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**Supporting Information**

# The Enhanced Dissociation and Associated Surface Structure of Anesthetic Propofol at the Water Interface: Vibrational Sum Frequency Generation Study

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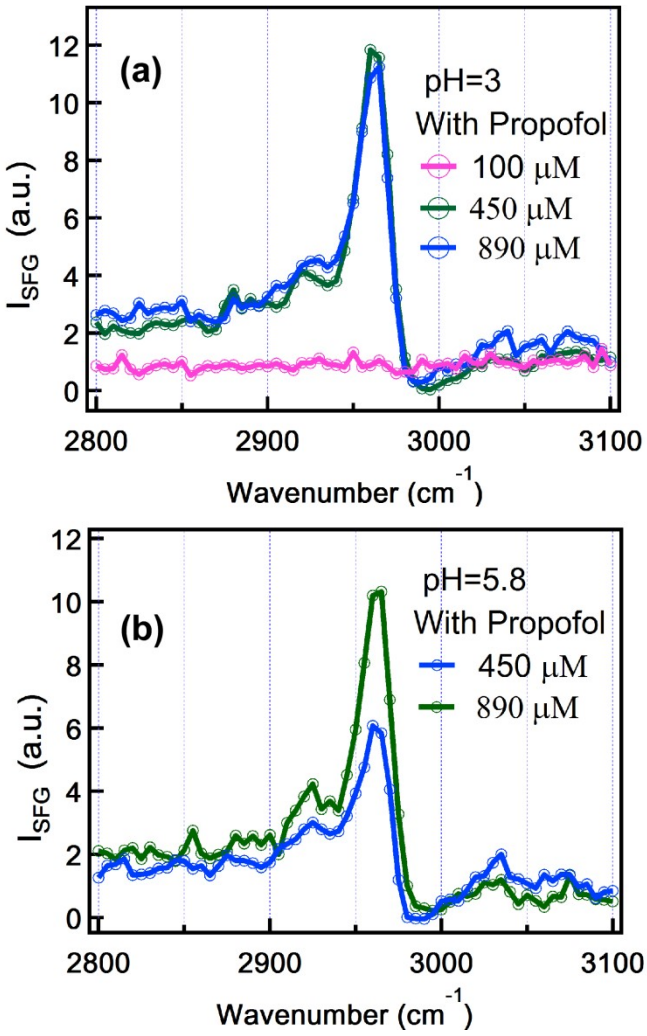


**Figure S1:** The PPP polarized VSFG spectra of the C-H stretch of propofol at pH 3 (a) and 5.8 (b), respectively.

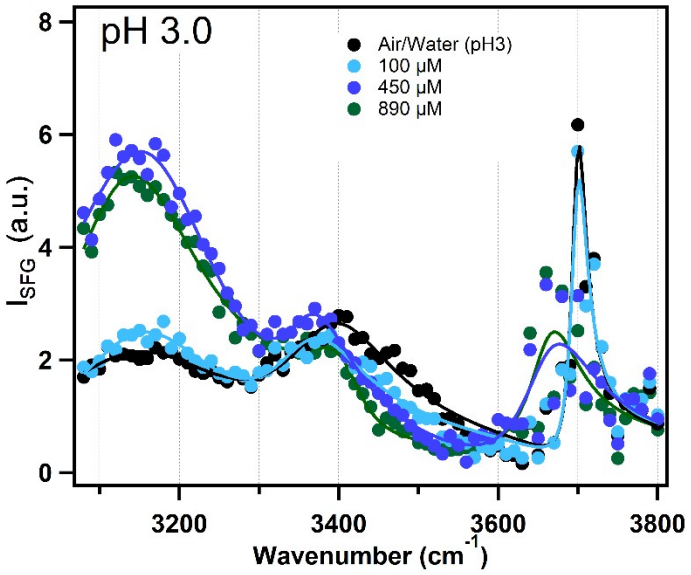


**Figure S2:** SSP polarized SFG spectra of water OH region at different concentrations of propofol at pH 3.0 along with fitted line (solid) using Lorentzian equation.

