Acta Crystallographica Section E

Structure Reports Online

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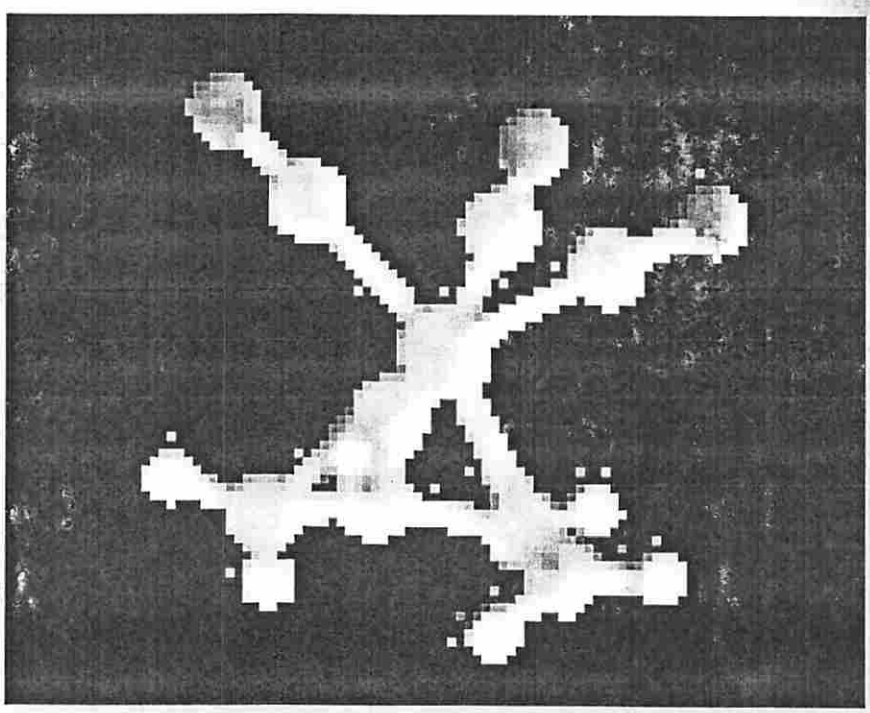

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(20*S*)-Dammar-24-ene-3β,20-diol monohydrate from the bark of *Aglaia exima* (Meliaceae)

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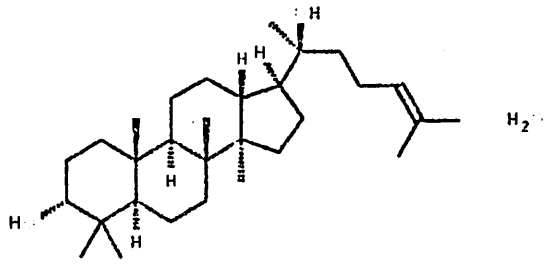
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.077; wR factor = 0.266; data-to-parameter ratio = 44.4.

In the title compound [systematic name: (1*R*,2*R*,5*R*,7*R*,10*R*,-11*R*,14*S*,15*R*)-14-[(2*S*)-2-hydroxy-6-methylhept-5-en-2-yl]-2,6,6,10,11-pentamethyltetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadecan-5-ol monohydrate], $C_{30}H_{52}O_2{\cdot}H_2O$, the three fused cyclohexane rings adopt chair conformations and the hydroxy substituent of one of these occupies an axial position. The fused cyclopentane ring adopts an envelope conformation (with the flap atom being the C atom bearing the methyl group) and the 3-methylbut-2-enyl portion of its substituent is disordered over three sets of sites in a 0.413 (7):0.250 (7):0.337 (7) ratio. The O atoms of both water molecules occupy special positions of 2 site symmetry. In the crystal, O$_s$—H$\cdots$O$_w$ and O$_w$—H$\cdots$O$_s$ (s = steroid and w = water) hydrogen bonds link hydroxy groups and water molecules, forming a three-dimensional network. The crystal studied was found to be a non-merohedral twin with a 0.518 (1):0.482 (1) component ratio.

Related literature

For the isolation of 20*S*-dammar-24-ene-3β,20-diol from other plants, see: Anjaneyulu *et al.* (1985); Bianchini *et al.* (1988); Huang *et al.* (2010); Leonti *et al.* (2004); Pakhathirathien *et al.* (2005); Ukiya *et al.* (2010).



Experimental

Crystal data

$C_{30}H_{52}O_2{\cdot}H_2O$
M_r = 462.73
Tetragonal, $P4_2$
a = 19.9229 (1) Å
c = 7.3302 (1) Å
V = 2909.52 (4) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.50 mm^{-1}
T = 100 K
0.30 × 0.10 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.864, T_{max} = 0.975
11893 measured reflections
15153 independent reflections
14049 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.266
S = 1.15
15153 reflections
341 parameters
45 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Absolute structure: Flack (1983), 2575 Friedel pairs
Flack parameter: 0.1 (3)

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D\cdots A$	D—H$\cdots$$A$
O1—H1$\cdots$O1w	0.84	1.96	2.745 (2)	154
O2—H2$\cdots$O2w	0.84	2.03	2.809 (2)	154
O1w—H1w$\cdots$O2^{i}	0.84	1.88	2.712 (2)	171
O2w—H2w$\cdots$O1^{ii}	0.84	1.95	2.786 (2)	171

Symmetry codes: (i) $-y+1, x+1, z-\frac{1}{4}$; (ii) $-y+1, x, z-\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6931).