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Cyclopent-3-ene-1,1-dicarboxylic acid

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.005 Å
R factor = 0.064
wR factor = 0.216
Data-to-parameter ratio = 15.6

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

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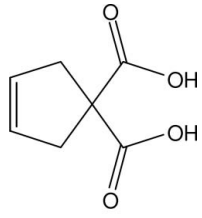
The cyclopentene ring of the title compound, $C_7H_8O_4$, is essentially planar. The molecules form zigzag chains *via* O—H···O hydrogen bonds.

Comment

The title compound, (I), is the product of a ring-closing metathesis (Rölle & Grubbs, 2002). A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27 plus one update; *MOGUL* Version 1.1; Allen, 2002). The cyclopentene ring is essentially planar (r.m.s. deviation of the ring atoms = 0.031 Å). The two carboxyl groups form dihedral angles of 67.2 (3) and 63.4 (4)° [for C11/O11/O12 and C21/O21/O22, respectively], with the cyclopentene ring. The molecules form zigzag chains *via* O—H···O hydrogen bonds (Fig. 2).



(I)

Experimental

The title compound was synthesized according to the procedure described by Rölle & Grubbs (2002). Colourless crystals suitable for X-ray diffraction were grown from a methanol solution of (I).

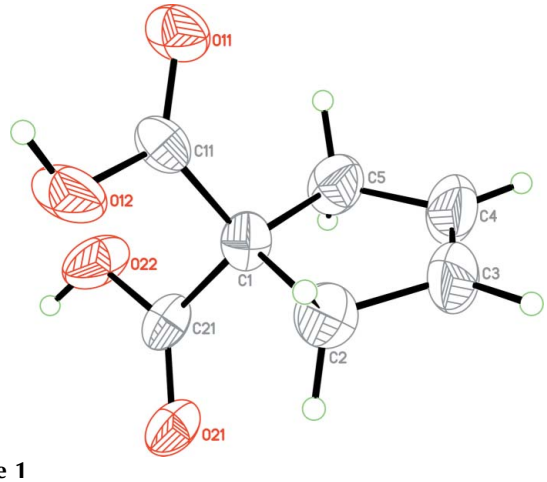


Figure 1
Perspective view of the title compound with the atom-numbering scheme; displacement ellipsoids are drawn at the 30% probability level.

Crystal data

$C_7H_8O_4$
M_r = 156.13
Monoclinic, $C2/c$
a = 20.543 (8) Å
b = 6.179 (2) Å
c = 12.394 (5) Å
β = 98.35 (3)°
V = 1556.6 (10) Å^3
Z = 8
D_x = 1.333 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4322 reflections
θ = 3.2–24.3°
μ = 0.11 mm^{-1}
T = 173 (2) K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD three-circle diffractometer
ω scans
Absorption correction: none
9705 measured reflections
1589 independent reflections
930 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 26.4°
$h = -25 \rightarrow 25$
$k = -7 \rightarrow 7$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.217
S = 0.95
1589 reflections
102 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1161P)^2 + 1.782P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C11—O11	1.208 (4)	C21—O21	1.210 (4)
C11—O12	1.294 (4)	C21—O22	1.315 (4)
O11—C11—O12	123.6 (3)	O21—C21—O22	124.2 (3)
O11—C11—C1	123.6 (3)	O21—C21—C1	124.5 (3)
O12—C11—C1	112.7 (3)	O22—C21—C1	111.3 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O12—H12···O11^{i}	0.84	1.79	2.619 (3)	168
O22—H22···O21^{ii}	0.84	1.81	2.650 (4)	173

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

H atoms were located in a difference map, but refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C)] using a riding model, with O—H = 0.84 Å, and C—H = 0.95 and 0.99 Å for Csp^2 and methylene C, respectively. In addtion, the torsion angles about the C—O bonds of the hydroxyl groups were refined.

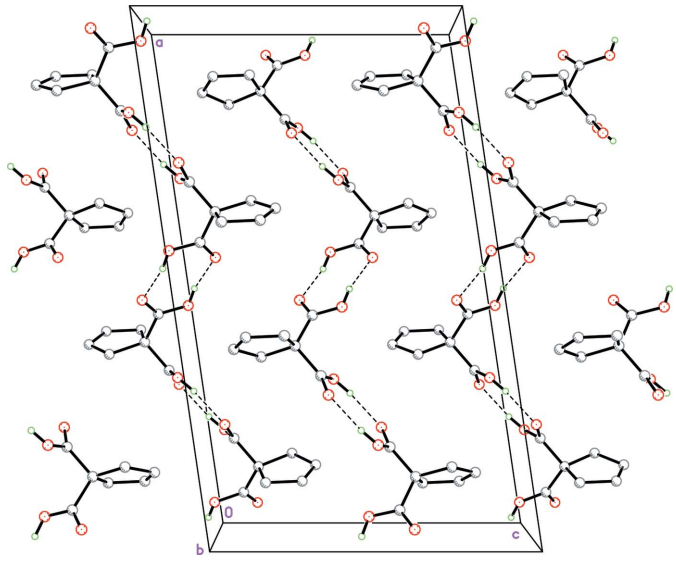


Figure 2
Packing diagram of the title compound, showing the hydrogen bonds as dashed lines. The view is projected on to the *ac* plane and H atoms not involved in hydrogen bonding have been omitted for clarity.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

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