**Table S1:** The peak center, amplitude (A), and peak width (Γ) values of SFG spectra different concentrations of propofol at pH 3.0, obtained from the fittings with equation 3.

| Sample | Peak Center ($cm^{-1}$) | Amplitude (A) | Width (Γ) |
|---|---|---|---|
| **Propofol (µM) at pH 3** | | | |
| **0** | 3148 ± 14.8 | 154.04 ± 59.5 | 153.2 ± 46. |
| | 3387 ± 9 | 73.913 ± 26.6 | 85.80 ± 18.8 |
| | 3698 ± 1.38 | 20.334 ± 2.09 | 11.46 ± 1.07 |
| **100** | 3149 ± 10.4 | 134.06 ± 36.7 | 120.5 ± 25.2 |
| | 3360 ± 9.39 | 48.756 ± 19.1 | 71.38 ± 19.2 |
| | 3698 ± 1.61 | 20.752 ± 2.32 | 12.61 ± 1.35 |
| **450** | 3160 ± 13.5 | 294.86 ± 53 | 130.2 ± 12.6 |
| | 3363 ± 11 | 39.203 ± 23.1 | 56.18 ± 20.9 |
| | 3658 ± 13.4 | 57.26 ± 17 | 54.89 ± 12.1 |
| **890** | 3130 ± 9.78 | 208.07 ± 29.5 | 111.0 ± 13.5 |
| | 3409 ± 10 | 21.014 ± 10.4 | 41.4 ± 16.9 |
| | 3661 ± 7.66 | 37.717 ± 10.1 | 38.8 ± 8.6 |

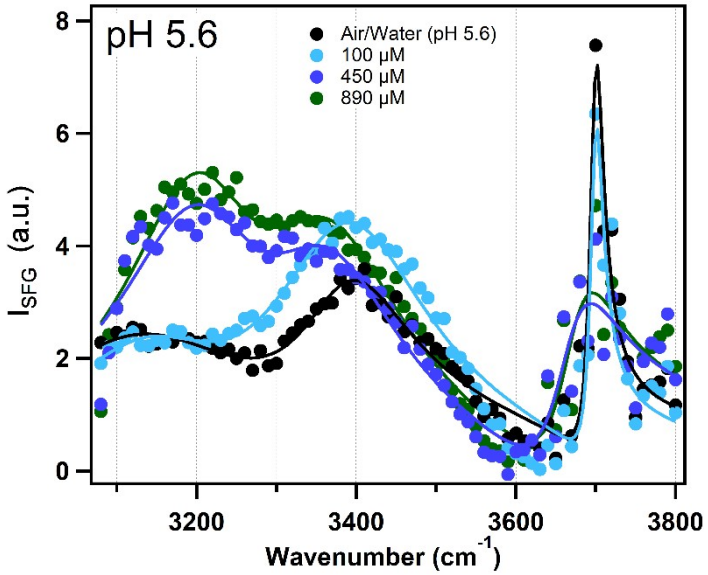


**Figure S3:** SSP polarized SFG spectra of water OH region at different concentrations of propofol at pH 5.6 along with fitted line (solid) using Lorentzian equation.

**Table S2:** The peak center, amplitude (A), and peak width (Γ) values of SFG spectra different concentrations of propofol at pH 5.6, obtained from the fittings with equation 3.

| Sample | Peak Center ($cm^{-1}$) | Amplitude (A) | Width (Γ) |
|---|---|---|---|
| **Propofol (μM) at pH 5.8** | | | |
| **0** | 3124 ± 24.2 | 207.3 ± 107 | 183.7 ± 73.6 |
| | 3383 ± 8.37 | 83.7 ± 29.8 | 87.6 ± 17.9 |
| | 3698 ± 1.23 | 20.8 ± 1.9 | 10.5 ± 0.873 |
| **100** | 3149 ± 19.5 | 109.7 ± 51.8 | 130.1 ± 46.9 |
| | 3383 ± 9.67 | 213.8 ± 16.9 | 125.7 ± 11.8 |
| | 3698 ± 1.67 | 18.1 ± 1.2 | 10.1 ± 1.14 |
| **450** | 3208 ± 21 | 243.9 ± 242 | 116.6 ± 52.4 |
| | 3353 ± 16 | 155.2 ± 253 | 106.8 ± 63.1 |
| | 3665 ± 10.8 | 61.5 ± 17.6 | 47.5 ± 9.93 |
| **890** | 3208 ± 18.3 | 219.4 ± 211 | 107.2 ± 45.9 |
| | 3352 ± 14.8 | 181.8 ± 247 | 111.4 ± 56.5 |
| | 3671 ± 10.1 | 55.6 ± 15.2 | 43.32 ± 9.26 |

