Carbon-Deuterium Vibrational Probes of Amino Acid Protonation State

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Supporting Information

Table S-1. Unscaled harmonic and anharmonic vibrational frequencies for neutral and charged Kdp as a function of the location of the C–D_2 probe in the lysine side chain. Harmonic intensities are reported relative to the asymmetric C_ε–D_2 stretch of the Kdp cation.

Probe	Charge	Harmonic (cm^{-1})		Anharmonic (cm^{-1})		Relative Intensity	
C_ε–D_2	0	2200.8	2274.2	2166.8	2236.3	6.9	5.7
	1	2249.6	2346.7	2211.7	2305.8	1.6	1.0
C_δ–D_2	0	2186.3	2256.2	2151.1	2219.9	3.7	3.6
	1	2194.5	2271.4	2162.1	2238.7	2.1	1.5
C_γ–D_2	0	2191.9	2259.6	2155.5	2222.4	3.1	3.3
	1	2204.4	2279.3	2170.1	2245.1	1.7	1.7
C_β–D_2	0	2215.1	2287.8	2181.6	2252.8	1.7	1.6
	1	2220.5	2291.8	2187.7	2258.8	1.3	1.3

Table S-2. Unscaled harmonic C–D stretch vibrational frequencies for neutral and charged Kdp-d_8. Harmonic intensities are reported relative to the weakest absorption in each molecule.

	Kdp (0)		Kdp (+1)	
	Frequency (cm^{-1})	Relative Intensity	Frequency (cm^{-1})	Relative Intensity
ω_{sym}	2185.9	114.4	2190.9	58.6
	2191.0	61.9	2196.3	112.3
	2201.7	366.4	2217.3	91.1
	2215.2	105.1	2219.6	25.5
ω_{asym}	2247.4	1.0	2253.5	1.5
	2261.4	76.3	2269.0	105.2
	2279.0	336.2	2292.0	106.7
	2289.7	194.3	2295.1	42.2