LARGE OLIGOMERS STABILIZED BY WHB NETWORKS: PENTAMERS OF DIFLUOROMETHANE AND ITS WATER CLUSTERS

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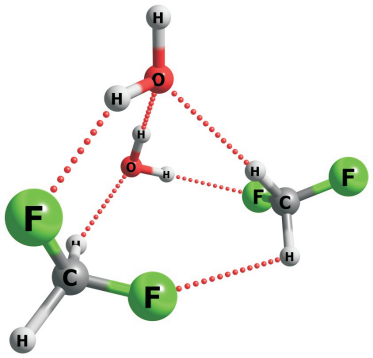

Microwave spectroscopy has been restricted to the investigation of small molecules in the last years. However, with the advent of FTMW and CP-FTMW spectroscopies coupled with laser vaporization techniques it has turned into a very competitive methodology in the studies of moderate-size molecules. In particular, the studies of relatively large molecular aggregates[a,b] are very interesting, being a bridge between microsystems and molecular bulk.

Here, we present the study of two pentarmers of difluoromethane $(CH_2F_2)_5$ and the water clusters $(CH_2F_2)_1\cdots(H_2O)_2$, $(CH_2F_2)_2\cdots(H_2O)_1$ and $(CH_2F_2)_2\cdots(H_2O)_2$ stabilized by weak hydrogen bonds networks (O-H···F, C-H···F and C-H···O interactions). The experiments were carried out in the CP-FTMW spectrometers of Bilbao (Spain)[c] and Virginia (USA). In addition, the experimental work was supported by theoretical calculations. The force fields were specifically parameterized for reproduce others oligomers where WHB interactions play a crucial role.

[a] T. Tang, Y. Xu, A. R. W. McKellar and W. Jäger, *Science* **29**, 297, 2002.
[b] C. Pérez, M. T. Muckle, D. P. Zaleski, N. A. Seifert, B. Temelso, G. H. Shields, Z. Kisiel and B. H. Pate, *Science* **336**, 897, 2012.
[c] I. Uriarte, C. Pérez, E. Caballero-Mancebo, F. J. Basterretxea, A. Lesarri, J. A. Fernández and E. J. Cocinero *Chem. Eur. J.* in press, 2017.