96.1 (4)
C13—N1—C2—O1	−175.1 (3)	C13—N1—C14—C15	82.0 (4)
C14—N1—C2—O1	2.9 (5)	N1—C14—C15—C20	86.5 (5)
C13—N1—C2—C3	4.6 (5)	N1—C14—C15—C16	−92.5 (4)
C14—N1—C2—C3	−177.4 (3)	C20—C15—C16—C17	−2.3 (5)
O1—C2—C3—C4	−5.1 (6)	C14—C15—C16—C17	176.8 (3)
N1—C2—C3—C4	175.2 (3)	C15—C16—C17—C18	−0.1 (5)
O1—C2—C3—C12	172.8 (4)	C16—C17—C18—C19	2.1 (5)
N1—C2—C3—C12	−6.8 (5)	C16—C17—C18—S1	−176.1 (3)
C12—C3—C4—C5	0.2 (6)	O4—S1—C18—C19	5.1 (3)
C2—C3—C4—C5	178.1 (4)	O3—S1—C18—C19	137.3 (3)
C3—C4—C5—C6	−1.7 (7)	N2—S1—C18—C19	−111.5 (3)
C4—C5—C6—C7	1.1 (7)	O4—S1—C18—C17	−176.8 (3)
C5—C6—C7—C8	179.7 (4)	O3—S1—C18—C17	−44.6 (3)

C5—C6—C7—C12	0.8 (5)	N2—S1—C18—C17	66.7 (3)
C6—C7—C8—C9	−179.1 (4)	C17—C18—C19—C20	−1.6 (5)
C12—C7—C8—C9	−0.2 (6)	S1—C18—C19—C20	176.6 (3)
C7—C8—C9—C10	1.2 (7)	C16—C15—C20—C19	2.8 (6)
C8—C9—C10—C11	−1.2 (7)	C14—C15—C20—C19	−176.2 (3)
C9—C10—C11—C12	0.2 (5)	C18—C19—C20—C15	−0.9 (6)
C9—C10—C11—C13	179.0 (4)	N2—N3—C21—C22	−179.6 (2)
C10—C11—C12—C3	−178.8 (3)	N3—C21—C22—C23	−173.8 (3)
C13—C11—C12—C3	2.5 (4)	N3—C21—C22—C27	3.6 (5)
C10—C11—C12—C7	0.7 (5)	C27—C22—C23—C24	−2.0 (5)
C13—C11—C12—C7	−178.0 (3)	C21—C22—C23—C24	175.5 (3)
C4—C3—C12—C11	−178.7 (3)	C22—C23—C24—C25	0.7 (5)
C2—C3—C12—C11	3.3 (5)	C23—C24—C25—C26	0.3 (5)
C4—C3—C12—C7	1.8 (5)	C23—C24—C25—N4	−177.2 (3)
C2—C3—C12—C7	−176.2 (3)	C24—C25—C26—C27	−0.1 (5)
C8—C7—C12—C11	−0.7 (5)	N4—C25—C26—C27	177.5 (3)
C6—C7—C12—C11	178.2 (3)	C25—C26—C27—C22	−1.2 (5)
C8—C7—C12—C3	178.8 (3)	C23—C22—C27—C26	2.2 (5)
C6—C7—C12—C3	−2.3 (5)	C21—C22—C27—C26	−175.3 (3)
C2—N1—C13—O2	−179.9 (3)	C24—C25—N4—O6	−0.8 (5)
C14—N1—C13—O2	2.1 (5)	C26—C25—N4—O6	−178.5 (4)
C2—N1—C13—C11	1.1 (5)	C24—C25—N4—O5	177.4 (4)
C14—N1—C13—C11	−176.9 (3)	C26—C25—N4—O5	−0.3 (5)
C10—C11—C13—O2	−2.5 (5)		

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the *p*-nitrophenyl (C22–C27) ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2N···O1S	0.80	1.99	2.764 (4)	163
C8—H8···Cg^{i}	0.93	2.90	3.799 (6)	162

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

Fig. 1

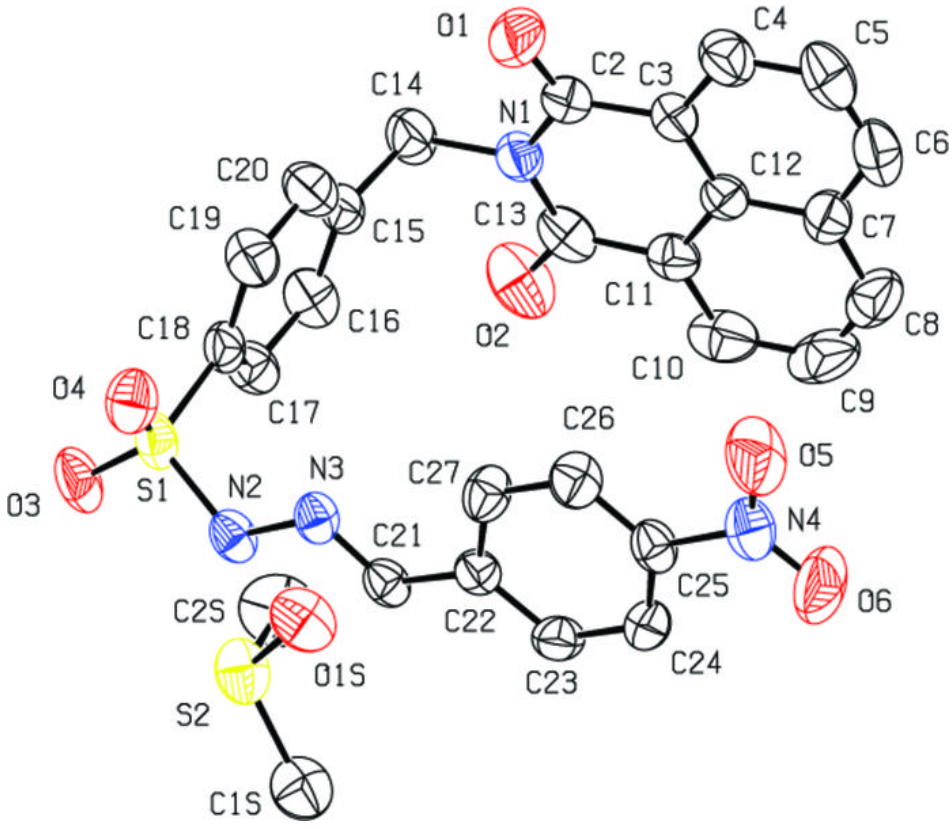
O1
C4
C5
C2
C3
C14
N1
C6
C20
C12
C19
C15
C13
C7
O2
C11
C16
C18
C8
O4
C17
C10
C9
C26
O5
O3
S1
N2
N3
C27
N4
C21
C25
O6
C2S
C22
O1S
C23
C24
S2
C1S

Fig. 2