THE STRUCTURE OF 1,2-DICYANOCYCLOBUTENE FROM MICROWAVE SPECTROSCOPY, ELECTRON DIFFRACTION AND AB INITIO CALCULATIONS.

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The microwave spectrum of 1,2-dicyanocyclobutene has been investigated by microwave Stark spectroscopy in the 11.0 - 34.0 GHz in Oslo. The normal species, the $^{15}N^{14}N$ and the ^{13}C isotopic species have been observed by molecular beam microwave Fourier transform spectroscopy in Lille. Hyperfine structures have been resolved and the quadrupole coupling constants have been determined. The molecule is found to have a symmetry plane (Cs symmetry). This structure is in good agreement with the ab initio structure, calculated at the MP2 6-311G** level, and the structure determined by electron diffraction experiments.