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[a]. 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[b]. Upper limits of 20 cm^{-1} (S_0) and 6 cm^{-1} (S_1) for the barriers hindering N_2 internal rotation have been obtained. Details about the problems in determing the equilibrium orientation and about implication on the structure determination will be discussed.

[a] Ch. Kang and D. W. Pratt, 54th International Symposium on Molecular Spectroscopy, OSU, Columbus, paper WJ12, 1999.
[b] M. Schäfer, J. Chem. Phys. **115**, 11139 (2001).