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Crystal structure of (*E*)-2-cyano-3-(12-methyl-12*H*-benzo[*b*]phenothiazin-11-yl)acrylic acid

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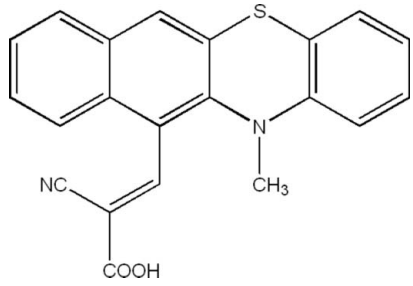
In the title compound, $C_{21}H_{14}N_2O_2S$, a donor–acceptor type of benzo[*b*]phenothiazine (bpz) derivative, the thiazine ring adopts a boat conformation and the bond-angle sum at the N atom is 360.0°. The dihedral angle between the benzene ring and the naphthelene ring system fused to the thiazine ring is 32.76 (5)°. In the crystal, carboxylic-acid inversion dimers linked by pairs of O—H···O hydrogen bonds generate $R_2^2(8)$ loops. Aromatic π–π stacking [shortest centroid–centroid separaton = 3.5242 (13)Å] consolidates the structure and very weak C—H···O and C—H···N interactions also occur.

Keywords: crystal structure; benzo[*b*]phenothiazine derivative; inversion dimers; hydrogen bonding; π–π stacking.

CCDC reference: 1018980

1. Related literature

For related structures, see: Bell *et al.* (1968), van de Waal & Feil (1977), Sun *et al.* (2004); Harrison *et al.* (2007). For applications of the title compound in dye-sensitized solar cells, see: Watanabe *et al.* (2014).



2. Experimental

2.1. Crystal data

$C_{21}H_{14}N_2O_2S$
M_r = 358.40
Triclinic, $P\overline{1}$
a = 6.7915 (17) Å
b = 9.196 (3) Å
c = 13.941 (3) Å
α = 95.831 (13)°
β = 101.214 (10)°
γ = 90.850 (15)°
V = 849.1 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 123 K
0.40 × 0.40 × 0.15 mm

2.2. Data collection

Rigaku R-AXIS RAPID CCD diffractometer
14164 measured reflections
3877 independent reflections
3663 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.100
S = 1.06
3877 reflections
290 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H14···O1^{i}	1.063 (18)	1.524 (18)	2.5856 (13)	176.8 (16)
C19—H10···N2^{ii}	0.958 (16)	2.699 (16)	3.5991 (18)	156.8 (13)
C19—H11···O1^{iii}	0.957 (17)	2.623 (17)	3.5518 (17)	163.7 (13)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *Yadokari-XG 2009* (Wakita, 2001; Kabuto *et al.*, 2009) and *POV-RAY* (Persistence of Vision Team, 2004).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7264).

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supporting information

Acta Cryst. (2014). E**70**, o1026–o1027 [doi:10.1107/S1600536814018388]

Crystal structure of (*E*)-2-cyano-3-(12-methyl-12*H*-benzo[*b*]phenothiazin-11-yl)acrylic acid

Motonori Watanabe and Tatsumi Ishihara

S1. Structural commentary

Phenothiazine, $C_{12}H_9NS$ showed stable redox properties. This crystal struture have been reported for the neutral state (Bell *et al.*, 1968, and van de Wall & Feli, 1977), and for the $C_{12}H_9NS$+ radical cation state (Sun *et al.*, 2004), and phenothiazine-picric acid (1/1) (Harrison *et al.*, 2007).

As part of our studies for understanding the donor-acceptor interaction type dye molecule for dye-sensitized solar cell (Watanabe *et al.*, 2014), we now report the title compound. In the title compound, $C_{21}H_{14}N_2O_2S$, consists a 12-methyl-12*H*-benzo[*b*]phenothiazine as a donor moiety, which has a (*E*)-2-cyanobut-2-enoic acid moiety as acceptor at C-11 position of 12-methyl-12*H*-benzo[*b*]phenothiazine.

Dark-red crystals were obtained from 0.013 g of title compound in tetrahydrofuran (10 ml) solution by slow diffusion.

