Solid state NMR study of 1,3-imidazolidine-2-thione, 1,3-imidazolidine-2-selenone and some of their N-substituted derivatives. Wazeer, Mohamed I. M.; Isab, Anvarhusein A.; El-Rayyes, Ali. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Spectroscopy (Amsterdam, Netherlands) (2004), 18(1), 113-119.

Abstract

Solid-state NMR spectra were recorded for 1,3-imidazolidine-2-thione, 1,3-imidazolidine-2selenone and some of their N-substituted derivs. Spinning side-bands of thione and selenone carbons were analyzed to yield chem. shift anisotropies for these carbons. The NMR spectrum of imidazolidine-2-thione (Imt) showed some evidence for the presence of thiol tautomer. Mol. computations were carried out for Imt and its N-Me deriv. to yield relative energies of various tautomers.