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2-(3,4-Dichlorophenoxy)propionic acid

Tashfeen Akhtar,[a] M. Khawar Rauf,[b] Masahiro Ebihara[b] and Shahid Hameed[a]*

[a]Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and [b]Department of Chemistry, Faculty of Engineering, Gifu University, Yanagido, Gifu 501-1193, Japan

Correspondence e-mail: shameed@qau.edu.pk

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Key indicators

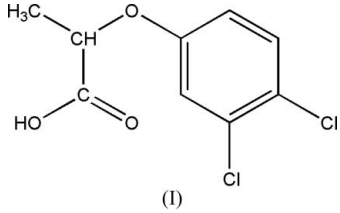
Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.005 Å
R factor = 0.067
wR factor = 0.149
Data-to-parameter ratio = 16.1

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

In the title compound, $C_9H_8Cl_2O_3$, the molecules are linked in dimers across centres of symmetry by O—H···O hydrogen bonds. The O···O distance and O—H···O angle compare well with values observed in other substituted phenoxy and benzoic acids.

Comment

Phenoxy acids have been used as intermediates in the synthesis of many valuable target molecules (Lupea *et al.*, 2006; Powers & Gotz, 2006). A series of aurones using phenoxy acids as intermediates has recently been synthesized and evaluated for insect antifeedant activity (Morimoto *et al.*, 2007). Phenoxy acids have also found applications in their own right in the agricultural industry (Heaton, 1994). A number of phenoxypropionic acid derivatives have been patented by some companies as herbicidal and plant-growth regulating agents (Takahashi *et al.*, 1977; Rempfler *et al.*, 1982; Ura *et al.*, 1994). We are interested in the synthesis of these phenoxyalkanoic acids as intermediates in the preparation of oxadiazoles and benzothiazole derivatives for the systematic study of bioactive drug-like molecules and we present here the crystal structure of the title compound, (I) (Fig. 1 and Table 1).



(I)

The C—Cl distances of 1.727 (4) and 1.731 (4) Å agree well with the values observed in a series of phenoxyalkanoic acids (Smith & Kennard, 1979; Smith *et al.*, 1981). Other interatomic distances and angles compare favourably with those reported for 2-(2,4,5-trichlorophenoxy)propionic acid (Smith *et al.*, 1977). The *exo*-C4 angles C9—C4—O3 [115.2 (3)°] and C5—C4—O3 [124.3 (3)°] deviate considerably from the trigonal value, as in several other members of this series of compounds (Smith & Kennard, 1979). The C═O and C—OH bond distances are very close to the normal values for the carboxylic acid group [1.216 (4) and 1.318 (4) Å, respectively; Leiserowitz, 1976]. The molecules are linked into centrosymmetric dimers by O—H···O hydrogen bonds (Fig. 2 and Table 2).

Experimental

A solution of 2-bromopropionic acid (1.53 g, 10 mmol) in 2 *M* NaOH (5.0 ml) was added to a solution of 3,4-dichlorophenol (1.63 g,

10 mmol) in 2 *M* NaOH (5.0 ml), and the mixture was refluxed. On completion of the reaction (thin-layer chromatography), it was cooled to room temperature, acidified with 5 *M* HCl and extracted with diethyl ether (3 × 25 ml). The combined ether extracts were washed with brine (25 ml), dried (anhydrous $MgSO_4$) and the solvent evaporated *in vacuo* after filtration. The product was recrystallized from diethyl ether/petroleum ether (7:3) (yield 80%) The spectroscopic and physical characterization will be reported separately.

Crystal data

$C_9H_8Cl_2O_3$
M_r = 235.07
Monoclinic, $P2_1/c$
a = 4.585 (5) Å
b = 6.412 (8) Å
c = 33.21 (4) Å
β = 90.471 (14)°
V = 976 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.64 mm^{-1}
T = 113 (2) K
0.40 × 0.30 × 0.22 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Absorption correction: none
6901 measured reflections
2119 independent reflections
1996 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.149
S = 1.28
2119 reflections
132 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C2—O2	1.216 (4)	C6—Cl1	1.727 (4)
C2—O1	1.318 (4)	C7—Cl2	1.731 (4)
O3—C4—C5	124.3 (3)	O3—C4—C9	115.2 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.79 (5)	1.88 (5)	2.665 (4)	171 (5)

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

The O-bound H atom was refined isotropically. All other H atoms were placed in idealized positions and treated as riding atoms, with C—H = 0.95–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *TEXSAN* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97* and *TEXSAN*.

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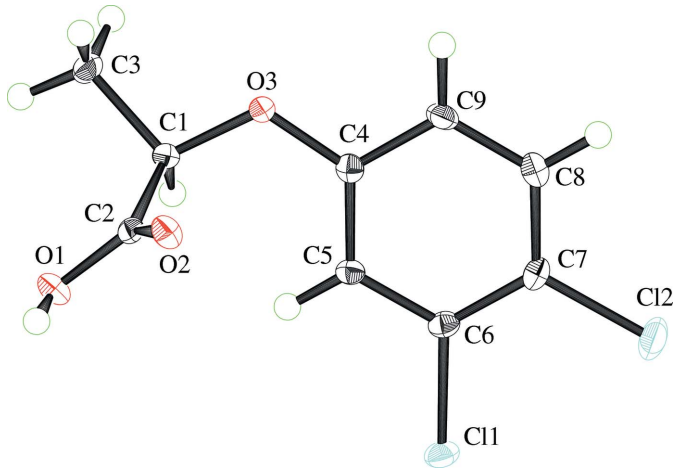

Figure 1
The molecular structure of (I), showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

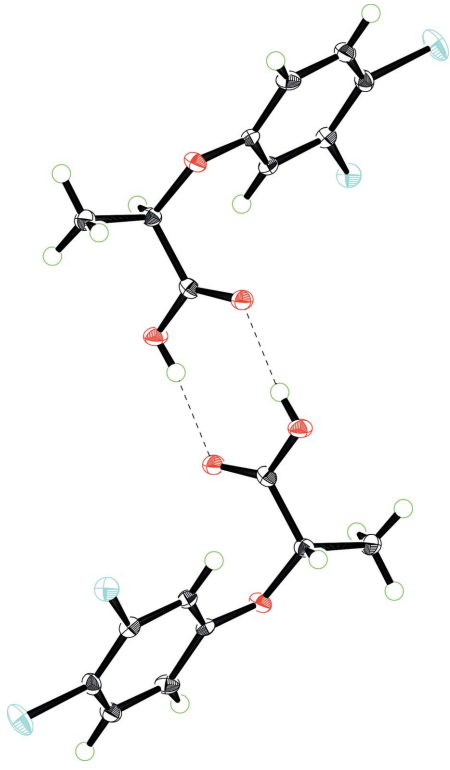

Figure 2
View of the hydrogen bonds (dashed lines) forming a centrosymmetric dimer. The unit cell has been omitted for clarity.

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