Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Costuslactone B[1]

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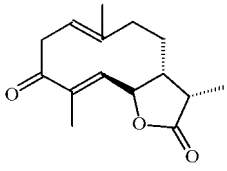
Received 1 April 1999
Accepted 6 December 1999

The crystal structure of 4,10,11α-trimethyl-3-oxocostuslactone, $C_{15}H_{20}O_3$, a new compound isolated from the dried root of *Vladimiria souliei* Liarke, has been determined and the compound has been named costuslactone B. The ten-membered ring takes a slightly distorted boat–chair–chair conformation typical of the substituents.

Comment

This work forms part of a series of studies on traditional Chinese medicinal herbs aimed at looking for bioactive drugs. The title compound, (I), was extracted from the dried root of *Vladimiria soulilei* Liarke, which is widespread in the west of Sichuan province and the south of neighbouring Gansu province. The herb is used in traditional Chinese medicine for relieving uneasiness and stomach ache, and it also has some antitumour function. Similar structures of sesquiterpene lactones have been reported (Breton *et al.*, 1985; Gomez-Rodriguez *et al.*, 1985).



(I)

The configuration shown in the scheme above and in Fig. 1 is the relative configuration. The conformation of the ten-membered ring of (I) is boat–chair–chair and it is slightly distorted owing to the influence of the substituents. The dihedral angles between planes 1 (C3/C2/C4) and 2 (C1/C2/C4/C5), 2 and 3 (C10/C1/C5/C6), 3 and 4 (C9/C10/C6/-C7), and 4 and 5 (C8/C7/C9) are 64.2 (3), 46.2 (1), 63.2 (1) and 62.9 (2)°, respectively. The lactone ring has an envelope conformation.

[1] Systematic name: 3,6,10-trimethyl-2,3,3a,4,5,8,9,11a-octahydrocyclodeca[1,2-*b*]furan-2,9-dione.

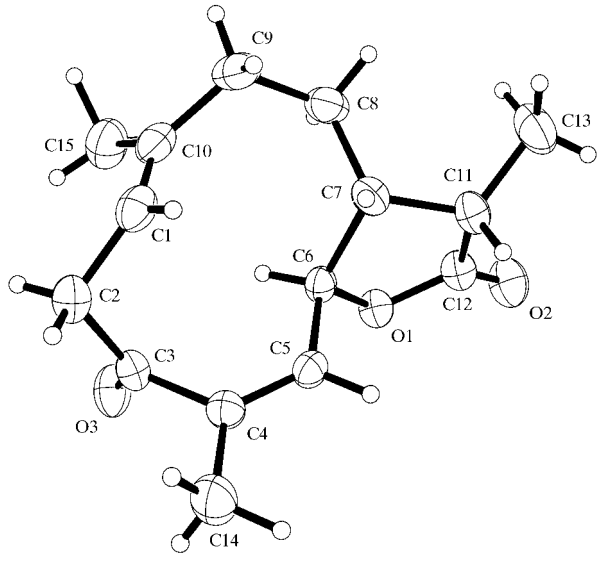


Figure 1
A view of (I) showing the labelling of the non-H atoms. Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as small circles of arbitrary radii.

Experimental

The air-dried powdered roots of *Vladimiria soulilei* Liarke (4.5 kg) were extracted with Et_2O for 7 d. When this Et_2O extract was concentrated, crystals of (I) were precipitated. The experimental sample was recrystallized from ethyl alcohol–acetone mixed solvent.

Crystal data

$C_{15}H_{20}O_3$
M_r = 248.31
Orthorhombic, $P2_12_12_1$
a = 5.553 (1) Å
b = 12.340 (1) Å
c = 20.875 (2) Å
V = 1430.4 (3) Å^3
Z = 4
D_x = 1.153 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–20°
μ = 0.079 mm^{-1}
T = 293 (2) K
Block, colourless
0.5 × 0.5 × 0.4 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
2409 measured reflections
2409 independent reflections
2194 reflections with $I > 2\sigma(I)$
θ_{max} = 30.63°
$h = 0 \rightarrow 7$
$k = 0 \rightarrow 17$
$l = 0 \rightarrow 29$
3 standard reflections
frequency: 60 min
intensity decay: <0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.137
S = 1.239
2409 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0644P)^2 + 0.1316P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.138 e Å^{-3}
$\Delta\rho_{min}$ = −0.137 e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.044 (5)

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1985); cell refinement: *CAD*-4 *Software*; data reduction: *MolEN* (Fair, 1987); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997);

program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL*/*PC* (Siemens, 1994).

Support for this research from the Science Foundation of Lanzhou University is gratefully acknowledged.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: TA1253). Services for accessing these data are described at the back of the journal.

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