Structural and Electrostatic Effects at the Surfaces of Size- and Charge-Selected Aqueous Nanodrops

Richard J. Cooper, Jeremy T. O'Brien, Terrence M. Chang and Evan R. Williams*

Department of Chemistry, University of California, Berkeley, California, 94720-1460

Supplementary Information

	La ³⁺	Ca ²⁺	Na⁺	Li+	ŀ	SO ₄ ²⁻
Fit 1 – small						
cluster sizes (n)	20-102	20-100	20-30	20-36	-	50-80
slope	-313.0	-132.8	-21.8	-50.3	-	59.8
intercept (cm ⁻¹)	3708.0	3703.8	3704.1	3703.5	-	3706.1
Fit 2 - large						
cluster sizes (n)	102-550	100-300	30-250	36-120	20-250	80-300
slope	-66.1	4.1	51.2	8.4	111.6	130.1
intercept (cm ⁻¹)	3696.5	3697.5	3696.5	3698.2	3699.4	3701.0

Table S1. Calculated slopes and intercepts from linear fits of the Stark shifting data in Figure 5

 at both small and large cluster sizes.



Figure S1. Calculated infrared spectra of $(H_2O)_{50}$ and $M(H_2O)_{50}$ where $M = Mo^{3+}$, Ca^{2+} , Na^+ , I⁻ and SO_4^{2-} . Spectra are calculated from 1000 structures identified by MD simulations using an electrostatic point charge model that accounts for intramolecular coupling and frequency-dependent transition intensities. The sharp bands between 3600–3800 cm⁻¹ arise from free OH stretches at the surfaces of the nanodrops whereas the broad resonances at lower energy correspond to hydrogen bonded OH stretches throughout the nanodrops.