THE MICROWAVE SPECTRA AND STRUCTURE OF THE 1,4-DIFLUOROBENZENE· · ·WATER DIMER

KAI BRENDEL AND HEINRICH MÄDER, *Institut für Physikalische Chemie, Universität Kiel, Olshausenstr. 40, D-24098 Kiel, Germany*.

We report the microwave spectra of the 1,4-difluorobenzene· · ·water dimer in the frequency region 3-20 GHz which were recorded using a pulsed molecular beam Fourier transform microwave spectrometer with a confocal Fabry-Perot resonator.
This dimer of a doubly fluorinated organic ring compound with water is of special interest as different structures may result from various types of intermolecular interaction.
In the case of the benzene· · ·water dimer, a microwave study yielded a structure where the water is located above the ring corresponding to a π-type interaction[a]. However, *ab initio* calculations performed for 1,4-difluorobenzene· · ·water by Brutschy and co-workers[b] predict in addition to this π-type structure a slightly more stable so-called σ-type structure which results from the formation of two H-bonds (water hydrogen and fluorine, water oxygen and benzene hydrogen) and leads to a planar configuration of the dimer.
Our results support the theoretical predictions and are in good agreement with the experimental results from fluorescence excitation spectroscopy which were presented earlier by C. Kang and D.W. Pratt[c].
The structure, refined rotational constants and the results of the analysis of the observed splittings of the rotational transitions will be presented.

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[a] H.S. Gutowsky, T. Emilsson, and E. Arunan, *J. Chem. Phys.* **99**, 4883 (1993).
[b] P. Tarakeshwar, Kwang S. Kim, B. Brutschy, *J. Chem. Phys.* **110**, 8501 (1999).
[c] Cheolhwa Kang and David W. Pratt, *55th International Symposium on Molecular Spectroscopy*, **RB06** (2000).