Supporting Information

Lysine-based amino-functionalized lipids for gene transfection: A study of the protonation state at the air-liquid interface

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1. Additional Data

1.1 π/A-Isotherms and Surface Gibbs Elasticity

The surface Gibbs elasticity ε_0 (also called surface compressional modulus C_s^{-1}) defines the elastic modulus representing a rheological quantity related to the monolayer rigidity and the capacity of a monolayer for energy storage. It can be obtained from the π/A – isotherms by the first derivation:

$$\varepsilon_0 = -A(d\pi/dA)_T$$

where A is the molecular area and dπ/dA is the slope of the isotherm at given molecular area. ε_0 is plotted versus the lateral pressure or the molecular area.

$\varepsilon_0 < 12.5$ mN/m: gas-analogue phase state (G)

$\varepsilon_0 \approx 13 – 100$ mN/m: liquid-expanded phase state (LE)

$\varepsilon_0 \approx 100 – 250$ mN/m: liquid-condensed phase state (LC) with tilted alkyl chains

$\varepsilon_0 > 250$ mN/m: solid phase state (SC, liquid-condensed phase state with untilted alkyl chains)

References

1 J. T. Davis and E. K. Rideal, *Interfacial Phenomena*, Academic Press, New York, 2nd Edition, 1963.

2 G. L. Gaines, *Insoluble monolayers at liquid-gas interfaces*, John Wiley & Sons Inc, 1st Edition., 1966.

2.1.1 **DODAB**

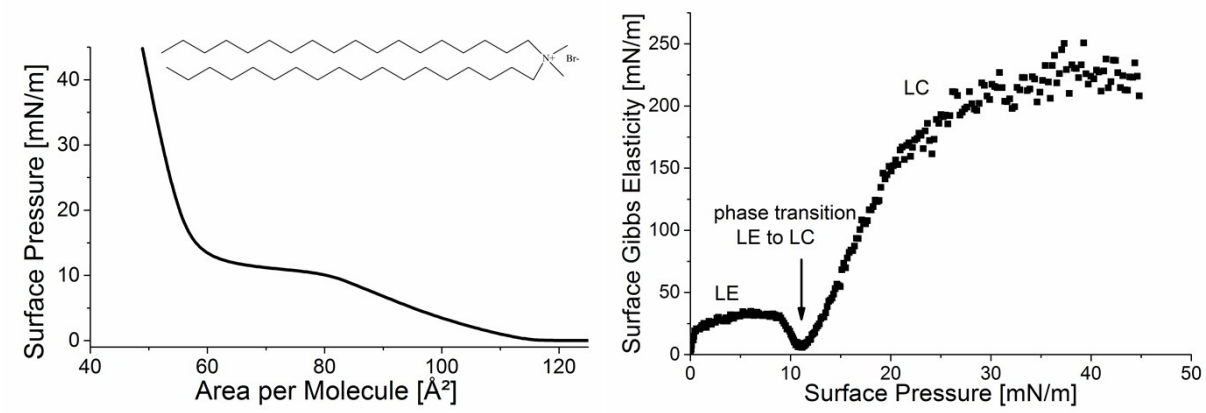

Figure S1: π/A-isotherm and surface Gibbs elasticity of **DODAB** at 20 °C on KCl buffer (c =10 mM)

2.1.2 **TH10**

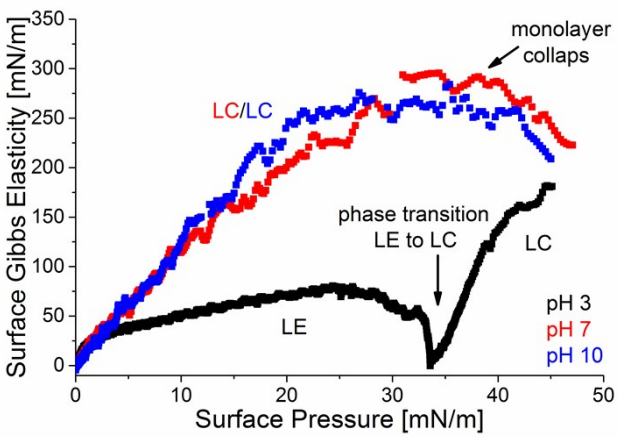

Figure S2: Surface Gibbs elasticity of **TH10** at 20 °C on HBr buffer (c =2 mM)

