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4,4′-Sulfonyldibenzoic acid

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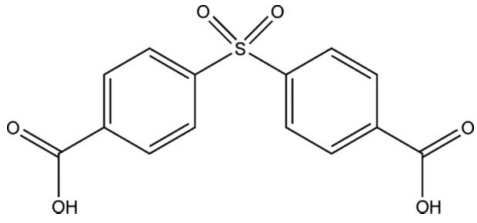
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.104; data-to-parameter ratio = 14.9.

In the title compound, $C_{14}H_8O_6S$, the dihedral angle of the two phthalic fragments is 76.41 (10) Å. The molecule lies on a mirror plane. The C atoms of the benzene rings have bond lengths in the range 1.384 (2)–1.490 (2) Å and bond angles in the range 118.80 (16)–121.64 (15)°. Centrosymmetric rings of hydrogen-bonded carboxyl groups connect molecules into a zigzig chain.

Related literature

For related literature, see: Chen & Lin (2002); Kitagawa & Kitaura (2004); Moulton & Zaworotko (2001); Fujita *et al.* (1994).



Experimental

Crystal data

$C_{14}H_{10}O_6S$
M_r = 306.29
Monoclinic, $P2_1/m$
a = 5.0019 (4) Å
b = 23.3653 (17) Å
c = 5.7871 (5) Å
β = 110.151 (3)°
V = 634.94 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 293 (2) K
0.21 × 0.13 × 0.10 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.943, T_{max} = 0.972
4922 measured reflections
1493 independent reflections
1287 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.104
S = 1.13
1493 reflections
100 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2^{i}	0.90	1.74	2.6390 (19)	172

Symmetry code: (i) $-x, -y, -z+1$.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: KP2097).

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supplementary materials

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4,4'-Sulfonyldibenzoic acid

F.-Y. Lian, D.-Q. Yuan, F.-L. Jiang and M.-C. Hong

Comment

Recently, the design and synthesis of the metal-organic frameworks (MOFs) have led to a large number of coordination polymers (Moulton *et al.*, 2001; Kitagawa *et al.*, 2004; Yaghi *et al.*, 2003). 4,4'-sulfonyldibenzoic acid is a typical V-shaped dicarboxylate ligand, which is important in construction of some novel frameworks (Jin *et al.*, 2006; Chen *et al.*, 2002). Here we report the crystal structure of (I) (Fig. 1). The central atom S_1 has a tetrahedral arrangement, with the S1—O3=1.4353 (17) Å, S1—O4=1.4405 (18) Å. The atoms S1,O3 and O4 are located at the special position on the mirror plane (x,1/4-y,z) and the molecular symmetry is C_m. An intermolecular O1—H1A···O2 hydrogen bond connects molecules into a infinite zig-zag chain (Fig. 2).

Experimental

The title compound (I), was prepared by the hydrothermal reaction of $Mn(OAc)_2{\cdot}4H_2O$(0.050 g, 0.20 mmol), 4,4'-sulfonyldibenzoic acid (0.062 g, 0.20 mmol) and in water (8 ml). The reaction was performed in 23 ml Teflon-lined stainless steel Parr bombs under autogeneous pressure. After heating at 423 K for 3 days and cooling to room temperature at 5 K h^{-1}, green crystals of (I) were obtained.

Refinement

The H atoms were positioned geometrically with C—H = 0.93 Å; they were constrained to ride on their parent atoms with $U_{iso}(H) = 1.2U_{eq}$.

Figures

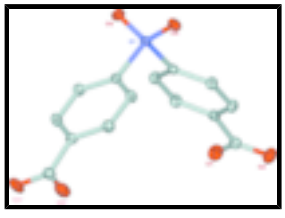

Fig. 1. The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level.

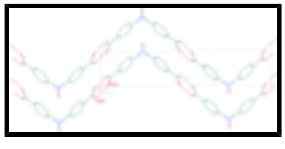

Fig. 2. Crystal packing of (I), showing the hydrogen-bonded (dashed lines) chain. H atoms not involved in the hydrogen bonds have been omitted for clarity.

