organic compounds

4,4'-Bis[2-(benzylsulfanyl)phenylhydra-zono]-2,2'-binaphthalene-1,1'(4H,4'H)-dione

Achintesh Narayan Biswas, Purak Das, Debatra Narayan Neogi, Rupa Bhawmick and Pinaki Bandyopadhyay*

Department of Chemistry, University of North Bengal, Siliguri 734 013, India
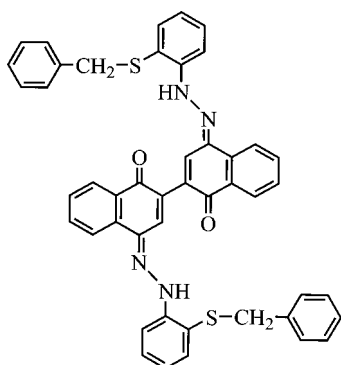Correspondence e-mail: pbchem@rediffmail.com

The crystal structure of the title compound, $C_{46}H_{34}N_4O_2S_2$, shows that the molecules exist in the hydrazone form and not the azo form. The title compound is actually a centrosymmetric dimer of 3-dehydro-1-[2-(benzylsulfanyl)phenylhydrazono]naphthalene-4-one connected through the C-3 position of the naphthalene unit. The hydrazone H atom and the sulfanyl S atom are linked by an intramolecular N—H···S hydrogen bond. In each molecule, there are two intramolecular C—H···O interactions. The crystal packing is stabilized by three weak intermolecular π–π interactions; the centroid–centroid distances are 3.808 (2), 3.955 (2) and 3.955 (2) Å; the corresponding perpendicular distances are 3.481, 3.535 and 3.584 Å.

Related literature

For related literature, see: Antonov et al. (1999); Bagchi et al. (2007); Liu et al. (2005); Sudesh Kumar & Neckers (1989).

Experimental

Crystal data

$C_{46}H_{34}N_4O_2S_2$	$V = 1743.0$ (7) Å^3
$M_r = 738.89$	$Z = 2$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 19.184$ (4) Å	$\mu = 0.20$ mm^{-1}
$b = 4.6066$ (10) Å	$T = 153$ (2) K
$c = 21.734$ (5) Å	$0.42 \times 0.31 \times 0.19$ mm
$\beta = 114.838$ (4)°	

Data collection

Bruker SMART APEX CCD area detector diffractometer	6195 measured reflections
	3027 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1893 reflections with $I > 2\sigma(I)$
$T_{min} = 0.926$, $T_{max} = 0.964$	$R_{int} = 0.061$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.065$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.139$	
$S = 0.97$	
3027 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
248 parameters	$\Delta\rho_{min} = -0.29$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H02···S1	0.88 (4)	2.54 (4)	3.012 (4)	115 (3)
C2—H2···O1^i	0.93	2.03	2.752 (5)	133

Symmetry code: (i) $-x + 1, -y + 2, -z + 1$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

References

Antonov, L., Kawauchi, S., Satoh, M. & Komiyama, J. (1999). *Dyes Pigm.* **40**, 163–170.
Bagchi, V., Das, P. & Bandyopadhyay, D. (2007). *Acta Cryst.* E**63**, m2130.
Bruker (1997). *SHELXTL.* Bruker AXS Inc. Madison, Wisconsin, USA.
Bruker (1998). *SMART.* Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2000). *SAINT.* Version 6.02a. Bruker AXS Inc., Madison, Wisconsin, USA.
Liu, X.-G., Feng, Y.-Q., Liang, Z.-P. & Wang, W. (2005). *Acta Cryst.* E**61**, o3857-o3858.
Sheldrick, G. M. (1996). *SADABS.* University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97.* University of Göttingen, Germany.
Sudesh Kumar, G. & Neckers, D. C. (1989). *Chem. Rev.* **89**, 1915–1925.

supplementary materials

4,4'-Bis[2-(benzylsulfanyl)phenylhydrazono]-2,2'-binaphthalene-1,1'(4*H*,4'*H*)-dione

A. N. Biswas, P. Das, D. N. Neogi, R. Bhawmick and P. Bandyopadhyay

Comment

Aryl diazenes are among the largest group of dyes. The extensive application of azo dyes in industry and analytical chemistry have attracted attention for decades (Sudesh Kumar & Neckers, 1989). Optically active azobenzene polymers are very important functional materials because of their photoresponsive properties. Generally arylazonaphthalenes have been found to exist in the hydrazo-keto form in the solid state (Liu *et al.*, 2005). The position of azo and hydroxyl groups in arylazo compounds brings into play the azo-hydrazo equilibrium, which has been the subject of intensive investigation in recent years (Antonov *et al.*, 1999). Here in, we report the crystal structure of the title compound where the hydrazo-keto form is dominant over the azo-enol form in the solid state.