The $C_{21}H_{14}N_2O_2S$ of 12-methyl-12*H*-benzo[*b*]phenothiazine moiety takes pyramidal structure, in which benzene and naphthalene had 147.2°, while the olefin bond at the cyanoacrylic moiety existed 123.8° from the naphthalene plane (Figure 1). The title compounds showed an intermolecular hydrogen bonding at O1—H14 - O2′ (1.520 Å) in the two molecule structure of carboxylic acid moiety (Figure 2). Furthermore, title compound have π-π stacking orientation along with *a* axis, where the two-naphthalene moieties oriented the parallel structures, which has a transannular distance at 3.273 Å (Figure 3).

S2. Crystallization

The chloroform solution (10 ml) of title compound (0.013 g) was standing under ambient condition until the desired single crystal was produced.

S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All the hydrogen atoms of the compound are fixed geometrically (C—H = 0.95 - 1.01 Å) and allowed to ride on their parent atoms. Structure was refined with unique reflections and with a cut-off sigma = 2.00.

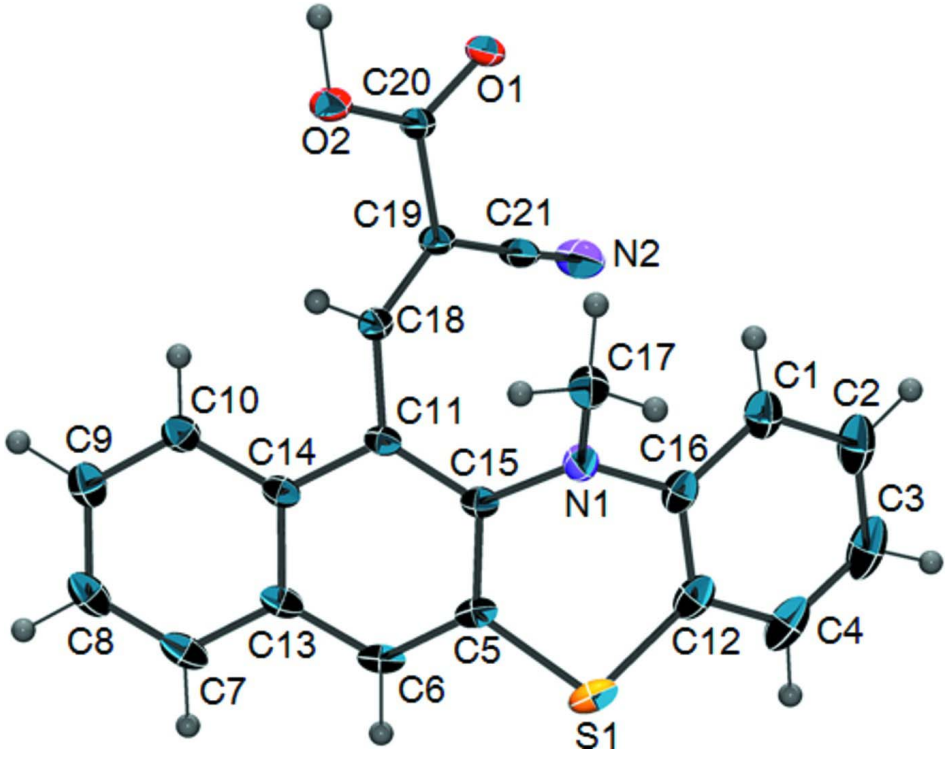

Figure 1

The molecular structure of $C_{21}H_{14}N_2O_2S$ with displacement ellipsoids drawn at the 50% probability level.

