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Synthesis and structure of 10,10′-[2,5-bis(octyloxy)-1,4-phenylene]bis(10*H*-phenothiazine)

Naohiro Takahashi,[a] Shota Fujii[a] and Takashi Okubo[b]*

[a]Department of Chemistry, Kindai University, Osaka, Japan, and [b]Department of Energy and Materials, Kindai University, Osaka, Japan. *Correspondence e-mail: okubo_t@emat.kindai.ac.jp

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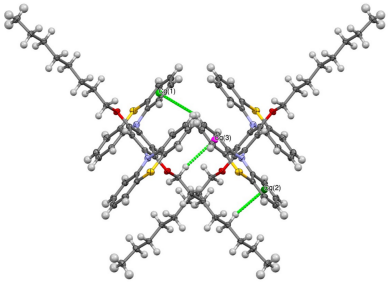
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The asymmetric unit of the title compound, $C_{46}H_{52}N_2O_2S_2$, contains one half of the molecule, with the complete molecule generated by crystallographic inversion symmetry. The molecule comprises two phenothiazine units attached to a central benzene ring bearing two octyloxy substituents. The phenothiazine moieties exhibit nearly planar conformations, with a butterfly angle of 2.31 (7)°, which is considerably smaller than those reported for related compounds. The dihedral angle between each phenothiazine unit and the central benzene ring is 87.23 (5)°. In the crystal, adjacent phenothiazine units form slipped π–π stacking interactions, accompanied by weak C—H$\cdots\pi$ contacts and van der Waals interactions between the alkyl chains. In $CHCl_3$ solution, the compound exhibits a strong absorption band at around 250 nm and a weak broad absorption band at 300–350 nm, together with photoluminescence centered at 450 nm. Cyclic voltammetry revealed an estimated HOMO energy level of −5.13 eV, while the LUMO energy level was estimated to be −1.72 eV from the optical absorption onset. These results provide insights into the molecular structure, crystal packing, and optoelectronic properties of this phenothiazine derivative.

1. Chemical context

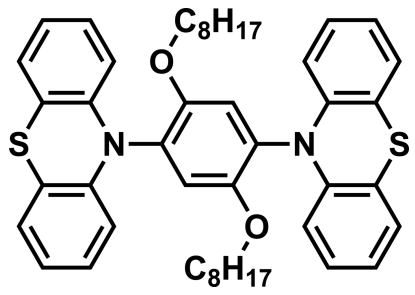
Phenothiazine is an electron-rich heterocyclic compound containing nitrogen and sulfur atoms. Owing to its characteristic non-planar structure and favorable electronic properties, it has been widely incorporated into functional organic molecules. In addition to its electron-donating ability arising from the nitrogen and sulfur atoms, the phenothiazine framework generally adopts a folded, butterfly-like conformation (Elliott *et al.*, 2021). This molecular geometry is characterized by the dihedral angle between the two outer benzene rings, known as the butterfly angle. Furthermore, the non-planar structure contributes to the formation of twisted molecular architectures and can influence the luminescence properties in the solid state (Huang *et al.*, 2021, Ekbote *et al.*, 2020). In addition, phenothiazine has attracted considerable attention as a donor building block for optoelectronic materials owing to its electron-donating ability, with potential applications in light-emitting organic materials and charge-transport materials used in organic light-emitting diodes (OLEDs), perovskite solar cells (PSCs), and organic solar cells (OSCs) (Castriotta *et al.*, 2023, Revoju *et al.*, 2018, Wang *et al.*, 2021).

This study reports the crystal structure of the title compound, $C_{46}H_{52}N_2O_2S_2$, (**1**), a phenothiazine derivative bearing flexible octyloxy chains, determined by single-crystal X-ray diffraction analysis. Particular attention was paid to the molecular conformation, including the butterfly angles of the phenothiazine units, and the molecular arrangement in the crystal. Furthermore, the effects of the octyloxy chains on the molecular structure and crystal packing were investigated to



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provide structural insights into phenothiazine-based functional organic materials.



2. Structural commentary

The molecular structure of compound **1** is shown in Fig. 1. The asymmetric unit contains one half of the molecule, with the complete molecule generated by an inversion operation centred at $[-x+\frac{3}{2}, -y+\frac{3}{2}, -z+\frac{1}{2}]$. The molecule consists of a central benzene ring bearing two octyloxy substituents and two phenothiazine units. Both phenothiazine moieties adopt nearly planar conformations, with a butterfly angle of 2.31 (7)°. The C12—N1 and C1—N1 bond lengths are 1.4046 (16) and 1.4062 (18) Å, respectively, while the C6—S1 and C7—S1 bond lengths are 1.7599 (16) and 1.7607 (15) Å, respectively. These values are comparable to those reported for the corresponding C—N (1.409–1.426 Å) and C—S (1.754–1.759 Å) bond lengths in the phenothiazine framework of a related compound (Sun *et al.*, 2004, Skhirtladze *et al.*, 2022). In contrast, the butterfly angle of 2.31 (5)° is considerably smaller than the reported values of 25.6 and 30.1°, indicating that the phenothiazine moieties in the title compound adopt substantially more planar conformations than those in the related compounds (Skhirtladze *et al.*, 2022, Wang *et al.*, 2021). The C14—N1 bond connecting the central benzene ring to the phenothiazine unit measures 1.4396 (17) Å, which is close to the corresponding bond lengths reported for related phenothiazine derivatives (Sun *et al.*, 2004; Song *et al.*, 2024).

