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# 2,2′-Thiodibenzoic acid

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.006 Å
*R* factor = 0.077
*wR* factor = 0.149
Data-to-parameter ratio = 12.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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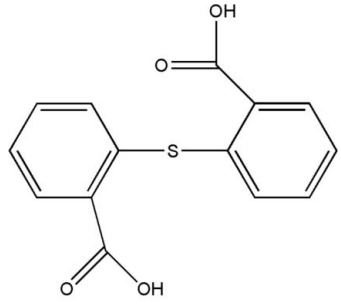
In the title molecule, $C_{14}H_{10}O_4S$, all bond lengths and angles are normal. In the crystal structure, strong intermolecular O—H···O hydrogen bonds between the carboxyl groups link the molecules into zigzag chains extending along the *c* axis.

## Comment

The current interest focused on the crystal engineering of coordination polymeric frameworks not only stems from their potential properties as functional solid materials, in host–guest chemistry, ion exchange, catalysis and for the development of optical, magnetic and electronic devices, but also from their intriguing variety of architectures and topologies (Chui *et al.*, 1999; Matsumoto *et al.*, 1999). Some organic S-donors, such as thiosalicylic acid or related species, attracted our attention for the process of constructing coordination polymers. However, an unexpected organic ligand was obtained as a result of the desulfurization of the thiosalicylic acid ligand. We report here the synthesis and crystal structure of the title compound, $C_{14}H_{10}O_4S$, (I).




(I)

In (I) (Fig. 1), the bond lengths and angles (Table 1) are normal. In the crystal structure, strong intermolecular O—H···O hydrogen bonds between the carboxyl groups (Table 2)

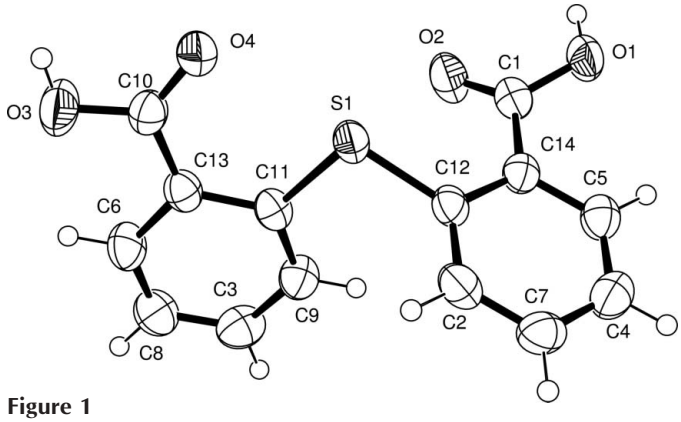



**Figure 1**
View of (I), showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

link the molecules into zigzag chains extending along the *c* axis (Fig. 2).

## Experimental

$CuCl_2{\cdot}2H_2O$ (0.17 g, 1 mmol), thiosalicylic acid (0.15 g, 1 mmol), and NaOH (0.04 g, 1 mmol), were mixed in water (15 ml) and heated at 433 K for 3 d in a sealed 25 ml Teflon-lined stainless steel vessel under autogenous pressure. After cooling to room temperature at a rate of 5 K $h^{-1}$, yellow block crystals were isolated, washed with water and dried in air.

*Crystal data*

$C_{14}H_{10}O_4S$
$M_r$ = 274.29
Monoclinic, $P2_1/c$
$a$ = 13.9126 (6) Å
$b$ = 6.4708 (2) Å
$c$ = 14.4664 (7) Å
$\beta$ = 103.134 (2)°
$V$ = 1268.28 (9) Å$^3$
$Z$ = 4
$D_x$ = 1.436 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 2271 reflections
$\theta$ = 2.9–25.0°
$\mu$ = 0.26 mm$^{-1}$
$T$ = 293 (2) K
Prism, yellow
0.60 × 0.36 × 0.30 mm

*Data collection*

Siemens SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multiscan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.621, $T_{max}$ = 0.924
4026 measured reflections
2250 independent reflections
2023 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 25.0°
$h = -16 \rightarrow 15$
$k = -7 \rightarrow 7$
$l = -10 \rightarrow 17$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.149
$S$ = 1.33
2250 reflections
176 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0139P)^2 + 2.6198P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.27 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C1—O2 | 1.223 (5) | C10—O3 | 1.318 (5) |
| C1—O1 | 1.315 (5) | C11—S1 | 1.778 (4) |
| C10—O4 | 1.225 (5) | C12—S1 | 1.790 (4) |
| | | | |
| O2—C1—O1 | 122.2 (4) | O4—C10—C13 | 122.6 (4) |
| O2—C1—C14 | 124.1 (4) | C11—S1—C12 | 102.46 (19) |
| O4—C10—O3 | 122.1 (4) | | |

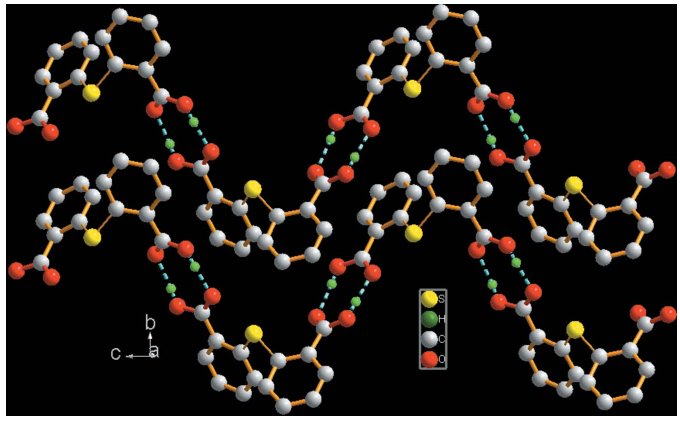



**Figure 2**
The one-dimensional zigzag chains of hydrogen-bonded (dashed lines) molecules extending along the *c* axis. C-bound H atoms have been omitted for clarity.

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···O4$^{i}$ | 0.92 (7) | 1.70 (7) | 2.621 (4) | 177 (7) |
| O3—H10$A$···O2$^{ii}$ | 0.82 (7) | 1.82 (7) | 2.640 (5) | 175 (7) |

Symmetry codes: (i) $x, -y+\frac{5}{2}, z-\frac{1}{2}$; (ii) $x, -y+\frac{5}{2}, z+\frac{1}{2}$.

The C-bound H atoms were positioned geometrically and refined as riding on their parent atoms, with C—H = 0.93 Å and $U_{iso}$ = 1.5$U_{eq}$(C). The carboxy H atoms were located in a difference Fourier map and refined isotropically.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996) and *XPREP* (Siemens, 1996); data reduction: *XPREP*; program(s) used to solve structure: *SHELXTL* (Siemens, 1996); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *ORTEP-3* in *WinGX* (Farrugia, 1999); software used to prepare material for publication: *SHELXTL*.

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