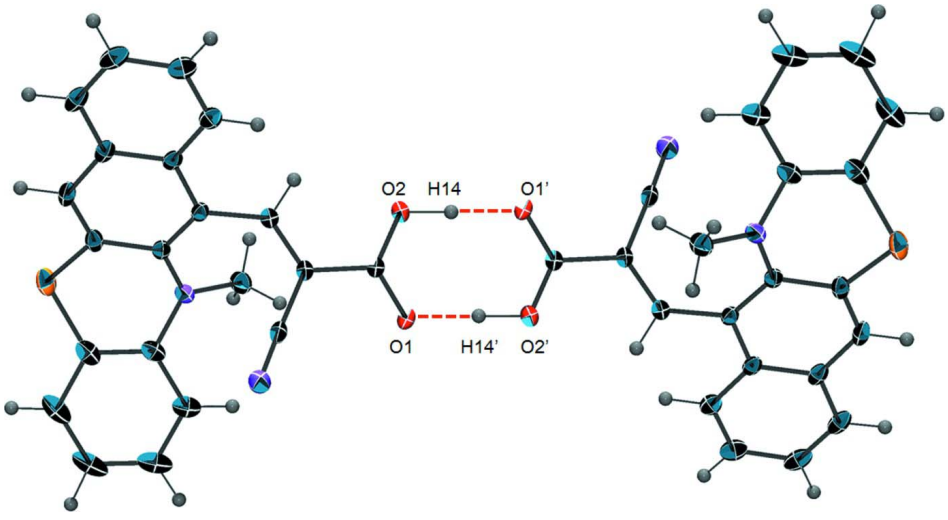

Figure 2

Intermolecular hydrogen bonding O1—H14—O2′ (1.520 Å) in the two molecule structure of carboxylic acid moiety.

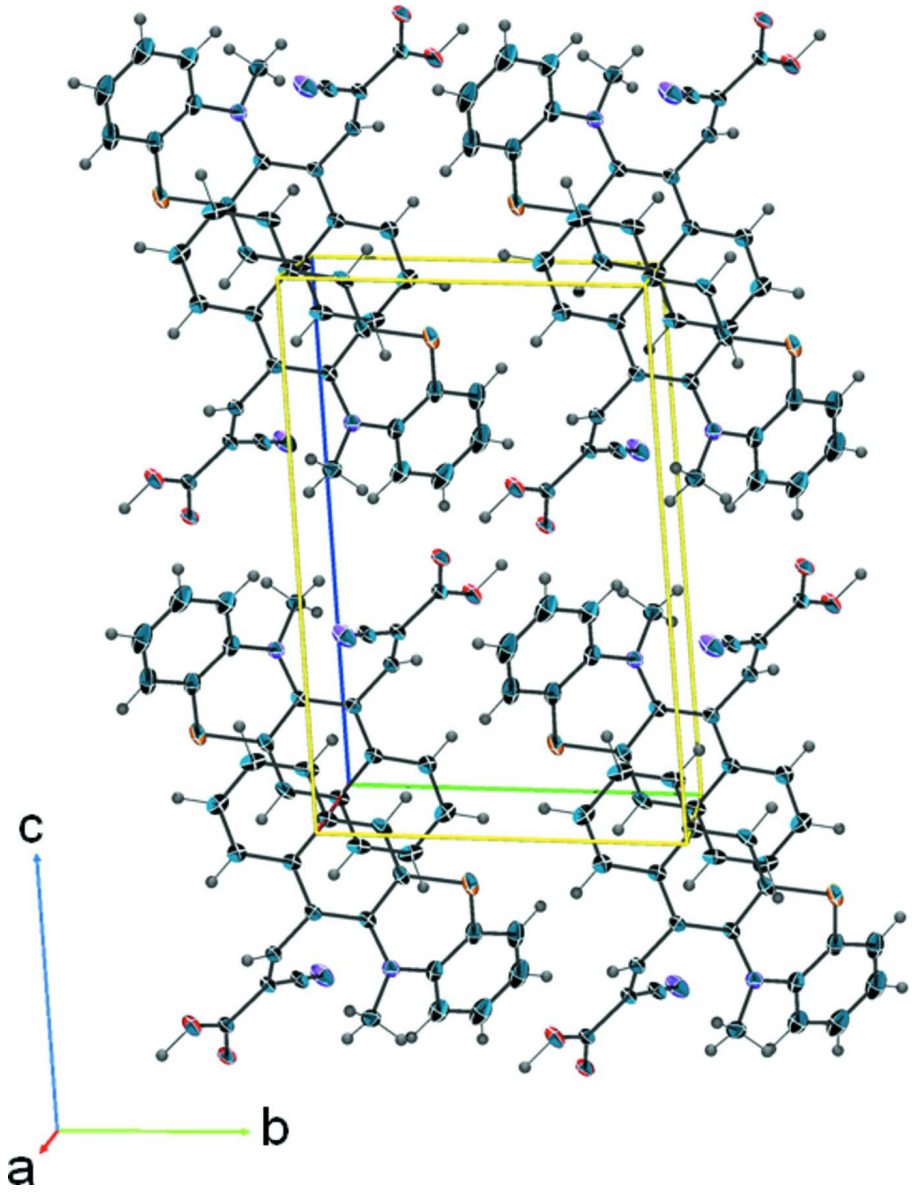

Figure 3

Packing diagram of $C_{21}H_{14}N_2O_2S$.

