Supplementary data

Chirality transfer through hydrogen-bonding: experimental and *ab initio* analyses of vibrational circular dichroism spectra of methyl lactate in water

Martin Losada and Yunjie Xu*

Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2G2

Email: yunjie.xu@ualberta.ca

TABLE S1: Raw (D_e) and counterpoise-corrected (D_e^{CPC}) binding energies, absolute ZPE differences (ΔZPE), absolute (D_0) and relative (ΔD_0) dissociation energies for the ML-$(H_2O)_n$ complexes, with $n = 2, 3$, calculated at the B3PW91/6-311++G(d,p) level of theory. All energy values are in kcal/mol.

Conformer	D_e	D_e^{CPC}	ΔZPE[a]	D_0[b]	ΔD_0	bf[c]
ML-$(H_2O)_2$:						
ML-2w-I	−15.197	−13.021	4.750	−8.271	0.0	0.910
ML-2w-II	−12.162	−10.435	4.176	−6.259	2.012	0.030
ML-2w-III	−12.367	−10.625	4.387	−6.238	2.033	0.029
ML-2w-IV	−12.326	−10.457	4.237	−6.220	2.051	0.028
ML-2w-V	−10.504	−8.942	4.026	−4.916	3.355	0.003
ML-$(H_2O)_3$:						
ML-3w-I	−25.824	−23.000	5.766	−17.233	0.0	0.522
ML-3w-II	−25.540	−22.710	5.530	−17.180	0.053	0.478

[a] ΔZPE=ZPE(complex)−ZPE(solute)−ZPE(solvent).

[b] $D_0 = D_e^{CPC} + \Delta$ZPE.

[c] The normalized Boltzmann factor at 298 K.

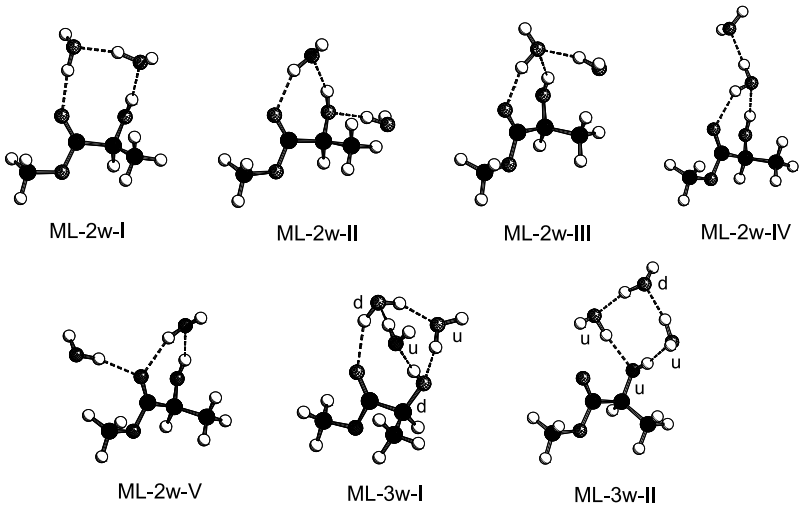

Figure S1. The optimized geometries of the most stable conformers of the ML-$(H_2O)_{2,3}$ complexes at the B3LYP/6-311++G(d,p) level of theory.

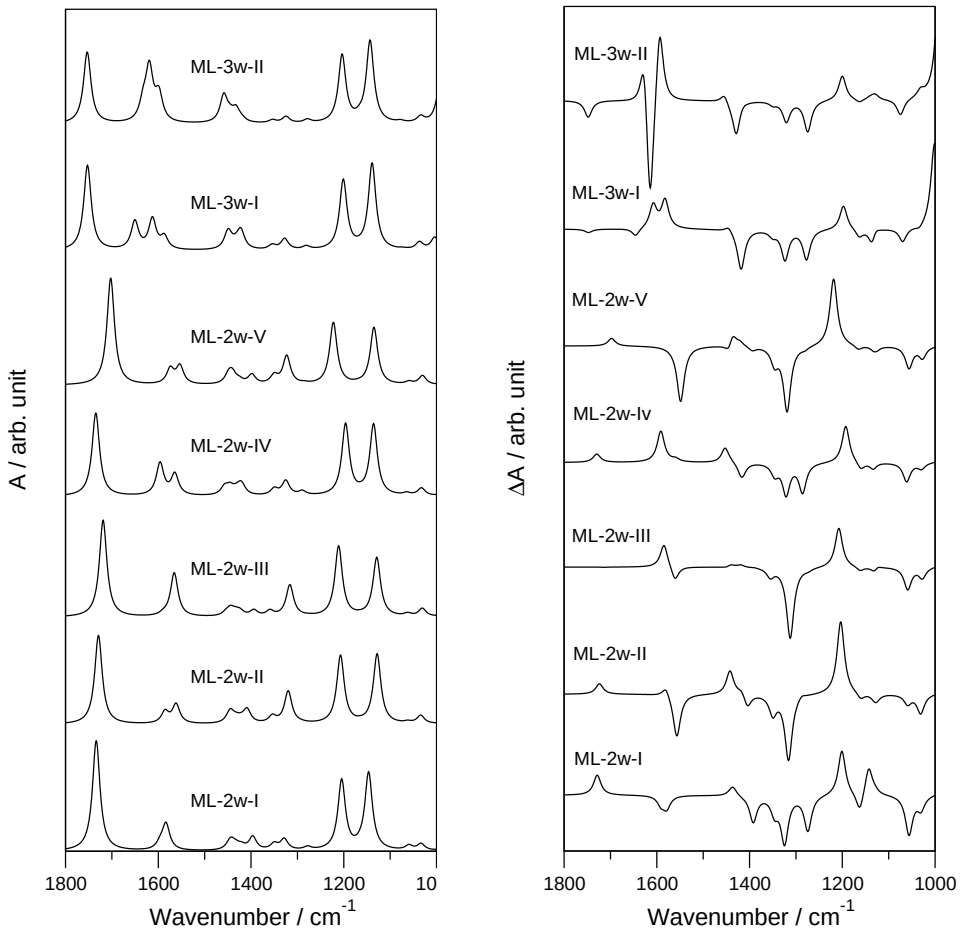

Figure S2. The predicted VA and VCD spectra of the ML-$(H_2O)_{2,3}$ conformers at the B3PW91/6-311++G(d,p) level of theory.