

Crystal structure of (2*E*)-*N*-methyl-2-(2-oxo-1,2-dihydroacenaphthylen-1-ylidene)hydrazinecarbothioamide

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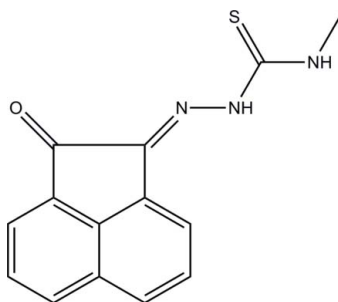
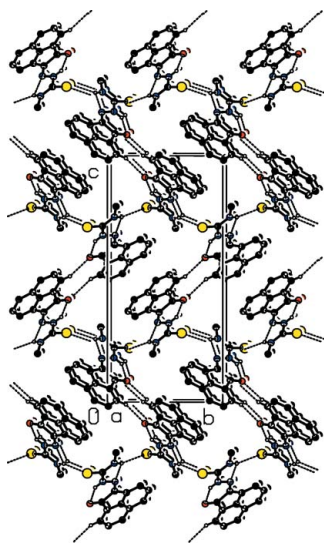
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In the title compound, C₁₄H₁₁N₃OS, the acenaphthylene ring system and hydrazinecarbothioamide unit (=N—NH—C=S—NH—) are essentially coplanar [with maximum deviations from their mean planes of -0.009 (2) and 0.033 (2) Å, respectively], and make a dihedral angle of 1.59 (9)°. The molecular conformation is stabilized by two weak intramolecular hydrogen bonds (N—H···O and N—H···N), which generate *S*(6) and *S*(5) ring motifs. In the crystal, molecules are linked by N—H···S hydrogen bonds, forming chains along [010]. The chains are linked *via* pairs of C—H···O hydrogen bonds, enclosing *R*₂²(10) ring motifs, and C—H··· π interactions, forming a three-dimensional framework. The absolute structure of the title compound was determined by resonant scattering.

1. Chemical context

The design and synthesis of thiosemicarbazones are of considerable interest because of their versatile chemistry and various biological activities, such as antitumor, antibacterial, antiviral, antiamebic and antimalarial (Kelly *et al.*, 1996). They comprise an intriguing class of chelating molecules, which possess a wide range of beneficial medicinal properties (Prabhakaran *et al.* 2008). Thiosemicarbazones are a versatile class of ligands that have been studied for their biological activity (Chellan *et al.*, 2010), their interesting binding motifs (Lobana *et al.*, 2009) and their use as ligands in catalysis (Xie *et al.*, 2010). In view of their biological importance, the crystal structure of the title compound has been determined and the results are presented herein.



2. Structural commentary

The molecular structure of the title compound is illustrated in Fig. 1. The atoms of both the acenaphthylene ring system and the =N—NH—C=S—NH— segment are essentially coplanar, the maximum deviations from their mean planes being -0.009 (2) and 0.033 (2) Å for atoms C12 and C14, respec-

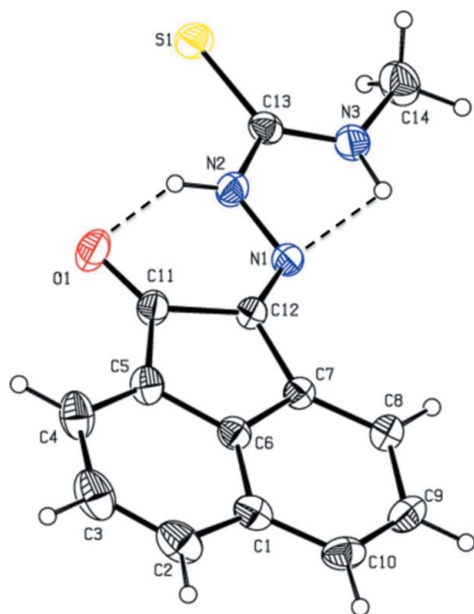


Figure 1
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines (see Table 1 for details).

tively. The dihedral angle between the benzene and cyclopentane rings of the acenaphthalene unit is $1.59(9)^\circ$. The molecular structure is stabilized by $N-H\cdots O$ and $N-H\cdots N$ hydrogen bonds, forming $S(6)$ and $S(5)$ ring motifs, respectively (Table 1 and Fig. 1).