(*E*)-2-Cyano-3-(12-methyl-12*H*-benzo[*b*]phenothiazin-11-yl)acrylic acid

Crystal data

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c = 13.941 (3) Å
α = 95.831 (13)°
β = 101.214 (10)°
γ = 90.850 (15)°
V = 849.1 (4) Å^3
Z = 2
$F(000)$ = 372
D_x = 1.402 Mg m^{-3}
Melting point: 351 K
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 14164 reflections
θ = 3.0–27.5°
μ = 0.21 mm^{-1}

T = 123 K
Block, dark red

0.40 × 0.40 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID CCD diffractometer
$\omega/2\theta$ scans
14164 measured reflections
3877 independent reflections
3663 reflections with $I > 2\sigma(I)$

R_{int} = 0.020
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −8→8
k = −11→11
l = −18→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.100
S = 1.06
3877 reflections
290 parameters
0 restraints

Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 0.2744P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
H2	0.953 (3)	−0.333 (2)	0.4654 (13)	0.041 (5)*
H3	0.968 (3)	−0.526 (2)	0.3462 (15)	0.056 (6)*
C1	0.71497 (19)	−0.23569 (15)	0.38906 (10)	0.0297 (3)
H10	0.213 (2)	−0.0357 (18)	0.3396 (12)	0.029 (4)*
C2	0.8586 (2)	−0.34194 (17)	0.40418 (12)	0.0371 (3)
C3	0.8644 (2)	−0.45592 (16)	0.33152 (13)	0.0402 (3)
C4	0.7256 (2)	−0.46500 (15)	0.24404 (12)	0.0353 (3)
C5	0.12589 (17)	0.17296 (15)	−0.11405 (9)	0.0274 (3)
H5	0.290 (2)	−0.2245 (18)	−0.0436 (12)	0.033 (4)*
H6	0.163 (2)	−0.0447 (18)	−0.1546 (12)	0.031 (4)*
H9	0.238 (2)	0.3227 (18)	0.1163 (12)	0.031 (4)*
C6	0.22142 (17)	0.24648 (13)	0.06076 (9)	0.0223 (2)
C7	0.34176 (15)	0.06021 (12)	0.17662 (8)	0.0173 (2)
S1	0.39308 (5)	−0.37579 (3)	0.12102 (2)	0.02878 (11)
O1	0.65112 (12)	0.36226 (9)	0.47776 (6)	0.02296 (18)
H7	0.075 (3)	0.1979 (19)	−0.1817 (13)	0.038 (4)*
H1	0.714 (2)	−0.1535 (19)	0.4397 (12)	0.029 (4)*
H8	0.124 (3)	0.386 (2)	−0.0451 (13)	0.040 (4)*
C8	0.24793 (16)	−0.00669 (13)	−0.00306 (8)	0.0202 (2)
H4	0.725 (3)	−0.541 (2)	0.1909 (13)	0.041 (5)*
C9	0.26789 (15)	0.10113 (12)	0.07897 (8)	0.0181 (2)