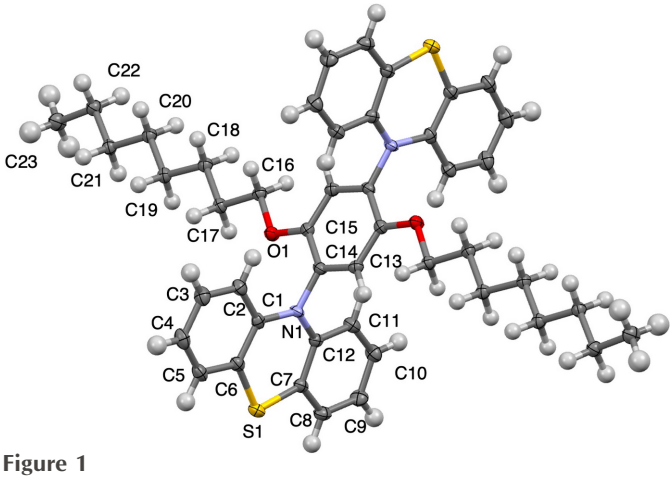


Figure 1
The molecular structure of compound **1** with displacement ellipsoids drawn at the 50% probability level. Unlabelled atoms are generated by the symmetry operation $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+\frac{1}{2}$.

Table 1
C—H···π interactions (Å, °).

*Cg*1, *Cg*2 and *Cg*3 are the centroids of rings C1–C6, C1–C6 and C7–C12, respectively.

C—H···*Cg*	C—H	H···*Cg*	C···*Cg*	C—H···*Cg*
C10—H10···*Cg*1^{i}	0.95	3.372	4.2732 (17)	159
C20—H20A···*Cg*2^{ii}	0.99	2.798	3.6177 (16)	141
C16—H16A···*Cg*3^{ii}	0.99	2.809	3.7090 (14)	151

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

The dihedral angle between each phenothiazine unit and the central benzene ring is 87.23 (5)°, close to the reported value of approximately 90° for a related compound (Deng *et al.*, 2022; Sugamata *et al.*, 2025). These results indicate that the relative orientation of the phenothiazine units with respect to the central benzene ring is essentially unchanged, whereas their internal conformations differ considerably. The octyloxy substituents adopt extended conformations, with their alkyl chains extending approximately parallel to the plane of the central benzene ring and perpendicular to the phenothiazine units.

3. Supramolecular features

The crystal packing is characterized by slipped π–π stacking interactions between adjacent phenothiazine units (Fig. 2). The plane-to-centroid separation and centroid–centroid distance are 3.6026 (4) and 4.3892 (6) Å, respectively, corresponding to a lateral slippage of 2.507 Å. These values indicate

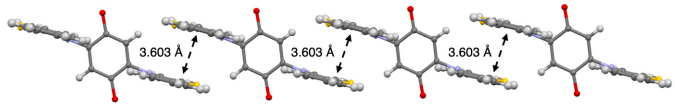


Figure 2
A view of the face-to-face π-stacking geometrical arrangement in compound **1**.

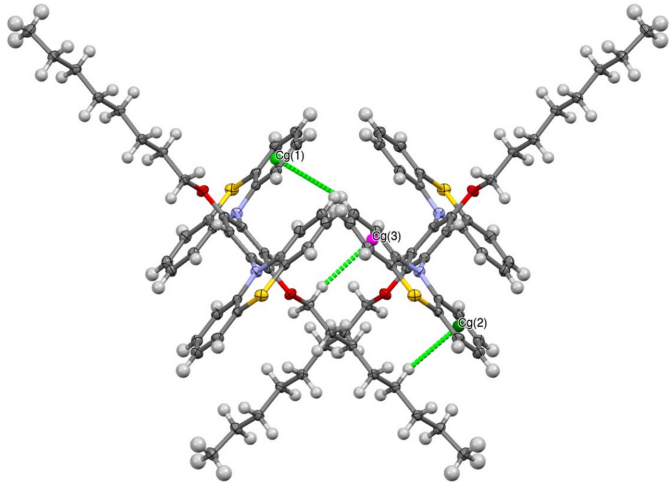


Figure 3
A view of the weak C—H···π interactions in compound **1**. Details are given in Table 1.

