A Molecular Orbital Treatment of the Electronic Structure and Spectra of Aryl Nitrones.

S. G. Aziz, Hassan Al-Bar and Rifaat Hilal, J. King Abdulaziz University (Science), Vol. 7, (1995) 47-56.

Abstract

The electronic structures of some aryl nitrones have been investigate using the MNDO-MO method. Equilibrium geometries, and charge density distribution have been computed. Various electronic differences between nitrones and the corresponding imines have been analyzed and discussed. The electronic absorption spectra of the studied nitrones have been analyzed and interpreted using the result of MO computation. Charge density distribution, dipole moments and the extent of delocalizedion of the MO's were used to interpret the observed solvent effects. Comparison between the spectra of aryl nitrones and that of the corresponding imines led to conclusions regarding the structural differences between the tow classes of compounds.