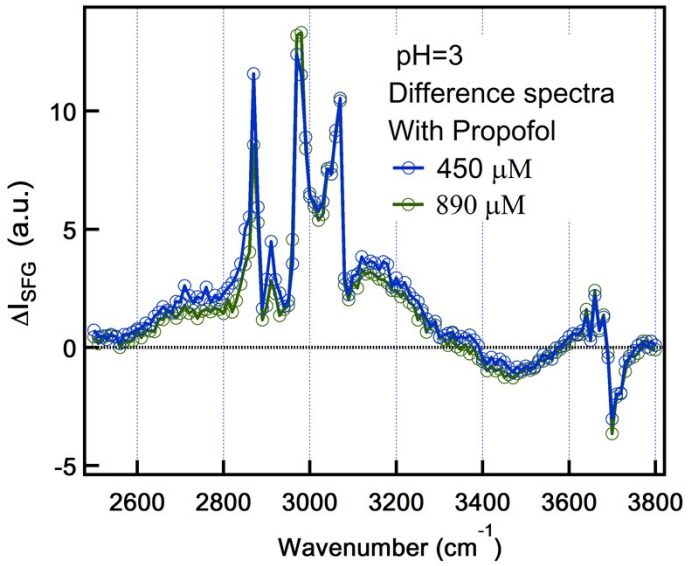


**Figure S4:** The difference VSFG spectra (VSFG spectra of propofol at different concentrations-VSFG spectra of air/water) for the different concentrations of propofol at pH=3.

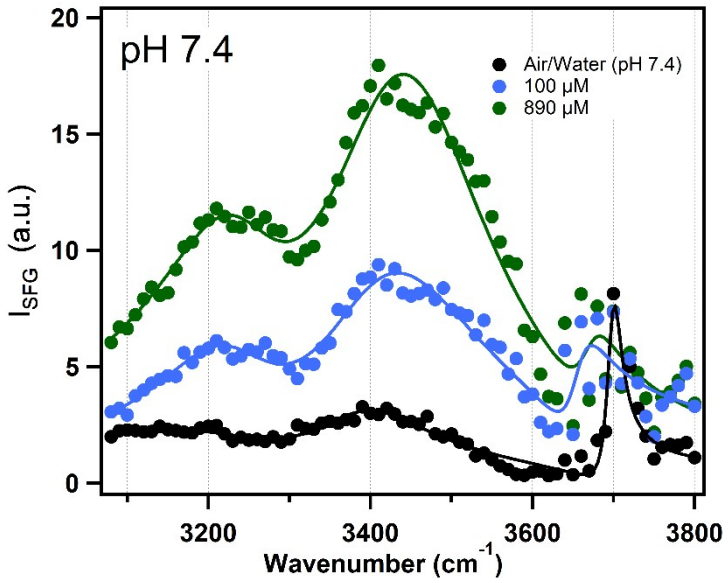


**Figure S5:** SSP polarized SFG spectra of water OH region at different concentrations of propofol at pH 7.4 along with fitted line (solid) using Lorentzian equation.

