organic compounds

4,4′-Methylenedianilinium 2,2′-dithio-dibenzoate

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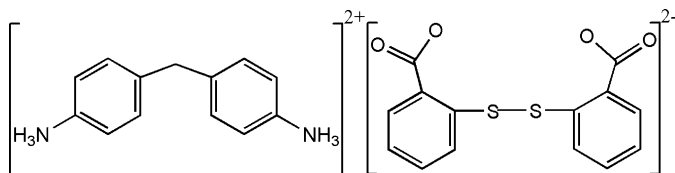
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In the title molecular salt, $C_{13}H_{16}N_2^{2+} \cdot C_{14}H_8O_4S_2^{2-}$, the component species are linked into an infinite three-dimensional framework by N—H···O hydrogen bonds. The dihedral angles between the aromatic rings in the cation and the anion are 72.8 (3) and 79.5 (3)°, respectively.

Related literature

For related literature, see: Tan *et al.* (2006).

Experimental

Crystal data

$C_{13}H_{16}N_2^{2+} \cdot C_{14}H_8O_4S_2^{2-}$
$M_r = 504.62$
Tetragonal, $P\bar{4}2_1c$
$a = 24.4620\ (15)$ Å
$c = 8.8325\ (10)$ Å
$V = 5285.3\ (8)$ Å^3

$Z = 8$
Mo $K\alpha$ radiation
$\mu = 0.24$ mm^{-1}
$T = 292\ (2)$ K
$0.40 \times 0.11 \times 0.09$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min} = 0.912$, $T_{max} = 0.979$

28154 measured reflections
5162 independent reflections
4092 reflections with $I > 2\sigma(I)$
$R_{int} = 0.081$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.086$
$wR(F^2) = 0.174$
$S = 1.17$
5162 reflections
316 parameters
H-atom parameters constrained

$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Absolute structure: Flack (1983), 2266 Friedel pairs
Flack parameter: 0.14 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2	0.89	1.85	2.722 (6)	166
N1—H1B···O3^i	0.89	1.84	2.724 (5)	174
N1—H1C···O1^{ii}	0.89	1.89	2.753 (5)	163
N2—H2A···O4^{iii}	0.89	1.95	2.804 (5)	161
N2—H2B···O1^{iv}	0.89	2.03	2.834 (5)	150
N2—H2B···O2^{iv}	0.89	2.50	3.231 (5)	140
N2—H2C···O4	0.89	1.87	2.734 (5)	164

Symmetry codes: (i) $-y+1, x, -z+1$; (ii) $y-\frac{1}{2}, x+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-y+\frac{3}{2}, -x+\frac{3}{2}, z-\frac{1}{2}$; (iv) $y, -x+1, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2607).

References

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supplementary materials

4,4'-Methylenedianilinium 2,2'-dithiodibenzoate

Q. Han

Comment

Crystallization for salt-like molecular crystals through hydrogen bonding interaction is a powerful tool for designing absolute asymmetric syntheses and new functional solid materials (Tan *et al.*, 2006). Herein we report a molecular salt containing 4,4'-methylene bis(benzenammonium) ($C_{13}H_{16}N_2^{2+}$) dications and 2,2'-dithiobis(benzoate) ($C_{14}H_8O_4S_2^{2-}$) dianions, (I). The asymmetric unit of (I) contains one dication and one dianion (Fig. 1). The dihedral angles between the aromatic rings of the dication and the dianion are 72.8 (3)° and 79.5 (3)°, respectively. The C2—S1—S2—C9 torsion angle is −86.2 (2)°.

The six hydrogen atoms bound to the two N atoms act as hydrogen bonds donors and interact with carboxylate O atoms as acceptors (Table 1). These components ions are finally organized into an infinite three-dimensional framework (Fig. 2). Large voids propagating in [001] are apparent in the structure, but the final difference map yielded no features that could be modelled as atoms occupying these spaces.

