



Figure 2. A perspective view of the molecular structure of abruslactone A (**1**). The O atoms are represented by shaded spheres, and all H atoms have been omitted for clarity.

$3\sigma(|F|)$ converged at $R = \Sigma\Delta/\Sigma|F_0| = 0.063$ and $R_w = [\Sigma w\Delta^2/\Sigma w|F_0|^2]^{1/2} = 0.064$, where $\Delta \equiv ||F_0| - |F_c||$ and $w = [\sigma^2(|F_0|) + 0.0005|F_0|^2]^{-1}$.[†] All computations were performed on a DGC Nova 3 minicomputer with the SHELXTL package of crystallographic programs.¹¹ Analytic expressions of complex atomic scattering factors were employed.¹² The final difference map was virtually flat, with residual maxima and minima lying between 0.25 and -0.25 e \AA^{-3} .

The measured molecular dimensions of (**1**) are normal, and molecules related by the 2_1 screw axis parallel to a are linked by O(1)–H . . . O(3') hydrogen bonds (2.872 \AA) to form infinite zigzag chains in the crystal lattice. A perspective view of the stereochemistry of (**1**) is illustrated in Figure 2. The six-membered rings A, B, and D are in the chair form, and C assumes a twist conformation owing to the presence of the ethylenic double bond at C-12 (see torsion angles displayed in the molecular formula). The most notable feature is that ring E adopts a boat conformation, which differs markedly from the usual chair conformation observed in the basic olean-12-ene skeletons of hederagenin,¹³ 3β -acetoxy-olean-12-en-28-oic

acid,¹⁴ sophoradiol,¹⁵ cantoniensistriol,¹⁵ and soyasapogenol B.¹⁶ Examination of a molecular model shows that formation of the γ -lactone ring is facilitated by manipulating ring E into the observed boat conformation.

In the light of the conditions used for its isolation, the new triterpene abruslactone A (**1**) is shown to be present as such in the corresponding naturally occurring saponin rather than derived from the hitherto unknown $3\beta,22\alpha$ -dihydroxy-olean-12-en-29 α -oic acid, which we have subsequently prepared from the alkali hydrolysis of (**1**) with dilute NaOH in MeOH–EtOH.

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[†] The atomic co-ordinates for this work are available on request from the Director of the Cambridge Crystallographic Data Centre, University Chemical Laboratory, Lensfield Rd., Cambridge CB2 1EW. Any request should be accompanied by the full literature citation for this communication. The structure factor table is available as Supplementary Publication No. SUP 23448 (11 pp) from the British Library Lending Division. For details of how to obtain this material, see Notice to Authors No. 7, *J. Chem. Soc., Dalton or Perkin Trans.*, Index Issues.