**Table S3:** The peak center, amplitude (A), and peak width (Γ) values of SFG spectra different concentrations of propofol at pH 5.6, obtained from the fittings with equation 3.

| Sample | Peak Center ($cm^{-1}$) | Amplitude (A) | Width (Γ) |
|---|---|---|---|
| **Propofol (µM) at pH 7.4** | | | |
| **0** | 3140 ± 22 | 242.44 ± 131 | 185.37 ± 77.4 |
| | 3384.3 ± 10.6 | 85.568 ± 41.8 | 88.407 ± 23.6 |
| | 3698.1 ± 1.3 | 24.213 ± 2.52 | 10.934 ± 0.965 |
| **100** | 3229.9 ± 28.1 | 181.75 ± 203 | 98.702 ± 49.1 |
| | 3408.4 ± 18.3 | 428.81 ± 239 | 128.94 ± 25.2 |
| | 3655.2 ± 6.13 | 22.852 ± 8.66 | 25.346 ± 9.01 |
| **890** | 3241.2 ± 13.1 | 183.97 ± 30.3 | 99.021 ± 7.52 |
| | 3437.1 ± 10.3 | 605.14 ± 57.7 | 132.01 ± 8.85 |
| | 3670.5 ± 9.65 | 17.454 ± 12.2 | 27.4 ± 16.9 |

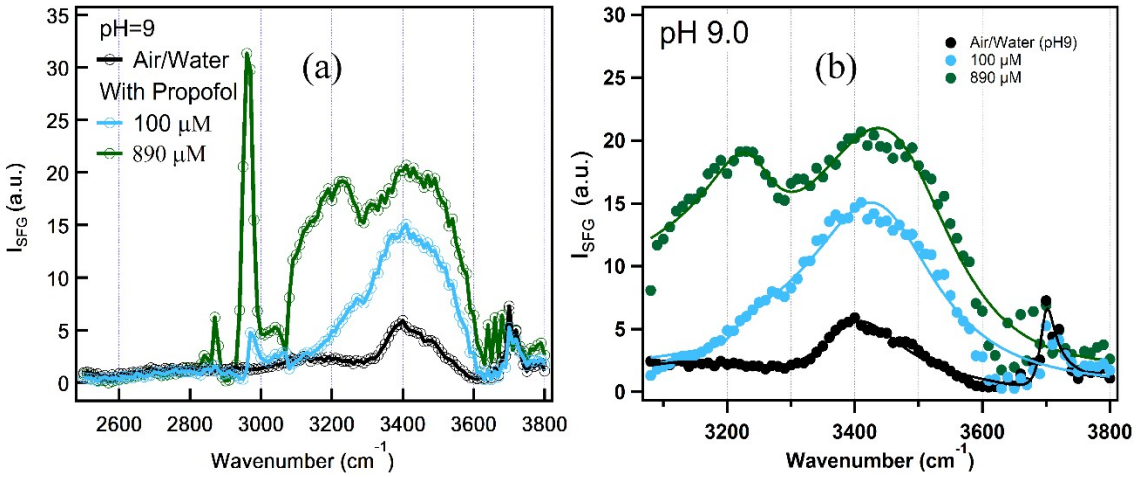


**Figure S6:** (a) SSP polarized SFG spectra at different concentrations of propofol at pH 9.0, and (b) fitted line (solid) of water OH region using Lorentzian equation.

**Table S4:** The peak center, amplitude (A), and peak width (Γ) values of SFG spectra different concentrations of propofol at pH 9.0, obtained from the fittings with equation 3.

| Sample | Peak Center ($cm^{-1}$) | Amplitude (A) | Width (Γ) |
|---|---|---|---|
| **Propofol (µM) at pH 9.0** | | | |
| **0** | 3147 ± 19.9 | 169.2 ± 77.2 | 152.4 ± 51.7 |
| | 3399 ± 5.64 | 146.0 ± 27.8 | 81.2 ± 8.83 |
| | 3698 ± 1.68 | 27.3 ± 3.1 | 14.0 ± 1.48 |
| **100** | 3282 ± 14.6 | 216.9 ± 134 | 148.8 ± 42.3 |
| | 3476 ± 6.19 | 573.7 ± 37.4 | 120.2 ± 8.42 |
| | 3698 ± 2.1 | 15.6 ± 1.44 | 8.5 ± 1.07 |
| **890** | 3245 ± 8.31 | 66.3 ± 36.3 | 64.8 ± 21.7 |
| | 3476 ± 13.6 | 449.5 ± 55.7 | 144.1 ± 11.9 |

