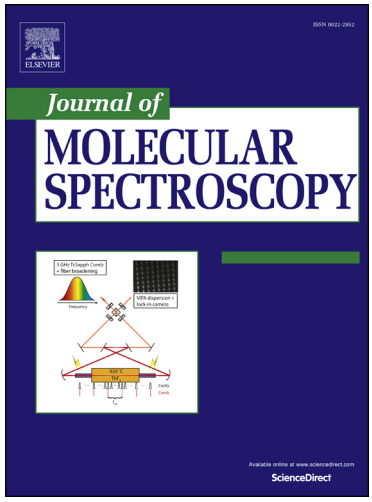

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On the competition between weak O-H···F and C-H···F hydrogen bonds, in cooperation with C-H···O contacts, in the difluoromethane – *tert*-butyl alcohol cluster

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Abstract

The 1:1 complex of tert-butyl alcohol with difluoromethane has been characterized by means of a joint experimental-computational investigation. Its rotational spectrum has been recorded by using a pulsed-jet Fourier-Transform microwave spectrometer. The experimental work has been guided and supported by accurate quantum-chemical calculations. In particular, the computed potential energy landscape pointed out the formation of three stable isomers. However, the very low interconversion barriers explain why only one isomer, showing one O-H···F and two C-H···O weak hydrogen bonds, has been experimentally characterized. The effect of the H → *tert*-butyl- group substitution has been analyzed from the comparison to the difluoromethane-water adduct.

Keywords: Weak hydrogen bonds; rotational spectroscopy; quantum chemistry; DFT calculations; Non-covalent interactions.

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