3. Supramolecular features

In the crystal, molecules are linked by $N-H\cdots S$ hydrogen bonds (Table 1 and Fig. 2), forming chains along [010]. The chains are linked *via* pairs of $C-H\cdots O$ hydrogen bonds, enclosing $R_2^2(10)$ ring motifs, and $C-H\cdots\pi$ interactions, forming a three-dimensional framework (Table 1 and Fig. 2).

4. Database survey

A search of the Cambridge Structural Database (Version 5.35, last update May 2014; Groom & Allen, 2014) for the substructure 2-(imino)acenaphthylene-1(2*H*)-one gave 13 hits, including that of the ethyl analogue of the title compound,

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

C_g is the centroid of ring C1/C6–C10.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H2\cdots O1$	0.86	2.03	2.7178 (19)	136
$N3-H3\cdots N1$	0.86	2.26	2.6437 (19)	107
$N3-H3\cdots S1^i$	0.86	2.64	3.4407 (15)	156
$C4-H4\cdots O1^{ii}$	0.93	2.47	3.246 (2)	141
$C2-H2A\cdots C_g^{iii}$	0.93	2.76	3.502 (2)	137

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

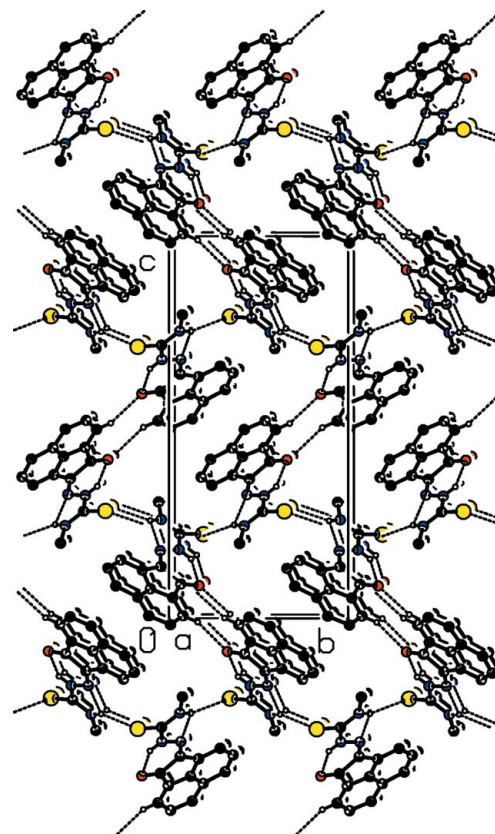


Figure 2
The crystal packing of the title compound viewed along the a axis. Hydrogen bonds are shown as dashed lines (see Table 1 for details; H atoms not involved in hydrogen bonding have been omitted for clarity).

acenaphthylene-1,2-dione 4-ethylthiosemicarbazone (GURHAD; Pascu *et al.*, 2010). The two molecules differ in the dihedral angle between the mean planes of the acenaphthylene ring system and hydrazinecarbothioamide unit ($=N-NH-C=S-NH-$) which is $1.59(9)^\circ$ in the title compound but $9.14(6)^\circ$ in the ethyl analogue (GURHAD; Pascu *et al.*, 2010). In the crystals of both compounds, molecules are linked *via* $N-H\cdots S$ hydrogen bonds, forming chains along [010].

5. Synthesis and crystallization

An ethanolic solution of *N*-methylhydrazinecarbothioamide (0.01 mol) was added to an ethanolic solution (50 ml) containing acenaphthylene-1,2-dione (0.01 mol). The mixture was refluxed for 2 h during which time a yellow precipitate separated out. The reaction mixture was then cooled to room temperature and the precipitate was filtered off. It was then washed with ethanol and dried under vacuum. The yield of the isolated product was 89%. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution of the title compound in ethanol at room temperature.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were fixed geom-

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₄ H ₁₁ N ₃ OS
<i>M</i> _r	269.33
Crystal system, space group	Orthorhombic, <i>P</i> 2 ₁ 2 ₁ 2 ₁
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.1110 (6), 10.0547 (11), 21.497 (2)
<i>V</i> (Å ³)	1320.8 (2)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.24
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractionmeter	Bruker <i>SMART</i> APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2008)
<i>T</i> _{min} , <i>T</i> _{max}	0.932, 0.954
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	23135, 3941, 2929
<i>R</i> _{int}	0.030
(sin θ/λ) _{max} (Å ⁻¹)	0.708
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.035, 0.100, 0.99
No. of reflections	3941
No. of parameters	173
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.19, -0.21
Absolute structure	Flack (1983); Friedel pairs
Absolute structure parameter	-0.02 (8)

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

etrically and allowed to ride on their parent atoms: N–H = 0.86 and C–H = 0.93–0.97 Å and with *U*_{iso}(H) = 1.5*U*_{eq}(C) for

methyl H atoms and = 1.2*U*_{eq}(C) for other H atoms. The absolute structure of the title compound was determined by resonant scattering, with a Flack parameter of 0.02 (8).

