Electronic Supplementary Material (ESI) for Soft Matter.

Propofol adsorption at the air/water interface: a combined vibrational sum frequency spectroscopy, nuclear magnetic resonance and neutron reflectometry study.

Petru Niga[1], Petra M. Hansson-Mille[1], Agne Swerin[1,2], Per M. Claesson[1,2], Joachim Schoelkopf[3], Patrick A. C. Gane[3,4], Jing Dai[5], István Furó[5], Richard A. Campbell[6,7] and C. Magnus Johnson[2*]*

[1]RISE Research Institutes of Sweden – Chemistry, Materials and Surfaces, Box 5607, SE-114 86 Stockholm, Sweden.

[2]KTH Royal Institute of Technology, Department of Chemistry, Division of Surface and Corrosion Science, SE - 100 44 Stockholm, Sweden.

[3]Omya International AG, Baslerstrasse 42, CH-4665 Oftringen, Switzerland.

[4]Aalto University, School of Chemical Technology, Department of Bioproducts and Biosystems, FI-00076 Aalto, Helsinki, Finland.

[5] KTH Royal Institute of Technology, Department of Chemistry, Division of Applied Physical Chemistry, SE - 100 44 Stockholm, Sweden.

[6] Institut Laue-Langevin, 71 Avenue des Martyrs, CS20156, 38042 Grenoble Cedex 9, France.

[7] Division of Pharmacy and Optometry, University of Manchester, Manchester M13 9PT, UK.

Supporting Information

Fitting of the propofol spectrum at 0.89 mM concentration

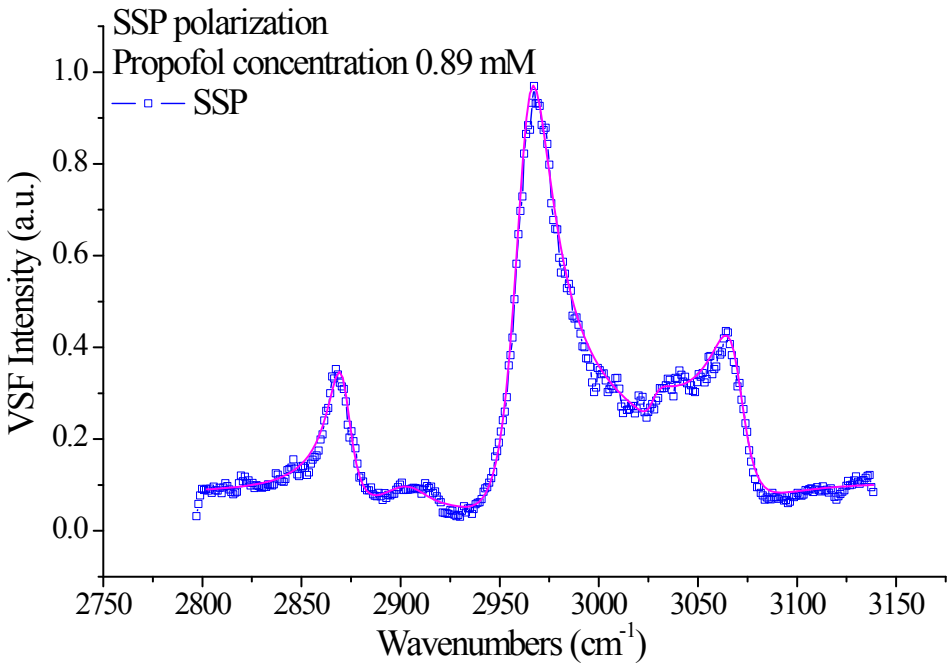

Figure S1. VSF spectra for propofol at a concentration of 0.89 mM in SSP polarization including the fitting curve.

Table S1. Fitting parameters for CH stretches of propofol at increasing concentrations

Concentration mM	Assignments	Peak position	Amplitude	Gamma
SSP				
0.22	sCH_3	2875	0.154	9
	CH isoprop.	2910	0,114	14
	aCH_3	2965	-0.349	12
	arCH	3035	-0.047	11
	arCH	3071	0.010	11
SSP				
0.28	sCH_3	2875	0.162	9
	CH isoprop.	2910	0,063	14
	aCH_3	2965	-0.410	12
	arCH	3035	-0.002	11
	arCH	3071	0.002	11

SSP				
0.39	sCH_3	2875	0.207	9
	CH isoprop.	2910	0,032	14
	aCH_3	2965	-0.484	12
	arCH	3035	-0,018	13
	arCH	3071	0,022	11
SSP				
0.56	sCH_3	2875	0.189	9
	CH isoprop.	2910	0,176	14
	aCH_3	2965	-0.524	12
	arCH	3035	-0.062	11
	arCH	3071	0.070	11
SSP				
0.73	sCH_3	2875	0,213	9
	CH isoprop.	2910	0,152	14
	aCH_3	2965	-0,526	12
	arCH	3035	-0,038	11
	arCH	3071	0,139	11
SSP				
0.89	sCH_3	2875	0,212	9
	CH isoprop.	2910	0,128	14
	aCH_3	2965	-0,547	12
	arCH	3035	-0.018	11
	arCH	3071	0.162	11

Details on the derivation of the area per molecule from the surface tension measurements.

The data of the surface tension isotherm was fitted using a second order polynomial function as shown below:

$$y = B1*x + B2*x^2 + C$$

where x = ln(c) and C is the intercept.

B1		B2		C		Statistics
Value	Standard Error	Value	Standard Error	Value	Standard Error	Adj. R-Square
-21.071	1.023	5.529	0.921	72	0.226	0.998

We have used a common approach to place the interfacial plane so that the surface excess of water is zero and the surface excess of propofol as determined from surface tensiometry, Γ_{ST}, is calculated as follows:[SI1]

$$\frac{d\gamma}{d\mu} = -\Gamma_{ST}$$

where γ is the surface tension, and μ is the chemical potential of propofol, which can be expressed as

$$\mu = \mu^0 + RTlna \approx \mu^0 + RTlnc$$

where μ^0 is the chemical potential of pure water, and a is the activity and c the bulk concentration of propofol. Γ_{ST} was calculated based on Gibb's equation:

$$\Gamma_{ST} = -\frac{1}{RT}\frac{d\gamma}{dlnc}$$

where R is the gas constant, and T is the absolute temperature. To calculate the derivative, the second order polynomial that was fitted to the data was used. The values of the area per molecule, A, reported in main text were calculated from the following relation

$$A = 1/(\Gamma_{ST} N_A)$$

where N_A is Avogadro's number.

Reference

SI1. D. Fennell Evans, H. W. (1999). The Colloidal Domain: Where Physics, Chemistry, Biology, and Technology Meet.