SIZING THE UBBELHODE EFFECT: THE ROTATIONAL SPECTRUM OF *TERT*-BUTYLALCOHOL DIMER

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We measured the molecular beam Fourier transform microwave spectra of four isotopic species of of the dimer of *tert*-butanol, that is C_4H_9-OH$\cdots$O(H)-C_4H_9, C_4H_9-OH$\cdots$O(D)-C_4H_9, C_4H_9-OD$\cdots$O(H)-C_4H_9, and C_4H_9-OD$\cdots$O(D)-C_4H_9. We observed that the H – D isotopic substitution of the hydroxylic hydrogen participating in the O-H$\cdots$O Hydrogen bond in the *tert*-butanol dimer produces an increase of the B and C rotational constants, according to the shrinkage of the O$\cdots$O distance, underlying and sizing the associated Ubbelhode effect.[a] The conformation and structure of the complex, and an estimation of the Ubbelhode effect have been obtained by combining the experimental data with the results of MP2/6-311++G** ab initio calculations.

[a] A. R. Ubbelhode, K. J. Gallagher, *Acta Crystallogr.* , 1955, 8, 71