The molecular structure of the title compound, (I), is shown in Fig. 1, with the atom-numbering scheme. Selected bond lengths are listed in Table 1. The packing arrangement of (I) is shown in Fig. 2. The title compound is actually the centro symmetric dimer of the asymmetric unit, 3-dehydro-1-[2-(benzylsulfanyl)phenylhydrazono]naphthalene-4-one and the centre of symmetry exists at the centre of the C3—C3^i [symmetry code: (i) −*x* + 1, −*y* + 2, −*z* + 1] bond. In each dimer the asymmetric units are inter-connected by a C3—C3^i [symmetry code: (i) −*x* + 1, −*y* + 2, −*z* + 1] bond of the naphthalene moiety and two C2—H···O1 interactions (Table 2, Fig. 1). Naphthyl and phenyl rings around the hydrazone group adopt a *trans* configuration. The hydrazone H atom and the sulfanyl S atom are linked by an intramolecular N—H···S hydrogen bond (Table 2, Fig. 1). The crystal packing is stabilized by three weak intermolecular π–π interactions (Bagchi *et al.*, 2007); the *Cg*1—*Cg*1^{ii}, *Cg*1—*Cg*2^{iii} and *Cg*2—*Cg*1^{iv} [Symmetry codes: (ii) 1 − *x*, 1 − *y*, 1 − *z*; (iii) *x*, 1 + *y*, *z*; (iv) *x*, −1 + *y*, *z*. *Cg*1 and *Cg*2 are the centroids of C1—C10 and C5—C9 rings respectively.] distances are 3.808 (2), 3.955 (2) and 3.955 (2) Å (Fig. 3); the corresponding perpendicular distances are 3.481 (with slippage of 1.544 Å), 3.535 and 3.584 Å, respectively.

Experimental

The title compound, (I) was prepared by coupling diazotized 2-benzylthioaniline with 1-naphthol at around 273–278 K. The product was isolated by column chromatography and crystallized from ethanol. Suitable crystals of (I) were obtained by slow diffusion of a dichloromethane solution into *n*-hexane.

Refinement

The N-bound H atom was located in a difference Fourier map and its coordinates and isotropic displacement parameter were freely refined. C-bound H atoms were included at calculated positions as riding atoms with C—H set to 0.93 Å for aromatic and 0.97 Å for CH$_2$. H atoms, with U_{iso} (H) = 1.2U_{eq}(C). Some low-angle reflections were excluded from the refinement, as they were probably obscured by the beam stop.
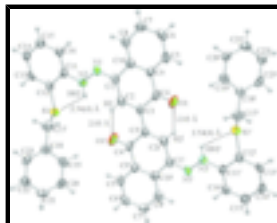
supplementary materials

Figures

Fig. 1. The asymmetric unit of (I), with displacement ellipsoids drawn at the 75% probability level. The C—H···O and N—H···S interactions are shown by dotted lines [symmetry code: (i) $-x + 1, -y + 2, -z + 1$].
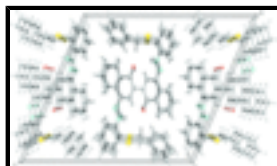
Fig. 2. The molecular arrangement of (I) in the *ac* plane.
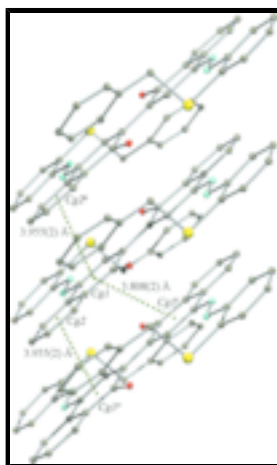
Fig. 3. The inter molecular π—π interaction for (I), indicated by the dotted line. [Symmetry codes: (ii) $1 - x, 1 - y, 1 - z$; (iii) $x, 1 + y, z$; (iv) $x, -1 + y, z$. *Cg*1 and *Cg*2 are the centroids of C1—C10 and C5—C9 rings respectively.]

