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Enhanced Tetrahedral Order in Hydrophobic Hydration-Shells¹

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The influence of oily molecules on water structure has long been a subject of speculation. Early thermodynamic evidence was interpreted as indicating the formation of "icebergs" around oily molecules, while later simulations and neutron scattering studies found no evidence of such structures. More recently, Raman multivariate curve resolution (Raman-MCR) studies of the OH stretch band of water in hydrophobic hydration-shells have found evidence of both hydrogen bond strengthening and the formation of broken hydrogen bonds (dangling OH groups). Here we use Raman-MCR to show that the enhanced tetrahedral order in cold liquid water, as well as in solid clathrate-hydrates, gives rise to the emergence of a peak near 200 cm^{-1} whose intensity is correlated with the OH stretch shoulder near 3200 cm^{-1} . Moreover, we observe the same two correlated bands in the hydration-shells of oily molecules, thus providing clear experimental evidence of enhanced tetrahedral order in hydrophobic hydration-shells.

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