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(4-Chlorophenyl)thioglycolic acid

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Key indicators

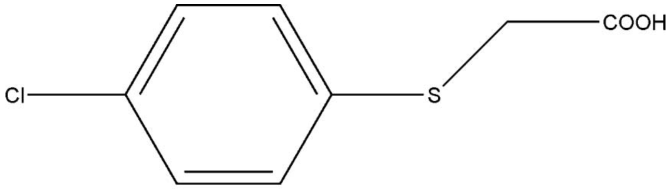
Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.117
Data-to-parameter ratio = 17.6

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

In the title compound, $C_8H_7ClO_2S$, all bond lengths and angles are normal. Inversion-related molecules are linked by paired O—H···O hydrogen bonds into dimers containing an $R_2^2(8)$ motif.

Comment

(4-Chlorophenyl)thioglycolic acid, (I), is a flexible ligand with versatile binding abilities and the capability of participating in hydrogen bonds as both a donor and an acceptor, thus representing an excellent candidate for the construction of supramolecular complexes. The crystal structure of (4-chlorophenyl)thioglycolic acid was first reported by Shklover *et al.* (1983); it consists of a tris(2-hydroxyethyl)ammonium cation and a 4-chlorophenylthioacetate anion. Two crystal structures of (4-chlorophenyl)thioglycolic acid derivatives have also been reported previously, namely 2,4-dichloro-5-methylphenylthioacetic acid (Mak *et al.*, 1989) and 4-dichloro-2,5-methylphenylthioacetic acid (Kennard *et al.*, 1989).



(I)

Interestingly, in contrast to the previously reported structures, the molecular skeleton of (I) is almost planar, the largest deviation being 0.2759 (19) Å for atom O2; however, the sulfanylacetate group is slightly twisted with a C1—S1—C7—C8 torsion angle of 4.94 (18)°. In two of the previous structures, the acetate group is approximately perpendicular to the benzene ring (Shklover *et al.*, 1983; Kennard *et al.*, 1989), but it is approximately parallel to the benzene ring in the third (Mak *et al.*, 1989) and in (I) (Fig. 1).

A familiar carboxylic acid centrosymmetric dimer, containing an $R_2^2(8)$ motif, is built up by O—H···O hydrogen-bonding interactions between the carboxylic acid groups (Fig. 2 and Table 1).

Experimental

(4-Chlorophenyl)thioglycolic acid was prepared by nucleophilic reaction of chloroacetic acid with 4-chlorothiophenol under basic conditions (Nobles *et al.*, 1965). Crystals of (I) suitable for single-crystal X-ray diffraction were grown by slow evaporation of an ethanol solution.

Crystal data

$C_8H_7ClO_2S$
$M_r = 202.65$
Monoclinic, $P2_1/n$
$a = 5.5743\ (11)$ Å
$b = 5.3123\ (11)$ Å
$c = 29.086\ (6)$ Å
$\beta = 90.60\ (3)°$
$V = 861.2\ (3)$ Å^3
$Z = 4$
$D_x = 1.563$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.64$ mm^{-1}
$T = 291\ (2)$ K
Block, colourless
0.33 × 0.32 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.817$, $T_{\max} = 0.907$
7327 measured reflections
1935 independent reflections
1324 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.048$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.118$
$S = 1.07$
1935 reflections
110 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.32$ e Å^{-3}
$\Delta\rho_{\min} = -0.22$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H7···O1$^{\rm i}$	0.82	1.88	2.689 (3)	171

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

All H atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 (aromatic) or 0.97 Å (methylene), O—H = 0.82 Å (carboxyl), and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) or 1.5$U_{\rm eq}$(O).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); 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: *SHELXL97*.

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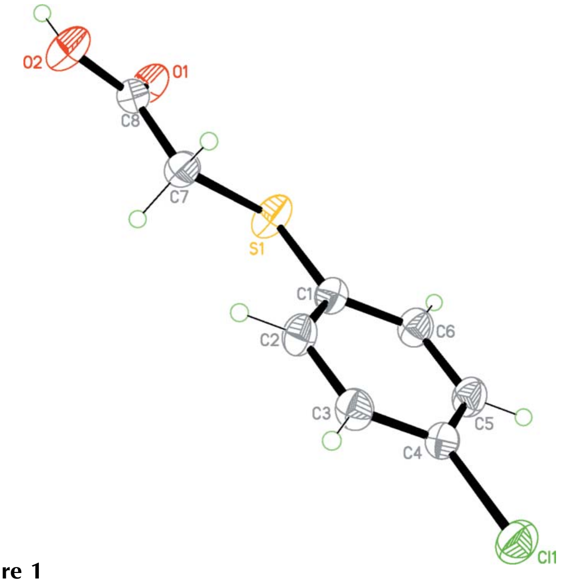

Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radius.

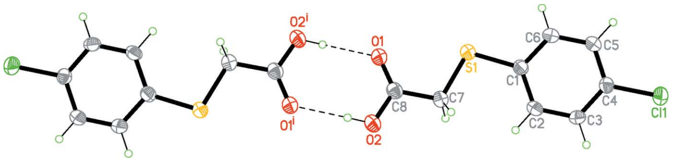

Figure 2
A view of the hydrogen-bonded (dashed lines) dimer [symmetry code: (i) $-x+1, -y-1, -z$].

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