An NMR study of conformational behaviour and nitrogen inversion process in 3-acyloxytetrahydro-1,3-oxazines

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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 DG .dbldag. 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.