Nitrogen inversion and N-O bond rotation in some hydroxylamine and isoxazolidine derivatives.

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Abstract

A series of trisubstituted hydroxylamine derivs., both cyclic and acyclic, has been prepd. The energy barriers in these hydroxylamines are found to be dominated either by nitrogen inversion or N-O bond rotation depending on the nature of the substituents attached to the nitrogen. In several series of compds., having XC6H4CH2 substituents attached to nitrogen, Hammett free energy correlations are obtained with pos. ρ values, indicating increased electron d. at the transition state for the inversion process. Isoxazolidines with C(5) ethoxy substituents demonstrate a strong anomeric effect.