2.1.3 **OO10**

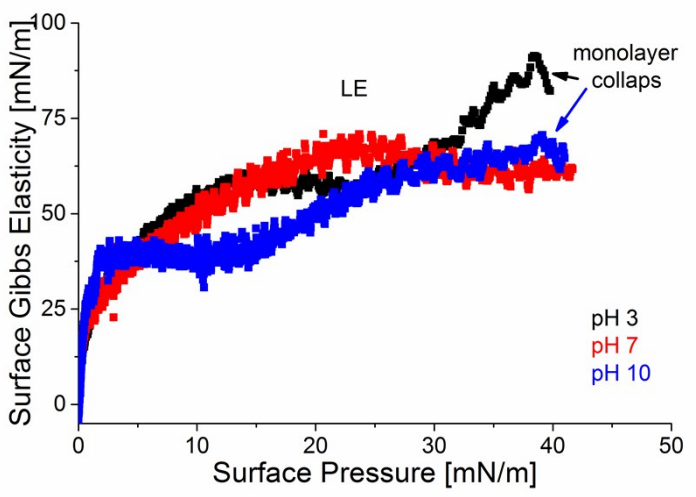

Figure S3: Surface Gibbs elasticity of **OO10** at 20 °C on HBr buffer (c =2 mM)

2.1.4 **TH4**

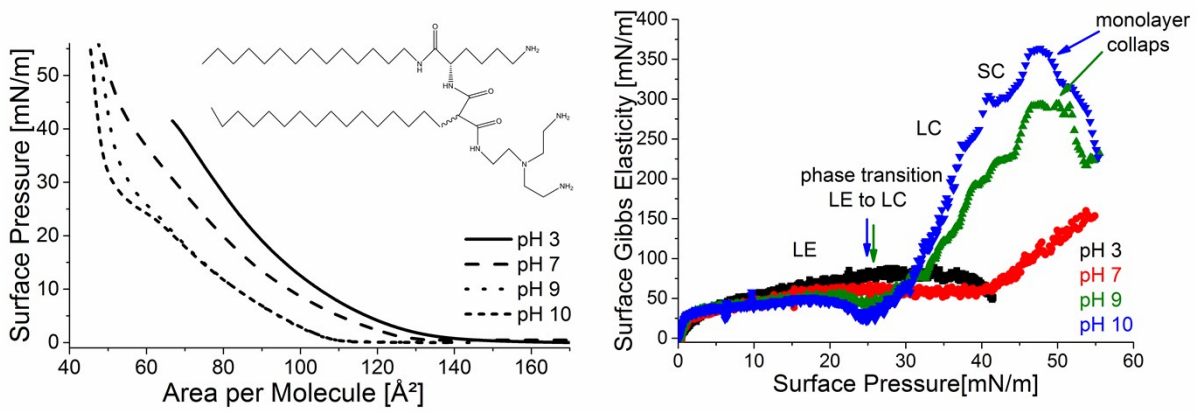

Figure S4: π/A-isotherm and surface Gibbs elasticity of **TH4** at 20 °C on HBr buffer (c =2 mM)

