

NMR study of nitrogen inversion process in some isoxazolidines. Wazeer, Mohammed I. M.; Ali, Sk. Asrof. Chemistry Dep., King Fahd Univ. Petroleum and Minerals, Dhahran, Saudi Arabia. Canadian Journal of Applied Spectroscopy (1995), 40(2), 53-60. Publisher: Polyscience Publications, Inc.

Abstract

A series of isoxazolidines I and II ($R_1 = \text{Me, CHMe}_2, \text{CMe}_3, \text{CH}_2\text{Ph, Ph}$, $R_2 = \text{H, Et}$, $R_3 = \text{H, CO}_2\text{Me, Me}$, $R_4 = \text{H, Me, CO}_2\text{Me}$, $R_5 = \text{CH}_2\text{OH, CH}_2\text{OSiMe}_2\text{CMe}_3, \text{Ph, CH}_2\text{CH}_2\text{OH, Ph, CO}_2\text{Me}$) with substituents at various ring positions has been synthesized and their NMR spectra recorded over a range of temps. The NMR spectra at low temps. indicate the presence of two isomers due to slow nitrogen inversion, except in I ($R_1 = \text{Ph, } R_2 = R_3 = R_4 = \text{H, } R_5 = \text{Ph}$; $R_1 = \text{CHMe}_2, R_2 = \text{Et, } R_3 = R_4 = \text{H, } R_5 = \text{Ph}$) and II ($R_1 = \text{CHMe}_2, R_2 = \text{Et, } R_3 = R_5 = \text{H, } R_4 = \text{Ph}$). The nitrogen inversion barriers are detd. using complete line-shape anal., and their dependence on solvent and steric factors is discussed. For the isoxazolidines with substitutions at the 2,5 and 2,3 positions, the trans compds. become the major and the sole isomer, resp.

