

## 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 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 Ubbelohde effect.<sup>a</sup> The conformation and structure of the complex, and an estimation of the Ubbelohde effect have been obtained by combining the experimental data with the results of MP2/6-311++G\*\* ab initio calculations.

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<sup>a</sup>A. R. Ubbelohde, K. J. Gallagher, *Acta Crystallogr.*, 1955, 8, 71