OLIGOMERS BASED ON A WEAK HYDROGEN BOND NETWORK: THE ROTATIONAL SPECTRUM OF THE TETRAMER OF DIFLUOROMETHANE

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Following the investigation of the rotational spectra of three conformers (so-called "book", "prism" and "cage") of the water hexamer, and of some other water oligomers, [a] we report here the rotational spectrum of the tetramer of a freon molecule.
The pulse jet Fourier transform microwave (pj-FTMW) spectrum of an isomer of the difluoromethane tetramer has been assigned. This molecular system is made of units of a relatively heavy asymmetric rotor, held together by a network of weak hydrogen bonds. The search of the rotational spectrum has been based on a high-level reference method, the CCSD(T)/CBS protocol.
It is interesting to outline that the rotational spectrum of the water tetramer was not observed, probably because the minimum energy structures of this oligomer is effectively nonpolar in its ground states, or because of high energy tunnelling splittings.
The rotational spectra of the monomer, dimer, trimer and tetramer of difluoromethane have been assigned in 1952, [b] 1999, [c] 2007, [d] and 2013 (present work), with a decreasing time spacing between the various steps, looking then promising for a continuous and rapid extension of the size limits of molecular systems accessible to MW spectroscopy.

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