Nitrogen inversion and N-O bond rotation processes in di- and trisubstituted hydroxylamines. A dynamic NMR study. Ali, Sk. Asrof; Hassan, Azfar; Wazeer, Mohammed I. M.. Chem. Dep., King Fahd Univ. Petr. Minerals, Dhahran, Saudi Arabia. Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1996), (7), 1479-1483. Publisher: Royal Society of Chemistry.

Abstract

The barriers to inversion in several acyclic di- and trisubstituted hydroxylamines are detd. by 1H NMR band shape anal. The barriers range from 49.1 to 66.8 kJ mol-1 and are discussed in terms of a conformational process which involves nitrogen inversion and rotation around the N-O bond. The N-benzyl group with an ortho hydroxy substituent increases the nitrogen inversion barrier by 10 kJ mol-1, which indicates the requirement of breaking of the intramol. hydrogen bond prior to inversion.