4,4'-Bis[2-(benzylsulfanyl)phenylhydrazono]-2,2'-binaphthalene- 1,1'(4*H*,4'H)-dione

Crystal data

$C_{46}H_{34}N_4O_2S_2$	$F_{000} = 772$
$M_r = 738.89$	$D_x = 1.408$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3027 reflections
$a = 19.184\ (4)$ Å	$\theta = 2.1–25.0°$
$b = 4.6066\ (10)$ Å	$\mu = 0.20$ mm^{-1}
$c = 21.734\ (5)$ Å	$T = 153\ (2)$ K
$\beta = 114.838\ (4)°$	Needle, red
$V = 1743.0\ (7)$ Å^3	$0.42 \times 0.31 \times 0.19$ mm
$Z = 2$	

Data collection

Bruker SMART APEX CCD area detector	3027 independent reflections

diffractometer

Radiation source: fine-focus sealed tube	1893 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.061$
$T = 298(2)$ K	$\theta_{max} = 25.0°$
phi and ω scans	$\theta_{min} = 2.1°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -14 \rightarrow 22$
$T_{min} = 0.926$, $T_{max} = 0.964$	$k = -5 \rightarrow 5$
6195 measured reflections	$l = -24 \rightarrow 25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.065$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.139$	$w = 1/[\sigma^2(F_o^2) + (0.0594P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{max} < 0.001$
3027 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
248 parameters	$\Delta\rho_{min} = -0.29$ 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 $F^2 > 2sigma(F^2)$ 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 ($\mathring{A}^2$)

	x	y	z	$U_{iso}*/U_{eq}$
H02	0.298 (2)	0.649 (8)	0.5023 (18)	0.035 (12)*
S1	0.15711 (5)	0.7308 (2)	0.42556 (4)	0.0214 (3)
N1	0.37643 (16)	0.4567 (6)	0.58144 (14)	0.0228 (8)
C12	0.1686 (2)	0.4824 (8)	0.49127 (17)	0.0201 (9)
C1	0.43806 (19)	0.5734 (8)	0.57898 (17)	0.0204 (9)
C3	0.50221 (19)	0.8952 (8)	0.52663 (16)	0.0189 (8)
C10	0.5114 (2)	0.4860 (8)	0.63407 (17)	0.0195 (9)
C11	0.2422 (2)	0.4009 (8)	0.53961 (17)	0.0196 (8)