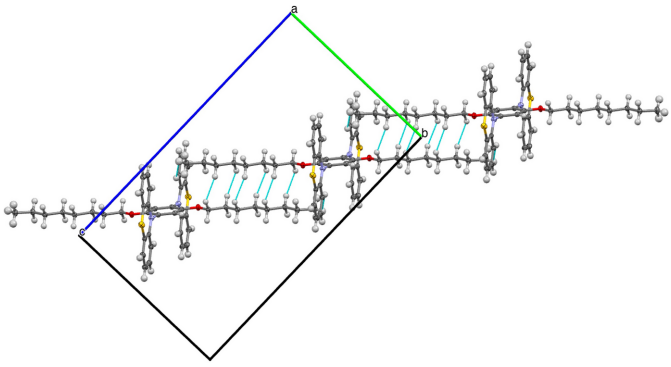


Figure 4
A view of the weak van der Waals interactions of the alkyl chains in compound **1**.

a significantly offset, non-cofacial stacking arrangement. In addition, weak C—H···π interactions between neighboring molecules provide further intermolecular contacts (Table 1 and Fig. 3). Weak van der Waals interactions between the alkyl chains also contribute to the crystal packing (Fig. 4).

4. Optical properties

The UV-vis absorption and photoluminescence spectra of the title compound **1** in $CHCl_3$ solution are shown in Fig. 5. The absorption spectrum exhibits a sharp absorption band at around 250nm and a weak broad absorption band in the range of 300–350nm. Based on studies of related compounds, the higher-energy absorption band is assigned to the n–π^* and π–π^* transitions of the phenothiazine unit, whereas the lower-energy band is attributed to charge-transfer (^{1}CT) transitions from the phenothiazine to the benzene units (Skhirtladze *et al.*, 2022). The photoluminescence spectrum exhibits a maximum at 450 nm, which is assigned to emission from the ^{1}CT state.

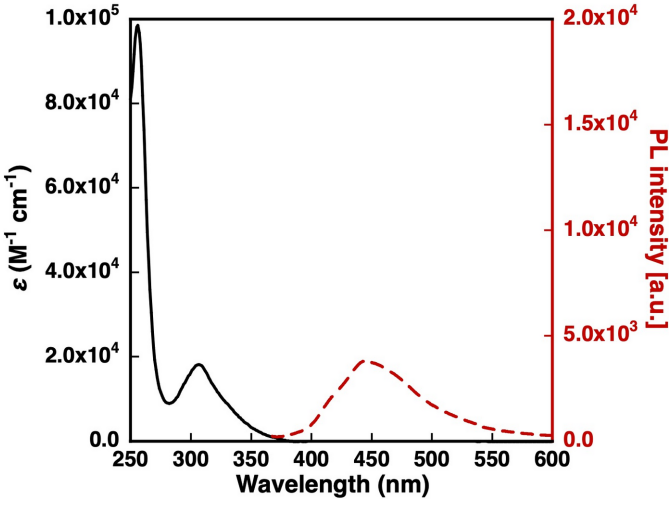


Figure 5
UV–vis absorption and photoluminescence spectra of the title compound **1** in $CHCl_3$ solution. The photoluminescence spectrum was measured at an excitation wavelength of 350 nm.

The HOMO level of the title compound **1** was determined from its oxidation potential obtained by cyclic voltammetry (CV) in $CHCl_3$, using the vacuum energy level of ferrocene/ferrocenium$^+$ (−4.8 eV) as a reference (Fig. 6). The LUMO level was estimated from the absorption onset wavelength (λ_{edge}). Accordingly, the HOMO and LUMO energy levels of the title compound 1 were estimated to be −5.13 and −1.72 eV, respectively. These results indicate that the title compound **1** exhibits donor character. The reported HOMO level of unsubstituted phenothiazine is −5.04 eV, suggesting that the HOMO of the title compound is primarily derived from the phenothiazine units (Zhou *et al.*, 2022). In comparison, the HOMO level of 2,6-di(phenothiazinyl)naphthalene (DPTZN), a naphthalene derivative bearing two phenothiazine units, has been reported to be −5.35 eV (Wang *et al.*, 2019). The relatively higher HOMO level of the title compound may be attributed to the electron-donating effect of the introduced alkoxy groups.

5. Database survey

A search of the Cambridge Structural Database (CSD, accessed *via* the CCDC Access Structures web interface on 25 October 2026; Groom *et al.*, 2016) was performed to identify structurally related compounds. Three structurally related phenothiazine derivatives were identified (Skhirtladze *et al.*, 2022, refcode RECBAG; Sun *et al.*, 2004, refcode AVISED; Wang *et al.*, 2021, refcode AVISED01). These compounds feature either an unsubstituted central benzene ring or one substituted with trifluoromethyl groups. Comparison with these compounds revealed that the corresponding bond lengths are similar to those of the title compound. However, the title compound exhibits a markedly reduced butterfly angle, indicating that the characteristic butterfly conformation of the phenothiazine moieties is suppressed, resulting in a more planar structure.

