Supporting Information for: Infrared spectra of small anionic water clusters from density functional theory and wavefunction theory calculations†

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1 Calculated IR spectra with other DFT functionals

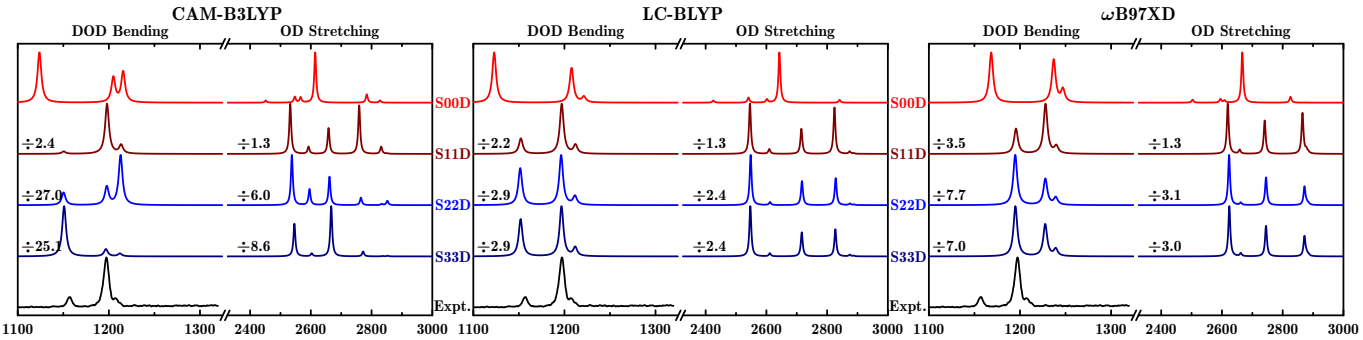

Fig. S1 Calculated IR spectra for anionic water trimer at the CAM-B3LYP/S*mn*D, LC-BLYP/S*mn*D, and ωB97XD/S*mn*D levels. All calculated spectra were broadened by a Lorentzian function with a fwhm of 5.0 cm^{-1} in the bending region and 7.5 cm^{-1} in the stretching region. The frequency scaling factors are 0.985, 0.995, and 1.0 in the bending region for the CAM-B3LYP/S*mn*D, LC-BLYP/P*mn*D, and ωB97XD/S*mn*D, respectively. The values are the corresponding scale factor for the spectra with respect to the maximum intensity of bending and stretching regions with S00D, respectively. The experimental IR spectrum in the bending region extracted from Ref. 1 was also included for comparison.

References

1 N. I. Hammer, J. R. Roscioli, M. A. Johnson, E. M. Myshakin and K. D. Jordan, *J. Phys. Chem. A*, 2005, **109**, 11526–11530.