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(±)-2,5-Dioxoperhydrocycloocta[*b*]furan-3-carboxylic acid

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Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.095
Data-to-parameter ratio = 18.0

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

The *anti* stereochemistry between the fused rings of the bicyclic lactone (±)-2,5-dioxoperhydrocycloocta[*b*]furan-3-carboxylic acid, $C_{11}H_{14}O_5$, has been established. Intermolecular hydrogen bonds are observed between the carboxylic acid group and the carbonyl O atom of an adjacent molecule.

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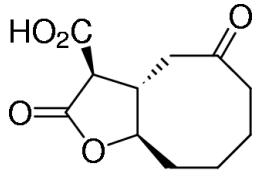
Comment

The *anti* stereochemistry of the fused rings of the title compound, (I), has been established. The molecular structure of (I) is shown in Fig. 1. A hydrogen-bonded chain structure is formed through an intermolecular hydrogen bond between the carboxylic acid group and the ketone O atom of an adjacent molecule.



(I)

Experimental

The title compound was prepared by base-catalysed hydrolysis of the parent ethyl ester as previously described (Greatrex *et al.*, 2002). Crystals suitable for X-ray analysis were grown by slow evaporation from an ethyl acetate/hexane (1:1) solution of the compound.

Crystal data

$C_{11}H_{14}O_5$
M_r = 226.22
Orthorhombic, *Pbca*
a = 8.0792 (1) Å
b = 10.6879 (2) Å
c = 24.5704 (5) Å
V = 2121.65 (6) Å^3
Z = 8
D_x = 1.416 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25701 reflections
θ = 3–28.3°
μ = 0.11 mm^{-1}
T = 123 (2) K
Tabular, colourless
0.24 × 0.14 × 0.04 mm

Data collection

KappaCCD diffractometer
Thick-slice scans
23 956 measured reflections
2630 independent reflections
1847 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 28.3°
h = −10 → 10
k = −14 → 14
l = −32 → 32

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.095$
$S = 1.06$
2630 reflections
146 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 0.2022P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···O3^{i}	0.84	1.81	2.6292 (13)	164

Symmetry code: (i) $-x, y-\frac{1}{2}, \frac{1}{2}-z$.

The H atoms were included in the riding-model approximation. The torsion angle about the C—O bond of the carboxylic acid group was refined.

Data collection: *COLLECT* (Nonius, 1997–2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

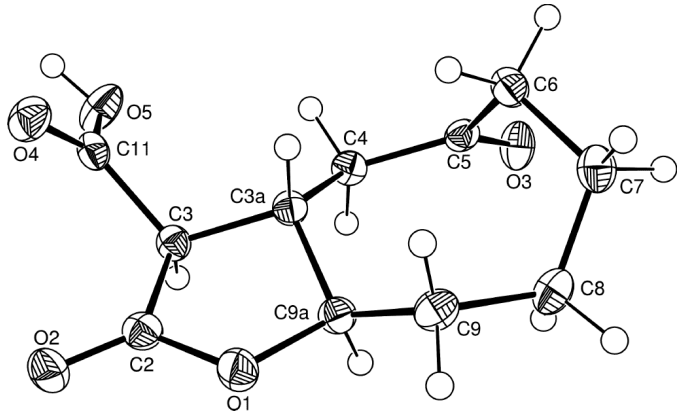


Figure 1
View of (I) (50% probability displacement ellipsoids).

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