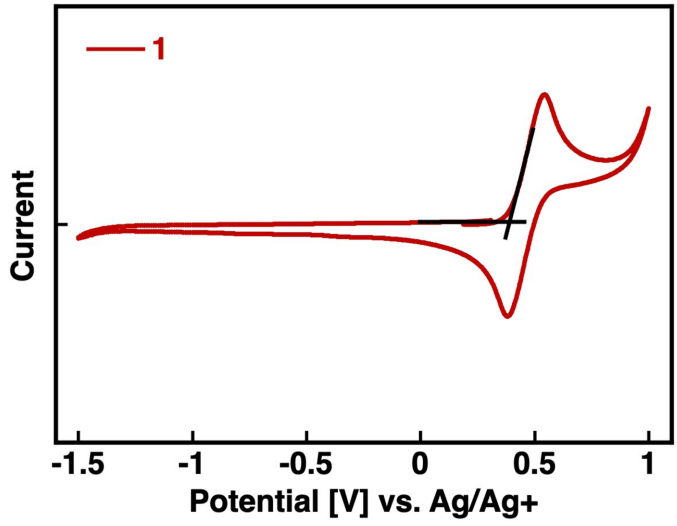


Figure 6
Cyclic voltammogram of the title compound **1** in $CHCl_3$ solution.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{46}H_{52}N_2O_2S_2$
M_r	729.07
Crystal system, space group	Monoclinic, *I*2/*a*
Temperature (K)	100
a, *b*, *c* (Å)	10.1447 (2), 14.8550 (2), 25.4074 (3)
β (°)	94.298 (1)
V (Å^3)	3818.12 (10)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.58
Crystal size (mm)	0.10 × 0.05 × 0.05
Data collection	
Diffractometer	Rigaku Saturn724+ (2x2 bin mode)
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2018)
T_{min}, T_{max}	0.696, 1.000
No. of measured, independent and observed [$I \geq 2u(I)$] reflections	10698, 3748, 3258
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.621
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.106, 1.02
No. of reflections	3748
No. of parameters	236
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.26, −0.44

Computer programs: *CrystalClear-SM Expert* (Rigaku, 2011), *SHELXT2018/2* (Sheldrick, 2015), *OLEX2.refine* (Bourhis *et al.*, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

6. Synthesis and crystallization

1,4-Dibromo-2,5-bis(octyloxy)benzene

2,5-Dibromo-1,4-hydroquinone (500 mg, 1.87 mmol) and K_2CO_3 (516 mg, 2 eq) were added to a round-bottom flask and was purged with N_2 for 15min. DMF (10 mL) was added and stirred at room temperature for 1 h. After then, 1-iodooctane (2.5 eq) was added to the reaction mixture and stirred at 353 K for 24 h. The reaction mixture was added to H_2O (30mL), extracted with hexane, dehydrated with $MgSO_4$ and concentrated using an evaporator. The crude product was purified by silica gel column eluted with hexane to give clear oil. Yield: 76%

10,10′-[2,5-Bis(octyloxy)-1,4-phenylene]bis(10*H*-phenothiazine) (1)

1,4-Dibromo-2,5-bis(octyloxy)benzene (800 mg, 1.62 mmol), phenothiazine (712 mg, 2.5 eq) and *t*-BuONa (936.9 mg, 6 eq) were added to round-bottom flask and flowed N_2 for 15min. Toluene (60 mL), $Pd_2(dba)_3$ (74.4 mg, 5 mol%; dba = dibenzylideneacetone) and *t*-Bu_3P (40 µL, 20mol%) were added to the reaction mixture and stirred at 383 K for 3 h. To the solution, 1*M* HCl aq (10mL) was added to quench the reaction, extracted with $CHCl_3$, dehydrated with $MgSO_4$ and concentrated using an evaporator. The crude product was purified by silica gel column eluted $CHCl_3$:hexane to give white solid. Yield: 55%

Single crystals suitable for single-crystal X-ray diffraction analysis were obtained by slow evaporation of a hexane solution of the sample. ^{1}H NMR ($CDCl_3$, 400MHz); 7.166 (2H, *s*), 7.040 (4H, *dd*, *J* = 7.6, 1.6Hz), 6.990–6.800 (8H, *m*), 6.250 (4H, *d*, *J* = 6.8Hz), 3.896 (4H, *t*, *J* = 6.0Hz), 1.519 (4H, *m*), 1.300–1.050 (20H, *m*), 0.866 (6H, *t*, *J* = 7.2Hz).

HR-MS(ESI); *m*/*z* calculated for $C_{46}H_{53}N_2O_2S_2$ ($[M + H]^+$) 729.3543, found: 729.3543.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All hydrogen atoms were placed in geometrically calculated positions and refined using a riding model, with their isotropic displacement parameters set to $1.2U_{eq}$(C) for aromatic and methylene hydrogen atoms and $1.5U_{eq}$(C) for methyl hydrogen atoms.

