

ELECTRONIC AND NMR SPECTRA OF SOME PYRAZINES AND THEIR N-OXIDES

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The electronic structures of some pyrazines including their N-oxides were systematically investigated by means of the modified CNDO/2 or INDO method. The results of these calculations were compared with the experimental results. The modified CNDO/2 method gives a reasonable interpretation of the electronic spectra of some pyrazines. The calculated chemical shifts obtained with an INDO method nearly reproduced the experimental shifts. Also, the electronic structure of these compounds is discussed.