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1-Chloro-4-hydroxyanthraquinone

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.061
wR factor = 0.200
Data-to-parameter ratio = 16.9

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

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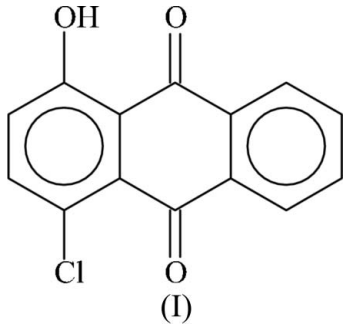
In the title crystal structure, $C_{14}H_7ClO_3$, the molecules are linked by weak intermolecular hydrogen bonds to form a one-dimensional chain.

Comment

1-Hydroxyanthraquinone in its deprotonated form should function as a bidentate chelate to metal ions. However, there is little interest in this class of ligands, and only a small number of metal complexes of 1-hydroxyanthraquinone and its derivatives have been reported to date (Ali *et al.*, 2005). A recent study has documented the structure of 1,4-dihydroxyanthraquinone (Zain & Ng, 2005). The title compound, (I), has a Cl substituent in the 4-position of 1-hydroxyanthraquinone (Fig. 1), and it exists in a nearly planar conformation.



(I)

The hydroxy group forms an intramolecular hydrogen bond. Adjacent molecules are linked by weak interactions (Table 1) into a chain motif (Fig. 2). Other chloroanthraquinones that have been reported are limited to 1-chloroanthraquinone (Klimasenko & Gol'der, 1969; Meng *et al.*, 1999) and 1,5-dichloroanthraquinone (Bailey, 1958; Nakata & Takaki, 1984; Wang, 1979) only.

Experimental

Crystals of 1-chloro-4-hydroxyanthraquinone were obtained by recrystallizing the commerically available compound from pyridine.

Crystal data

$C_{14}H_7ClO_3$
M_r = 258.65
Monoclinic, $P2_1/n$
a = 7.4180 (7) Å
b = 10.2724 (9) Å
c = 14.262 (1) Å
β = 90.588 (2)°
V = 1086.7 (2) Å^3
Z = 4
D_x = 1.581 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1782 reflections
θ = 2.4–26.1°
μ = 0.35 mm^{-1}
T = 295 (2) K
Block, red
0.42 × 0.34 × 0.16 mm

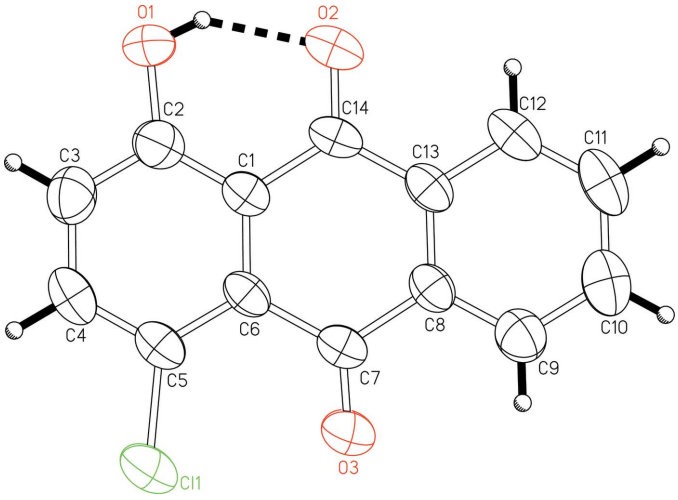


Figure 1
A plot of the molecule of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. The dashed line indicates a hydrogen bond.

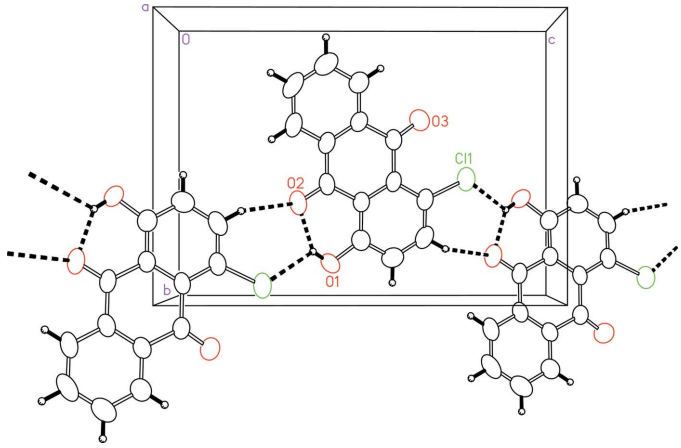


Figure 2
A plot showing the weak interactions (dashed lines) that link adjacent molecules of (I) into a chain.

Data collection

Bruker SMART area-detector diffractometer	$R_{int} = 0.030$
φ and ω scans	$\theta_{max} = 27.1^\circ$
6405 measured reflections	$h = -9 \rightarrow 9$
2366 independent reflections	$k = -13 \rightarrow 12$
1306 reflections with $I > 2\sigma(I)$	$l = -12 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.113P)^2 + 0.225P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.061$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.200$	$\Delta\rho_{max} = 0.54$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -0.40$ e Å^{-3}
2366 reflections	
140 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.82	1.87	2.569 (3)	143
O1—H1···Cl1^{i}	0.82	3.16	3.655 (2)	122
C4—H4···O2^{ii}	0.93	2.55	3.397 (3)	152

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

The two aromatic rings were refined as rigid hexagons of side 1.39 Å in order to raise the reflections-to-parameters ratio, as the crystal was not a strongly diffracting specimen. The H atoms were placed in calculated positions (C—H = 0.93 Å and O—H = 0.82 Å), and they were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C,O)$. The hydroxy group was rotated to fit the electron density.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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