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Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINTE* (Bruker, 2008); data reduction: *SAINTE* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

(2*E*)-*N*-Methyl-2-(2-oxo-1,2-dihydroacenaphthylen-1-ylidene)hydrazinecarbothioamide

Crystal data

$C_{14}H_{11}N_3OS$	$Z = 4$
$M_r = 269.33$	$F(000) = 560$
Orthorhombic, $P2_12_12_1$	$D_x = 1.354 \text{ Mg m}^{-3}$
Hall symbol: P 2ac 2ab	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 6.1110 (6) \text{ \AA}$	$\mu = 0.24 \text{ mm}^{-1}$
$b = 10.0547 (11) \text{ \AA}$	$T = 293 \text{ K}$
$c = 21.497 (2) \text{ \AA}$	Block, yellow
$V = 1320.8 (2) \text{ \AA}^3$	$0.30 \times 0.25 \times 0.20 \text{ mm}$

Data collection

Bruker SMART APEXII CCD diffractometer	23135 measured reflections
Radiation source: fine-focus sealed tube	3941 independent reflections
Graphite monochromator	2929 reflections with $I > 2\sigma(I)$
ω and φ scans	$R_{\text{int}} = 0.030$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2008)	$\theta_{\text{max}} = 30.2^\circ$, $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.932$, $T_{\text{max}} = 0.954$	$h = -8 \rightarrow 8$
	$k = -13 \rightarrow 14$
	$l = -29 \rightarrow 29$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2 + 0.2048P]$
$S = 0.99$	where $P = (F_o^2 + 2F_c^2)/3$
3941 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
173 parameters	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Absolute structure: Flack (1983); Friedel pairs

Absolute structure parameter: -0.02 (8)