4,4'-Sulfonyldibenzoic acid

Crystal data

$C_{14}H_{10}O_6S$	$F_{000} = 316$
$M_r = 306.29$	$D_x = 1.602$ Mg m^{-3}
Monoclinic, $P2_1/m$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.0019$ (4) Å	Cell parameters from 1385 reflections
$b = 23.3653$ (17) Å	$\theta = 2.6$–27.5°
$c = 5.7871$ (5) Å	$\mu = 0.28$ mm^{-1}
$\beta = 110.151$ (3)$^\circ$	$T = 293$ (2) K
$V = 634.94$ (9) Å^3	Prism, white
$Z = 2$	0.21 × 0.13 × 0.10 mm

Data collection

Mercury CCD diffractometer	1493 independent reflections
Radiation source: fine-focus sealed tube	1287 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
Detector resolution: 14.6306 pixels mm^{-1}	$\theta_{max} = 27.5^\circ$
$T = 293(2)$ K	$\theta_{min} = 3.5^\circ$
CCD_Profile_fitting scans	$h = -6 \rightarrow 6$
Absorption correction: multi-scan PROGRAM? (Reference?)	$k = -30 \rightarrow 28$
$T_{min} = 0.943$, $T_{max} = 0.972$	$l = -6 \rightarrow 7$
4922 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 0.2393P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.041$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.104$	$\Delta\rho_{max} = 0.27$ e Å^{-3}
$S = 1.13$	$\Delta\rho_{min} = -0.36$ e Å^{-3}
1493 reflections	Extinction correction: none
100 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
S1	1.01179 (12)	0.2500	0.38263 (11)	0.02846 (19)
O1	0.0581 (3)	0.04204 (6)	0.2645 (3)	0.0538 (4)
C1	0.2637 (4)	0.05520 (7)	0.4617 (3)	0.0349 (4)
O2	0.3019 (3)	0.03297 (6)	0.6669 (3)	0.0519 (4)
C2	0.4609 (4)	0.10079 (7)	0.4376 (3)	0.0304 (4)
O3	1.2667 (4)	0.2500	0.5955 (3)	0.0379 (4)
C3	0.6752 (4)	0.12019 (7)	0.6472 (3)	0.0347 (4)
H3	0.7043	0.1027	0.7982	0.042*
O4	1.0291 (4)	0.2500	0.1392 (3)	0.0380 (4)
C4	0.8453 (4)	0.16565 (7)	0.6310 (3)	0.0331 (4)
H4	0.9868	0.1794	0.7709	0.040*
C5	0.8018 (3)	0.19037 (6)	0.4031 (3)	0.0270 (4)
C6	0.5925 (4)	0.17070 (7)	0.1919 (3)	0.0335 (4)
H6	0.5664	0.1876	0.0403	0.040*
C7	0.4233 (4)	0.12549 (8)	0.2107 (3)	0.0353 (4)
H7	0.2832	0.1115	0.0703	0.042*
H1A	−0.0784	0.0181	0.2769	0.042*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0256 (3)	0.0241 (3)	0.0379 (4)	0.000	0.0138 (3)	0.000
O1	0.0453 (8)	0.0515 (9)	0.0588 (10)	−0.0231 (7)	0.0107 (7)	0.0021 (7)
C1	0.0328 (9)	0.0277 (8)	0.0449 (10)	−0.0010 (7)	0.0145 (8)	0.0008 (7)
O2	0.0531 (9)	0.0486 (8)	0.0536 (9)	−0.0156 (7)	0.0179 (7)	0.0098 (7)
C2	0.0296 (9)	0.0238 (8)	0.0394 (10)	0.0003 (6)	0.0138 (8)	−0.0002 (7)
O3	0.0255 (9)	0.0354 (9)	0.0481 (11)	0.000	0.0068 (8)	0.000
C3	0.0388 (10)	0.0313 (9)	0.0344 (9)	−0.0030 (7)	0.0132 (8)	0.0038 (7)
O4	0.0439 (11)	0.0353 (9)	0.0435 (11)	0.000	0.0262 (9)	0.000
C4	0.0329 (9)	0.0314 (8)	0.0319 (9)	−0.0038 (7)	0.0071 (7)	−0.0005 (7)
C5	0.0251 (8)	0.0225 (7)	0.0347 (9)	0.0014 (6)	0.0119 (7)	−0.0004 (6)
C6	0.0356 (10)	0.0324 (9)	0.0317 (9)	−0.0012 (7)	0.0104 (8)	0.0024 (7)

C7	0.0331 (9)	0.0326 (9)	0.0353 (9)	−0.0050 (7)	0.0054 (8)	−0.0020 (7)

Geometric parameters (Å, °)