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supporting information

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Synthesis and structure of 10,10′-[2,5-bis(octyloxy)-1,4-phenylene]bis(10*H*-phenothiazine)

Naohiro Takahashi, Shota Fujii and Takashi Okubo

Computing details

10,10′-[2,5-bis(octyloxy)-1,4-phenylene]bis(10*H*-phenothiazine)

Crystal data

$C_{46}H_{52}N_2O_2S_2$
M_r = 729.07
Monoclinic, *I*2/*a*
a = 10.1447 (2) Å
b = 14.8550 (2) Å
c = 25.4074 (3) Å
β = 94.298 (1)°
V = 3818.12 (10) Å^3
Z = 4
F(000) = 1566.969
D_x = 1.268 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 6309 reflections
θ = 3.4–72.9°
μ = 1.58 mm^{-1}
T = 100 K
Needle, clear whiteish white
0.1 × 0.05 × 0.05 mm

Data collection

Rigaku Saturn724+ (2x2 bin mode) diffractometer
Detector resolution: 28.5714 pixels mm^{-1}
profile data from *ω*–scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2018)
T_{min} = 0.696, T_{max} = 1.000
10698 measured reflections
3748 independent reflections
3258 reflections with $I \geq 2u(I)$
R_{int} = 0.032
θ_{max} = 73.2°, θ_{min} = 3.5°
h = −12→7
k = −17→18
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.106
S = 1.02
3748 reflections
236 parameters
0 restraints
43 constraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 3.1081P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.0002
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.22306 (4)	0.70950 (3)	0.335034 (14)	0.02457 (13)
O1	0.73399 (10)	0.62994 (7)	0.33279 (4)	0.0216 (2)

N1	0.50981 (12)	0.72322 (8)	0.29710 (5)	0.0188 (3)
C1	0.48179 (15)	0.77538 (9)	0.34108 (5)	0.0195 (3)
C6	0.35691 (15)	0.77482 (9)	0.36139 (6)	0.0208 (3)
C15	0.74617 (14)	0.68848 (9)	0.29216 (5)	0.0180 (3)
C14	0.63410 (14)	0.73722 (9)	0.27446 (5)	0.0180 (3)
C13	0.63781 (14)	0.79774 (9)	0.23294 (5)	0.0190 (3)
H13	0.56024 (14)	0.83021 (9)	0.22147 (5)	0.0227 (4)*
C12	0.42534 (14)	0.65813 (9)	0.27274 (5)	0.0182 (3)
C7	0.29476 (14)	0.64581 (9)	0.28619 (6)	0.0198 (3)
C17	0.81546 (14)	0.51917 (10)	0.39509 (5)	0.0207 (3)
H17a	0.78550 (14)	0.55643 (10)	0.42421 (5)	0.0248 (4)*
H17b	0.74175 (14)	0.47899 (10)	0.38264 (5)	0.0248 (4)*
C2	0.57891 (15)	0.83075 (10)	0.36541 (6)	0.0233 (3)
H2	0.66474 (15)	0.83086 (10)	0.35280 (6)	0.0279 (4)*
C11	0.46961 (15)	0.60476 (10)	0.23256 (6)	0.0227 (3)
H11	0.55848 (15)	0.61074 (10)	0.22366 (6)	0.0273 (4)*
C16	0.85028 (14)	0.57965 (9)	0.35037 (5)	0.0199 (3)
H16a	0.88047 (14)	0.54309 (9)	0.32100 (5)	0.0239 (4)*
H16b	0.92244 (14)	0.62123 (9)	0.36263 (5)	0.0239 (4)*
C18	0.93389 (14)	0.46237 (9)	0.41557 (5)	0.0206 (3)
H18a	0.96209 (14)	0.42418 (9)	0.38652 (5)	0.0247 (4)*
H18b	1.00831 (14)	0.50281 (9)	0.42680 (5)	0.0247 (4)*
C19	0.90346 (14)	0.40244 (10)	0.46181 (5)	0.0210 (3)
H19a	0.87639 (14)	0.44094 (10)	0.49092 (5)	0.0252 (4)*
H19b	0.82778 (14)	0.36303 (10)	0.45063 (5)	0.0252 (4)*
C20	1.01912 (15)	0.34381 (10)	0.48253 (6)	0.0215 (3)
H20a	1.04808 (15)	0.30643 (10)	0.45327 (6)	0.0258 (4)*
H20b	1.09397 (15)	0.38310 (10)	0.49490 (6)	0.0258 (4)*
C21	0.98508 (15)	0.28233 (10)	0.52768 (6)	0.0222 (3)
H21a	0.95696 (15)	0.31998 (10)	0.55698 (6)	0.0266 (4)*
H21b	0.90925 (15)	0.24389 (10)	0.51534 (6)	0.0266 (4)*
C5	0.33249 (16)	0.82978 (11)	0.40398 (6)	0.0268 (3)
H5	0.24772 (16)	0.82876 (11)	0.41752 (6)	0.0321 (4)*
C10	0.38817 (16)	0.54342 (10)	0.20527 (6)	0.0258 (3)
H10	0.42088 (16)	0.50862 (10)	0.17771 (6)	0.0310 (4)*
C9	0.25898 (16)	0.53266 (10)	0.21808 (6)	0.0271 (3)
H9	0.20193 (16)	0.49135 (10)	0.19909 (6)	0.0326 (4)*
C3	0.55349 (17)	0.88582 (10)	0.40764 (6)	0.0274 (3)
H3	0.62129 (17)	0.92347 (10)	0.42326 (6)	0.0329 (4)*
C22	1.09900 (15)	0.22191 (10)	0.54874 (6)	0.0246 (3)
H22a	1.13305 (15)	0.18837 (10)	0.51894 (6)	0.0295 (4)*
H22b	1.17163 (15)	0.26005 (10)	0.56451 (6)	0.0295 (4)*
C8	0.21405 (15)	0.58291 (10)	0.25894 (6)	0.0249 (3)
H8	0.12627 (15)	0.57431 (10)	0.26861 (6)	0.0299 (4)*
C4	0.42958 (17)	0.88595 (11)	0.42701 (6)	0.0299 (4)
H4	0.41131 (17)	0.92395 (11)	0.45564 (6)	0.0359 (4)*
C23	1.05843 (17)	0.15506 (11)	0.59000 (6)	0.0296 (4)
H23a	0.9863 (8)	0.1172 (5)	0.57469 (16)	0.0444 (5)*

