

Simulation of Raman optical activity of multi-component monosaccharide samples

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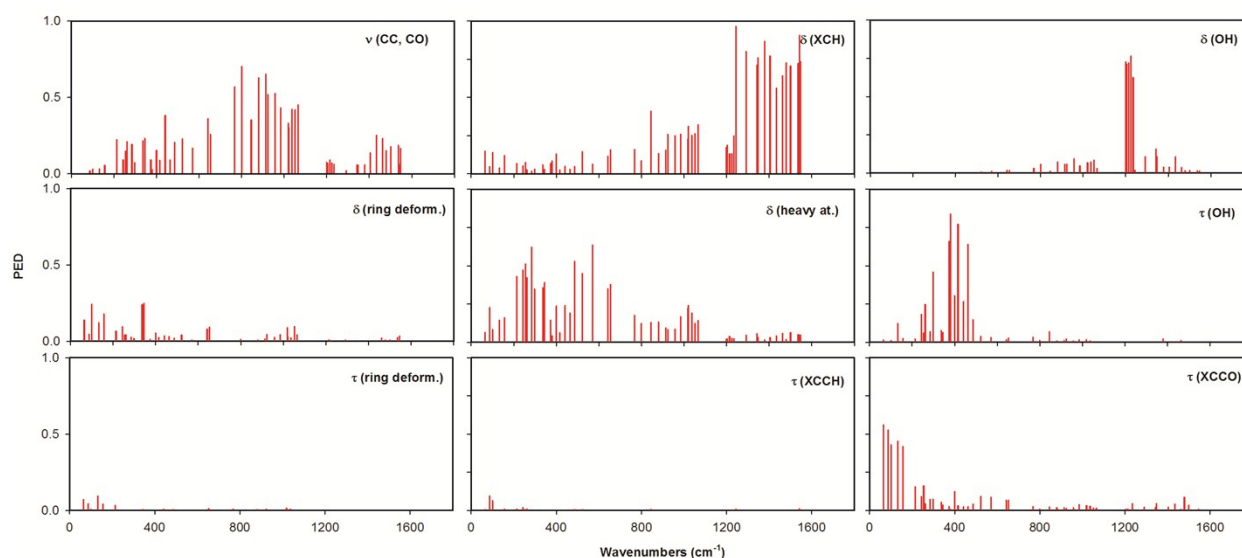


Fig. S1. Calculated (B3LYP/6-311++G**/CPCM) relative potential energy distributions (PED) of selected stretching (ν), bending (δ), and torsion (τ) coordinates in **DG** vibrations.

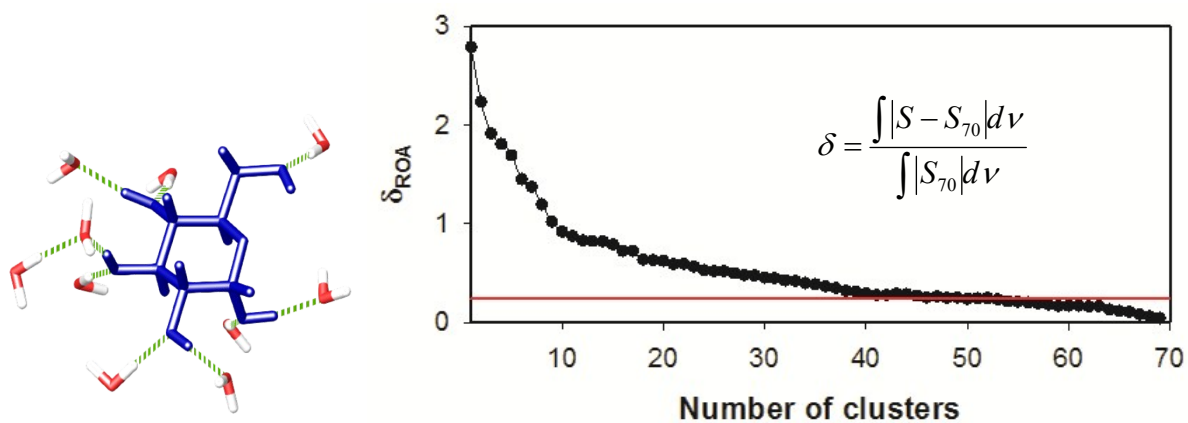


Fig. S2. Example of a cluster of α -D-glucose with water molecules, and dependence of ROA spectral error (in %) on the number of averaged snapshots, preselected from 1000 ones by the parallel variable selection approach (J. Kessler, M. Dračinský and P. Bouř, *J. Comput. Chem.*, 2012, **34**, 366-371).

