

Supporting Information

Assembly and molecular order of two-dimensional peptoid nanosheets through the oil-water interface

Robertson et al.

Table S1. Physical properties (at 25 °C) of nonpolar phases found to produce peptoid nanosheets in water.

	Dielectric constant ϵ_r	Viscosity, cP	Density, g/cm ³	Miscibility with water, w/w	IFT ^a with water, mN/m	IFP ^b with 20 μ M aqueous peptoid 1, mN/m	Enthalpy of mixing with benzene, J/mol
Air	1.0	n/a	n/a	n/a	72	33	n/a
Hexane	1.8	0.3	0.65	0.001	50	36	900 ^c
CCl ₄	2.2	0.9	1.6	0.08	45	36	100 ^d

^a Interfacial tension (IFT).

^b Interfacial pressure (IFP), which is defined as the (IFT of pure water) – (IFT of peptoid 1 in water).

^c Reference 1.

^d References 2 & 3.

Vibrational Sum Frequency Spectra Fitting Routine

All spectra shown were fit using a convolution of a Gaussian and Lorentzian distribution described by Bain *et al.*,⁽⁴⁾ shown in Equation S1.

$$\left| \chi^{(2)}(\omega_{SF}) \right|^2 = \left| \sum_v \int_{-\infty}^{\infty} \frac{A_v e^{i\phi_v} e^{-[(\omega_L - \omega_v)/\Gamma_v]^2}}{\omega_L - \omega_{IR} - i\Gamma_L} d\omega_L \right|^2 \quad (\text{S1})$$

This line shape takes into account both homogenous broadening due to the inherent nature of the transition, as well as inhomogeneous broadening due to the local environments of the molecules. For the fits, the Lorentzian line widths were held at constant values consistent with typical vibrational lifetimes, while the Gaussian line widths were allowed to vary to account for the wide array of complex molecular environments.

References

1. Hwang C-A, Elkabule AS, Whitman DL, & Miller RC (1987) Excess molar enthalpies of (benzene + cyclohexane + n-hexane). *J. Chem. Thermodyn.* 19:1031-1036.

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3. Ahmed A (1973) Complex-formation between carbon tetrachloride and alkyl-substituted benzenes. *J. Chem. Soc., Faraday Trans.* 69(3):540-545.
4. Bain CD, Davies PB, Ong TH, Ward RN, & Brown MA (1991) The structure of interfaces probed by sum-frequency spectroscopy. *Surf. Interface Anal.* 17(7):529-530.