

## Accepted Manuscript

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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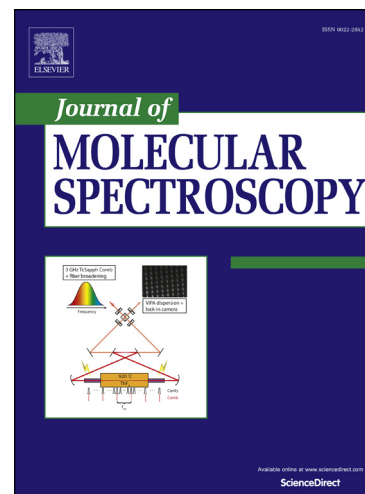
PII: S0022-2852(17)30058-9  
DOI: <http://dx.doi.org/10.1016/j.jms.2017.04.001>  
Reference: YJMSP 10876

To appear in: *Journal of Molecular Spectroscopy*

Received Date: 30 January 2017  
Revised Date: 13 March 2017  
Accepted Date: 1 April 2017

Please cite this article as: L. Spada, N. Tasinato, G. Bosi, F. Vazart, V. Barone, C. Puzzarini, 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, *Journal of Molecular Spectroscopy* (2017), doi: <http://dx.doi.org/10.1016/j.jms.2017.04.001>

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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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