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2-[(2-Carboxyphenyl)sulfanyl]acetic acid

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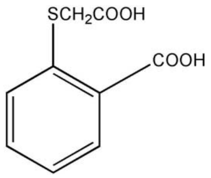
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; R factor = 0.074; wR factor = 0.222; data-to-parameter ratio = 15.9.

The title compound, $C_9H_8O_4S$, affords a zigzig chain in the crystal structure by intermolecular O—H⋯O hydrogen bonds. The molecular geometry suggests that extensive but not uniform π-electron delocalization is present in the benzene ring and extends over the exocyclic C—S and C—C bonds.

Related literature

For background to the coordination chemistry of rigid carboxylate system, see: Sagatys *et al.* (2003); Sokolov *et al.* (2001).



Experimental

Crystal data

$C_9H_8O_4S$
M_r = 212.22
Triclinic, $P\bar{1}$
a = 5.1786 (5) Å
b = 9.2973 (9) Å
c = 10.4776 (11) Å
α = 69.980 (4)°
β = 81.959 (6)°
γ = 79.732 (6)°
V = 464.69 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 296 K
0.33 × 0.24 × 0.15 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.910, $T_{\max}$ = 0.952
6609 measured reflections
2110 independent reflections
1941 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.222
S = 1.19
2110 reflections
133 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$ = 0.65 e Å^{-3}
$\Delta\rho_{\min}$ = −0.34 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O2—H2⋯O1$^{\rm i}$	0.86 (7)	1.92 (5)	2.687 (6)	149 (8)
O3—H3⋯O4$^{\rm ii}$	0.85 (2)	1.80 (5)	2.634 (4)	167 (6)

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

Data collection: *APEX2* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2858).

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supporting information

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S1. Comment

Thioacetatebenzoic acid (I) is an interesting ligand from a structural point of view since it can display a wide range of coordination patterns with metal ions. The ligand (I) belongs to dicarboxylic acids. The characteristic coordination chemistry of the rigid carboxylate system may facilitate the formation of inorganic-organic materials with high thermal stability and form large channels, while the peculiar coordination chemistry of the flexible carboxylate system employed in the self-assembly reaction has versatile coordination behavior and may be favorable for the formation of the helical structure (Sagatys *et al.*, 2003; Sokolov *et al.*, 2001). As shown in Fig.1, the bond lengths within the benzene ring exhibit the expected pattern with C—C bonds (1.368 (8)–1.399 (6) Å) between the single and double bonds. And the bond distance of C1—C7 (1.476 (5) Å) and S1—C6 (1.768 (4) Å) also fall between the double and single bonds. All these interatomic distances suggest that extensive but not uniform π electron delocalization is present in the benzene ring and extends over the exocyclic C—S and C—C bonds. The torsion angle of C6—S1—C8—C9 is -71.7 (4)°. O—H···O hydrogen bonds link independent molecules to form a zigzig chain.

S2. Experimental

To an aqueous solution of 2-thiobenzoic acid (1.54 g, 10.0 mmol) and NaOH (0.80 g, 20.0 mmol) were sequentially added the aqueous solution of chloroactic acid (2.835 g, 30.0 mmol) and NaOH (1.400 g, 35.0 mmol). After stirring for 4 h at 353 K under nitrogen atmosphere, the mixture was cooled to room temperature slowly. Adjusted the pH to 2 by adding 1.0 mol/*L* HCl, the pink deposit appeared rapidly. The solids were filtered and washed with water. The single crystals suitable for X-ray diffraction were obtained by the recrystallization of sieved solid in the ethanol.

S3. Refinement

The H atoms bonded to C atoms were positioned geometrically [aromatic C—H = 0.93 Å and aliphatic C—H = 0.97 Å, U_{iso}(H) = 1.2U_{eq}(C)]. The H atoms bonded to O atoms were located in a difference Fourier map and refined freely.

