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4,4′,6,6′-Tetrabromo-2,2′-[dithiobis(*o*-phenylenenitrilomethylidyne)]diphenol

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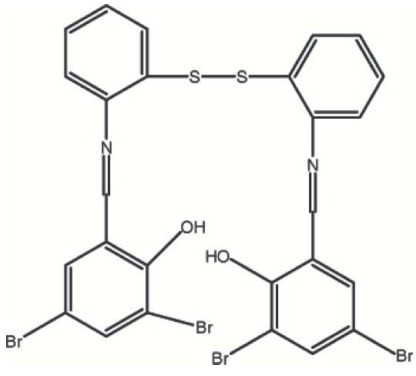
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.048; wR factor = 0.103; data-to-parameter ratio = 14.5.

The title Schiff base, $C_{26}H_{16}Br_4N_2O_2S_2$, was synthesized from 3,5-dibromosalicylaldehyde and 2-aminobenzenethiol. C—H···Br hydrogen bonds link the molecules into a one-dimensional chain which resembles a staircase. The chains are further joined to form a three-dimensional supramolecular network *via* C—H···Br hydrogen bonds and S···Br interactions.

Related literature

For a related structure, see: Elmali *et al.* (1995). For related literature, see: Ghosh & Bharadwaj (2004); Ghosh *et al.* (2005); Lv *et al.* (2006); Raghuraman *et al.* (2003); Rahaman *et al.* (2005); Ravoof *et al.* (2007); Taylor & Kennard (1984); Zhong *et al.* (2006).



Experimental

Crystal data

$C_{26}H_{16}Br_4N_2O_2S_2$
M_r = 772.17
Triclinic, $P\overline{1}$
a = 10.4361 (17) Å
b = 11.4199 (18) Å
c = 12.938 (2) Å
α = 89.721 (3)°
β = 71.536 (2)°
γ = 68.211 (2)°
V = 1346.9 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 6.16 mm^{-1}
T = 298 (2) K
0.28 × 0.16 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.277, T_{max} = 0.578
(expected range = 0.259–0.540)
7083 measured reflections
4705 independent reflections
2583 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.103
S = 1.00
4705 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···Br3^{i}	0.93	3.06	3.942 (7)	158
C1—H1A···Br4^{ii}	0.93	3.01	3.753 (6)	138

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2337).

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supplementary materials

Acta Cryst. (2007). E**63**, o3854 [**doi:10.1107/S1600536807037932**]

4,4',6,6'-Tetrabromo-2,2'-[dithiobis(*o*-phenylenenitrilomethylidyne)]diphenol

L.-X. Jin, Z. Liu, J.-H. Xia and G.-Z. Li

Comment

Schiff bases, the organic ligands, have recently been focused by the coordination chemists as versatile spacers because of their preparative accessibilities, structural varieties and varied denticities (Rahaman *et al.*, 2005). The potential biological activity of compounds containing sulfur and nitrogen may be better than other compounds, such as antitumor, antibacterial and *et al.* (Zhong *et al.*, 2006; Ravoof *et al.*, 2007; Lv *et al.*, 2006), and applies of Schiff base in analysis are very comprehensive today. So we report herein the ligand 3,5-dibromosalicylaldehyde (2-aminobenzenethiol), (I).

One molecule is composed by two Schiff bases which are boned by S1—S2 (Elmali *et al.*, 1995). Two Schiff bases are not in one face, and distances between O, N, S are not far away, so it is conferred that two metal atoms can be coordinated at least (Fig.1). As shown in Fig. 2 and Fig. 3, weak C—H···Br hydrogen bonds and S···Br are also found in this ligand. The C—H···Br hydrogen bonds line the molecules like a chain (Fig. 2). The S···Br weak interaction connected each adjacent ligand to form a two-dimensional network structure (Fig. 3). Both supramolecular role contribute to the stability of the structure (Taylor *et al.*, 1984).

This new Schiff base (I) is a new analysis reagent, put forward the spectrophotometric determination of copper^{II}. The new reagent gives yellow coloured water solution with copper^{II} at room temperature. The complex shows an absorbance maximum at 400 nm. and a higher absorption peak if more copper^{II} was added. So an analysis method can be established.