Experimental

A 5-ml ethanol solution of 4,4'-methylene bis(benzenamine) (0.25 mmol, 0.050 g) was added to an aqueous solution (25 ml) of 2,2'-dithiobis(benzoic acid) (0.25 mmol, 0.075 g). The mixture was stirred for 10 minutes at 373 K. The solution was filtered, and the filtrate was kept at room temperature. After a week, pink rods of (I) were obtained.

Refinement

All the H atoms were placed in calculated positions with C—H = 0.93Å and N—H = 0.89 Å, respectively, and were refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $U_{iso} = 1.5U_{eq}(N)$.
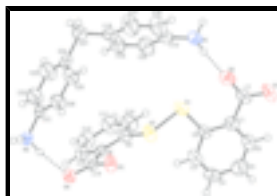
Figures

Fig. 1. The molecular structure unit of (I). Displacement ellipsoids for the non-H atoms are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.
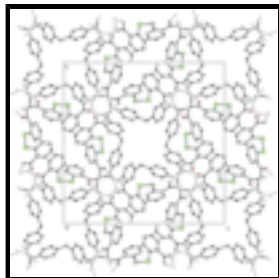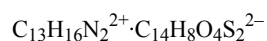
Fig. 2. The infinite three-dimensional framework in (I) viewed down the c axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity.

4,4'-Methylenedianilinium 2,2'-dithiodibenzoate

Crystal data

$C_{13}H_{16}N_2^{2+}{\cdot}C_{14}H_8O_4S_2^{2-}$	$Z = 8$
$M_r = 504.62$	$F_{000} = 2112$
Tetragonal, $P\bar{4}2_1c$	$D_x = 1.268$ Mg m^{-3}
Hall symbol: P -4 2n	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 24.4620\,(15)$ Å	Cell parameters from 5675 reflections
$b = 24.4620\,(15)$ Å	$\theta = 2.1{-}28.2°$
$c = 8.8325\,(10)$ Å	$\mu = 0.24$ mm^{-1}
$\alpha = 90°$	$T = 292\,(2)$ K
$\beta = 90°$	Bar, pink
$\gamma = 90°$	$0.40 \times 0.11 \times 0.09$ mm
$V = 5285.3\,(8)$ Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	5162 independent reflections
Radiation source: fine-focus sealed tube	4092 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.081$
$T = 292(2)$ K	$\theta_{max} = 26.0°$
ω scans	$\theta_{min} = 1.7°$
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -30 \rightarrow 30$
$T_{min} = 0.912$, $T_{max} = 0.979$	$k = -30 \rightarrow 13$
28154 measured reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.086$	$w = 1/[\sigma^2(F_o^2) + (0.0782P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.174$	$(\Delta/\sigma)_{max} < 0.001$

$S = 1.17$	$\Delta\rho_{max} = 0.43$ e Å^{-3}
5162 reflections	$\Delta\rho_{min} = -0.23$ e Å^{-3}
316 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 2266 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.14 (14)

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 $F^2 > 2\text{sigma}(F^2)$ 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	$U_{iso}*/U_{eq}$
N1	0.33512 (16)	0.73080 (15)	0.4507 (5)	0.0451 (10)
H1A	0.3521	0.7343	0.5393	0.054*
H1B	0.3066	0.7085	0.4612	0.054*
H1C	0.3236	0.7635	0.4197	0.054*
N2	0.70205 (14)	0.71797 (14)	0.0445 (4)	0.0363 (9)
H2A	0.7105	0.7347	−0.0418	0.044*
H2B	0.7251	0.6904	0.0599	0.044*
H2C	0.7046	0.7416	0.1208	0.044*
C15	0.3726 (2)	0.7084 (2)	0.3410 (6)	0.0444 (13)
C16	0.3866 (3)	0.6543 (2)	0.3499 (9)	0.076 (2)
H16	0.3717	0.6324	0.4254	0.091*
C17	0.4225 (3)	0.6324 (3)	0.2484 (9)	0.082 (2)
H17	0.4328	0.5960	0.2584	0.098*
C18	0.4438 (2)	0.6627 (3)	0.1324 (8)	0.0619 (16)
C19	0.4293 (3)	0.7165 (3)	0.1219 (8)	0.0711 (18)
H19	0.4438	0.7382	0.0454	0.085*
C20	0.3925 (2)	0.7388 (3)	0.2270 (7)	0.0635 (16)
H20	0.3818	0.7751	0.2175	0.076*
C21	0.64643 (17)	0.69709 (18)	0.0351 (5)	0.0327 (10)
C22	0.6135 (2)	0.7135 (3)	−0.0764 (7)	0.0618 (16)
H22	0.6263	0.7372	−0.1507	0.074*
C23	0.5596 (3)	0.6947 (3)	−0.0802 (7)	0.079 (2)
H23	0.5365	0.7069	−0.1566	0.095*
C24	0.5400 (2)	0.6590 (3)	0.0250 (7)	0.0577 (15)
C25	0.5752 (2)	0.6430 (2)	0.1395 (8)	0.0605 (16)
H25	0.5631	0.6191	0.2140	0.073*

