THE RADIO SPECTRA AND -VE INERTIAL DEFECTS BEHAVIOR OF PLANAR AROMATIC HETEROCYCLES

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The simplest tricyclic aromatic nitrogen heterocyclic molecules 5,6 benzoquinoline and 7,8 benzoquinoline are possible candidates for detection of aromatic systems in the interstellar medium. Therefore the pure rotational spectra have been recorded using frequency-scanned Stark modulated, jet-cooled millimetre wave absorption spectroscopy (48-87 GHz) and Fourier Transform Microwave (FT MW) spectroscopy (2-26 GHz) of a supersonic rotationally cold molecular jet. Guided by ab initio molecular orbital predictions, spectral analysis of mm wave spectra, and higher resolution FT MW spectroscopy provided accurate rotational and centrifugal distortion constants together with 14N nuclear quadrupole coupling constants for both species. The determined inertial defects, along with those of similar species are used to develop an empirical formula for calculation of inertial defects of aromatic ring systems. The predictive ability of the formula is shown to be excellent for planar species with a number of pronounced out of plane vibrations. The resultant constants are of sufficient accuracy to be used in potential astrophysical searches.[a]

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