SUPPLEMENT

Chirality-dependent balance between hydrogen bonding and London dispersion in isolated (±)-1-indanol clusters

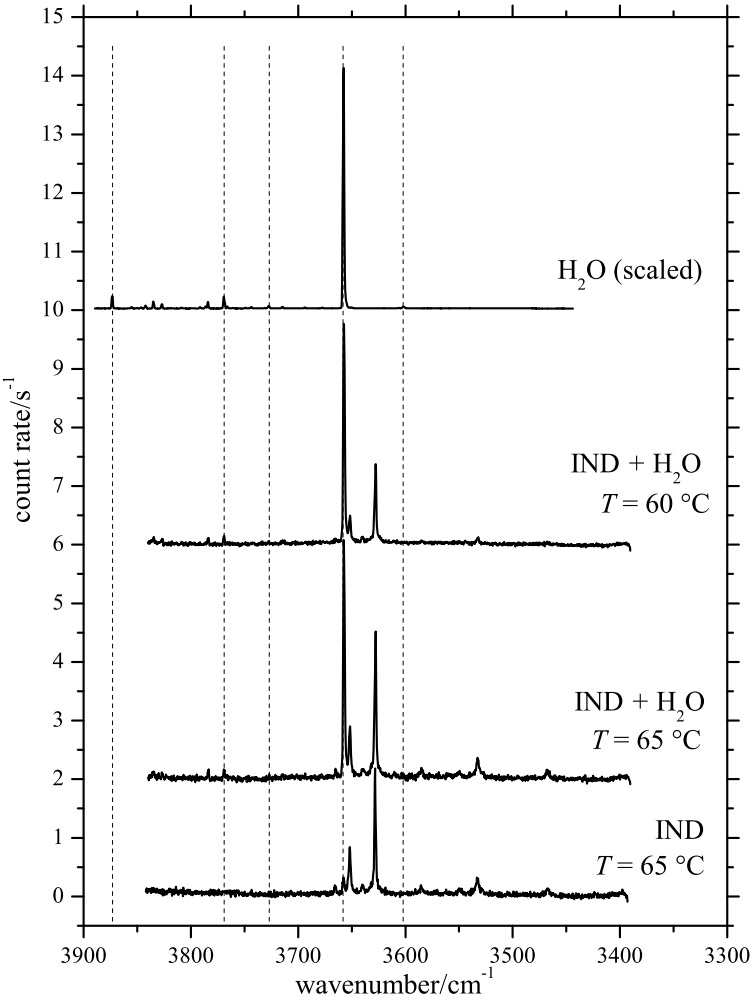
Jonas Altnöder[a], Aude Bouchet[b,c], Juhyon J. Lee[a], Katharina E. Otto[a], Martin A. Suhm[a,*], Anne Zehnacker-Rentien[b,c,*]

a) Institut für Physikalische Chemie, Universität Göttingen, Tammannstr. 6, 37077 Göttingen, Germany;

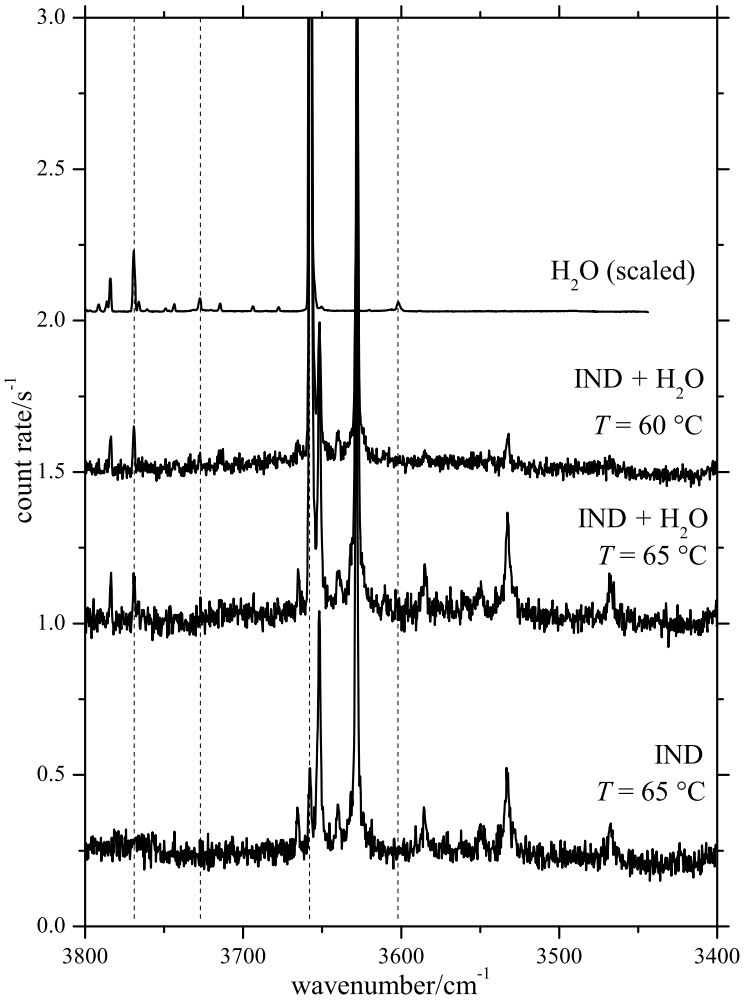
b) Institut des Sciences Moléculaires d'Orsay, Université Paris-Sud, France;

c) CLUPS (Centre Laser de l'Université Paris Sud/LUMAT FR 2764), Univ Paris-Sud, Orsay, F-91405, France

*corresponding authors (msuhm@gwdg.de, anne.zehnacker-rentien@u-psud.fr)



S 1: Raman jet spectra of enantiopure 1-indanol (sample temperature T, nozzle temperature 100 °C) in helium with and without deliberately added water. Some important water monomer bands are marked with vertical dashed lines. The pure water spectrum (sample/nozzle temperature 10/120 °C) is scaled to similar water content as the mixed ones.



S 2: Raman jet spectra of enantiopure 1-indanol with and without deliberately added water; same spectra as in S 1, vertical scale optimized for interpreting small bands. Some important water monomer bands are marked with vertical dashed lines.

structure	dispersion type	B97D-opt	B3LYPD3-opt	Δ
eq	E_{D2}	–64.1	–64.0	–0.2
	E_{D3}	–39.3	–39.5	0.1
ax	E_{D2}	–63.7	–63.6	–0.1
	E_{D3}	–39.2	–39.3	0.1
HetOΠ	E_{D2}	–187.0	–182.8	–4.2
	E_{D3}	–125.1	–123.4	–1.7
HomΠΠ	E_{D2}	–192.1	–184.4	–7.7
	E_{D3}	–126.8	–123.7	–3.1
HomOΠ	E_{D2}	–190.2	–185.6	–4.6
	E_{D3}	–126.7	–124.8	–2.0

S 3: Analysis of absolute dispersion corrections as a function of the correction type (E_{D2},E_{D3}) and the molecule/dimer structure (B97D-optimized or B3LYP-D3-optimized) in kJ/mol.