NMR study of inversion isomerism in 1-oxa-10-azabicyclo[5.3.0]decanes. Wazeer, Mohammed I. M.; Ali, S. Asrof. Chem. Dep., King Fahd Univ. Pet. Miner., Dhahran, Saudi Arabia. Canadian Journal of Applied Spectroscopy (1993), 38(1), 22-5. Publisher: Polyscience Publications, Inc.

Abstract

The NMR spectra of title compds. I (R1, R2 = H, Ph, CH2OH, OEt, CO2Me; R3, R4 = H, CO2Me, CO2Et) showed the presence of two isomers of unequal populations at -40°. The major isomer is the trans conformer, which is in equil. with the cis conformer by a relatively slow nitrogen inversion process. The barriers to nitrogen inversion were detd. by NMR band shape anal. and were in the 53-56 kJ/mol-1 range.

$$\begin{array}{c|c}
 & R^3 \\
 & R^4 \\
 & R^2 \\
 & I
\end{array}$$