N2	0.30659 (17)	0.5246 (7)	0.53532 (16)	0.0234 (8)
C8	0.5156 (2)	0.2926 (8)	0.68462 (17)	0.0237 (9)
H8	0.4709	0.2088	0.6834	0.028*
C9	0.5792 (2)	0.6001 (8)	0.63453 (17)	0.0210 (9)
C15	0.1852 (2)	0.0758 (9)	0.59165 (18)	0.0258 (9)
H15	0.1905	−0.0625	0.6245	0.031*
O1	0.64011 (15)	0.8716 (7)	0.58070 (15)	0.0543 (10)
C16	0.2494 (2)	0.1971 (8)	0.58925 (17)	0.0225 (9)
H16	0.2979	0.1429	0.6210	0.027*
C4	0.5785 (2)	0.7989 (8)	0.58052 (18)	0.0249 (9)
C14	0.1119 (2)	0.1591 (8)	0.54492 (18)	0.0255 (10)
H14	0.0686	0.0787	0.5471	0.031*
C20	0.1604 (2)	0.9702 (8)	0.22193 (18)	0.0243 (9)
H20	0.1898	1.1158	0.2148	0.029*
C2	0.4387 (2)	0.7774 (8)	0.52924 (17)	0.0231 (9)
H2	0.3913	0.8339	0.4959	0.028*
C6	0.6527 (2)	0.3442 (8)	0.73783 (18)	0.0268 (10)
H6	0.6998	0.2997	0.7731	0.032*
C18	0.1411 (2)	0.6237 (8)	0.29665 (17)	0.0196 (8)
C13	0.1043 (2)	0.3600 (8)	0.49592 (17)	0.0207 (9)
H13	0.0555	0.4158	0.4652	0.025*
C7	0.5857 (2)	0.2237 (9)	0.73672 (17)	0.0260 (9)
H7	0.5880	0.0974	0.7709	0.031*
C5	0.6494 (2)	0.5284 (8)	0.68709 (18)	0.0250 (9)
H5	0.6945	0.6060	0.6878	0.030*
C17	0.1672 (2)	0.4796 (8)	0.36412 (17)	0.0266 (10)
H17A	0.2204	0.4212	0.3798	0.032*
H17B	0.1366	0.3070	0.3602	0.032*
C23	0.0728 (2)	0.5399 (8)	0.24326 (18)	0.0244 (9)
H23	0.0428	0.3965	0.2503	0.029*
C22	0.0486 (2)	0.6662 (8)	0.17986 (18)	0.0238 (9)
H22	0.0032	0.6062	0.1445	0.029*
C21	0.0926 (2)	0.8822 (8)	0.16946 (18)	0.0254 (9)
H21	0.0764	0.9686	0.1270	0.031*
C19	0.1846 (2)	0.8421 (8)	0.28492 (17)	0.0225 (9)
H19	0.2304	0.9018	0.3200	0.027*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0238 (5)	0.0194 (5)	0.0204 (5)	0.0035 (4)	0.0086 (4)	0.0017 (4)
N1	0.0170 (17)	0.0224 (18)	0.0239 (17)	−0.0004 (14)	0.0036 (14)	0.0034 (15)
C12	0.018 (2)	0.020 (2)	0.0208 (19)	0.0020 (16)	0.0069 (16)	−0.0019 (17)
C1	0.0156 (19)	0.019 (2)	0.026 (2)	0.0027 (16)	0.0077 (16)	−0.0025 (18)
C3	0.0184 (19)	0.018 (2)	0.021 (2)	−0.0009 (16)	0.0090 (16)	−0.0041 (16)
C10	0.025 (2)	0.017 (2)	0.0181 (19)	0.0009 (17)	0.0109 (16)	−0.0053 (17)
C11	0.018 (2)	0.022 (2)	0.0200 (19)	−0.0032 (17)	0.0095 (16)	−0.0048 (17)
N2	0.0192 (18)	0.027 (2)	0.0222 (18)	0.0024 (15)	0.0066 (15)	0.0085 (16)

C8	0.023 (2)	0.020 (2)	0.028 (2)	0.0010 (17)	0.0105 (17)	−0.0042 (18)
C9	0.023 (2)	0.018 (2)	0.024 (2)	−0.0042 (17)	0.0116 (17)	−0.0008 (17)
C15	0.029 (2)	0.026 (2)	0.024 (2)	−0.0030 (19)	0.0118 (18)	0.0000 (18)
O1	0.0198 (16)	0.075 (2)	0.059 (2)	−0.0034 (16)	0.0080 (14)	0.0415 (19)
C16	0.0178 (19)	0.026 (2)	0.021 (2)	−0.0006 (17)	0.0057 (16)	0.0018 (17)
C4	0.018 (2)	0.023 (2)	0.033 (2)	−0.0027 (18)	0.0111 (17)	0.0056 (18)
C14	0.019 (2)	0.034 (3)	0.026 (2)	−0.0074 (17)	0.0110 (17)	−0.0045 (19)
C20	0.025 (2)	0.024 (2)	0.027 (2)	−0.0033 (18)	0.0136 (18)	0.0017 (19)
C2	0.0180 (19)	0.024 (2)	0.025 (2)	0.0024 (18)	0.0062 (16)	−0.0033 (19)
C6	0.019 (2)	0.031 (2)	0.023 (2)	0.0045 (18)	0.0014 (17)	−0.0008 (19)
C18	0.024 (2)	0.016 (2)	0.021 (2)	0.0086 (17)	0.0121 (17)	0.0006 (17)
C13	0.0169 (19)	0.029 (2)	0.0130 (19)	−0.0043 (17)	0.0029 (15)	−0.0055 (17)
C7	0.032 (2)	0.028 (2)	0.021 (2)	0.007 (2)	0.0128 (17)	0.0062 (19)
C5	0.018 (2)	0.022 (2)	0.031 (2)	−0.0033 (17)	0.0066 (17)	−0.0005 (19)
C17	0.037 (2)	0.020 (2)	0.025 (2)	0.0061 (18)	0.0153 (18)	−0.0008 (18)
C23	0.024 (2)	0.023 (2)	0.033 (2)	−0.0011 (18)	0.0192 (18)	−0.0004 (19)
C22	0.021 (2)	0.031 (2)	0.022 (2)	0.0067 (18)	0.0108 (16)	0.0009 (18)
C21	0.030 (2)	0.029 (2)	0.020 (2)	0.0127 (19)	0.0142 (18)	0.0057 (18)
C19	0.024 (2)	0.021 (2)	0.021 (2)	0.0052 (17)	0.0083 (17)	−0.0019 (17)