O2	0.35247 (13)	0.41863 (10)	0.39083 (6)	0.0275 (2)
H14	0.353 (3)	0.507 (2)	0.4467 (13)	0.041*
N1	0.42827 (14)	−0.13630 (10)	0.28349 (7)	0.0208 (2)
C10	0.38246 (15)	−0.08478 (12)	0.19057 (8)	0.0177 (2)
H13	0.246 (2)	0.2398 (16)	0.2575 (11)	0.023 (3)*
C11	0.35977 (16)	0.17829 (12)	0.25662 (8)	0.0186 (2)
C12	0.50856 (16)	0.34153 (12)	0.40510 (8)	0.0185 (2)
N2	0.86564 (16)	0.10083 (13)	0.34623 (9)	0.0336 (3)
H11	0.312 (2)	−0.1618 (18)	0.3995 (12)	0.031 (4)*
H12	0.420 (3)	−0.003 (2)	0.4129 (13)	0.041 (5)*
C13	0.30285 (16)	−0.15078 (13)	0.01314 (8)	0.0219 (2)
C14	0.36473 (16)	−0.18954 (12)	0.10592 (8)	0.0201 (2)
C15	0.17442 (17)	0.03230 (15)	−0.09906 (8)	0.0250 (2)
C16	0.15205 (18)	0.28132 (14)	−0.03332 (9)	0.0266 (3)
C17	0.57900 (18)	−0.36047 (13)	0.22895 (10)	0.0262 (2)
C18	0.57427 (17)	−0.24412 (12)	0.30077 (9)	0.0231 (2)
C19	0.33548 (19)	−0.08052 (14)	0.36491 (9)	0.0248 (2)
C20	0.51890 (16)	0.21732 (12)	0.32950 (8)	0.0186 (2)
C21	0.70959 (17)	0.14883 (13)	0.33855 (8)	0.0222 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0244 (6)	0.0300 (6)	0.0354 (7)	0.0032 (5)	0.0037 (5)	0.0107 (5)
C2	0.0239 (6)	0.0388 (7)	0.0513 (8)	0.0065 (5)	0.0052 (6)	0.0218 (6)
C3	0.0290 (6)	0.0339 (7)	0.0655 (10)	0.0136 (5)	0.0183 (6)	0.0231 (7)
C4	0.0344 (7)	0.0229 (6)	0.0559 (9)	0.0083 (5)	0.0227 (6)	0.0106 (6)
C5	0.0187 (5)	0.0433 (7)	0.0200 (5)	−0.0067 (5)	0.0017 (4)	0.0078 (5)
C6	0.0189 (5)	0.0240 (6)	0.0231 (5)	−0.0022 (4)	0.0023 (4)	0.0017 (4)
C7	0.0140 (4)	0.0198 (5)	0.0168 (5)	−0.0007 (4)	0.0021 (4)	−0.0026 (4)
S1	0.03269 (18)	0.01645 (16)	0.03660 (19)	−0.00299 (11)	0.00977 (13)	−0.00517 (11)
O1	0.0245 (4)	0.0230 (4)	0.0180 (4)	0.0017 (3)	−0.0007 (3)	−0.0045 (3)
C8	0.0143 (4)	0.0278 (6)	0.0176 (5)	−0.0054 (4)	0.0043 (4)	−0.0026 (4)
C9	0.0130 (4)	0.0223 (5)	0.0177 (5)	−0.0028 (4)	0.0019 (4)	−0.0009 (4)
O2	0.0262 (4)	0.0258 (4)	0.0262 (4)	0.0094 (3)	−0.0004 (3)	−0.0080 (3)
N1	0.0208 (4)	0.0211 (5)	0.0207 (4)	0.0053 (4)	0.0046 (4)	0.0015 (3)
C10	0.0137 (4)	0.0198 (5)	0.0186 (5)	−0.0008 (4)	0.0034 (4)	−0.0020 (4)
C11	0.0195 (5)	0.0178 (5)	0.0179 (5)	0.0024 (4)	0.0034 (4)	−0.0003 (4)
C12	0.0197 (5)	0.0177 (5)	0.0170 (5)	0.0013 (4)	0.0028 (4)	−0.0012 (4)
N2	0.0236 (5)	0.0391 (6)	0.0338 (6)	0.0074 (4)	0.0017 (4)	−0.0098 (5)
C13	0.0183 (5)	0.0251 (6)	0.0210 (5)	−0.0056 (4)	0.0065 (4)	−0.0083 (4)
C14	0.0174 (5)	0.0178 (5)	0.0247 (5)	−0.0024 (4)	0.0065 (4)	−0.0042 (4)
C15	0.0176 (5)	0.0392 (7)	0.0171 (5)	−0.0080 (4)	0.0042 (4)	−0.0018 (5)
C16	0.0204 (5)	0.0320 (6)	0.0276 (6)	−0.0026 (4)	0.0024 (4)	0.0089 (5)
C17	0.0241 (5)	0.0197 (5)	0.0381 (6)	0.0017 (4)	0.0131 (5)	0.0055 (5)
C18	0.0191 (5)	0.0209 (5)	0.0312 (6)	0.0027 (4)	0.0077 (4)	0.0066 (4)
C19	0.0270 (6)	0.0275 (6)	0.0218 (5)	0.0055 (5)	0.0086 (4)	0.0035 (4)
C20	0.0197 (5)	0.0177 (5)	0.0176 (5)	0.0020 (4)	0.0034 (4)	−0.0026 (4)

