

Conformational assignments and a nitrogen inversion process in some 3-acyloxy-1,3-oxazinanes by NMR and X-ray analysis. Hashmi, Syed M. A.; Wazeer, Mohammed I. M.; Hussain, M. Sakhawat; Reibenspies, Joseph H.; Perzanowski, Herman P.; Ali, Sk. Asrof. Chemistry Department, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1999), (4), 877-884. Publisher: Royal Society of Chemistry

Abstract

The stereochem. of the preferred conformers of several 3-acyloxy-1,3-oxazinanes has been established by NMR spectroscopy. A strong anomeric effect stabilizes the conformation having an equatorial orientation of the lone pair on nitrogen. A nitrogen inversion process was found to be the rate-limiting process in the conformational equil. The range of ΔG values was found to be 60-71 kJ mol⁻¹. Solid state structures as detd. by X-ray diffraction confirm the findings of the NMR study.