1.1.5 **OH4**

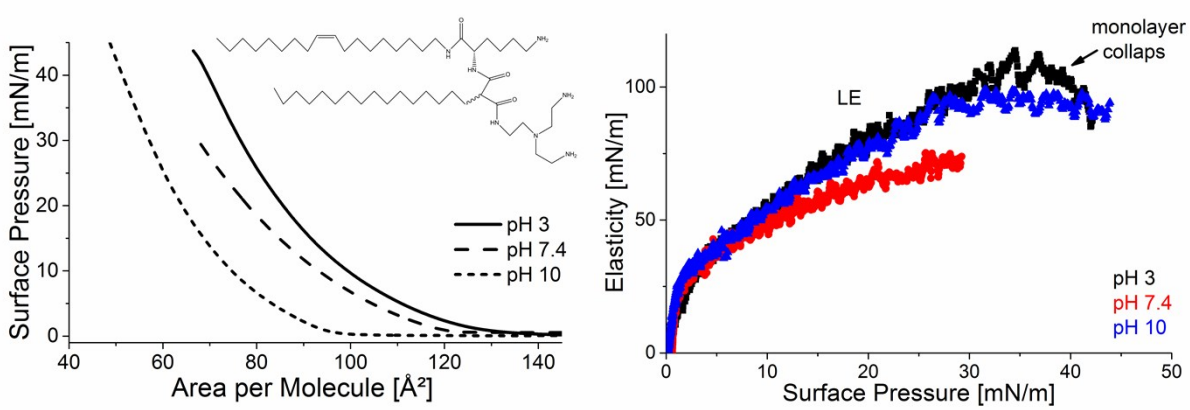

Figure S5: π/A-isotherm and surface Gibbs elasticity of **OH4** at 20 °C on HBr buffer (c =2 mM)

1.1.6 **OO4**

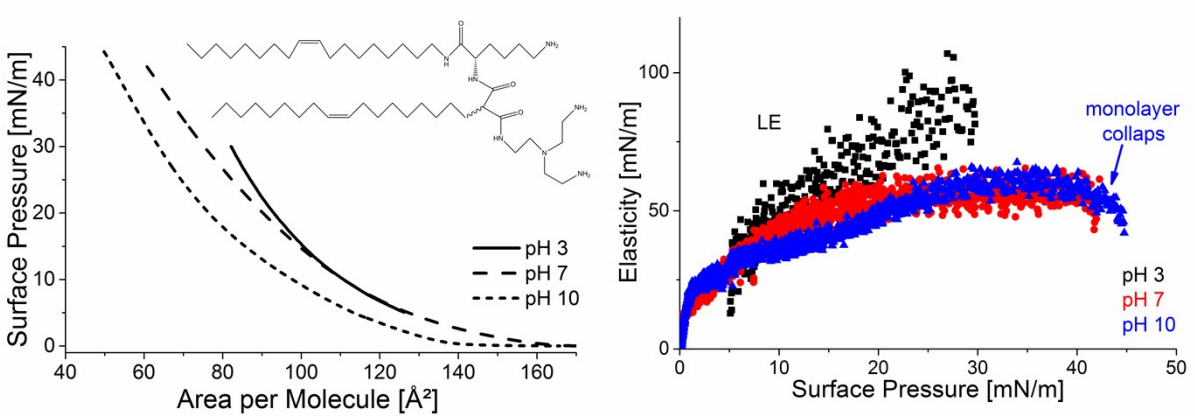

Figure S6: π/A-isotherm and surface Gibbs elasticity of **OO4** at 20 °C on HBr buffer (c =2 mM)

