THE MICROWAVE SPECTRA OF FLUOROBENZENE$\cdots$H$_2$O AND 1,4-DIFLUOROBENZENE$\cdots$H$_2$O: STRUCTURE AND INTERNAL ROTATION ANALYSIS[a]

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Large amplitude motions often occur in weakly bound molecular dimers because the attractive forces involved are at least an order of magnitude smaller than those in chemically bound species. These motions can have noticeable effects on the rotational spectra as obtained by FTMW spectroscopy. In the case of the 1,4-difluorobenzene$\cdots$ H$_2$O dimer a small splitting of the rotational transitions can be observed which can be interpreted as the result of a hindered rotation of the water moiety about its C_2 axis. The two transitions then correspond to the $\sigma = 0$ and the $\sigma = 1$ component of the ground internal rotor state, respectively. A similar splitting was also observed in the newly assigned microwave spectrum of the fluorobenzene$\cdots$ H$_2$O dimer, suggesting that the corresponding interaction potentials share common features. In order to achieve a better understanding of the resulting intermolecular dynamics we used the flexible model developed by Meyer[b] to analyse the experimental data. This model yields a potential function for the internal rotation and effective rotational constants for the respective internal rotor states.
The results of the analysis and a comparison with the data obtained from high level *ab initio* calculations will be presented.

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[b] R. Meyer, *J. Mol. Spectrosc.* **76**, 266 (1979)