

NMR study of inversion isomerism in some isoxazolidines. Wazeer, Mohammed I. M.; Ali, S. Asrof. Chem. Dep., King Fahd Univ. Pet. Miner., Dhahram, Saudi Arabia. Magnetic Resonance in Chemistry (1993), 31(1), 12-16.

Abstract

Carbon-13 NMR spectra were recorded for two series of isoxazolidines, I (R1, R2, R3, R4 = H, CH2OH, CH2OAc, etc.) (a 5/5 fused system) and II (R1, R2, R3, R4 = H, CH2OH, CH2OAc, CO2Me, etc.) (a 6/5 fused system), over the temp. range -100 to +60°. Whereas all the compds. in series I existed solely as one isomer throughout this temp. range, some compds. in series II showed the presence of two isomers of unequal population at low temps. The major isomer was the trans conformer, which is in equil. with the minor isomer (cis conformer) through a relatively slow nitrogen inversion. The monosubstituted isoxazolidine II having endo substituents at either C-2 or C-3 and 2,3-di- and 2,3,3-trisubstituted compds. showed the presence of only one isomer throughout the temp. range. The barriers to nitrogen inversion were detd. by band shape anal. and were in the range 65.2-69.0 kJ mol⁻¹.