1.1.7 **TH14**

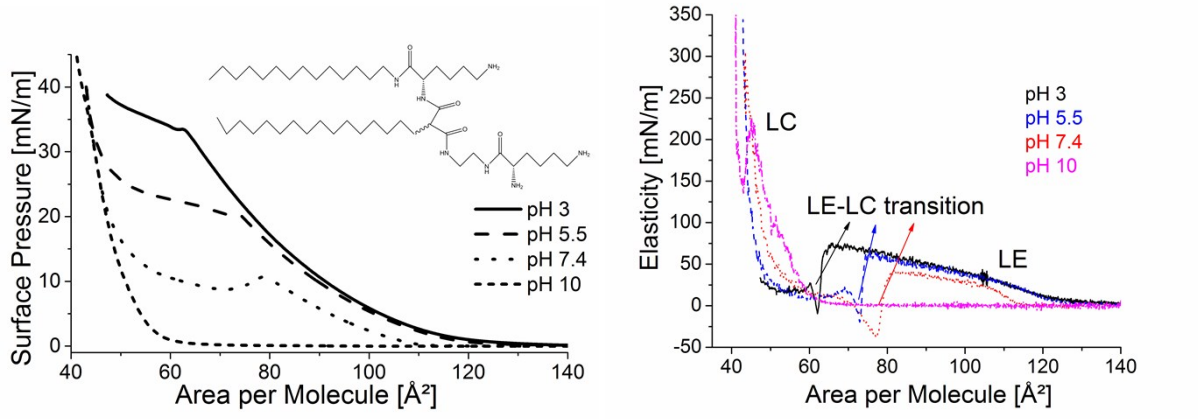

Figure S7: π/A-isotherm and surface Gibbs elasticity of **TH14** at 20 °C on HBr buffer (c =2 mM)

1.1.8 **OH14**

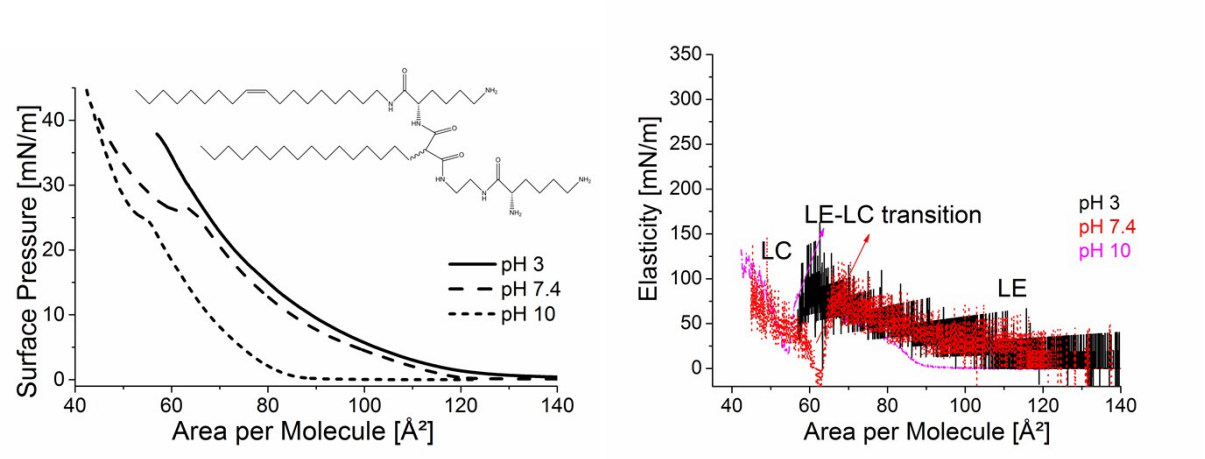

Figure S8: π/A-isotherm and surface Gibbs elasticity of **OH14** at 20 °C on HBr buffer (c =2 mM)

