MICROWAVE SPECTRUM AND STRUCTURE OF THE 2,6-DIFLUOROPYRIDINE-CO_2 COMPLEX

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The microwave spectrum of the weakly bound complex formed from 2,6-difluoropyridine and CO_2 has been obtained using the Amherst broadband microwave spectrometer. Preliminary analysis indicates a structure in which the nitrogen of the 2,6-difluoropyridine is directed toward the carbon of the CO_2. However, unlike the related complex pyridine-CO_2, which is planar, the CO_2 is rotated out of the plane of the heterocycle. The nitrogen-carbon van der Waals distance is 2.916 Å, significantly larger than the 2.7977(64) Å value previously reported for pyridine-CO_2. *Ab initio* calculations at the MP2/6-311++G(2d,2p) level support a nitrogen bound geometry, but indicate an equilibrium structure in which the CO_2 lies off the C_2 axis of the 2,6-difluoropyridine. One dimensional discrete variable representation (DVR) calculations using an *ab initio* potential restricted to rotation of CO_2 about the C_2 axis of the difluoropyridine indicate that the complex is in the high-barrier limit to internal rotation and that no splittings due to internal rotation will be observed in the spectrum.