C21	0.0218 (5)	0.0226 (5)	0.0195 (5)	0.0005 (4)	0.0018 (4)	−0.0064 (4)

Geometric parameters (Å, º)

C1—C2	1.3933 (18)	C8—C15	1.4185 (16)
C1—C18	1.3982 (18)	C8—C9	1.4192 (15)
C1—H1	0.982 (17)	O2—C12	1.2786 (14)
C2—C3	1.388 (2)	O2—H14	1.063 (18)
C2—H2	0.959 (18)	N1—C10	1.4042 (14)
C3—C4	1.383 (2)	N1—C18	1.4174 (14)
C3—H3	0.97 (2)	N1—C19	1.4553 (14)
C4—C17	1.3956 (17)	C10—C14	1.4301 (15)
C4—H4	0.963 (19)	C11—C20	1.3478 (15)
C5—C15	1.366 (2)	C11—H13	0.964 (15)
C5—C16	1.4072 (19)	C12—C20	1.4855 (15)
C5—H7	0.990 (17)	N2—C21	1.1440 (16)
C6—C16	1.3764 (17)	C13—C14	1.3650 (17)
C6—C9	1.4145 (16)	C13—H5	0.978 (17)
C6—H9	0.978 (17)	C15—H6	0.985 (17)
C7—C10	1.3908 (16)	C16—H8	1.006 (18)
C7—C9	1.4458 (15)	C17—C18	1.3942 (18)
C7—C11	1.4611 (15)	C19—H10	0.958 (16)
S1—C14	1.7556 (13)	C19—H11	0.957 (17)
S1—C17	1.7581 (14)	C19—H12	1.013 (19)
O1—C12	1.2544 (14)	C20—C21	1.4376 (15)
C8—C13	1.4101 (17)		
C2—C1—C18	120.09 (13)	C20—C11—C7	128.50 (10)
C2—C1—H1	120.2 (9)	C20—C11—H13	114.1 (9)
C18—C1—H1	119.7 (9)	C7—C11—H13	117.3 (9)
C3—C2—C1	120.34 (14)	O1—C12—O2	125.12 (10)
C3—C2—H2	121.5 (11)	O1—C12—C20	118.13 (10)
C1—C2—H2	118.2 (11)	O2—C12—C20	116.75 (9)
C4—C3—C2	119.87 (12)	C14—C13—C8	121.34 (10)
C4—C3—H3	123.7 (12)	C14—C13—H5	120.0 (10)
C2—C3—H3	116.5 (12)	C8—C13—H5	118.6 (10)
C3—C4—C17	120.17 (14)	C13—C14—C10	121.42 (10)
C3—C4—H4	123.1 (11)	C13—C14—S1	118.47 (8)
C17—C4—H4	116.8 (11)	C10—C14—S1	119.66 (9)
C15—C5—C16	119.59 (11)	C5—C15—C8	120.96 (11)
C15—C5—H7	119.6 (10)	C5—C15—H6	121.2 (9)
C16—C5—H7	120.8 (10)	C8—C15—H6	117.8 (9)
C16—C6—C9	121.02 (11)	C6—C16—C5	120.73 (12)
C16—C6—H9	119.9 (9)	C6—C16—H8	119.9 (10)
C9—C6—H9	119.1 (9)	C5—C16—H8	119.4 (10)
C10—C7—C9	120.36 (9)	C18—C17—C4	120.36 (13)
C10—C7—C11	123.92 (10)	C18—C17—S1	118.84 (9)
C9—C7—C11	115.66 (10)	C4—C17—S1	120.77 (11)

