Supporting Information: Reduced Acid Dissociation of Amino-Acids at the Surface of Water

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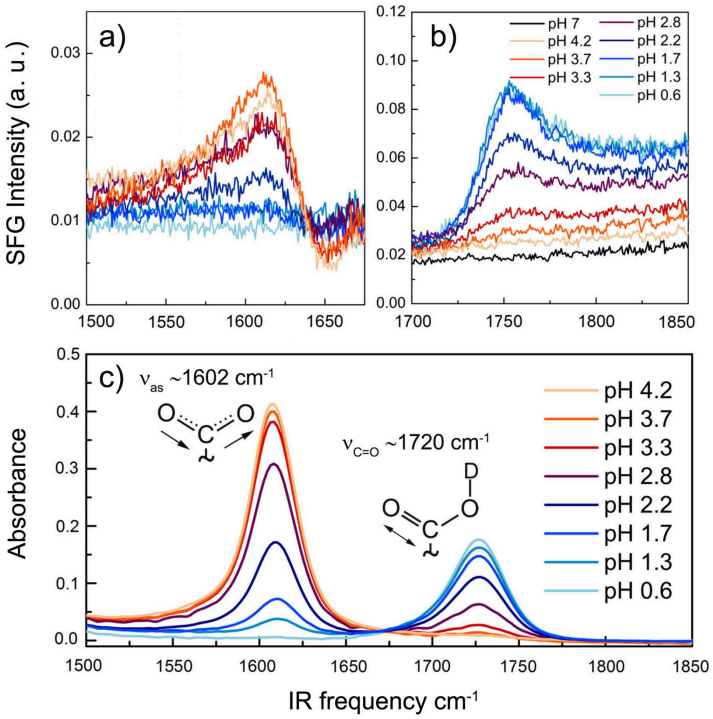

Figure S1: VSFG spectra of L-alanine in the frequency regions of the $\nu_{\mathrm{AS,COO^-}}$ (a) and the ν_{COOD} (b) vibrations. ATR spectra in the region 1500 - 1850 $\mathrm{cm^{-1}}$ (c).

Fitting L-alanine VSFG Spectra

Table 1: Fitting parameters for the L-alanine in ν_{COOD} and $\nu_{\mathrm{AS,COO^-}}$ vibrational regions.

	ν_{COOD} ω_0=1740 cm^{-1} Γ=17 cm^{-1}			$\nu_{\mathrm{AS,COO^-}}$ ω_0=1630 cm^{-1} Γ=18 cm^{-1}		
pH	A_{NR}	φ_{NR}	A_{R}	A_{NR}	φ_{NR}	A_{R}
0.6	0.18 ± 0.01	7 ± 1	2.6 ± 0.1	–	– ± 2	–
1.3	0.17 ± 0.01	6 ± 1	2.7 ± 0.1	0.12 ± 0.01	141 ± 16	0.08 ± 0.01
1.7	0.17 ± 0.01	4 ± 1	2.45 ± 0.04	0.10 ± 0.01	162 ± 1	0.22 ± 0.01
2.3	0.16 ± 0.01	10 ± 1	2.18 ± 0.04	0.11 ± 0.01	170 ± 2	0.44 ± 0.02
2.8	0.15 ± 0.01	9 ± 1	1.38 ± 0.04	0.11 ± 0.01	178 ± 1	0.83 ± 0.02
3.3	0.12 ± 0.01	2 ± 1	0.82 ± 0.03	0.12 ± 0.01	181 ± 1	1.14 ± 0.02
3.7	0.10 ± 0.01	5 ± 1	0.43 ± 0.05	0.11 ± 0.01	191 ± 1	1.38 ± 0.02
4.2	–	–	–	0.11	170	1.43 ± 0.02

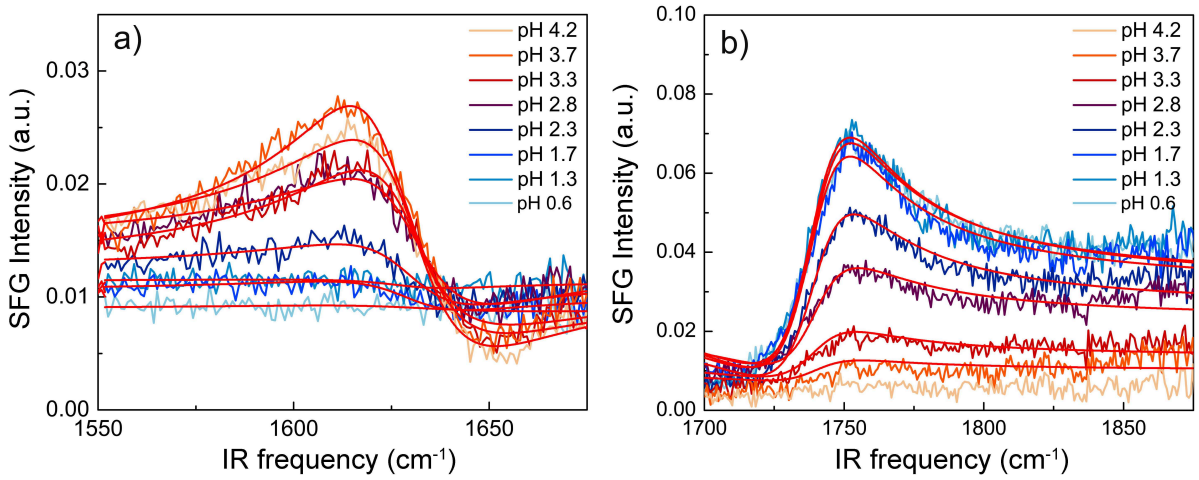

Figure S2: VSFG spectra of L-alanine in the frequency regions of the $\nu_{\mathrm{AS,COO^-}}$ (a) and the ν_{COOD} (b) vibrations.