Experimental

The schiff base was prepared as follows: a solution of 3,5-dibromosalicyaldehyde in ethanol was put in a flask. To this solution, 2-aminobenzenethiol in ethanol was added slowly. After stirring at 323 K for 1 h, the title compound (I) was obtained as Red–brown crystalline solid by slow evaporation of ethanol from the reaction mixture at room temperature.

Refinement

All H atoms were positioned geometrically and refined as riding on their carrier C and O atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) and O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

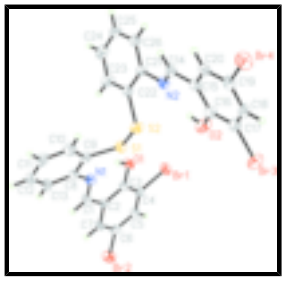

Fig. 1. The molecular structure of the ligand (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

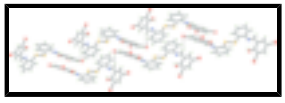

Fig. 2. one-dimensional chain structure of the ligand (I).

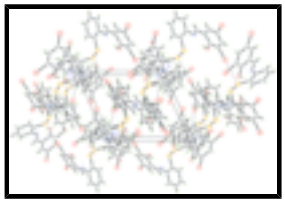

Fig. 3. two-dimensional layer structure of the ligand (I).

4,4',6,6'-Tetrabromo-2,2'-[dithiobis(*o*-phenylenenitrilomethylidyne)]diphenol

Crystal data

$C_{26}H_{16}Br_4N_2O_2S_2$	V = 1346.9 (4) Å^3
M_r = 772.17	Z = 2
Triclinic, $P\overline{1}$	F_{000} = 748
Hall symbol: -P 1	D_x = 1.904 Mg m^{-3}
a = 10.4361 (17) Å	Mo $K\alpha$ radiation λ = 0.71073 Å
b = 11.4199 (18) Å	μ = 6.16 mm^{-1}
c = 12.938 (2) Å	T = 298 (2) K
α = 89.721 (3)º	Block, red
β = 71.536 (2)º	0.28 × 0.16 × 0.10 mm
γ = 68.211 (2)º	

Data collection

Bruker SMART CCD area-detector diffractometer	4705 independent reflections
Radiation source: fine-focus sealed tube	2583 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→12
T_{min} = 0.277, T_{max} = 0.578	k = −12→13
7083 measured reflections	l = −12→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.103$	$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
4705 reflections	$\Delta\rho_{max} = 0.67$ e Å^{-3}
325 parameters	$\Delta\rho_{min} = -0.52$ 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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.93027 (8)	0.39861 (7)	0.41754 (6)	0.0631 (3)
Br2	1.44706 (8)	−0.03777 (8)	0.21997 (6)	0.0723 (3)
Br3	0.86654 (8)	0.71957 (8)	1.26383 (6)	0.0698 (3)
Br4	0.43115 (9)	0.78697 (8)	1.67614 (6)	0.0690 (3)
N1	0.9772 (5)	0.0487 (5)	0.7093 (4)	0.0394 (13)
N2	0.4884 (5)	0.5127 (5)	1.2167 (4)	0.0421 (13)
O1	0.8957 (4)	0.2397 (4)	0.6008 (3)	0.0470 (11)
H1	0.8877	0.1962	0.6512	0.071*
O2	0.6965 (5)	0.5945 (5)	1.1942 (4)	0.0650 (14)
H2	0.6494	0.5604	1.1752	0.098*
S1	0.79827 (19)	0.24089 (17)	0.88492 (13)	0.0501 (5)
S2	0.70339 (18)	0.33660 (18)	1.03865 (14)	0.0532 (5)
C1	1.0880 (7)	−0.0061 (6)	0.6243 (5)	0.0430 (17)
H1A	1.1525	−0.0880	0.6251	0.052*
C2	1.1179 (6)	0.0547 (6)	0.5251 (5)	0.0374 (16)
C3	1.0214 (7)	0.1775 (6)	0.5193 (5)	0.0382 (16)
C4	1.0596 (7)	0.2332 (6)	0.4252 (5)	0.0422 (16)
C5	1.1858 (7)	0.1714 (6)	0.3370 (5)	0.0446 (17)