C26	0.6282 (2)	0.6623 (2)	0.1440 (6)	0.0518 (14)
H26	0.6515	0.6514	0.2215	0.062*
C27	0.4827 (2)	0.6370 (3)	0.0164 (8)	0.077 (2)
H27A	0.4837	0.5978	0.0322	0.092*
H27B	0.4684	0.6436	−0.0845	0.092*
S1	0.47191 (5)	0.76473 (6)	0.60874 (17)	0.0493 (4)
S2	0.55352 (5)	0.76056 (6)	0.55829 (16)	0.0490 (4)
O1	0.33785 (14)	0.80258 (17)	0.9168 (5)	0.0677 (11)
O2	0.37348 (15)	0.75345 (17)	0.7332 (5)	0.0619 (10)
O3	0.65762 (13)	0.74742 (15)	0.5071 (4)	0.0495 (9)
O4	0.70770 (12)	0.77377 (13)	0.3123 (4)	0.0449 (8)
C1	0.41755 (18)	0.8370 (2)	0.7978 (5)	0.0385 (11)
C2	0.46407 (18)	0.82736 (19)	0.7109 (6)	0.0382 (11)
C3	0.5034 (2)	0.8683 (2)	0.7033 (6)	0.0518 (14)
H3	0.5348	0.8626	0.6457	0.062*
C4	0.4972 (2)	0.9165 (2)	0.7778 (7)	0.0616 (16)
H4	0.5240	0.9433	0.7701	0.074*
C5	0.4508 (2)	0.9257 (2)	0.8661 (8)	0.0657 (17)
H5	0.4463	0.9586	0.9171	0.079*
C6	0.4125 (2)	0.8862 (2)	0.8766 (7)	0.0532 (14)
H6	0.3821	0.8919	0.9377	0.064*
C7	0.37240 (19)	0.7948 (2)	0.8169 (7)	0.0475 (13)
C8	0.61475 (19)	0.80094 (18)	0.3180 (5)	0.0357 (11)
C9	0.56232 (18)	0.79766 (19)	0.3847 (6)	0.0393 (11)
C10	0.5198 (2)	0.8239 (2)	0.3138 (7)	0.0587 (16)
H10	0.4852	0.8225	0.3569	0.070*
C11	0.5272 (2)	0.8521 (2)	0.1804 (7)	0.0628 (17)
H11	0.4974	0.8684	0.1333	0.075*
C12	0.5776 (2)	0.8564 (2)	0.1169 (7)	0.0558 (15)
H12	0.5826	0.8760	0.0279	0.067*
C13	0.6213 (2)	0.8311 (2)	0.1867 (6)	0.0442 (13)
H13	0.6560	0.8344	0.1444	0.053*
C14	0.66339 (18)	0.77186 (17)	0.3853 (5)	0.0327 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.046 (2)	0.036 (2)	0.054 (3)	−0.0068 (18)	0.002 (2)	0.008 (2)
N2	0.040 (2)	0.034 (2)	0.035 (2)	0.0021 (17)	0.0033 (18)	−0.0010 (17)
C15	0.039 (3)	0.046 (3)	0.049 (3)	−0.008 (2)	−0.002 (2)	−0.004 (3)
C16	0.080 (4)	0.050 (4)	0.098 (5)	0.005 (3)	0.029 (4)	0.018 (4)
C17	0.082 (5)	0.053 (4)	0.110 (6)	0.012 (4)	0.029 (5)	−0.003 (4)
C18	0.035 (3)	0.078 (4)	0.073 (4)	−0.014 (3)	0.002 (3)	−0.027 (4)
C19	0.069 (4)	0.088 (5)	0.056 (4)	−0.013 (3)	0.018 (3)	0.008 (4)
C20	0.065 (4)	0.064 (4)	0.062 (4)	−0.002 (3)	0.005 (3)	0.013 (3)
C21	0.028 (2)	0.035 (2)	0.035 (3)	0.005 (2)	0.004 (2)	−0.008 (2)
C22	0.047 (3)	0.091 (4)	0.047 (3)	−0.011 (3)	−0.005 (3)	0.021 (3)
C23	0.055 (4)	0.133 (6)	0.050 (4)	−0.006 (4)	−0.015 (3)	0.016 (4)