H23b	1.1342 (4)	0.1171 (6)	0.6015 (4)	0.0444 (5)*
H23c	1.0286 (11)	0.18787 (11)	0.6204 (2)	0.0444 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0170 (2)	0.0318 (2)	0.0255 (2)	0.00172 (14)	0.00607 (14)	−0.00095 (14)
O1	0.0188 (5)	0.0242 (5)	0.0220 (5)	0.0029 (4)	0.0039 (4)	0.0070 (4)
N1	0.0136 (6)	0.0226 (6)	0.0208 (6)	−0.0007 (5)	0.0059 (5)	−0.0011 (5)
C1	0.0236 (8)	0.0178 (7)	0.0176 (7)	0.0030 (5)	0.0036 (6)	0.0037 (5)
C6	0.0208 (7)	0.0205 (7)	0.0214 (7)	0.0044 (6)	0.0044 (6)	0.0044 (5)
C15	0.0175 (7)	0.0195 (7)	0.0171 (6)	−0.0004 (5)	0.0020 (5)	0.0005 (5)
C14	0.0152 (7)	0.0201 (7)	0.0190 (7)	−0.0015 (5)	0.0044 (5)	−0.0014 (5)
C13	0.0171 (7)	0.0192 (7)	0.0205 (7)	0.0015 (5)	0.0012 (5)	−0.0000 (5)
C12	0.0169 (7)	0.0180 (6)	0.0196 (7)	0.0009 (5)	0.0017 (5)	0.0047 (5)
C7	0.0178 (7)	0.0207 (7)	0.0213 (7)	0.0021 (5)	0.0031 (5)	0.0056 (5)
C17	0.0209 (7)	0.0223 (7)	0.0191 (7)	−0.0003 (6)	0.0034 (6)	0.0010 (5)
C2	0.0247 (8)	0.0229 (7)	0.0227 (7)	−0.0012 (6)	0.0050 (6)	0.0021 (6)
C11	0.0208 (7)	0.0219 (7)	0.0262 (7)	0.0006 (6)	0.0069 (6)	0.0010 (6)
C16	0.0179 (7)	0.0214 (7)	0.0204 (7)	0.0015 (5)	0.0015 (5)	0.0018 (5)
C18	0.0212 (7)	0.0215 (7)	0.0192 (7)	0.0003 (6)	0.0018 (5)	0.0007 (5)
C19	0.0217 (7)	0.0225 (7)	0.0189 (7)	0.0001 (6)	0.0022 (5)	0.0008 (5)
C20	0.0225 (8)	0.0225 (7)	0.0195 (7)	0.0003 (6)	0.0021 (6)	0.0014 (5)
C21	0.0232 (8)	0.0239 (7)	0.0196 (7)	0.0011 (6)	0.0030 (6)	0.0010 (6)
C5	0.0288 (8)	0.0281 (8)	0.0247 (7)	0.0049 (6)	0.0107 (6)	0.0020 (6)
C10	0.0281 (8)	0.0226 (7)	0.0274 (8)	−0.0017 (6)	0.0065 (6)	−0.0026 (6)
C9	0.0264 (8)	0.0248 (7)	0.0300 (8)	−0.0066 (6)	0.0010 (6)	−0.0008 (6)
C3	0.0337 (9)	0.0237 (8)	0.0252 (7)	−0.0033 (6)	0.0049 (6)	−0.0017 (6)
C22	0.0230 (8)	0.0256 (7)	0.0251 (7)	0.0019 (6)	0.0020 (6)	0.0041 (6)
C8	0.0184 (7)	0.0268 (8)	0.0297 (8)	−0.0017 (6)	0.0036 (6)	0.0046 (6)
C4	0.0394 (10)	0.0256 (8)	0.0258 (8)	0.0024 (7)	0.0102 (7)	−0.0029 (6)
C23	0.0289 (9)	0.0285 (8)	0.0315 (8)	0.0035 (7)	0.0031 (7)	0.0096 (6)