H5	1.2081	0.2108	0.2745	0.054*
C6	1.2785 (7)	0.0504 (7)	0.3425 (5)	0.0480 (18)
C7	1.2461 (7)	−0.0082 (6)	0.4356 (5)	0.0423 (16)
H7	1.3097	−0.0896	0.4388	0.051*
C8	0.9465 (6)	−0.0068 (6)	0.8074 (5)	0.0369 (15)
C9	0.8537 (7)	0.0765 (6)	0.9017 (5)	0.0420 (17)
C10	0.8122 (7)	0.0326 (7)	1.0005 (5)	0.0555 (19)
H10	0.7491	0.0892	1.0635	0.067*
C11	0.8654 (8)	−0.0968 (8)	1.0051 (7)	0.064 (2)
H11	0.8363	−0.1277	1.0714	0.077*
C12	0.9606 (8)	−0.1799 (7)	0.9129 (7)	0.059 (2)
H12	0.9987	−0.2666	0.9176	0.071*
C13	1.0006 (7)	−0.1362 (7)	0.8129 (6)	0.0528 (19)
H13	1.0632	−0.1930	0.7500	0.063*
C14	0.4397 (7)	0.5530 (6)	1.3193 (5)	0.0420 (16)
H14	0.3578	0.5407	1.3646	0.050*
C15	0.5082 (7)	0.6176 (6)	1.3676 (5)	0.0397 (16)
C16	0.6351 (7)	0.6344 (6)	1.3020 (5)	0.0448 (17)
C17	0.6972 (7)	0.6964 (6)	1.3508 (6)	0.0496 (18)
C18	0.6378 (7)	0.7390 (6)	1.4610 (6)	0.0485 (18)
H18	0.6819	0.7789	1.4926	0.058*
C19	0.5134 (7)	0.7235 (6)	1.5254 (5)	0.0452 (17)
C20	0.4499 (7)	0.6628 (6)	1.4787 (5)	0.0407 (16)
H20	0.3663	0.6517	1.5223	0.049*
C21	0.4218 (7)	0.4508 (6)	1.1691 (5)	0.0355 (15)
C22	0.5164 (6)	0.3641 (6)	1.0753 (5)	0.0379 (16)
C23	0.4613 (7)	0.3024 (7)	1.0211 (5)	0.0533 (19)
H23	0.5238	0.2431	0.9596	0.064*
C24	0.3122 (8)	0.3284 (7)	1.0579 (6)	0.060 (2)
H24	0.2752	0.2869	1.0205	0.072*
C25	0.2190 (7)	0.4150 (7)	1.1490 (6)	0.0525 (19)
H25	0.1190	0.4325	1.1727	0.063*
C26	0.2731 (7)	0.4755 (6)	1.2052 (5)	0.0462 (17)
H26	0.2100	0.5332	1.2676	0.055*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0645 (5)	0.0435 (5)	0.0624 (5)	−0.0110 (4)	−0.0094 (4)	0.0119 (4)
Br2	0.0602 (5)	0.0741 (6)	0.0529 (5)	−0.0136 (4)	0.0046 (4)	−0.0175 (4)
Br3	0.0690 (6)	0.0919 (7)	0.0651 (5)	−0.0507 (5)	−0.0212 (5)	0.0118 (5)
Br4	0.0817 (6)	0.0751 (6)	0.0438 (5)	−0.0226 (5)	−0.0222 (4)	−0.0088 (4)
N1	0.045 (3)	0.039 (3)	0.029 (3)	−0.016 (3)	−0.006 (3)	−0.008 (3)
N2	0.047 (3)	0.040 (3)	0.036 (3)	−0.015 (3)	−0.012 (3)	−0.004 (3)
O1	0.045 (3)	0.039 (3)	0.037 (3)	−0.004 (2)	−0.003 (2)	0.005 (2)
O2	0.067 (3)	0.098 (4)	0.036 (3)	−0.049 (3)	−0.005 (3)	−0.008 (3)
S1	0.0536 (12)	0.0460 (12)	0.0376 (10)	−0.0185 (9)	0.0003 (9)	−0.0019 (8)
S2	0.0445 (11)	0.0661 (13)	0.0423 (11)	−0.0238 (10)	−0.0031 (9)	−0.0131 (9)

