

## INTERNAL ROTATION IN THE NITROGEN COMPLEX OF 1,4-DIFLUOROBENZENE

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The rotationally resolved  $S_1 \leftarrow S_0$  spectrum of the 1,4-difluorobenzene- $N_2$  van der Waals complex has been measured by Kang and Pratt<sup>a</sup>. Due to internal motion, the spectrum is split into two subbands, of which only the stronger one can be fit with a rigid rotor Hamiltonian. The analysis of the stronger subband has revealed that  $N_2$  is located above the ring plane of 1,4-difluorobenzene.

In order to obtain information about the internal motion, both subbands were analyzed with a semirigid  $C_{2v}$  frame- $C_{2v}$  top internal rotor model<sup>b</sup>. Upper limits of  $20 \text{ cm}^{-1}$  ( $S_0$ ) and  $6 \text{ cm}^{-1}$  ( $S_1$ ) for the barriers hindering  $N_2$  internal rotation have been obtained. Details about the problems in determining the equilibrium orientation and about implication on the structure determination will be discussed.

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<sup>a</sup>Ch. Kang and D. W. Pratt, 54th International Symposium on Molecular Spectroscopy, OSU, Columbus, paper WJ12, 1999.

<sup>b</sup>M. Schäfer, J. Chem. Phys. **115**, 11139 (2001).