ROTATIONAL SPECTRA AND NUCLEAR QUADRUPOLE COUPLING CONSTANTS OF IODOIMIDAZOLES

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The microwave spectra of two isomers of iodoimidazole have been recorded and assigned with resolution of their nuclear quadrupole coupling constants. These constants have been analysed in terms of the conjugation between the lone pairs on the iodine atom and the aromatic π -bonding system, and the effect of this conjugation on the distribution of π -electron density in the ring. A comparison of these properties has been made between iodoimidazole and other 5- and 6-membered aromatic rings bonded to halogen atoms.