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Organic molecules on the surface of water droplets - an energetic perspective - Supporting Information

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1 Liquid properties

In Table 1 seven properties of neat liquids of 1000 molecules are given, following the protocols given in ref. [1]. Simulations were performed using GROMACS version 4.5.5 [2] and the input files used are available from the GROMACS Molecule & Liquid database [3]. Most analyses are quite standard (see e.g. Allen and Tildesly [4]) but for the calculation of the heat capacity a new method based on the density of states was used [5, 6]. For a consistent derivation of this method we refer to the supporting information of Caleman *et al.* [1].

Table S1: Liquid properties for six molecules used in the droplet PMF calculations: MOH (methanol), EOH (ethanol), PAC (propanoic acid), DEE (diethyl ether), NBA (N-butylamine) and NPT (neopentane). The properties are the density ρ, the enthalpy of vaporization ΔH_{vap}, the surface tension γ, the static dielectric constant $\epsilon(0)$, the volumetric expansion coefficient α_P, the isothermal compressibility κ_T, and the heat capacity at constant pressure c_P.

Molecule		MOH	EOH	PAC	DEE	NBA	NPT
T (K)		298.15	298.15	298.15	298.15	298.15	298.15
ρ	Exper.	787.2[7]	784.8[7]	988[7]	708[7]	741[7]	586[8]
(g/l)	GAFF	807.5	797.3	1079.1	723.8	773.7	626.6
	OPLS	776.8	796.3	1011.0	711.0	747.0	637.6
ΔH_{vap}	Exper.	37.43 [7]	42.32[7]	30.97[7]	27.18[7]	45.83[7]	21.78[9]
(g/l)	GAFF	39.62	44.62	98.84	31.47	45.85	27.37
	OPLS	36.44	42.32	56.63	29.34	38.52	26.67
γ	Exper.	22[10]	22[10]	26[8]	17[8]	14.5[10]	13.3[8]
(0.001 N/m)	GAFF	21	19	26	13	18	9
	OPLS	20	19	26	11	15	9
$\epsilon(0)$	Exper.	32[1]	25[10]	3.44[10]	4.4[10]	5.2[10]	1.77[9]
	GAFF	25	14	55	3.3	5.3	1.0
	OPLS	25	-	3.1	3.0	4.9	1.0
α_P	Exper.	1.19[7]	1.09[7]	1.07[7]	1.61[7]	1.25[7]	2[11]
(1/Gpa)	GAFF	1.41	1.26	0.60	1.88	1.25	2.04
	OPLS	1.53	1.44	1.09	2.07	1.70	1.82
κ_T	Exper.	1.25[7]	1.15[1]	1.05[7]	1.97[7]	0.90[1]	-
(0.001/K)	GAFF	1.02	0.98	0.40	1.59	0.87	2.12
	OPLS	1.08	0.95	0.58	1.90	1.28	2.01
c_P	Exper.	81[7]	112[7]	153[7]	173[7]	171[7]	-
(J/mol K)	GAFF	73	106	141	148	171	171
	OPLS	76	109	152	141	173	176

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