Structure of 19-Hydroxyneohopane

Kenneth J Haller, *School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima, Thailand*. E-mail: haller@ccs.sut.ac.th

Several fused multicyclic natural product ring systems, especially those that are saturated or nearly saturated, are poorly represented in the Cambridge Structural Database of crystallographic determinations of organic compounds.

19-hydroxyneohopane, $C_{30}H_{48}O$, is one such compound consisting of a five fused ring system (rings 1 to 4 containing six carbons and ring 5 containing five carbons) with two double bonds trans across the 2-3 ring junction. The compound was obtained from the rhizome of *Davallia solida* Sw and crystallizes in the monoclinic space group, $P2_1$, with two molecules in a cell of dimensions: a = 12.587(3), b = 7.558(3), c = 13.620(3) Å, and β = 102.68(3)^o at T = 113(2) K.

Crystal Data: $C_{30}H_{48}O$, MW = 424.68, clear colorless plate crystal, 0.50 x 0.50 x 0.02 mm, monoclinic, $P2_1$, a = 12.587(3), b = 7.558(3), c = 13.620(3) Å, β = 102.68(3)^o, V = 1264.10, Z = 2 T = 113(2) K, d_{calc} = 1.116 Mg m^{-3}, μ = 0.48 mm^{-1}, CuK$_\alpha$ radiation, F(000) = 472., $\sin\theta/\lambda_{max}$ = 0.545 Å^{-1}, R_{int} = 0.0688, 3876 unique data, 3404 observed $F_o > 4s(F_o)$, R_1 = 0.0737, goof = 1.126.

Keywords: fused ring system, natural product, hopane