Geometric parameters (Å, º)

S1—C6	1.7599 (16)	C18—H18b	0.9900
S1—C7	1.7607 (15)	C18—C19	1.5240 (19)
O1—C15	1.3624 (16)	C19—H19a	0.9900
O1—C16	1.4389 (17)	C19—H19b	0.9900
N1—C1	1.4062 (18)	C19—C20	1.523 (2)
N1—C14	1.4396 (17)	C20—H20a	0.9900
N1—C12	1.4046 (18)	C20—H20b	0.9900
C1—C6	1.403 (2)	C20—C21	1.5260 (19)
C1—C2	1.392 (2)	C21—H21a	0.9900
C6—C5	1.393 (2)	C21—H21b	0.9900
C15—C14	1.394 (2)	C21—C22	1.528 (2)
C15—C13^{i}	1.395 (2)	C5—H5	0.9500
C14—C13	1.3886 (19)	C5—C4	1.386 (2)

C13—H13	0.9500	C10—H10	0.9500
C12—C7	1.4046 (19)	C10—C9	1.383 (2)
C12—C11	1.3932 (19)	C9—H9	0.9500
C7—C8	1.392 (2)	C9—C8	1.383 (2)
C17—H17a	0.9900	C3—H3	0.9500
C17—H17b	0.9900	C3—C4	1.384 (2)
C17—C16	1.5108 (19)	C22—H22a	0.9900
C17—C18	1.527 (2)	C22—H22b	0.9900
C2—H2	0.9500	C22—C23	1.523 (2)
C2—C3	1.389 (2)	C8—H8	0.9500
C11—H11	0.9500	C4—H4	0.9500
C11—C10	1.381 (2)	C23—H23a	0.9800
C16—H16a	0.9900	C23—H23b	0.9800
C16—H16b	0.9900	C23—H23c	0.9800
C18—H18a	0.9900		

C7—S1—C6	102.52 (7)	C19—C18—H18b	109.05 (8)
C16—O1—C15	116.61 (10)	H19a—C19—C18	108.77 (8)
C14—N1—C1	118.23 (12)	H19b—C19—C18	108.77 (8)
C12—N1—C1	125.20 (12)	H19b—C19—H19a	107.7
C12—N1—C14	116.56 (11)	C20—C19—C18	113.90 (12)
C6—C1—N1	122.05 (13)	C20—C19—H19a	108.77 (7)
C2—C1—N1	119.99 (13)	C20—C19—H19b	108.77 (8)
C2—C1—C6	117.95 (13)	H20a—C20—C19	108.99 (7)
C1—C6—S1	123.74 (11)	H20b—C20—C19	108.99 (8)
C5—C6—S1	116.22 (11)	H20b—C20—H20a	107.8
C5—C6—C1	120.02 (14)	C21—C20—C19	112.96 (12)
C14—C15—O1	117.26 (12)	C21—C20—H20a	108.99 (8)
C13^{i}—C15—O1	124.58 (13)	C21—C20—H20b	108.99 (8)
C13^{i}—C15—C14	118.16 (13)	H21a—C21—C20	108.75 (8)
C15—C14—N1	120.91 (12)	H21b—C21—C20	108.75 (8)
C13—C14—N1	118.13 (13)	H21b—C21—H21a	107.6
C13—C14—C15	120.90 (13)	C22—C21—C20	114.02 (12)
C14—C13—C15^{i}	120.93 (13)	C22—C21—H21a	108.75 (8)
H13—C13—C15^{i}	119.53 (8)	C22—C21—H21b	108.75 (8)
H13—C13—C14	119.53 (8)	H5—C5—C6	119.38 (9)
C7—C12—N1	122.54 (12)	C4—C5—C6	121.24 (14)
C11—C12—N1	119.67 (12)	C4—C5—H5	119.38 (9)
C11—C12—C7	117.76 (13)	H10—C10—C11	120.00 (9)
C12—C7—S1	123.26 (11)	C9—C10—C11	119.99 (14)
C8—C7—S1	116.91 (11)	C9—C10—H10	120.00 (9)
C8—C7—C12	119.79 (13)	H9—C9—C10	120.48 (9)
H17b—C17—H17a	108.0	C8—C9—C10	119.04 (14)
C16—C17—H17a	109.38 (8)	C8—C9—H9	120.48 (9)
C16—C17—H17b	109.38 (8)	H3—C3—C2	119.94 (9)
C18—C17—H17a	109.38 (7)	C4—C3—C2	120.12 (15)
C18—C17—H17b	109.38 (8)	C4—C3—H3	119.94 (9)
C18—C17—C16	111.26 (12)	H22a—C22—C21	109.02 (8)