C14—S1—C17	99.34 (6)	C17—C18—C1	119.14 (11)
C13—C8—C15	121.48 (10)	C17—C18—N1	119.89 (11)
C13—C8—C9	118.85 (10)	C1—C18—N1	120.97 (11)
C15—C8—C9	119.67 (11)	N1—C19—H10	109.2 (9)
C6—C9—C8	117.97 (10)	N1—C19—H11	107.3 (10)
C6—C9—C7	122.69 (10)	H10—C19—H11	111.2 (14)
C8—C9—C7	119.29 (10)	N1—C19—H12	114.0 (10)
C12—O2—H14	113.7 (10)	H10—C19—H12	106.4 (14)
C10—N1—C18	119.48 (9)	H11—C19—H12	108.7 (14)
C10—N1—C19	122.62 (9)	C11—C20—C21	123.98 (10)
C18—N1—C19	117.88 (9)	C11—C20—C12	120.73 (10)
C7—C10—N1	123.61 (9)	C21—C20—C12	115.25 (9)
C7—C10—C14	118.54 (10)	N2—C21—C20	176.72 (13)
N1—C10—C14	117.73 (10)		

C18—C1—C2—C3	0.6 (2)	C7—C10—C14—S1	−174.34 (8)
C1—C2—C3—C4	−0.7 (2)	N1—C10—C14—S1	1.83 (13)
C2—C3—C4—C17	−0.4 (2)	C17—S1—C14—C13	152.24 (9)
C16—C6—C9—C8	2.30 (16)	C17—S1—C14—C10	−35.38 (10)
C16—C6—C9—C7	179.77 (10)	C16—C5—C15—C8	0.99 (17)
C13—C8—C9—C6	176.94 (9)	C13—C8—C15—C5	−178.54 (10)
C15—C8—C9—C6	−2.82 (15)	C9—C8—C15—C5	1.22 (16)
C13—C8—C9—C7	−0.62 (15)	C9—C6—C16—C5	−0.12 (18)
C15—C8—C9—C7	179.61 (9)	C15—C5—C16—C6	−1.56 (18)
C10—C7—C9—C6	179.09 (9)	C3—C4—C17—C18	1.62 (19)
C11—C7—C9—C6	1.88 (15)	C3—C4—C17—S1	−176.53 (10)
C10—C7—C9—C8	−3.47 (15)	C14—S1—C17—C18	36.16 (10)
C11—C7—C9—C8	179.32 (9)	C14—S1—C17—C4	−145.67 (10)
C9—C7—C10—N1	−171.10 (9)	C4—C17—C18—C1	−1.66 (17)
C11—C7—C10—N1	5.86 (16)	S1—C17—C18—C1	176.53 (9)
C9—C7—C10—C14	4.83 (15)	C4—C17—C18—N1	178.19 (11)
C11—C7—C10—C14	−178.20 (9)	S1—C17—C18—N1	−3.63 (15)
C18—N1—C10—C7	−142.33 (11)	C2—C1—C18—C17	0.53 (18)
C19—N1—C10—C7	35.94 (16)	C2—C1—C18—N1	−179.31 (11)
C18—N1—C10—C14	41.71 (14)	C10—N1—C18—C17	−41.32 (15)
C19—N1—C10—C14	−140.02 (11)	C19—N1—C18—C17	140.33 (11)
C10—C7—C11—C20	53.51 (17)	C10—N1—C18—C1	138.52 (11)
C9—C7—C11—C20	−129.39 (12)	C19—N1—C18—C1	−39.83 (16)
C15—C8—C13—C14	−176.93 (10)	C7—C11—C20—C21	2.65 (19)
C9—C8—C13—C14	3.31 (16)	C7—C11—C20—C12	−179.85 (10)
C8—C13—C14—C10	−1.94 (16)	O1—C12—C20—C11	171.53 (10)
C8—C13—C14—S1	170.30 (8)	O2—C12—C20—C11	−7.97 (16)
C7—C10—C14—C13	−2.19 (15)	O1—C12—C20—C21	−10.77 (15)
N1—C10—C14—C13	173.98 (10)	O2—C12—C20—C21	169.73 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H14···O1^{i}	1.063 (18)	1.524 (18)	2.5856 (13)	176.8 (16)
C19—H10···N2^{ii}	0.958 (16)	2.699 (16)	3.5991 (18)	156.8 (13)
C19—H11···O1^{iii}	0.957 (17)	2.623 (17)	3.5518 (17)	163.7 (13)

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