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.25692 (8)	0.16757 (4)	0.21243 (2)	0.04960 (13)
N1	0.7542 (2)	-0.05741 (12)	0.17414 (6)	0.0365 (3)
C6	1.2232 (3)	-0.09719 (15)	0.07905 (7)	0.0371 (3)
O1	0.8428 (2)	0.16301 (14)	0.08374 (6)	0.0550 (4)
N2	0.6084 (2)	0.04380 (14)	0.17558 (7)	0.0416 (3)
H2	0.6259	0.1109	0.1513	0.050*
C7	1.0847 (3)	-0.14650 (15)	0.12619 (7)	0.0342 (3)
C13	0.4342 (3)	0.04074 (16)	0.21510 (8)	0.0380 (3)
N3	0.4208 (2)	-0.06205 (15)	0.25248 (7)	0.0445 (3)
H3	0.5225	-0.1210	0.2506	0.053*
C12	0.9103 (3)	-0.04864 (16)	0.13442 (7)	0.0350 (3)
C5	1.1533 (3)	0.02565 (17)	0.05510 (8)	0.0425 (4)
C11	0.9539 (3)	0.06370 (17)	0.08912 (8)	0.0403 (4)
C8	1.1346 (3)	-0.26514 (17)	0.15336 (8)	0.0416 (4)
H8	1.0445	-0.3015	0.1838	0.050*
C9	1.3268 (3)	-0.3313 (2)	0.13404 (9)	0.0492 (4)
H9	1.3632	-0.4114	0.1530	0.059*
C14	0.2450 (4)	-0.0824 (2)	0.29673 (10)	0.0634 (5)
H14A	0.2421	-0.0099	0.3258	0.095*
H14B	0.2686	-0.1642	0.3187	0.095*
H14C	0.1080	-0.0866	0.2750	0.095*
C1	1.4122 (3)	-0.16161 (19)	0.05877 (8)	0.0435 (4)
C2	1.5292 (4)	-0.0968 (2)	0.01114 (10)	0.0604 (6)
H2A	1.6559	-0.1356	-0.0045	0.072*
C4	1.2699 (4)	0.0860 (2)	0.00894 (9)	0.0578 (5)
H4	1.2252	0.1668	-0.0078	0.069*
C3	1.4596 (4)	0.0221 (2)	-0.01250 (11)	0.0671 (6)
H3A	1.5408	0.0621	-0.0439	0.080*
C10	1.4618 (3)	-0.2829 (2)	0.08867 (9)	0.0505 (5)
H10	1.5867	-0.3300	0.0775	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0421 (2)	0.0413 (2)	0.0654 (3)	0.0080 (2)	0.0033 (2)	-0.01024 (19)
N1	0.0345 (6)	0.0331 (6)	0.0420 (7)	0.0008 (6)	0.0020 (7)	-0.0007 (5)
C6	0.0373 (9)	0.0370 (8)	0.0369 (8)	-0.0031 (7)	-0.0004 (7)	-0.0047 (6)
O1	0.0621 (8)	0.0423 (7)	0.0605 (8)	0.0123 (7)	0.0046 (7)	0.0140 (6)
N2	0.0397 (7)	0.0361 (7)	0.0488 (8)	0.0054 (6)	0.0055 (7)	0.0043 (6)
C7	0.0353 (8)	0.0338 (8)	0.0336 (7)	0.0004 (6)	-0.0001 (6)	-0.0013 (6)
C13	0.0337 (8)	0.0365 (8)	0.0438 (8)	-0.0028 (6)	0.0001 (7)	-0.0089 (7)
N3	0.0401 (8)	0.0406 (7)	0.0528 (8)	0.0015 (6)	0.0077 (7)	-0.0009 (7)
C12	0.0356 (8)	0.0326 (7)	0.0368 (7)	0.0007 (6)	-0.0014 (7)	0.0021 (6)
C5	0.0498 (10)	0.0395 (9)	0.0381 (8)	-0.0029 (8)	0.0047 (8)	-0.0009 (7)
C11	0.0436 (9)	0.0357 (8)	0.0415 (8)	-0.0005 (7)	-0.0003 (7)	0.0040 (7)
C8	0.0454 (10)	0.0386 (9)	0.0407 (9)	0.0029 (8)	0.0000 (8)	0.0019 (7)
C9	0.0523 (10)	0.0432 (9)	0.0521 (10)	0.0129 (9)	-0.0088 (8)	-0.0013 (8)
C14	0.0583 (12)	0.0610 (12)	0.0707 (13)	-0.0037 (11)	0.0226 (12)	0.0021 (9)
C1	0.0388 (9)	0.0476 (9)	0.0441 (9)	-0.0044 (8)	0.0042 (7)	-0.0129 (8)
C2	0.0513 (12)	0.0702 (14)	0.0596 (12)	-0.0090 (10)	0.0196 (10)	-0.0180 (10)
C4	0.0742 (14)	0.0496 (10)	0.0495 (10)	-0.0103 (11)	0.0164 (11)	0.0068 (8)
C3	0.0747 (16)	0.0684 (15)	0.0581 (12)	-0.0179 (12)	0.0285 (12)	-0.0009 (10)
C10	0.0397 (10)	0.0547 (11)	0.0572 (11)	0.0100 (8)	-0.0044 (8)	-0.0157 (9)

Geometric parameters (Å, °)

S1—C13	1.6744 (17)	C5—C11	1.472 (3)
N1—C12	1.283 (2)	C8—C9	1.412 (2)
N1—N2	1.3528 (19)	C8—H8	0.9300
C6—C1	1.394 (2)	C9—C10	1.367 (3)
C6—C5	1.405 (2)	C9—H9	0.9300
C6—C7	1.410 (2)	C14—H14A	0.9600
O1—C11	1.213 (2)	C14—H14B	0.9600
N2—C13	1.362 (2)	C14—H14C	0.9600
N2—H2	0.8600	C1—C2	1.409 (3)
C7—C8	1.363 (2)	C1—C10	1.411 (3)
C7—C12	1.461 (2)	C2—C3	1.367 (3)
C13—N3	1.312 (2)	C2—H2A	0.9300
N3—C14	1.449 (2)	C4—C3	1.403 (3)
N3—H3	0.8600	C4—H4	0.9300
C12—C11	1.515 (2)	C3—H3A	0.9300
C5—C4	1.364 (3)	C10—H10	0.9300
C12—N1—N2	116.93 (13)	C7—C8—H8	120.9
C1—C6—C5	123.08 (16)	C9—C8—H8	120.9
C1—C6—C7	123.95 (16)	C10—C9—C8	122.95 (18)
C5—C6—C7	112.96 (15)	C10—C9—H9	118.5
N1—N2—C13	120.78 (14)	C8—C9—H9	118.5
N1—N2—H2	119.6	N3—C14—H14A	109.5

