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Methyl 2-(2-hydroxy-1,3-dioxoinden-2-yl)acrylate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.114
Data-to-parameter ratio = 12.5

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

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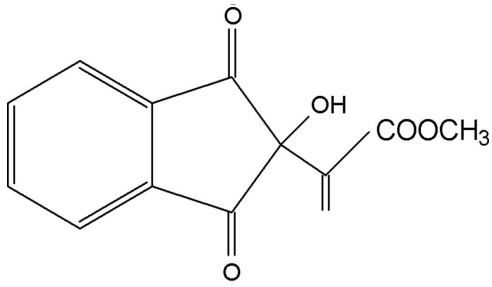
In the title compound, $C_{13}H_{10}O_5$, the five-membered ring adopts an envelope conformation. The crystal structure is stabilized by intermolecular C—H···O and O—H···O hydrogen bonds.

Comment

Methacrylate monomers with bulky ester substituents have been synthesized in order to study stereospecific and asymmetric polymerization, in which the ester group plays an important role. Okamoto and co-workers (Okamoto *et al.*, 1983; Okamoto & Nakano, 1994) reported on a series of bulky methacrylates and found that many of these types of monomers yield highly isotactic optically active polymers with one-handed helical conformations by asymmetric anionic polymerization. The anions of tetrabutylammonium salts of CH-acidic compounds are initiators for the metal free anionic polymerization of acrylates, methacrylates and acrylonitrile (Reetz *et al.*, 1995). Against this background and in order to obtain detailed information on its molecular conformation, the structure of the title compound, (I), has been determined and the results are presented here.



(I)

Fig. 1 shows the molecular structure of (I) with its atom-numbering scheme. (I) consists of a 2-hydroxy-1*H*-indene-1,3(2*H*)-dione unit connected to a methyl acrylate group *via* atom C2. The five-memberd ring (atoms C1, C2, C3, C3*A* and C7*A*) of the indene group adopts an envelope conformation; the puckering parameters are q_2 = 0.167 (2) Å and φ = −5.6 (5)° (Cremer & Pople, 1975), and the lowest displacement asymmetry parameter Δ_S(C1) is 0.013 (1)° (Nardelli, 1983), with atoms O1 and O3 deviating by 0.278 (1) and 0.236 (1) Å from the least-squares plane of the ring. The crystal structure is stabilized by two intermolecular hydrogen bonds (Table 1). The O—H···O and C—H···O bonds each generate centrosymmetric hydrogen-bonded dimers with a cyclic $R_2^2(10)$ ring system (Bernstein *et al.*, 1995).

Experimental

To a stirred solution of ninhydrin (178 mg, 1.0 mmol) and methyl acrylate (2.0 ml) was added DABCO (11 mg, 0.1 mmol), and the solution was stirred at 323–333 K for 1 h. After the removal of methyl acrylate in vacuum, the compound was purified by flash column chromatography using hexane–ethyl acetate (1:1) as the eluant, and the desired compound was isolated in an 86% yield as a white solid. Single crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation of a solution in ethanol.

Crystal data

$C_{13}H_{10}O_5$
M_r = 246.21
Triclinic, $P\overline{1}$
a = 7.1194 (5) Å
b = 8.7236 (4) Å
c = 9.7519 (11) Å
α = 83.838 (8)°
β = 88.921 (8)°
γ = 74.015 (6)°
V = 578.84 (8) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 0.93 mm^{-1}
T = 293 (2) K
0.26 × 0.21 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
2239 measured reflections
2054 independent reflections
1917 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
2 standard reflections
frequency: 60 min
intensity decay: 4%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.114
S = 1.08
2054 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O3^{i}	0.93	2.50	3.431 (2)	174
O2—H2···O1^{ii}	0.82	2.00	2.808 (2)	171

Symmetry codes: (i) $-x+1, -y, -z+2$; (ii) $-x, -y+1, -z+1$.

All H atoms were positioned geometrically and allowed to ride on their parent C atoms, with C—H distances fixed in the range 0.93–0.96 Å and an O—H distance of 0.82 Å, with U_{iso}(H) = 1.5U_{eq}(C,O) for methyl and hydroxy H atoms and U_{iso}(H) = 1.2U_{eq}(C) for other H atoms.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

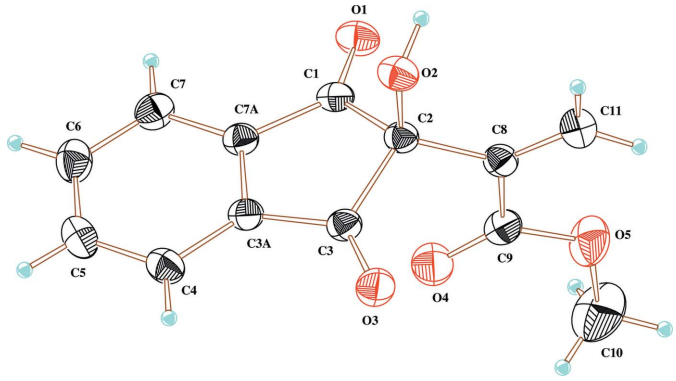


Figure 1
The molecular structure and atom-numbering scheme for (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radius.

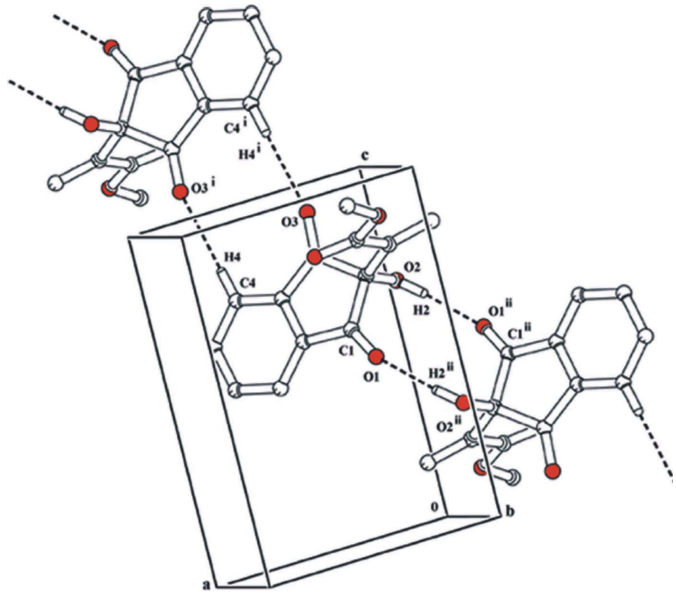


Figure 2
Part of the crystal structure of (I), showing the $R_2^2(10)$ rings. For the sake of clarity, H atoms not participating in the hydrogen bonding have been omitted. Hydrogen bonding is shown as dashed lines. [Symmetry codes: (i) $1-x, -y, 2-z$; (ii) $-x, 1-y, 1-z$.]

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