1.1.9 **OO14**

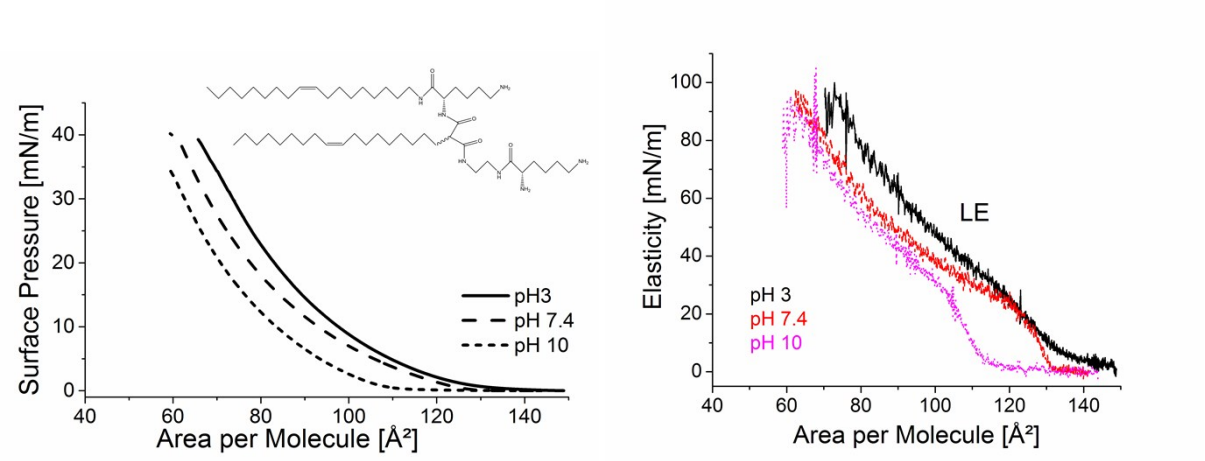

Figure S9: π/A-isotherm and surface Gibbs elasticity of **OO14** at 20 °C on HBr buffer (c =2 mM)

1.2 Total Reflection X-Ray Fluorescence

1.2.1 Titration curve of **OO10** (5 mN·m^{-1} and 30 mN·m^{-1})

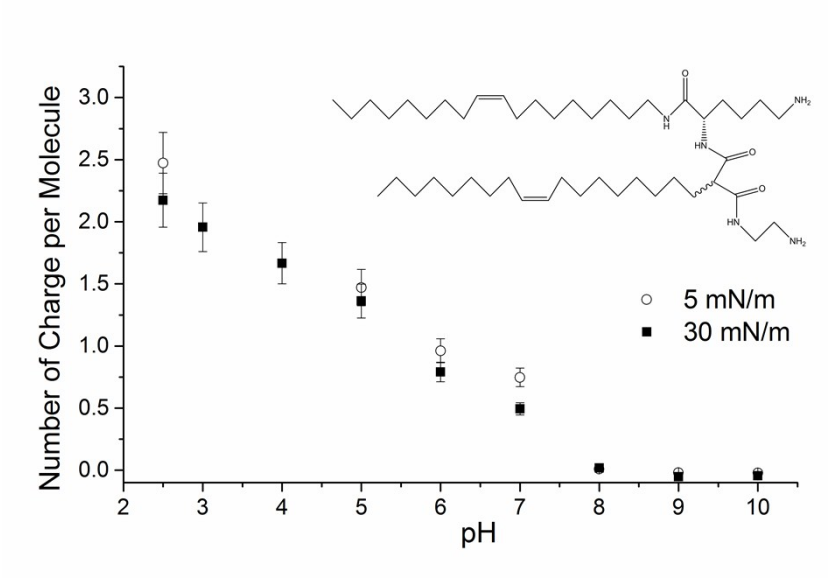

Figure S10: Number of Charge per Molecule for **OO10** on HBr buffer (2 mM, different pH values) at room temperature, π = 5 mN·m^{-1} (o) and π = 30 mN·m^{-1} (▪)

