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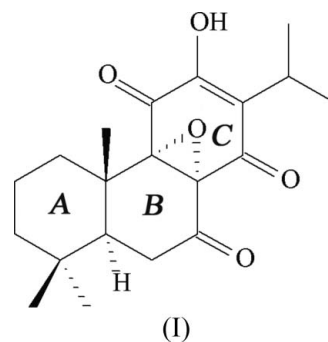
Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å
 R factor = 0.060
 wR factor = 0.152
Data-to-parameter ratio = 9.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.8 α ,9 α -Epoxy-7-oxoroleanonThe title compound, $\text{C}_{20}\text{H}_{26}\text{O}_5$, is a naturally occurring diterpenoid epoxyquinone. Its geometrical parameters are normal. The hydroxy group forms an intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond which links the molecules into infinite chains extended along the b axis.

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Comment

The title compound, (I), was isolated from an Abyssinian *Plectranthus* species (Rüedi, 1984). Recently, we have obtained this compound from *Lycopodium japonicum* Thunb. Here we report its crystal structure.Compound (I) crystallizes in the monoclinic space group $P2_1$ with one molecule in the asymmetric unit (Fig. 1). The geometrical parameters for (I) fall within their expected ranges (Allen *et al.*, 1987). The six-membered ring *A* adopts the usual chair conformation, while ring *B* adopts a twist-boat conformation. Ring *C* is essentially planar with an r.m.s. deviation of 0.042 (2) Å. The dihedral angle between the ring *C* and the three-membered ring C8/C9/O22 is 81.2 (3)°.In the crystal structure, the hydroxy group forms an intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond (Table 21), which links the molecules into infinite chains extended along the b axis (Fig. 2).

Experimental

The air-dried and powdered whole plants (2.0 kg) were extracted with acetone (3×15 l) at room temperature and concentrated *in vacuo* to give a crude extract (50 g), which was directly subjected to column chromatography over MCI-gel CHP-20P, eluting with 95% ethanol. The elute from 95% ethanol (40 g) was concentrated *in vacuo* and then repeatedly subjected to column chromatography over silica gel. Further purification with silica gel column chromatography yielded 8 α ,9 α -epoxy-7-oxoroleanon (3 mg). A single crystal of the title compound was obtained by recrystallization from methanol by slow evaporation at 283 K.

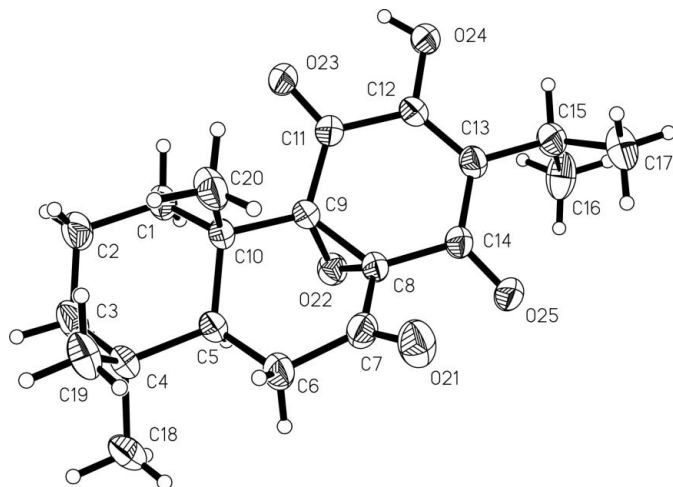


Figure 1
View of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by circles of arbitrary size.

Crystal data

$C_{20}H_{26}O_5$
 $M_r = 346.41$
 Monoclinic, $P2_1$
 $a = 10.336(2) \text{ \AA}$
 $b = 7.4770(15) \text{ \AA}$
 $c = 11.760(2) \text{ \AA}$
 $\beta = 101.61(3)^\circ$
 $V = 890.2(3) \text{ \AA}^3$

$Z = 2$
 $D_x = 1.292 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 0.09 \text{ mm}^{-1}$
 $T = 296(2) \text{ K}$
 Block, yellow
 $0.30 \times 0.20 \times 0.10 \text{ mm}$

Data collection

MAC DIP 2030K diffractometer
 ω scans
 Absorption correction: none
 5289 measured reflections

2066 independent reflections
 1845 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.038$
 $\theta_{max} = 27.1^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.060$
 $wR(F^2) = 0.152$
 $S = 1.09$
 2066 reflections
 227 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.071P)^2 + 0.3757P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.25 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.18 \text{ e \AA}^{-3}$

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O24-H24A\cdots O25^i$	0.82	2.20	2.820 (4)	132

Symmetry code: (i) $x, y - 1, z$.

In the absence of significant anomalous scatterers, Friedel pairs were merged. All H atoms were constrained to an ideal geometry,

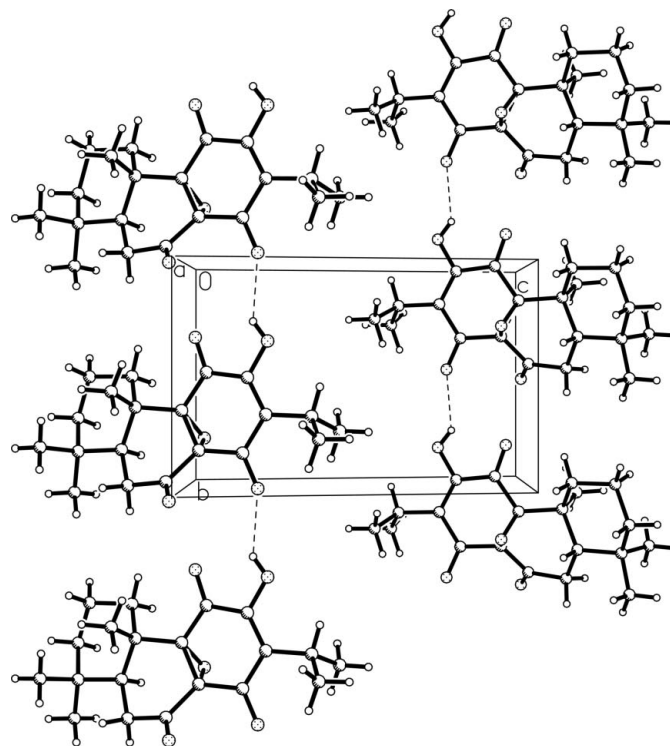


Figure 2
The molecular packing of (I), viewed along the b axis. Dashed lines indicate hydrogen-bonding interactions.

with $C-H = 0.98 \text{ \AA}$ and $U_{iso}(H) = 1.2U_{eq}(C)$ for CH, $C-H = 0.97 \text{ \AA}$ and $U_{iso}(H) = 1.2U_{eq}(C)$ for CH_2 , $C-H = 0.96 \text{ \AA}$ and $U_{iso}(H) = 1.5U_{eq}(C)$ for CH_3 , and $O-H = 0.82 \text{ \AA}$ and $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *DENZO* (Otwinowski & Minor, 1997); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*

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