C1	0.048 (4)	0.034 (4)	0.044 (4)	−0.008 (3)	−0.021 (4)	0.004 (3)
C2	0.035 (4)	0.038 (4)	0.034 (4)	−0.010 (3)	−0.009 (3)	−0.007 (3)
C3	0.035 (4)	0.043 (4)	0.035 (4)	−0.013 (3)	−0.012 (3)	−0.004 (3)
C4	0.043 (4)	0.043 (4)	0.034 (4)	−0.014 (3)	−0.008 (3)	0.004 (3)
C5	0.047 (4)	0.046 (5)	0.038 (4)	−0.018 (4)	−0.012 (4)	0.009 (3)
C6	0.043 (4)	0.060 (5)	0.039 (4)	−0.024 (4)	−0.007 (4)	−0.009 (4)
C7	0.039 (4)	0.032 (4)	0.047 (4)	−0.005 (3)	−0.013 (4)	−0.007 (3)
C8	0.041 (4)	0.045 (5)	0.031 (4)	−0.022 (3)	−0.016 (3)	0.005 (3)
C9	0.045 (4)	0.051 (5)	0.039 (4)	−0.024 (4)	−0.019 (4)	0.014 (4)
C10	0.060 (5)	0.058 (5)	0.043 (5)	−0.024 (4)	−0.009 (4)	0.007 (4)
C11	0.064 (5)	0.081 (7)	0.066 (6)	−0.045 (5)	−0.027 (5)	0.042 (5)
C12	0.053 (5)	0.050 (5)	0.082 (6)	−0.023 (4)	−0.031 (5)	0.019 (5)
C13	0.059 (5)	0.045 (5)	0.059 (5)	−0.022 (4)	−0.023 (4)	0.005 (4)
C14	0.043 (4)	0.042 (4)	0.041 (4)	−0.019 (3)	−0.011 (4)	−0.002 (3)
C15	0.044 (4)	0.044 (4)	0.030 (4)	−0.018 (3)	−0.010 (3)	0.003 (3)
C16	0.051 (5)	0.048 (5)	0.035 (4)	−0.022 (4)	−0.011 (4)	0.004 (3)
C17	0.051 (5)	0.047 (5)	0.057 (5)	−0.022 (4)	−0.023 (4)	0.010 (4)
C18	0.060 (5)	0.045 (5)	0.056 (5)	−0.025 (4)	−0.034 (4)	0.004 (4)
C19	0.056 (5)	0.043 (4)	0.041 (4)	−0.018 (4)	−0.023 (4)	0.001 (3)
C20	0.042 (4)	0.036 (4)	0.037 (4)	−0.010 (3)	−0.011 (3)	0.001 (3)
C21	0.037 (4)	0.041 (4)	0.028 (4)	−0.015 (3)	−0.010 (3)	−0.003 (3)
C22	0.042 (4)	0.042 (4)	0.030 (4)	−0.020 (3)	−0.006 (3)	0.001 (3)
C23	0.052 (5)	0.070 (5)	0.035 (4)	−0.033 (4)	0.000 (4)	−0.013 (4)
C24	0.075 (6)	0.077 (6)	0.051 (5)	−0.047 (5)	−0.030 (5)	0.004 (4)
C25	0.043 (4)	0.062 (5)	0.051 (5)	−0.027 (4)	−0.006 (4)	0.006 (4)
C26	0.044 (4)	0.049 (5)	0.040 (4)	−0.019 (4)	−0.005 (4)	0.002 (3)

Geometric parameters (Å, °)

Br1—C4	1.895 (6)	C10—C11	1.381 (9)
Br2—C6	1.886 (6)	C10—H10	0.9300
Br3—C17	1.882 (6)	C11—C12	1.368 (10)
Br4—C19	1.886 (6)	C11—H11	0.9300
N1—C1	1.265 (7)	C12—C13	1.379 (9)
N1—C8	1.414 (7)	C12—H12	0.9300
N2—C14	1.279 (7)	C13—H13	0.9300
N2—C21	1.415 (7)	C14—C15	1.458 (8)
O1—C3	1.333 (6)	C14—H14	0.9300
O1—H1	0.8200	C15—C20	1.386 (8)
O2—C16	1.337 (7)	C15—C16	1.409 (8)
O2—H2	0.8200	C16—C17	1.388 (9)
S1—C9	1.781 (6)	C17—C18	1.370 (8)
S1—S2	2.025 (2)	C18—C19	1.376 (8)
S2—C22	1.758 (6)	C18—H18	0.9300
C1—C2	1.458 (8)	C19—C20	1.373 (8)
C1—H1A	0.9300	C20—H20	0.9300
C2—C7	1.400 (8)	C21—C26	1.387 (8)
C2—C3	1.408 (8)	C21—C22	1.398 (8)
C3—C4	1.386 (8)	C22—C23	1.372 (8)