C24	0.048 (3)	0.077 (4)	0.048 (3)	−0.004 (3)	0.014 (3)	−0.027 (3)
C25	0.048 (3)	0.068 (4)	0.066 (4)	−0.015 (3)	0.012 (3)	0.005 (3)
C26	0.044 (3)	0.062 (3)	0.049 (3)	−0.001 (3)	−0.007 (3)	0.009 (3)
C27	0.040 (3)	0.107 (5)	0.083 (5)	−0.016 (3)	0.006 (3)	−0.040 (4)
S1	0.0340 (6)	0.0482 (8)	0.0656 (9)	−0.0046 (6)	0.0065 (6)	0.0004 (7)
S2	0.0371 (6)	0.0574 (8)	0.0524 (8)	0.0102 (6)	0.0075 (6)	0.0128 (7)
O1	0.036 (2)	0.091 (3)	0.077 (3)	−0.005 (2)	0.019 (2)	0.008 (2)
O2	0.055 (2)	0.066 (3)	0.065 (3)	−0.024 (2)	0.005 (2)	−0.002 (2)
O3	0.0407 (19)	0.062 (2)	0.046 (2)	0.0168 (17)	0.0056 (16)	0.0084 (18)
O4	0.0347 (18)	0.059 (2)	0.0410 (19)	0.0012 (16)	0.0013 (16)	−0.0055 (16)
C1	0.031 (3)	0.041 (3)	0.043 (3)	0.006 (2)	−0.009 (2)	0.011 (2)
C2	0.028 (2)	0.045 (3)	0.042 (3)	−0.003 (2)	−0.002 (2)	0.009 (2)
C3	0.034 (3)	0.055 (4)	0.066 (4)	−0.003 (2)	0.007 (3)	0.013 (3)
C4	0.058 (4)	0.043 (3)	0.083 (4)	−0.018 (3)	−0.006 (3)	0.005 (3)
C5	0.069 (4)	0.052 (3)	0.076 (4)	−0.005 (3)	0.005 (4)	−0.006 (3)
C6	0.042 (3)	0.061 (4)	0.057 (3)	0.006 (3)	0.009 (3)	0.006 (3)
C7	0.026 (3)	0.061 (4)	0.055 (3)	−0.005 (3)	−0.002 (3)	0.017 (3)
C8	0.040 (3)	0.031 (2)	0.036 (3)	0.008 (2)	−0.004 (2)	−0.011 (2)
C9	0.037 (3)	0.039 (3)	0.042 (3)	0.004 (2)	0.000 (2)	0.000 (2)
C10	0.039 (3)	0.069 (4)	0.068 (4)	0.006 (3)	−0.006 (3)	0.016 (3)
C11	0.055 (4)	0.066 (4)	0.068 (4)	0.015 (3)	−0.014 (3)	0.019 (3)
C12	0.069 (4)	0.052 (3)	0.046 (3)	0.007 (3)	−0.009 (3)	0.014 (3)
C13	0.052 (3)	0.040 (3)	0.041 (3)	0.000 (2)	0.006 (3)	−0.001 (2)
C14	0.036 (2)	0.031 (2)	0.031 (3)	0.001 (2)	−0.002 (2)	−0.007 (2)