Geometric parameters (Å, °)

S1—C12	1.770 (4)	C16—H16	0.9300
S1—C17	1.837 (4)	C14—C13	1.372 (5)
N1—C1	1.320 (4)	C14—H14	0.9300
N1—N2	1.330 (4)	C20—C19	1.380 (5)
C12—C13	1.398 (5)	C20—C21	1.383 (5)
C12—C11	1.411 (5)	C20—H20	0.9300
C1—C2	1.436 (5)	C2—H2	0.9300
C1—C10	1.469 (5)	C6—C5	1.372 (5)
C3—C2	1.357 (5)	C6—C7	1.392 (5)
C3—C3^i	1.482 (7)	C6—H6	0.9300
C3—C4	1.507 (5)	C18—C23	1.391 (5)
C10—C8	1.390 (5)	C18—C19	1.398 (5)
C10—C9	1.399 (5)	C18—C17	1.491 (5)
C11—C16	1.393 (5)	C13—H13	0.9300
C11—N2	1.398 (4)	C7—H7	0.9300
N2—H02	0.88 (4)	C5—H5	0.9300
C8—C7	1.382 (5)	C17—H17A	0.9700
C8—H8	0.9300	C17—H17B	0.9700
C9—C5	1.392 (5)	C23—C22	1.384 (5)
C9—C4	1.484 (5)	C23—H23	0.9300
C15—C16	1.372 (5)	C22—C21	1.383 (5)
C15—C14	1.399 (5)	C22—H22	0.9300
C15—H15	0.9300	C21—H21	0.9300
O1—C4	1.227 (4)	C19—H19	0.9300
C12—S1—C17	99.43 (17)	C19—C20—H20	120.0
C1—N1—N2	120.6 (3)	C21—C20—H20	120.0
C13—C12—C11	118.4 (3)	C3—C2—C1	125.8 (3)