C4—C5	1.378 (8)	C23—C24	1.386 (8)
C5—C6	1.378 (8)	C23—H23	0.9300
C5—H5	0.9300	C24—C25	1.373 (9)
C6—C7	1.385 (8)	C24—H24	0.9300
C7—H7	0.9300	C25—C26	1.371 (9)
C8—C9	1.382 (8)	C25—H25	0.9300
C8—C13	1.383 (8)	C26—H26	0.9300
C9—C10	1.370 (8)		
C1—N1—C8	123.7 (5)	C12—C13—C8	119.2 (7)
C14—N2—C21	122.5 (5)	C12—C13—H13	120.4
C3—O1—H1	109.5	C8—C13—H13	120.4
C16—O2—H2	109.5	N2—C14—C15	122.3 (6)
C9—S1—S2	105.9 (2)	N2—C14—H14	118.9
C22—S2—S1	105.3 (2)	C15—C14—H14	118.9
N1—C1—C2	122.3 (6)	C20—C15—C16	119.2 (6)
N1—C1—H1A	118.9	C20—C15—C14	120.5 (6)
C2—C1—H1A	118.9	C16—C15—C14	120.3 (6)
C7—C2—C3	119.6 (6)	O2—C16—C17	118.8 (6)
C7—C2—C1	119.6 (6)	O2—C16—C15	122.4 (6)
C3—C2—C1	120.8 (6)	C17—C16—C15	118.7 (6)
O1—C3—C4	119.9 (6)	C18—C17—C16	120.7 (6)
O1—C3—C2	121.9 (5)	C18—C17—Br3	120.2 (5)
C4—C3—C2	118.2 (6)	C16—C17—Br3	119.1 (5)
C5—C4—C3	122.3 (6)	C17—C18—C19	120.8 (6)
C5—C4—Br1	119.5 (5)	C17—C18—H18	119.6
C3—C4—Br1	118.2 (5)	C19—C18—H18	119.6
C6—C5—C4	119.2 (6)	C20—C19—C18	119.4 (6)
C6—C5—H5	120.4	C20—C19—Br4	120.7 (5)
C4—C5—H5	120.4	C18—C19—Br4	119.9 (5)
C5—C6—C7	120.5 (6)	C19—C20—C15	121.1 (6)
C5—C6—Br2	119.6 (5)	C19—C20—H20	119.4
C7—C6—Br2	119.9 (5)	C15—C20—H20	119.4
C6—C7—C2	120.2 (6)	C26—C21—C22	119.9 (6)
C6—C7—H7	119.9	C26—C21—N2	124.9 (6)
C2—C7—H7	119.9	C22—C21—N2	115.1 (5)
C9—C8—C13	119.7 (6)	C23—C22—C21	119.5 (6)
C9—C8—N1	116.1 (6)	C23—C22—S2	124.2 (5)
C13—C8—N1	124.2 (6)	C21—C22—S2	116.3 (5)
C10—C9—C8	120.9 (6)	C22—C23—C24	120.0 (6)
C10—C9—S1	123.7 (6)	C22—C23—H23	120.0
C8—C9—S1	115.4 (5)	C24—C23—H23	120.0
C9—C10—C11	119.0 (7)	C25—C24—C23	120.6 (7)
C9—C10—H10	120.5	C25—C24—H24	119.7
C11—C10—H10	120.5	C23—C24—H24	119.7
C12—C11—C10	120.6 (7)	C26—C25—C24	120.0 (6)
C12—C11—H11	119.7	C26—C25—H25	120.0
C10—C11—H11	119.7	C24—C25—H25	120.0
C11—C12—C13	120.5 (7)	C25—C26—C21	120.1 (6)
C11—C12—H12	119.7	C25—C26—H26	120.0