H2—C2—C1	119.17 (8)	H22b—C22—C21	109.02 (8)
C3—C2—C1	121.66 (14)	H22b—C22—H22a	107.8
C3—C2—H2	119.17 (9)	C23—C22—C21	112.82 (13)
H11—C11—C12	119.01 (8)	C23—C22—H22a	109.02 (9)
C10—C11—C12	121.98 (14)	C23—C22—H22b	109.02 (9)
C10—C11—H11	119.01 (9)	C9—C8—C7	121.39 (14)
C17—C16—O1	108.05 (11)	H8—C8—C7	119.31 (8)
H16a—C16—O1	110.09 (7)	H8—C8—C9	119.31 (9)
H16a—C16—C17	110.09 (8)	C3—C4—C5	118.99 (14)
H16b—C16—O1	110.09 (7)	H4—C4—C5	120.50 (9)
H16b—C16—C17	110.09 (8)	H4—C4—C3	120.50 (9)
H16b—C16—H16a	108.4	H23a—C23—C22	109.5
H18a—C18—C17	109.05 (8)	H23b—C23—C22	109.5
H18b—C18—C17	109.05 (8)	H23b—C23—H23a	109.5
H18b—C18—H18a	107.8	H23c—C23—C22	109.5
C19—C18—C17	112.70 (12)	H23c—C23—H23a	109.5
C19—C18—H18a	109.05 (8)	H23c—C23—H23b	109.5

S1—C6—C1—N1	0.39 (14)	C15—O1—C16—C17	−179.81 (12)
S1—C6—C1—C2	179.50 (12)	C15—C14—N1—C12	−90.81 (14)
S1—C6—C5—C4	−178.25 (11)	C15—C14—C13—C15^{i}	−0.09 (13)
S1—C7—C12—N1	−0.46 (14)	C14—N1—C1—C2	−7.58 (14)
S1—C7—C12—C11	−178.62 (11)	C14—N1—C12—C7	−171.47 (12)
S1—C7—C8—C9	176.78 (11)	C14—N1—C12—C11	6.65 (14)
O1—C15—C14—N1	−2.33 (14)	C14—C15—O1—C16	179.58 (12)
O1—C15—C14—C13	−179.46 (12)	C14—C15—C13^{i}—C14^{i}	−0.09 (13)
O1—C15—C13^{i}—C14^{i}	179.43 (14)	C14—C13—C15^{i}—O1^{i}	−179.43 (13)
O1—C16—C17—C18	179.27 (11)	C14—C13—C15^{i}—C14^{i}	0.09 (13)
N1—C1—C6—C5	−177.95 (13)	C13^{i}—C15—O1—C16	0.06 (17)
N1—C1—C2—C3	177.50 (13)	C13^{i}—C15—C14—C13	0.09 (13)
N1—C14—C15—C13^{i}	177.22 (13)	C13—C14—N1—C12	86.40 (14)
N1—C14—C13—C15^{i}	−177.30 (12)	C12—N1—C1—C2	172.93 (14)
N1—C12—C7—C8	177.10 (13)	C12—C7—C8—C9	−0.94 (16)
N1—C12—C11—C10	−176.21 (13)	C12—C11—C10—C9	−0.94 (17)
C1—N1—C14—C15	89.66 (13)	C7—S1—C6—C5	−176.38 (10)
C1—N1—C14—C13	−93.13 (13)	C7—C12—C11—C10	2.00 (16)
C1—N1—C12—C7	8.03 (16)	C7—C8—C9—C10	2.02 (17)
C1—N1—C12—C11	−173.85 (14)	C17—C18—C19—C20	179.06 (12)
C1—C6—S1—C7	5.22 (13)	C2—C1—C6—C5	1.16 (16)
C1—C6—C5—C4	0.21 (16)	C2—C3—C4—C5	0.68 (18)
C1—C2—C3—C4	0.73 (17)	C11—C12—C7—C8	−1.05 (15)
C6—S1—C7—C12	−5.18 (9)	C11—C10—C9—C8	−1.09 (18)
C6—S1—C7—C8	177.19 (10)	C16—C17—C18—C19	178.34 (12)
C6—C1—N1—C14	171.51 (13)	C18—C19—C20—C21	−178.24 (12)
C6—C1—N1—C12	−7.98 (16)	C19—C20—C21—C22	179.27 (12)

C6—C1—C2—C3	−1.63 (16)	C20—C21—C22—C23	−174.43 (13)
C6—C5—C4—C3	−1.14 (18)		

Symmetry code: (i) −*x*+3/2, −*y*+3/2, −*z*+1/2.