S1—O3	1.4357 (18)	C2—C3	1.389 (2)
S1—O4	1.4409 (19)	C3—C4	1.384 (2)
S1—C5^{i}	1.7732 (16)	C3—H3	0.9300
S1—C5	1.7732 (16)	C4—C5	1.386 (2)
O1—C1	1.283 (2)	C4—H4	0.9300
O1—H1A	0.9040	C5—C6	1.386 (2)
C1—O2	1.249 (2)	C6—C7	1.381 (2)
C1—C2	1.490 (2)	C6—H6	0.9300
C2—C7	1.386 (2)	C7—H7	0.9300
O3—S1—O4	120.27 (12)	C4—C3—H3	120.0
O3—S1—C5^{i}	108.31 (7)	C2—C3—H3	120.0
O4—S1—C5^{i}	107.57 (7)	C3—C4—C5	119.04 (16)
O3—S1—C5	108.31 (7)	C3—C4—H4	120.5
O4—S1—C5	107.57 (7)	C5—C4—H4	120.5
C5^{i}—S1—C5	103.59 (10)	C6—C5—C4	121.61 (15)
C1—O1—H1A	118.3	C6—C5—S1	119.12 (13)
O2—C1—O1	123.98 (16)	C4—C5—S1	119.24 (13)
O2—C1—C2	119.79 (16)	C7—C6—C5	118.80 (16)
O1—C1—C2	116.22 (16)	C7—C6—H6	120.6
C7—C2—C3	120.21 (16)	C5—C6—H6	120.6
C7—C2—C1	120.51 (16)	C6—C7—C2	120.39 (16)
C3—C2—C1	119.21 (16)	C6—C7—H7	119.8
C4—C3—C2	119.91 (16)	C2—C7—H7	119.8

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O2^{ii}	0.90	1.74	2.6390 (19)	172

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

Fig. 1

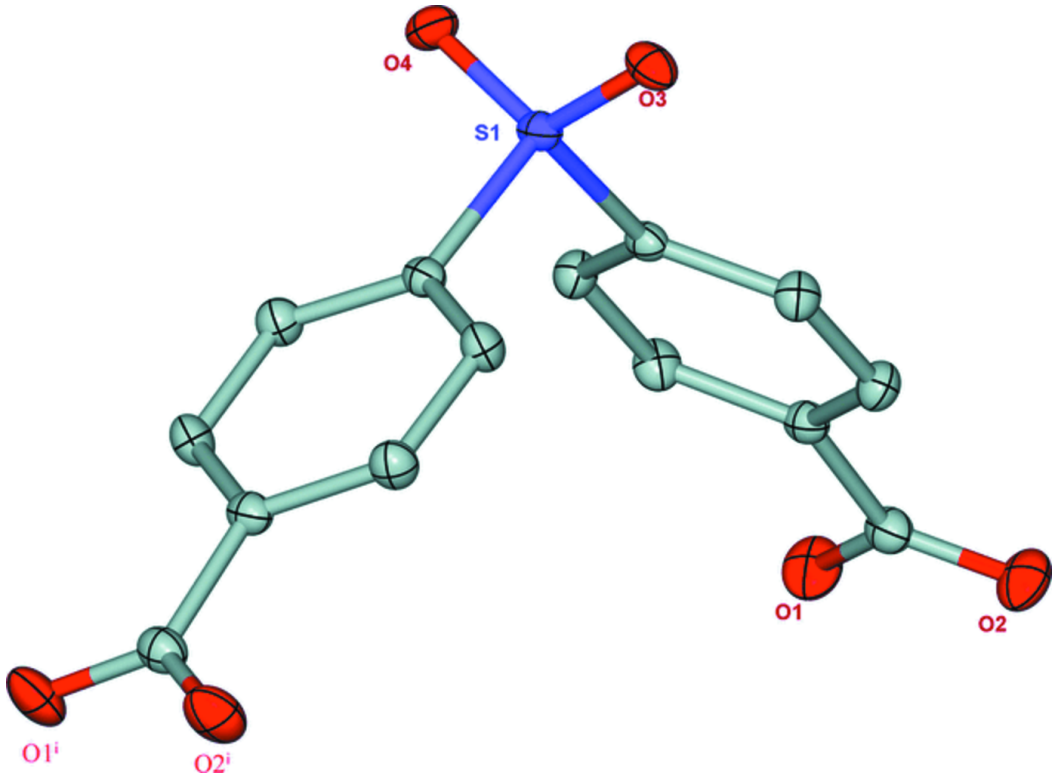

Fig. 2