C13—C12—H12	119.7	C21—C26—H26	120.0
C9—S1—S2—C22	−90.3 (3)	C21—N2—C14—C15	−179.5 (5)
C8—N1—C1—C2	−178.9 (5)	N2—C14—C15—C20	178.4 (6)
N1—C1—C2—C7	176.7 (6)	N2—C14—C15—C16	−1.9 (9)
N1—C1—C2—C3	−1.4 (9)	C20—C15—C16—O2	−179.3 (6)
C7—C2—C3—O1	177.8 (5)	C14—C15—C16—O2	0.9 (9)
C1—C2—C3—O1	−4.0 (9)	C20—C15—C16—C17	−0.3 (9)
C7—C2—C3—C4	−1.6 (9)	C14—C15—C16—C17	180.0 (6)
C1—C2—C3—C4	176.6 (5)	O2—C16—C17—C18	179.9 (6)
O1—C3—C4—C5	−177.7 (5)	C15—C16—C17—C18	0.9 (10)
C2—C3—C4—C5	1.7 (9)	O2—C16—C17—Br3	−0.8 (8)
O1—C3—C4—Br1	0.8 (8)	C15—C16—C17—Br3	−179.9 (4)
C2—C3—C4—Br1	−179.8 (4)	C16—C17—C18—C19	−1.2 (10)
C3—C4—C5—C6	−0.7 (9)	Br3—C17—C18—C19	179.5 (5)
Br1—C4—C5—C6	−179.2 (5)	C17—C18—C19—C20	1.0 (10)
C4—C5—C6—C7	−0.5 (9)	C17—C18—C19—Br4	−178.4 (5)
C4—C5—C6—Br2	177.3 (5)	C18—C19—C20—C15	−0.5 (9)
C5—C6—C7—C2	0.5 (9)	Br4—C19—C20—C15	179.0 (5)
Br2—C6—C7—C2	−177.3 (4)	C16—C15—C20—C19	0.1 (9)
C3—C2—C7—C6	0.6 (9)	C14—C15—C20—C19	179.9 (6)
C1—C2—C7—C6	−177.6 (6)	C14—N2—C21—C26	31.8 (9)
C1—N1—C8—C9	159.1 (6)	C14—N2—C21—C22	−151.8 (6)
C1—N1—C8—C13	−22.2 (9)	C26—C21—C22—C23	−1.2 (9)
C13—C8—C9—C10	−1.3 (9)	N2—C21—C22—C23	−177.8 (5)
N1—C8—C9—C10	177.5 (5)	C26—C21—C22—S2	−178.4 (4)
C13—C8—C9—S1	177.3 (4)	N2—C21—C22—S2	5.0 (7)
N1—C8—C9—S1	−4.0 (7)	S1—S2—C22—C23	15.4 (6)
S2—S1—C9—C10	10.7 (6)	S1—S2—C22—C21	−167.6 (4)
S2—S1—C9—C8	−167.8 (4)	C21—C22—C23—C24	1.5 (10)
C8—C9—C10—C11	0.5 (10)	S2—C22—C23—C24	178.4 (5)
S1—C9—C10—C11	−177.8 (5)	C22—C23—C24—C25	−0.5 (10)
C9—C10—C11—C12	1.3 (10)	C23—C24—C25—C26	−0.7 (10)
C10—C11—C12—C13	−2.5 (11)	C24—C25—C26—C21	0.9 (10)
C11—C12—C13—C8	1.8 (10)	C22—C21—C26—C25	0.0 (9)
C9—C8—C13—C12	0.1 (9)	N2—C21—C26—C25	176.3 (6)
N1—C8—C13—C12	−178.5 (6)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···Br3^{i}	0.93	3.06	3.942 (7)	158
C1—H1A···Br4^{ii}	0.93	3.01	3.753 (6)	138