Geometric parameters (Å, °)

N1—C15	1.443 (6)	C27—H27B	0.9700
N1—H1A	0.8900	S1—C2	1.788 (5)
N1—H1B	0.8900	S1—S2	2.0480 (17)
N1—H1C	0.8900	S2—C9	1.795 (5)
N2—C21	1.456 (5)	O1—C7	1.237 (6)
N2—H2A	0.8900	O2—C7	1.254 (7)
N2—H2B	0.8901	O3—C14	1.239 (5)
N2—H2C	0.8899	O4—C14	1.262 (5)
C15—C20	1.343 (7)	C1—C2	1.393 (6)
C15—C16	1.369 (7)	C1—C6	1.396 (7)
C16—C17	1.364 (9)	C1—C7	1.521 (7)
C16—H16	0.9300	C2—C3	1.392 (7)
C17—C18	1.367 (9)	C3—C4	1.357 (7)
C17—H17	0.9300	C3—H3	0.9300
C18—C19	1.366 (9)	C4—C5	1.396 (8)
C18—C27	1.532 (8)	C4—H4	0.9300
C19—C20	1.403 (9)	C5—C6	1.349 (7)
C19—H19	0.9300	C5—H5	0.9300
C20—H20	0.9300	C6—H6	0.9300
C21—C22	1.334 (7)	C8—C13	1.384 (7)
C21—C26	1.360 (7)	C8—C9	1.414 (6)
C22—C23	1.397 (8)	C8—C14	1.508 (6)

C22—H22	0.9300	C9—C10	1.373 (7)
C23—C24	1.362 (9)	C10—C11	1.377 (8)
C23—H23	0.9300	C10—H10	0.9300
C24—C25	1.385 (8)	C11—C12	1.358 (8)
C24—C27	1.504 (8)	C11—H11	0.9300
C25—C26	1.379 (7)	C12—C13	1.380 (7)
C25—H25	0.9300	C12—H12	0.9300
C26—H26	0.9300	C13—H13	0.9300
C27—H27A	0.9700		
C15—N1—H1A	109.2	C24—C27—H27A	108.9
C15—N1—H1B	109.6	C18—C27—H27A	108.9
H1A—N1—H1B	109.5	C24—C27—H27B	108.9
C15—N1—H1C	109.6	C18—C27—H27B	108.9
H1A—N1—H1C	109.5	H27A—C27—H27B	107.7
H1B—N1—H1C	109.5	C2—S1—S2	104.89 (16)
C21—N2—H2A	109.3	C9—S2—S1	106.11 (16)
C21—N2—H2B	109.6	C2—C1—C6	119.5 (5)
H2A—N2—H2B	109.5	C2—C1—C7	122.7 (5)
C21—N2—H2C	109.6	C6—C1—C7	117.7 (5)
H2A—N2—H2C	109.5	C1—C2—C3	118.1 (5)
H2B—N2—H2C	109.5	C1—C2—S1	120.7 (4)
C20—C15—C16	119.2 (5)	C3—C2—S1	121.2 (4)
C20—C15—N1	121.6 (5)	C4—C3—C2	121.6 (5)
C16—C15—N1	119.2 (5)	C4—C3—H3	119.2
C17—C16—C15	120.1 (6)	C2—C3—H3	119.2
C17—C16—H16	119.9	C3—C4—C5	120.1 (5)
C15—C16—H16	119.9	C3—C4—H4	119.9
C16—C17—C18	121.7 (6)	C5—C4—H4	119.9
C16—C17—H17	119.1	C6—C5—C4	119.2 (6)
C18—C17—H17	119.1	C6—C5—H5	120.4
C17—C18—C19	118.2 (6)	C4—C5—H5	120.4
C17—C18—C27	121.1 (6)	C5—C6—C1	121.5 (5)
C19—C18—C27	120.7 (6)	C5—C6—H6	119.3
C18—C19—C20	119.8 (6)	C1—C6—H6	119.3
C18—C19—H19	120.1	O1—C7—O2	124.0 (5)
C20—C19—H19	120.1	O1—C7—C1	118.1 (6)
C15—C20—C19	120.9 (6)	O2—C7—C1	117.8 (5)
C15—C20—H20	119.6	C13—C8—C9	119.0 (4)
C19—C20—H20	119.6	C13—C8—C14	119.4 (5)
C22—C21—C26	120.9 (5)	C9—C8—C14	121.7 (4)
C22—C21—N2	120.0 (5)	C10—C9—C8	118.1 (5)
C26—C21—N2	119.1 (4)	C10—C9—S2	122.3 (4)
C21—C22—C23	119.2 (6)	C8—C9—S2	119.6 (4)
C21—C22—H22	120.4	C9—C10—C11	121.6 (5)
C23—C22—H22	120.4	C9—C10—H10	119.2
C24—C23—C22	121.8 (6)	C11—C10—H10	119.2
C24—C23—H23	119.1	C12—C11—C10	120.7 (5)
C22—C23—H23	119.1	C12—C11—H11	119.6
C23—C24—C25	117.4 (5)	C10—C11—H11	119.6