Fitting L-alanine ATR Spectra

Table 2: Fitting parameters for the L-alanine ATR spectra.

	$\omega_0 = 1515$ cm^{-1} $\Gamma = 140$ cm^{-1}	$\omega_0 = 1608$ cm^{-1} $\Gamma = 30$ cm^{-1}	$\omega_0 = 1727$ cm^{-1} $\Gamma = 40$ cm^{-1}
pH	Peak Area	Peak Area	Peak Area
7	9.8 ± 0.4	20.8 ± 0.2	0.4 ± 0.1
4.2	9.4 ± 0.4	19.8 ± 0.1	0.6 ± 0.1
3.7	9.5 ± 0.3	19.4 ± 0.1	1.1 ± 0.1
3.3	9.2 ± 0.3	18.5 ± 0.1	1.9 ± 0.1
2.8	8.6 ± 0.3	14.9 ± 0.4	4.2 ± 0.1
2.3	7.2 ± 0.2	8.4 ± 0.1	7.5 ± 0.2
1.7	7.1 ± 0.3	3.5 ± 0.1	9.9 ± 0.1
1.3	7.3 ± 0.3	1.8 ± 0.08	11.0 ± 0.1
0.6	5.9 ± 0.3	0.5 ± 0.08	12 ± 0.1

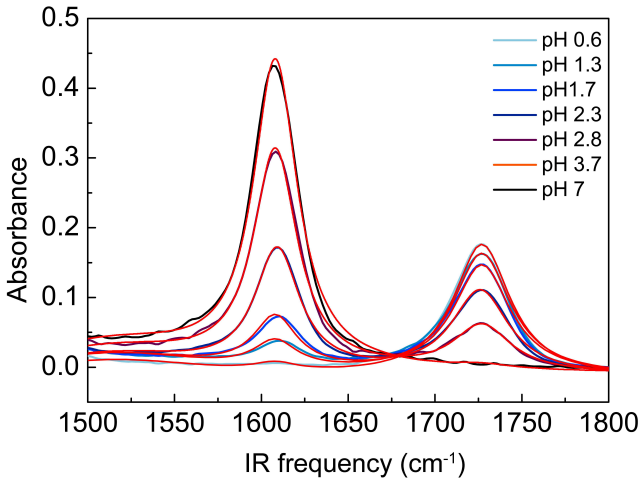

Figure S3: Experimentally measured ATR spectra of L-alanine and Lorentzian model fits.

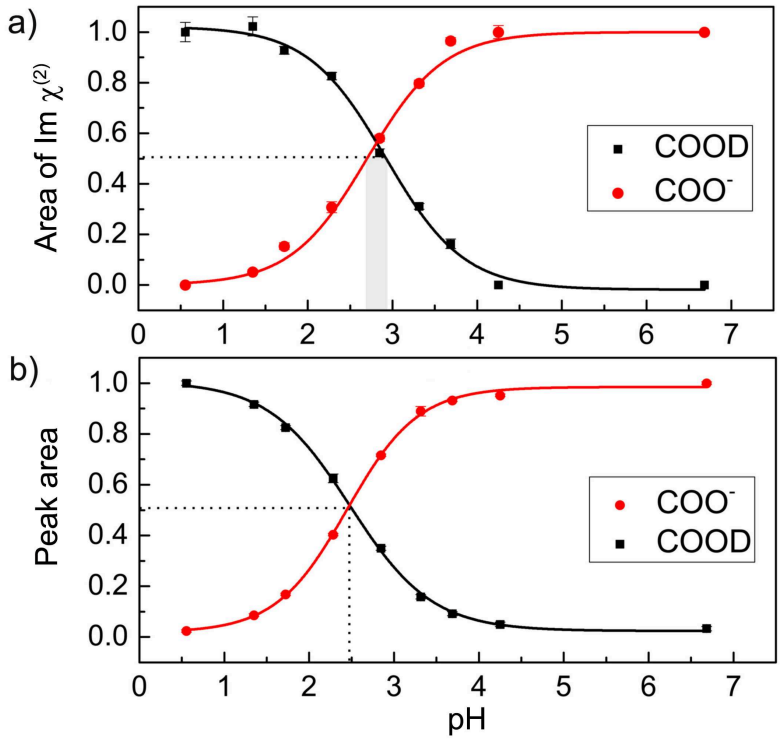

Figure S4: pH dependence of the peak areas of the $\nu_{\mathrm{AS,COO^-}}$ and ν_{COOD} vibrations obtained from fitting the VSFG (a) and ATR (b) spectra of L-alanine.