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3-(1*H*-1,2,4-Triazol-3-ylsulfanylmethyl)-benzoic acid

Lei Han, You-Fu Zhou, Rui-Hu Wang and Mao-Chun Hong*

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Fuzhou, Fujian 350002, People's Republic of China

Correspondence e-mail: hmc@fjirsm.ac.cn

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Key indicators

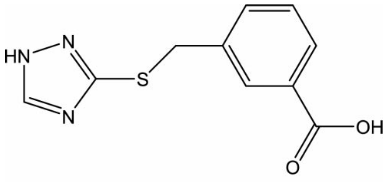
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.058
wR factor = 0.133
Data-to-parameter ratio = 12.6

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

The title compound, $C_{10}H_9N_3O_2S$, crystallizes in the orthorhombic non-centrosymmetric space group $P2_12_12_1$. The molecules are linked into a three-dimensional network through O—H···N and N—H···O hydrogen bonds and weak S···O interactions.

Comment

The construction of chiral coordination polymers combining asymmetric catalysis and optical activity is a rapidly developing area of supramolecular chemistry (Seo *et al.*, 2000; Evans & Lin, 2002). Generally, chiral compounds can be obtained either by stereoselective synthesis using chiral organic ligands or by spontaneous resolution upon crystallization without any chiral sources, and the chirally discriminative interactions may arise from coordination bonds and/or hydrogen bonds. We rationalize that the twisted binding sites of asymmetric bridging ligands containing sulfide moieties can induce the formation of chiral structures when linked by suitable metal nodes (Han *et al.*, 2003). Additionally, the incorporation of S atoms in the related ligands will lead to weak interactions between the chalcogen centers, which play an important role in the crystal structures. We report here the synthesis and crystal structure of the organic ligand 3-(1*H*-1,2,4-triazol-3-ylsulfanylmethyl)benzoic acid, (I) (Fig. 1).



(I)

Compound (I), prepared from 1*H*-1,2,4-triazole-3-thiol and 3-(chloromethyl)benzoic acid, crystallizes in the orthorhombic non-centrosymmetric space group $P2_12_12_1$. Intriguing features of the compound arise not only from its flexibility but also from the presence of triazole and benzenecarboxylate

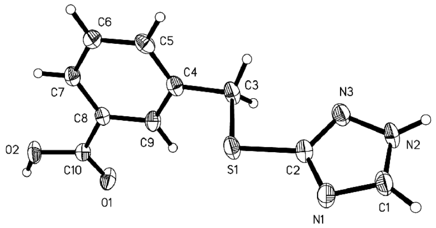


Figure 1
Perspective view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

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moieties connected by a $-CH_2S-$ spacer. The sp^3 configurations of the C and S atoms of the $-CH_2S-$ spacer force the molecule to be twisted. Actually, the C—C—S and C—S—C angles are 105.4 (3) and 101.3 (2)°, respectively. The dihedral angle between the benzene and triazole rings is 70.1 (2)°. The molecules are linked into a three-dimensional network through O—H···N and N—H···O hydrogen bonds (Table 2) and weak S···O (3.251 Å) interactions (Fig. 2).

Experimental

1*H*-1,2,4–Triazole-3-thiol (1.01 g, 10 mmol) was added to a stirred solution of NaOH (0.4 g, 10 mmol) in H_2O (20 ml). The mixture was warmed to reflux, then 3-(chloromethyl)benzoic acid (1.70 g, 10 mmol) was added and the mixture was refluxed for about 10 h with vigorous stirring. After cooling, the mixture was left to stand overnight. The precipitate was filtered off and washed with water, giving a fine white powder in 80% yield. Colorless needle-shaped crystals suitable for X-ray diffraction were isolated after recrystallization from a chloroform–ether solution.

Crystal data

$C_{10}H_9N_3O_2S$
$M_r = 235.26$
Orthorhombic, $P2_12_12_1$
$a = 5.5079$ (1) Å
$b = 13.1233$ (6) Å
$c = 14.3414$ (7) Å
$V = 1036.62$ (7) Å^3
$Z = 4$
$D_x = 1.507$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 3393 reflections
$\theta = 2.1$–25.1°
$\mu = 0.30$ mm^{-1}
$T = 293$ (2) K
Needle, colorless
0.20 × 0.10 × 0.08 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.972$, $T_{\max} = 0.978$
3393 measured reflections

1827 independent reflections
1460 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.044$
$\theta_{\max} = 25.1°$
$h = -6 \rightarrow 6$
$k = -10 \rightarrow 15$
$l = -17 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.133$
$S = 1.26$
1827 reflections
145 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2 + 1.1042P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.22$ e Å^{-3}
$\Delta\rho_{\min} = -0.27$ e Å^{-3}
Absolute structure: Flack (1983), 728 Friedel pairs
Flack parameter = 0.0 (2)

Table 1
Selected geometric parameters (Å, °).

S1—C2	1.760 (4)	C3—C4	1.524 (6)
S1—C3	1.818 (5)	C4—C5	1.384 (7)
O1—C10	1.220 (5)	C4—C9	1.390 (7)
O2—C10	1.317 (5)	C5—C6	1.396 (7)
N1—C1	1.338 (6)	C6—C7	1.381 (7)
N1—C2	1.352 (6)	C7—C8	1.383 (7)
N2—C1	1.314 (7)	C8—C9	1.403 (6)
N2—N3	1.373 (5)	C8—C10	1.486 (7)
N3—C2	1.318 (6)		
C2—S1—C3	101.3 (2)	C4—C3—S1	105.4 (3)

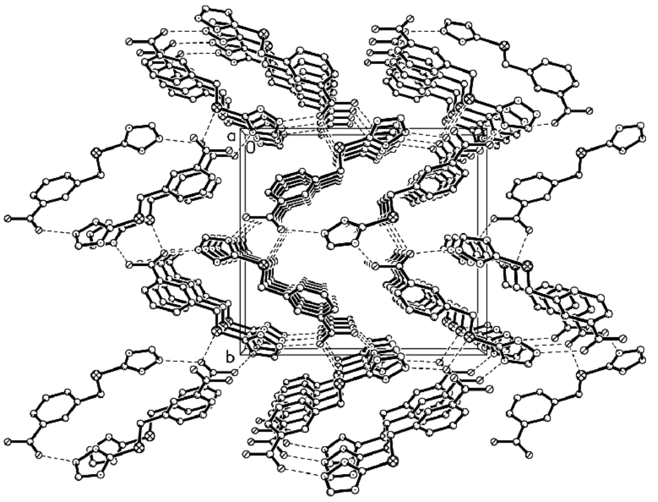

Figure 2
Packing diagram, viewed along the *a* axis. Hydrogen bonds and weak S···O interactions are indicated by dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*B*···N1$^{\rm i}$	0.84	1.89	2.707 (6)	163
N2—H2*A*···O1$^{\rm ii}$	0.88	1.90	2.767 (5)	170

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

H atoms were positioned geometrically and allowed to ride on their respective parent atoms with $U_{\rm iso} = 1.5$ (carboxyl H) or1.2 (other H atoms) times $U_{\rm eq}$ of the parent atoms

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *SAINT* and *SHELXTL* (Sheldrick, 1997*b*); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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