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

Fig. 1

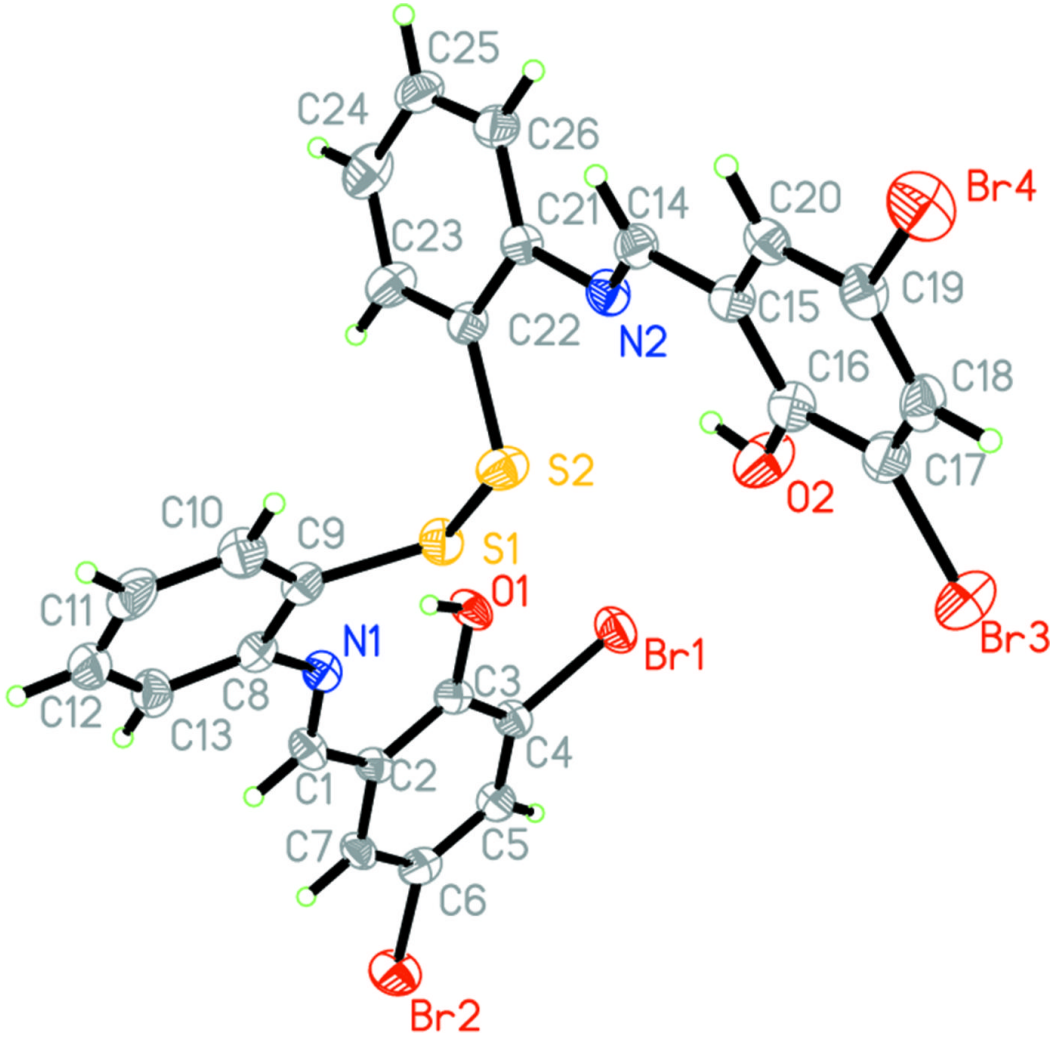
C25
C24
C26
C21
C14
C20
Br4
C23
C19
C15
C22
N2
C16
C18
S2
O2
C17
C10
C9
S1
O1
C11
N1
Br1
Br3
C8
C3
C12
C13
C4
C1
C2
C7
C5
C6
Br2

Fig. 2

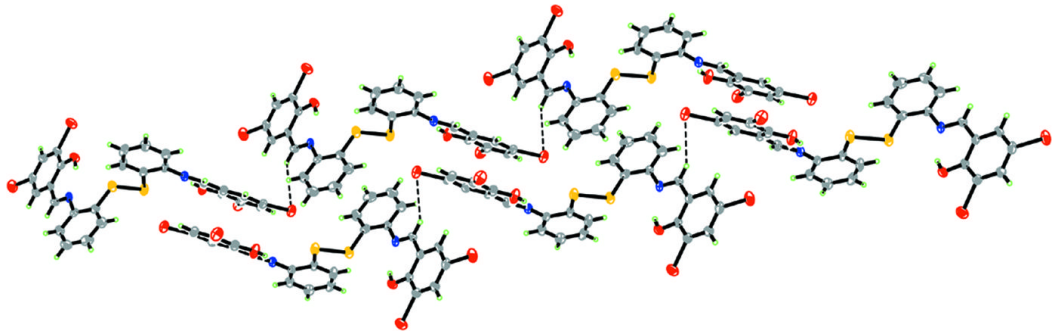

Fig. 3