C13—C12—S1	120.3 (3)	C3—C2—H2	117.1
C11—C12—S1	121.3 (3)	C1—C2—H2	117.1
N1—C1—C2	126.0 (3)	C5—C6—C7	120.2 (3)
N1—C1—C10	115.0 (3)	C5—C6—H6	119.9
C2—C1—C10	119.0 (3)	C7—C6—H6	119.9
C2—C3—C3^i	122.4 (4)	C23—C18—C19	118.2 (3)
C2—C3—C4	116.5 (3)	C23—C18—C17	120.4 (3)
C3^i—C3—C4	121.2 (4)	C19—C18—C17	121.3 (3)
C8—C10—C9	119.3 (3)	C14—C13—C12	121.3 (3)
C8—C10—C1	122.6 (3)	C14—C13—H13	119.4
C9—C10—C1	118.1 (3)	C12—C13—H13	119.4
C16—C11—N2	121.6 (3)	C8—C7—C6	119.7 (3)
C16—C11—C12	119.9 (3)	C8—C7—H7	120.1
N2—C11—C12	118.5 (3)	C6—C7—H7	120.1
N1—N2—C11	119.5 (3)	C6—C5—C9	120.5 (4)
N1—N2—H02	123 (3)	C6—C5—H5	119.7
C11—N2—H02	117 (3)	C9—C5—H5	119.7
C7—C8—C10	120.6 (4)	C18—C17—S1	109.9 (3)
C7—C8—H8	119.7	C18—C17—H17A	109.7
C10—C8—H8	119.7	S1—C17—H17A	109.7
C5—C9—C10	119.6 (3)	C18—C17—H17B	109.7
C5—C9—C4	118.6 (3)	S1—C17—H17B	109.7
C10—C9—C4	121.8 (3)	H17A—C17—H17B	108.2
C16—C15—C14	120.3 (4)	C22—C23—C18	121.2 (4)
C16—C15—H15	119.8	C22—C23—H23	119.4
C14—C15—H15	119.8	C18—C23—H23	119.4
C15—C16—C11	120.4 (3)	C21—C22—C23	119.6 (3)
C15—C16—H16	119.8	C21—C22—H22	120.2
C11—C16—H16	119.8	C23—C22—H22	120.2
O1—C4—C9	118.5 (3)	C22—C21—C20	120.2 (3)
O1—C4—C3	122.8 (3)	C22—C21—H21	119.9
C9—C4—C3	118.7 (3)	C20—C21—H21	119.9
C13—C14—C15	119.7 (4)	C20—C19—C18	120.8 (3)
C13—C14—H14	120.2	C20—C19—H19	119.6
C15—C14—H14	120.2	C18—C19—H19	119.6
C19—C20—C21	120.0 (4)		
C17—S1—C12—C13	−95.4 (3)	C2—C3—C4—O1	174.2 (4)
C17—S1—C12—C11	83.9 (3)	C3^i—C3—C4—O1	−5.1 (7)
N2—N1—C1—C2	0.0 (6)	C2—C3—C4—C9	−3.8 (5)
N2—N1—C1—C10	178.3 (3)	C3^i—C3—C4—C9	176.9 (4)
N1—C1—C10—C8	0.7 (5)	C16—C15—C14—C13	1.0 (5)
C2—C1—C10—C8	179.2 (3)	C3^i—C3—C2—C1	179.9 (4)
N1—C1—C10—C9	179.7 (3)	C4—C3—C2—C1	0.7 (5)
C2—C1—C10—C9	−1.8 (5)	N1—C1—C2—C3	−179.5 (3)
C13—C12—C11—C16	1.7 (5)	C10—C1—C2—C3	2.2 (6)
S1—C12—C11—C16	−177.7 (3)	C15—C14—C13—C12	0.5 (5)
C13—C12—C11—N2	−179.6 (3)	C11—C12—C13—C14	−1.8 (5)
S1—C12—C11—N2	1.0 (5)	S1—C12—C13—C14	177.6 (3)

C1—N1—N2—C11	−179.2 (3)	C10—C8—C7—C6	−1.4 (6)
C16—C11—N2—N1	−3.1 (5)	C5—C6—C7—C8	−0.6 (6)
C12—C11—N2—N1	178.2 (3)	C7—C6—C5—C9	0.9 (6)
C9—C10—C8—C7	3.1 (5)	C10—C9—C5—C6	0.9 (5)
C1—C10—C8—C7	−177.9 (3)	C4—C9—C5—C6	−179.6 (3)
C8—C10—C9—C5	−2.8 (5)	C23—C18—C17—S1	−108.6 (3)
C1—C10—C9—C5	178.1 (3)	C19—C18—C17—S1	72.3 (4)
C8—C10—C9—C4	177.7 (3)	C12—S1—C17—C18	166.4 (3)
C1—C10—C9—C4	−1.4 (5)	C19—C18—C23—C22	0.7 (5)
C14—C15—C16—C11	−1.1 (6)	C17—C18—C23—C22	−178.4 (3)
N2—C11—C16—C15	−179.0 (3)	C18—C23—C22—C21	−0.9 (5)
C12—C11—C16—C15	−0.3 (5)	C23—C22—C21—C20	0.4 (5)
C5—C9—C4—O1	6.6 (6)	C19—C20—C21—C22	0.1 (5)
C10—C9—C4—O1	−173.9 (4)	C21—C20—C19—C18	−0.2 (5)
C5—C9—C4—C3	−175.3 (3)	C23—C18—C19—C20	−0.2 (5)
C10—C9—C4—C3	4.2 (5)	C17—C18—C19—C20	178.9 (3)

Symmetry codes: (i) −x+1, −y+2, −z+1.

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N2—H02⋯S1	0.88 (4)	2.54 (4)	3.012 (4)	115 (3)
C2—H2⋯O1[i]	0.93	2.03	2.752 (5)	133

Symmetry codes: (i) −x+1, −y+2, −z+1.

Fig. 1

Fig. 2

Fig. 3