NMR study of the anomeric effect and nitrogen inversion in some isoxazolidines. Ali, Sk. Asrof; Hassan, Azfar; Wazeer, Mohammed I. M.. Chemistry Dep., King Fahd Univ. Petroleum and Minerals, Dhahran, Saudi Arabia. Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (1995), 51A(13), 2279-87. Publisher: Elsevier.

Abstract

A series of isoxazolidines with various alkyl substituents at N and an ethoxy group at C(5) have been synthesized and their NMR spectra recorded over a range of temps. The NMR spectra at low temp. indicate the presence of two isomers due to slow nitrogen inversion. The nitrogen inversion barriers are detd. using complete band shape anal. and are found to be in the range 59.3-65.6 kJ mol-1. The strong anomeric effect exerted by the C(5) ethoxy group locks the substituent in the pseudoaxial orientation. The cis isomers are found to be more stable than the trans isomers.