

Conformational Analysis of Substituted Perhydro-1,2-oxazolo[3,2-c][1,4]oxazines by NMR Spectroscopy

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ABSTRACT

The ^{13}C NMR spectra of most of the substituted perhydro-1,2-oxazolo[3,2-c][1,4]oxazines (3) at low temp. showed the presence of two isomers of unequal populations. The major isomer is shown to be the cis isomer {except in 2-hydroxymethyl-2-methylperhydro-1,2-oxazolo[3,2-c][1,4]oxazine (3e)}, which is in equil. with the minor isomer (trans conformer) by a relatively slow nitrogen inversion. Intramol. hydrogen bonding in oxazines, having 2-hydroxymethyl substituents, is shown to be an important factor in detg. the population ratio of the two isomers. The barrier to nitrogen inversion was detd. by detailed band-shape anal. of proton and carbon NMR spectra and were in the range 66.3-72.9 kJ mol⁻¹. The chair inversion had been slowed down, in one case, trans-dimethylperhydro-1,2-oxazol[3,2-c][1,4]oxazine-2,3-dicarboxylate (3j), to show the presence of the two forms of the cis isomers. The barrier to chair inversion is 41.5 kJ mol⁻¹ as detd. by proton NMR band-shape anal. of 3j.