RITZ ASSIGNMENT AND EVALUATION OF THE WATSONIAN PARAMETERS FOR THE ν_1 N−H STRETCHING BAND OF DIFLUOROMETHANIMINE, F_2C=NH

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Difluoromethanimine, F_2C=NH, is a planar, asymmetric rotor close to the oblate symmetric top limit, with $\kappa = 0.8928$. The first successful synthesis of this molecule was carried out by Bürger and Pawelke[a] in 1988. In the present work we present an investigation of the in-plane ν_1 fundamental, N−H stretching, centered at 3042.3 cm^{-1}; this band, of symmetry species A', presents a hybrid *ab*-type contour with a prominent Q head and wide P and R branches. The difficulties encountered in the assignment of this band are due both to systematic line overlappings and to interactions with dark states — consisting of combination bands in which at least three vibrational quanta are involved — these interactions being particularly strong for $13 \leq K_c \leq 16$. The capabilities of the "Multi-Molecule Ritz Program", presented at this conference in 1996,[b] have been enhanced by adding a "feed-back loop" which calculates the best-fit Watsonian parameters directly from the Ritz data-base. This has led to a list of approximately 2300 assigned lines belonging to the investigated band. These assignments, and the perturbations encountered, will be discussed.

[a] H. Bürger and G. Pawelke, J. Chem. Soc., Chem. Commun., 1988, 105

[b] G. Moruzzi, Ohio State University 51st International Symposium on Molecular Spectroscopy, TC06, p. 119 (1996).