C23—C24—C27	121.5 (6)	C11—C12—C13	118.9 (5)
C25—C24—C27	121.0 (6)	C11—C12—H12	120.5
C26—C25—C24	120.5 (5)	C13—C12—H12	120.5
C26—C25—H25	119.7	C12—C13—C8	121.6 (5)
C24—C25—H25	119.7	C12—C13—H13	119.2
C21—C26—C25	120.1 (5)	C8—C13—H13	119.2
C21—C26—H26	119.9	O3—C14—O4	124.0 (4)
C25—C26—H26	119.9	O3—C14—C8	118.7 (4)
C24—C27—C18	113.5 (5)	O4—C14—C8	117.3 (4)
C20—C15—C16—C17	3.2 (10)	S2—S1—C2—C3	18.8 (4)
N1—C15—C16—C17	−179.2 (6)	C1—C2—C3—C4	0.0 (8)
C15—C16—C17—C18	−2.6 (12)	S1—C2—C3—C4	178.6 (4)
C16—C17—C18—C19	1.6 (11)	C2—C3—C4—C5	0.6 (9)
C16—C17—C18—C27	−178.1 (6)	C3—C4—C5—C6	0.3 (9)
C17—C18—C19—C20	−1.4 (9)	C4—C5—C6—C1	−1.8 (9)
C27—C18—C19—C20	178.3 (5)	C2—C1—C6—C5	2.5 (8)
C16—C15—C20—C19	−3.0 (9)	C7—C1—C6—C5	179.9 (5)
N1—C15—C20—C19	179.5 (5)	C2—C1—C7—O1	167.0 (5)
C18—C19—C20—C15	2.1 (9)	C6—C1—C7—O1	−10.3 (7)
C26—C21—C22—C23	0.3 (9)	C2—C1—C7—O2	−10.9 (7)
N2—C21—C22—C23	−177.5 (5)	C6—C1—C7—O2	171.8 (5)
C21—C22—C23—C24	−1.6 (11)	C13—C8—C9—C10	1.2 (7)
C22—C23—C24—C25	1.8 (10)	C14—C8—C9—C10	−177.9 (5)
C22—C23—C24—C27	−177.2 (6)	C13—C8—C9—S2	−178.0 (4)
C23—C24—C25—C26	−0.9 (9)	C14—C8—C9—S2	2.8 (6)
C27—C24—C25—C26	178.2 (6)	S1—S2—C9—C10	2.4 (5)
C22—C21—C26—C25	0.6 (8)	S1—S2—C9—C8	−178.4 (3)
N2—C21—C26—C25	178.4 (5)	C8—C9—C10—C11	0.9 (8)
C24—C25—C26—C21	−0.3 (9)	S2—C9—C10—C11	−179.8 (4)
C23—C24—C27—C18	−105.1 (7)	C9—C10—C11—C12	−2.2 (9)
C25—C24—C27—C18	75.9 (8)	C10—C11—C12—C13	1.2 (9)
C17—C18—C27—C24	−112.8 (7)	C11—C12—C13—C8	1.0 (8)
C19—C18—C27—C24	67.5 (8)	C9—C8—C13—C12	−2.2 (7)
C2—S1—S2—C9	−86.2 (2)	C14—C8—C13—C12	177.0 (5)
C6—C1—C2—C3	−1.6 (7)	C13—C8—C14—O3	176.3 (4)
C7—C1—C2—C3	−178.8 (4)	C9—C8—C14—O3	−4.6 (6)
C6—C1—C2—S1	179.9 (4)	C13—C8—C14—O4	−4.2 (6)
C7—C1—C2—S1	2.7 (6)	C9—C8—C14—O4	174.9 (4)
S2—S1—C2—C1	−162.7 (3)		