C13—N2—H2	119.6	N3—C14—H14B	109.5
C8—C7—C6	118.78 (16)	H14A—C14—H14B	109.5
C8—C7—C12	134.48 (16)	N3—C14—H14C	109.5
C6—C7—C12	106.73 (13)	H14A—C14—H14C	109.5
N3—C13—N2	116.67 (15)	H14B—C14—H14C	109.5
N3—C13—S1	125.49 (13)	C6—C1—C2	115.65 (19)
N2—C13—S1	117.84 (13)	C6—C1—C10	115.92 (16)
C13—N3—C14	124.05 (16)	C2—C1—C10	128.43 (18)
C13—N3—H3	118.0	C3—C2—C1	121.1 (2)
C14—N3—H3	118.0	C3—C2—H2A	119.4
N1—C12—C7	125.20 (14)	C1—C2—H2A	119.4
N1—C12—C11	127.56 (15)	C5—C4—C3	117.9 (2)
C7—C12—C11	107.22 (14)	C5—C4—H4	121.1
C4—C5—C6	119.92 (18)	C3—C4—H4	121.1
C4—C5—C11	132.73 (18)	C2—C3—C4	122.4 (2)
C6—C5—C11	107.34 (15)	C2—C3—H3A	118.8
O1—C11—C5	129.05 (16)	C4—C3—H3A	118.8
O1—C11—C12	125.21 (16)	C9—C10—C1	120.19 (17)
C5—C11—C12	105.74 (14)	C9—C10—H10	119.9
C7—C8—C9	118.19 (17)	C1—C10—H10	119.9
C12—N1—N2—C13	178.14 (14)	C6—C5—C11—C12	-0.95 (18)
C1—C6—C7—C8	-1.1 (2)	N1—C12—C11—O1	-0.7 (3)
C5—C6—C7—C8	-179.95 (15)	C7—C12—C11—O1	-179.08 (17)
C1—C6—C7—C12	178.56 (15)	N1—C12—C11—C5	179.18 (16)
C5—C6—C7—C12	-0.34 (19)	C7—C12—C11—C5	0.76 (18)
N1—N2—C13—N3	2.3 (2)	C6—C7—C8—C9	1.7 (2)
N1—N2—C13—S1	-178.08 (12)	C12—C7—C8—C9	-177.74 (17)
N2—C13—N3—C14	-179.01 (17)	C7—C8—C9—C10	-1.3 (3)
S1—C13—N3—C14	1.4 (3)	C5—C6—C1—C2	-1.3 (2)
N2—N1—C12—C7	179.26 (15)	C7—C6—C1—C2	179.96 (16)
N2—N1—C12—C11	1.1 (2)	C5—C6—C1—C10	178.58 (16)
C8—C7—C12—N1	0.8 (3)	C7—C6—C1—C10	-0.2 (2)
C6—C7—C12—N1	-178.75 (15)	C6—C1—C2—C3	0.6 (3)
C8—C7—C12—C11	179.24 (18)	C10—C1—C2—C3	-179.2 (2)
C6—C7—C12—C11	-0.29 (17)	C6—C5—C4—C3	-0.7 (3)
C1—C6—C5—C4	1.4 (3)	C11—C5—C4—C3	178.57 (19)
C7—C6—C5—C4	-179.72 (17)	C1—C2—C3—C4	0.0 (4)
C1—C6—C5—C11	-178.08 (15)	C5—C4—C3—C2	0.1 (3)
C7—C6—C5—C11	0.83 (19)	C8—C9—C10—C1	0.0 (3)
C4—C5—C11—O1	-0.5 (4)	C6—C1—C10—C9	0.7 (2)
C6—C5—C11—O1	178.88 (19)	C2—C1—C10—C9	-179.5 (2)
C4—C5—C11—C12	179.7 (2)		

Hydrogen-bond geometry (Å, °)

Cg is the centroid of ring C1/C6–C10.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N2—H2···O1	0.86	2.03	2.7178 (19)	136
N3—H3···N1	0.86	2.26	2.6437 (19)	107
N3—H3···S1 ⁱ	0.86	2.64	3.4407 (15)	156
C4—H4···O1 ⁱⁱ	0.93	2.47	3.246 (2)	141
C2—H2A···Cg ⁱⁱⁱ	0.93	2.76	3.502 (2)	137

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