Access to full text denied by publisher.

Please contact your local library to acquire the following paper:

Citation:

Determining Absolute Configuration by Vibrational Circular Dichroism: (+)-(1S,5S,6S)- and (-)-(1R,5R,6R)-Spiro[4.4]nonane-1,6-diol
J. A. Nieman, B. A. Keay, M. Kubicki, D. Yang, A. Rauk, D. Tsankov, and H. Wieser
pp 1918 – 1919.

Figures:

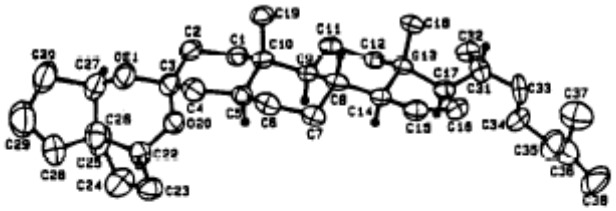


Figure 1. Thermal-ellipsoid representation of ketal **3** as defined by using optically pure (+)-5α-cholestan-3-one. Melting point 122−122.5 °C, orthorombic $P2_12_12$, $a = 41.261(2)$ Å, $b = 12.2083(8)$ Å, $c = 6.4622(4)$ Å, $Z = 4$. The ellipsoids are drawn at the 25% probability level; hydrogen atoms are represented as spheres with an arbitrary radius. Only relevant hydrogen atoms are drawn. The disordered parts are represented by those of larger occupancy factors. Bijvoet analysis was not performed since optically pure ketone **2** was used.

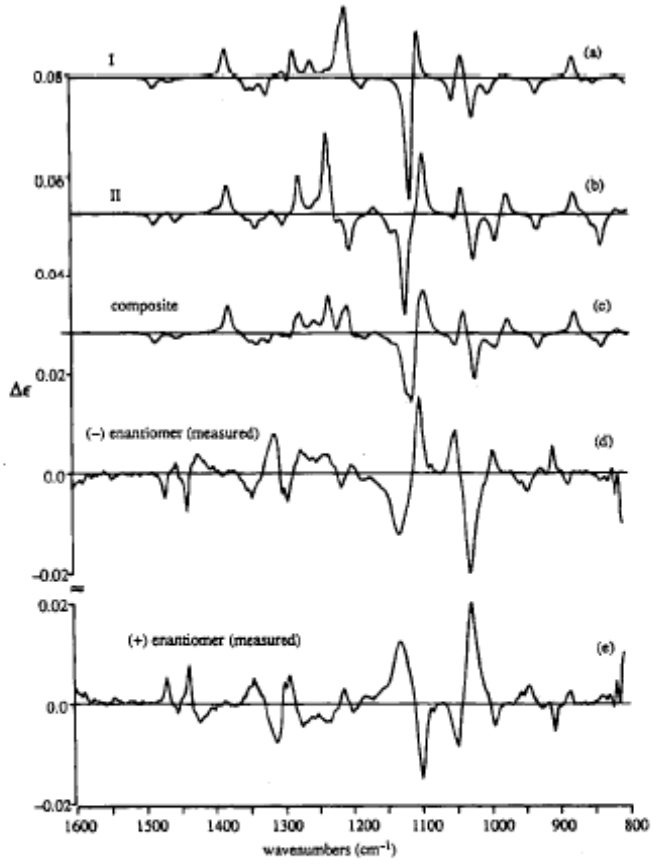


Figure 2. Calculated VCD spectra of (−)-(1*R*,5*R*,6*R*)-spiro-[4.4]nonane-1,6-diol: 6-31G*(0.3) geometry, force field, and atomic polar tensors; 6-31G atomic axial tensors; calculated frequencies scaled by 0.9; Lorentzian line shapes of 5 cm^{-1} half width at half height: (a) conformer I; (b) conformer II; (c) composite of six conformers. Measured VCD spectra of both enantiomers (see text for measurement conditions): (d) (−)-isomer, $[\alpha]23_D = -101.4$ (11.0, absolute ethanol), 100% ee; (e) (+)-isomer, $[\alpha]23_D = +97.1$ (9.0, absolute ethanol), 100% ee (ee as determined by ^1H NMR on the camphor ketal).[6]

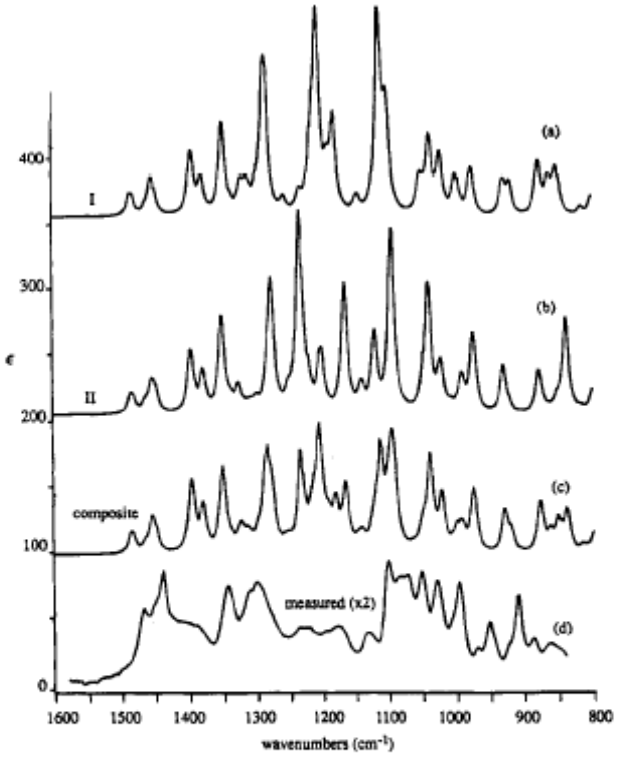
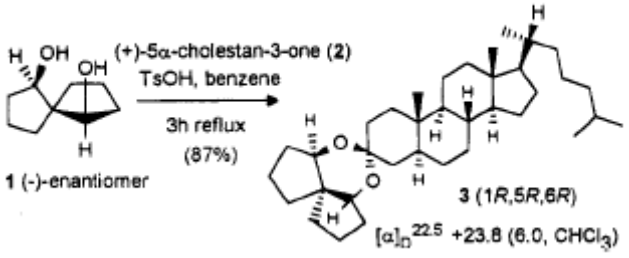


Figure 3. Calculated absorption spectra of spiro[4.4]nonane-1,6-diol; 6-31G*(0.3) geometry, force field, and atomic polar tensors; calculated frequencies scaled by 0.9; Lorentzian line shapes of 5 cm^{-1} half width at half height: (a) conformer I; (b) conformer II; (c) composite of six conformers. Measured absorption spectrum (d); see Figure 2 and text for measurement conditions.

Schemes:

Scheme 1



DOI: 10.1021/jo00112a004