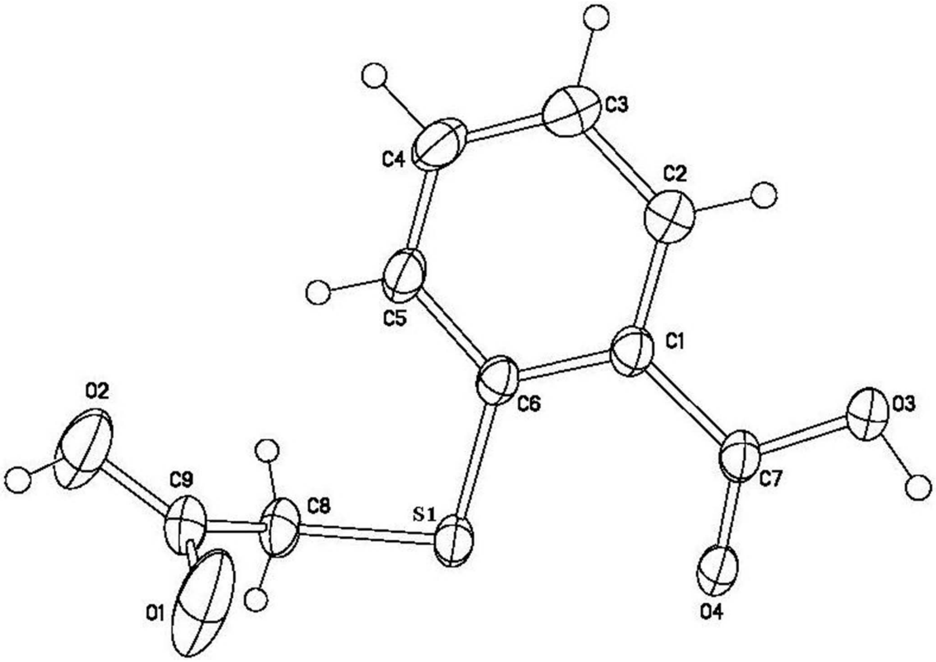

Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids

2-[(2-Carboxyphenyl)sulfanyl]acetic acid

Crystal data

$C_9H_8O_4S$
$M_r = 212.22$
Triclinic, $P\bar{1}$
Hall symbol: -P 1
$a = 5.1786\ (5)$ Å
$b = 9.2973\ (9)$ Å
$c = 10.4776\ (11)$ Å
$\alpha = 69.980\ (4)°$
$\beta = 81.959\ (6)°$
$\gamma = 79.732\ (6)°$
$V = 464.69\ (8)$ Å^3
$Z = 2$
$F(000) = 220$
$D_x = 1.517$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5343 reflections
$\theta = 2.1–27.7°$
$\mu = 0.33$ mm^{-1}
$T = 296$ K
Block, colourless
0.33 × 0.24 × 0.15 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.910$, $T_{\max} = 0.952$
6609 measured reflections
2110 independent reflections
1941 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.024$
$\theta_{\max} = 27.7°$, $\theta_{\min} = 2.1°$
$h = -6 \rightarrow 6$
$k = -12 \rightarrow 11$
$l = -13 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.074$
$wR(F^2) = 0.222$
$S = 1.19$
2110 reflections
133 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0736P)^2 + 1.2589P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.65$ e Å^{-3}
$\Delta\rho_{\min} = -0.34$ 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.