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1A⋯O2	0.89	1.85	2.722 (6)	166
N1—H1B⋯O3[i]	0.89	1.84	2.724 (5)	174
N1—H1C⋯O1[ii]	0.89	1.89	2.753 (5)	163
N2—H2A⋯O4[iii]	0.89	1.95	2.804 (5)	161
N2—H2B⋯O1[iv]	0.89	2.03	2.834 (5)	150

N2—H2B···O2^{iv}	0.89	2.50	3.231 (5)	140
N2—H2C···O4	0.89	1.87	2.734 (5)	164

Symmetry codes: (i) $-y+1, x, -z+1$; (ii) $y-1/2, x+1/2, z-1/2$; (iii) $-y+3/2, -x+3/2, z-1/2$; (iv) $y, -x+1, -z+1$.
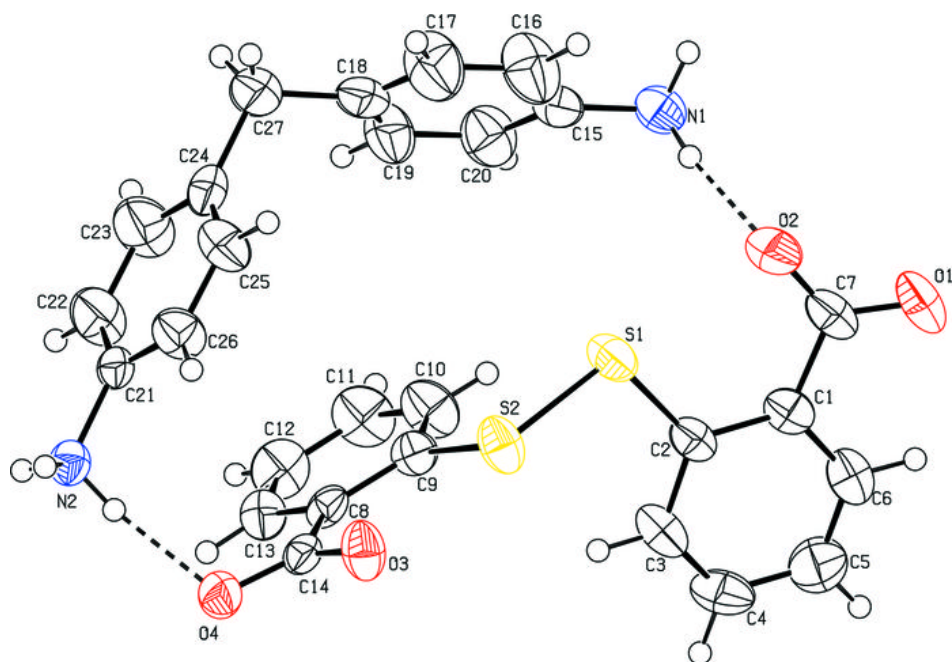
Fig. 1

Fig. 2