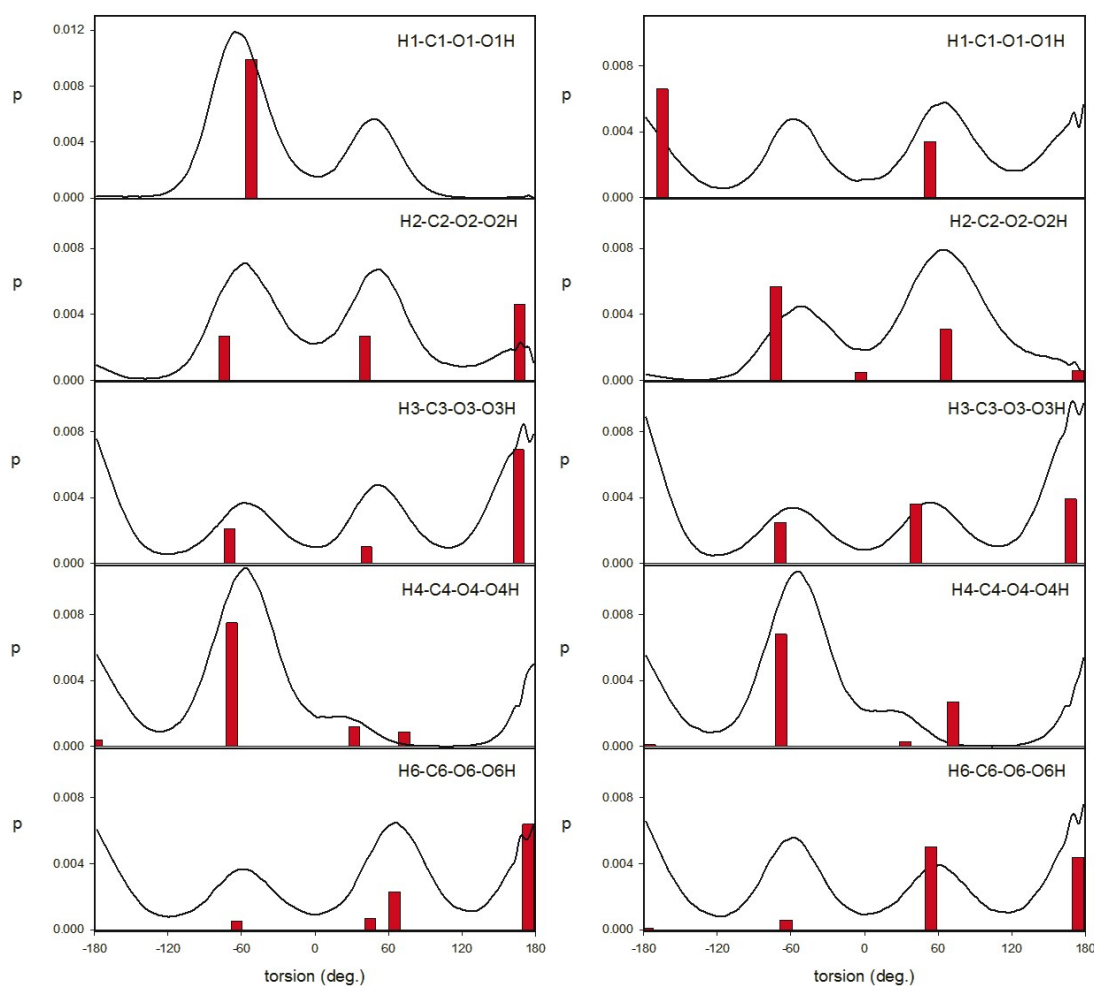


Fig. S3. Comparison of selected torsional angles as obtained by MD and DFT computations, for α -DM (left) and β -DM (right). MD probability histograms (black line) were obtained during 10 ns simulations with the GLYCAM06 force field. The DFT distribution bars (red, in arbitrary scale) were obtained from the B3LYP/6-311++G**/CPCM conformational scan and Boltzmann weighting.

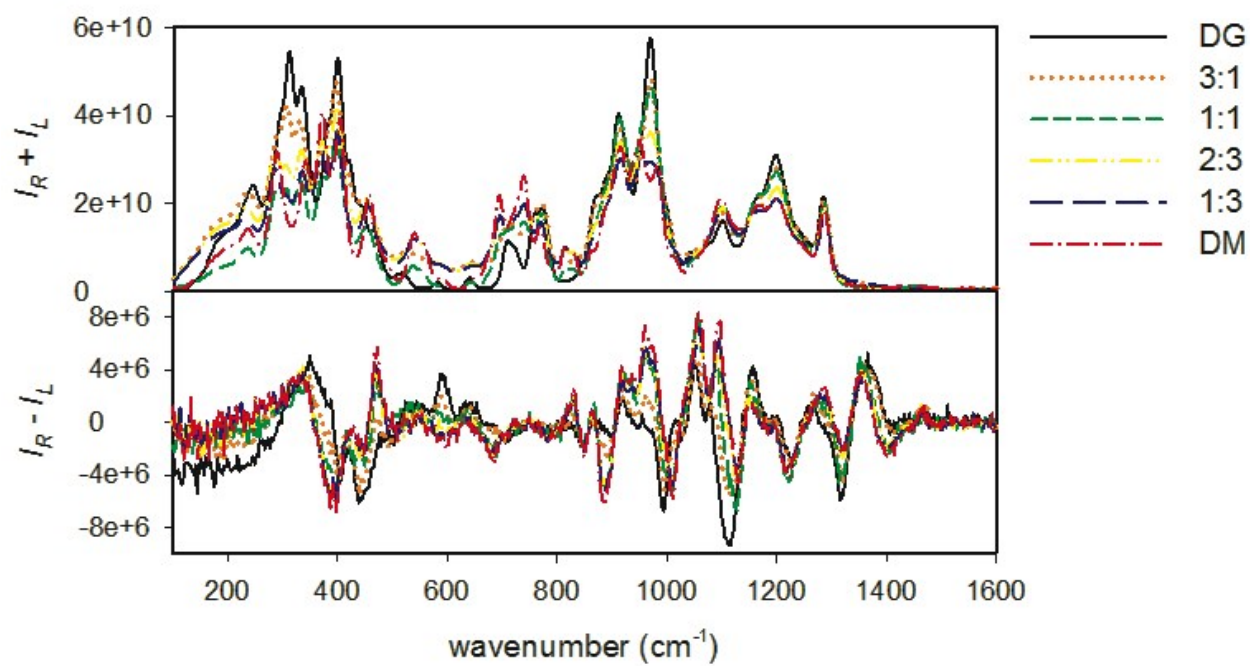


Fig. S4. Experimental Raman and ROA spectra of **DG** and **DM** mixtures.