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 $F^2 > \sigma(F^2)$ 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	$U_{\rm iso}$*/$U_{\rm eq}$
S1	0.2028 (2)	0.36823 (12)	0.11601 (11)	0.0417 (3)
O1	−0.0678 (11)	0.4660 (9)	0.3612 (6)	0.116 (2)
O2	0.2828 (9)	0.5474 (7)	0.3870 (5)	0.0891 (16)
H2	0.173 (12)	0.569 (10)	0.449 (6)	0.107*
O3	0.2508 (7)	−0.1074 (4)	0.1122 (4)	0.0549 (9)
H3	0.127 (8)	−0.107 (7)	0.067 (5)	0.066*
O4	0.0891 (7)	0.1410 (4)	0.0369 (3)	0.0506 (8)
C1	0.4065 (8)	0.0579 (5)	0.2004 (4)	0.0383 (9)
C2	0.5712 (9)	−0.0691 (6)	0.2747 (5)	0.0482 (10)
H2A	0.5667	−0.1659	0.2682	0.058*
C3	0.7421 (10)	−0.0540 (7)	0.3583 (5)	0.0571 (12)
H3A	0.8511	−0.1398	0.4081	0.068*
C4	0.7485 (10)	0.0890 (7)	0.3665 (5)	0.0571 (13)
H4A	0.8638	0.1000	0.4221	0.068*
C5	0.5879 (9)	0.2166 (6)	0.2942 (5)	0.0465 (10)
H5A	0.5959	0.3124	0.3018	0.056*
C6	0.4120 (8)	0.2051 (5)	0.2093 (4)	0.0365 (8)
C7	0.2342 (8)	0.0364 (5)	0.1093 (4)	0.0402 (9)
C8	0.2613 (11)	0.5208 (5)	0.1742 (5)	0.0488 (11)
H8A	0.4498	0.5209	0.1687	0.059*
H8B	0.1864	0.6192	0.1130	0.059*
C9	0.1482 (10)	0.5076 (6)	0.3179 (5)	0.0504 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0549 (7)	0.0366 (5)	0.0400 (6)	−0.0082 (4)	−0.0092 (4)	−0.0178 (4)
O1	0.093 (3)	0.210 (7)	0.109 (4)	−0.084 (4)	0.041 (3)	−0.121 (5)
O2	0.076 (3)	0.149 (5)	0.077 (3)	−0.034 (3)	0.002 (2)	−0.075 (3)
O3	0.064 (2)	0.0412 (17)	0.073 (2)	0.0014 (15)	−0.0322 (18)	−0.0301 (16)
O4	0.063 (2)	0.0398 (16)	0.060 (2)	−0.0022 (14)	−0.0285 (16)	−0.0241 (15)
C1	0.040 (2)	0.043 (2)	0.038 (2)	−0.0067 (17)	−0.0030 (16)	−0.0202 (17)
C2	0.052 (3)	0.046 (2)	0.050 (3)	−0.004 (2)	−0.012 (2)	−0.020 (2)
C3	0.056 (3)	0.062 (3)	0.055 (3)	0.000 (2)	−0.021 (2)	−0.020 (2)
C4	0.046 (3)	0.077 (3)	0.060 (3)	−0.005 (2)	−0.020 (2)	−0.033 (3)
C5	0.042 (2)	0.058 (3)	0.054 (3)	−0.012 (2)	−0.0053 (19)	−0.033 (2)
C6	0.0368 (19)	0.044 (2)	0.0344 (19)	−0.0082 (16)	−0.0008 (15)	−0.0194 (16)
C7	0.043 (2)	0.041 (2)	0.045 (2)	−0.0066 (17)	−0.0047 (17)	−0.0241 (18)
C8	0.067 (3)	0.038 (2)	0.050 (2)	−0.016 (2)	−0.008 (2)	−0.0189 (19)
C9	0.058 (3)	0.047 (2)	0.060 (3)	−0.010 (2)	−0.009 (2)	−0.032 (2)

Geometric parameters (Å, º)

S1—C6	1.768 (4)	C2—C3	1.385 (6)
S1—C8	1.809 (4)	C2—H2A	0.9300
O1—C9	1.224 (7)	C3—C4	1.368 (8)
O2—C9	1.251 (6)	C3—H3A	0.9300
O2—H2	0.86 (7)	C4—C5	1.372 (7)
O3—C7	1.315 (5)	C4—H4A	0.9300
O3—H3	0.85 (2)	C5—C6	1.399 (6)
O4—C7	1.216 (5)	C5—H5A	0.9300
C1—C2	1.388 (6)	C8—C9	1.509 (7)
C1—C6	1.409 (6)	C8—H8A	0.9700
C1—C7	1.476 (5)	C8—H8B	0.9700
C6—S1—C8	103.4 (2)	C6—C5—H5A	119.4
C9—O2—H2	105 (6)	C5—C6—C1	117.6 (4)
C7—O3—H3	105 (4)	C5—C6—S1	121.8 (3)
C2—C1—C6	120.0 (4)	C1—C6—S1	120.6 (3)
C2—C1—C7	118.8 (4)	O4—C7—O3	122.1 (4)
C6—C1—C7	121.2 (4)	O4—C7—C1	123.9 (4)
C3—C2—C1	121.0 (4)	O3—C7—C1	114.1 (4)
C3—C2—H2A	119.5	C9—C8—S1	114.5 (3)
C1—C2—H2A	119.5	C9—C8—H8A	108.6
C4—C3—C2	119.1 (5)	S1—C8—H8A	108.6
C4—C3—H3A	120.5	C9—C8—H8B	108.6
C2—C3—H3A	120.5	S1—C8—H8B	108.6
C3—C4—C5	121.1 (4)	H8A—C8—H8B	107.6
C3—C4—H4A	119.4	O1—C9—O2	122.5 (5)
C5—C4—H4A	119.4	O1—C9—C8	121.3 (4)
C4—C5—C6	121.2 (4)	O2—C9—C8	116.1 (5)

C4—C5—H5A	119.4

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.86 (7)	1.92 (5)	2.687 (6)	149 (8)
O3—H3···O4^{ii}	0.85 (2)	1.80 (5)	2.634 (4)	167 (6)

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