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9-Chloro-10-(dimethoxymethyl)anthracene

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.071
wR factor = 0.255
Data-to-parameter ratio = 11.3

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

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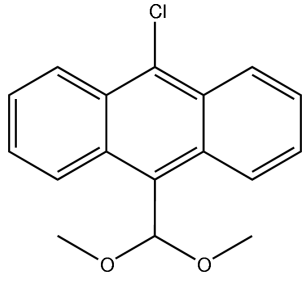
In the title compound, $C_{17}H_{15}ClO_2$, the anthracene ring system is planar and the bond lengths and angles are unexceptional. In the crystal structure, the molecules stack along the *a* axis and there are no significantly short intermolecular contacts.

Comment

In the course of complex syntheses, for instance, in the total syntheses of natural products, carbonyl groups must often be protected against nucleophilic attack, *e.g.* by organometallic compounds, strong bases, reduction and sometimes also oxidation. To achieve this, the carbonyl groups are generally transformed into appropriate acetals, hydrazones, oximes and cyanohydrins. Dialkyl acetals and ketals can easily be formed from carbonyl compounds with alcohols under acidic conditions.



(I)

We report here the structure of a new acetal, (I) (Fig. 1), formed by reacting 10-chloro-9-anthraldehyde with methanol in the presence of $CuCl_2$. The bond lengths and angles lie within normal ranges (You & Zhu, 2004). The dihedral angles between the anthracene plane and the groups C1—O1—C16 and C1—O2—C17 are 62.1 (4) and 83.5 (4)°, respectively; the dihedral angle between planes C1—O1—C16 and C1—O2—C17 is 79.1 (4)°. In the crystal structure, the molecules stack along the *a* axis and there are no significantly short intermolecular contacts.

Experimental

10-Chloro-9-anthraldehyde, methanol, ethanol and $CuCl_2$ are available commercially and were used without further purification. 10-Chloro-9-anthraldehyde (0.5 mmol, 120.3 mg) and $CuCl_2$ (0.1 mmol, 13.4 mg) were dissolved in MeOH–EtOH (1:1 *v*/*v*, 5 ml). The mixture was stirred for 2 h at room temperature, filtered, and the filtrate was left to evaporate. After 4 weeks, some crystals suitable for X-ray crystallographic analysis were formed; these were washed three times with the same ratio mixture of solvent (yield 63%). Analysis found: C 71.1, H 5.3%; calculated for $C_{17}H_{15}ClO_2$: C 71.2, H 5.2%.

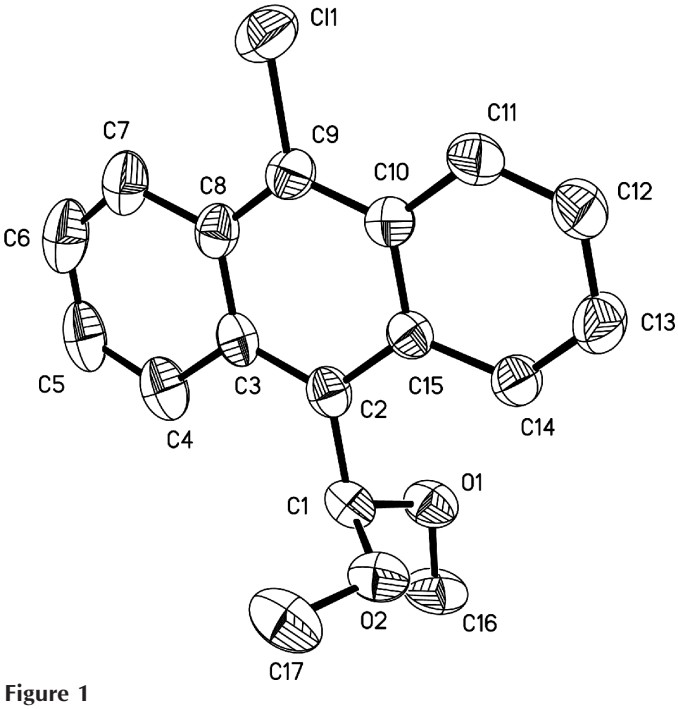


Figure 1
The structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted.

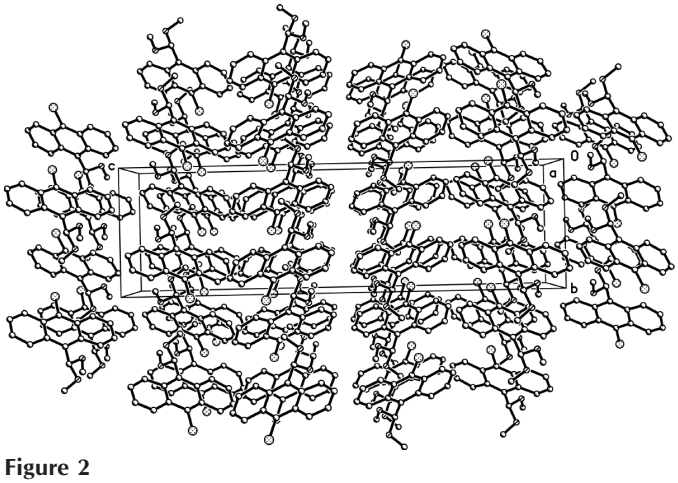


Figure 2
The crystal packing of the title compound, viewed along the *a* axis. H atoms have been omitted.

Crystal data

$C_{17}H_{15}ClO_2$
M_r = 286.74
Orthorhombic, *Pbca*
a = 10.553 (12) Å
b = 8.948 (10) Å
c = 30.84 (3) Å
V = 2912 (6) Å^3
Z = 8
D_x = 1.308 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1879 reflections
θ = 2.3–20.1°
μ = 0.26 mm^{-1}
T = 293 (2) K
Block, colourless
0.42 × 0.35 × 0.28 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.899, T_{max} = 0.931
13634 measured reflections
2550 independent reflections
1069 reflections with $I > 2\sigma(I)$
R_{int} = 0.087
θ_{max} = 25.0°
$h = -12 \rightarrow 12$
$k = -10 \rightarrow 10$
$l = -36 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.255
S = 0.95
2550 reflections
226 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.141P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

All H atoms were refined isotropically, giving C—H distances in the range 0.93 (2)–0.99 (2) Å; U_{iso}(H) values were fixed at 0.08 Å^2.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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