ROTATIONALLY RESOLVED ELECTRONIC SPECTRA OF 2,6-DIAMINOPYRIDINE: A FOUR-FOLD BARRIER PROBLEM[a]

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High resolution, rotationally resolved electronic spectra of four bands of 2,6-diaminopyridine were obtained. They were found to have zigzagging inertial defects that point to a double minimum excited state potential energy surface along the amino group inversion coordinate. The possibility of two isomers, differing in the position of the amino group hydrogens above or below the plane of the ring, leads to a four-fold barrier problem. The observed spectra, in combination with high level ab initio calculations, make it possible to distinguish which of the species is the more stable form, and provide information about the barrier heights that govern their interconversion.

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