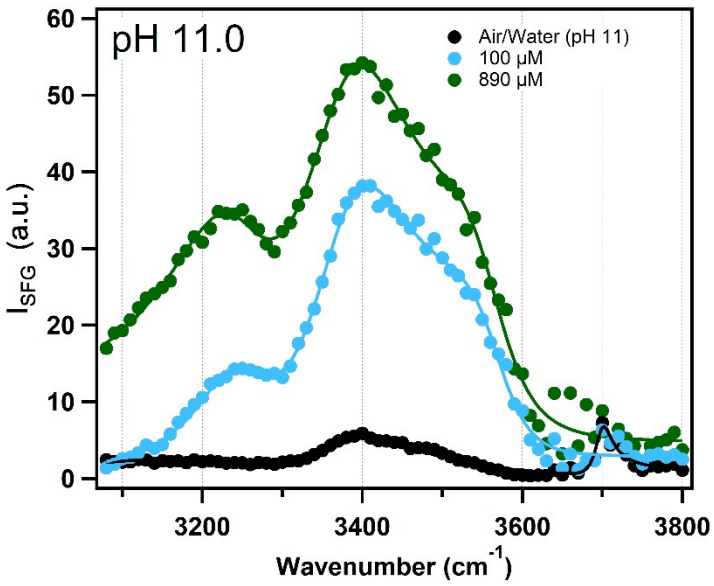


**Figure S7:** SSP polarized SFG spectra of water OH region at different concentrations of propofol at pH 11.0 along with fitted line (solid) using Lorentzian equation.

**Table S5:** The peak center, amplitude (A), and peak width (Γ) values of SFG spectra different concentrations of propofol at pH 11.0, obtained from the fittings with equation 3.

| Sample | Peak Center ($cm^{-1}$) | Amplitude (A) | Width (Γ) |
|---|---|---|---|
| **Propofol (µM) at pH 11.0** | | | |
| **0** | 3125 ± 19.1 | 121.42 ± 45.9 | 110.2 ± 39.1 |
| | 3410 ± 5.2 | 150.05 ± 23.7 | 78.7 ± 6.77 |
| | 3698 ± 1.6 | 24.345 ± 2.76 | 12.8 ± 1.42 |
| **100** | 3245 ± 10 | 173.56 ± 42.6 | 61.6 ± 8.59 |
| | 3376 ± 3.2 | 488.3 ± 56.4 | 82.2 ± 5.4 |
| | 3564 ± 4.3 | 153.7 ± 19.1 | 59.1 ± 5.16 |
| **890** | 3245 ± 6.5 | 328.0 ± 143 | 82.7 ± 15 |
| | 3377 ± 5.5 | 789.1 ± 163 | 93.9 ± 8.77 |
| | 3557 ± 6.2 | 216.6 ± 39.5 | 65.8 ± 6.63 |

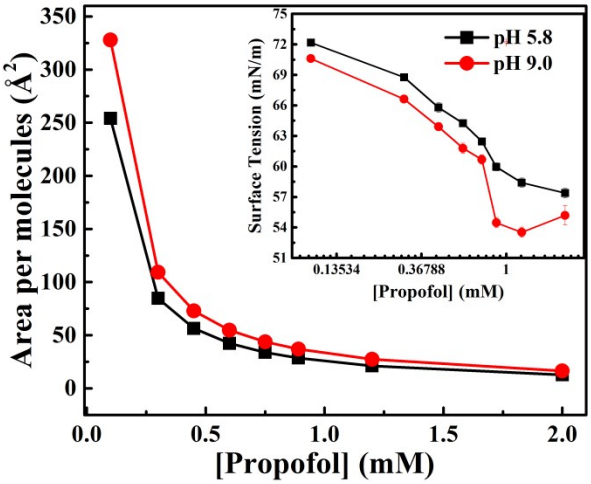


**Figure S8:** Concentration-dependent Area per molecule (Å$^2$) of propofol at different pHs. Inset shows the concentration-dependent change in surface tension (mN/m) of propofol at different pHs.