1.2.2 Titration curve of **OO4** (5 mN·m^{-1} and 30 mN·m^{-1})

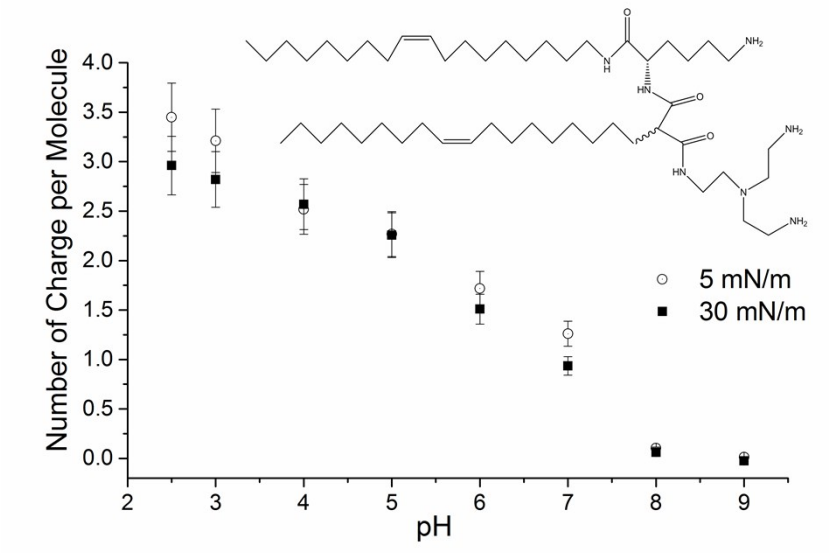

Figure S11: Number of Charge per Molecule for **OO4** on HBr buffer (2 mM, different pH values) at room temperature, π = 5 mN·m^{-1} (o) and π = 30 mN·m^{-1} (▪)

1.3 X-Ray Reflectivity

1.3.1 **OO10**

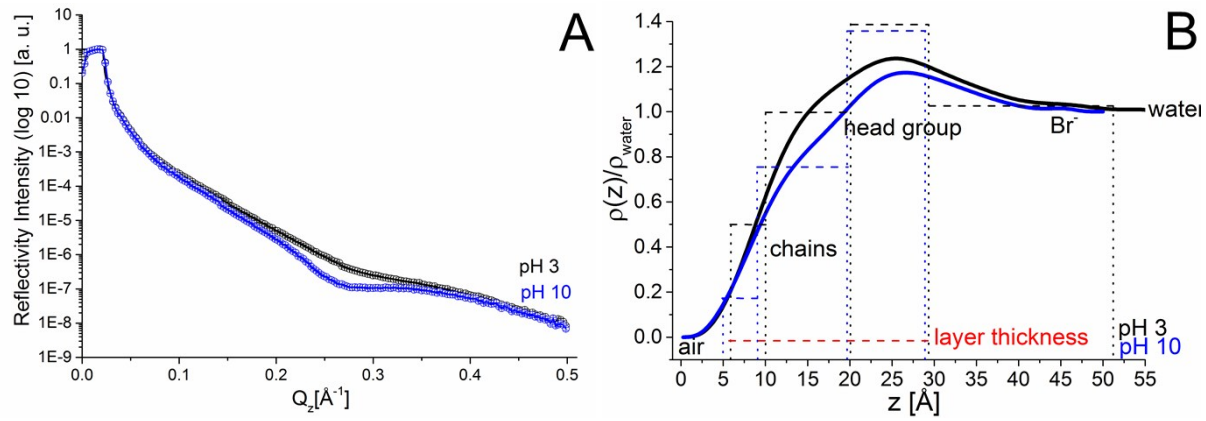

Figure S12: **A** X-ray reflectivity of **OO10** at 20 °C on HBr buffer at 30 mN·m^{-1}, **B** electron density normalized to that of water versus z. The box-model is shown.

Table S1: structural data obtained from fits of the specular X-ray reflectivity curves of OO10 on HBr buffer pH 3 and pH 10, 20 °C, 30 mN·m^{-1}.

	chain				head group				
	z [Å]	**ρ [e-/ Å^{-3}]**	**e$^-$ [e$^-$ / Å^{-2}]**	**theoretical number of electrons**	**z [Å]**	**ρ [e-/ Å^{-3}]**	**e$^-$ [e$^-$ / Å^{-2}]**	**theoretical number of electrons**	**measured numbers of electrons**
pH 3	14.222	1.24	3.668	286	9.429	1.39	4.382	146	287
pH 10	14.756	0.925	2.909	286	9.24	1.359	4.199	146	250

10 e$^-$ for H_2O; 36 e$^-$ for Br$^-$

1.3.2 **OO4**

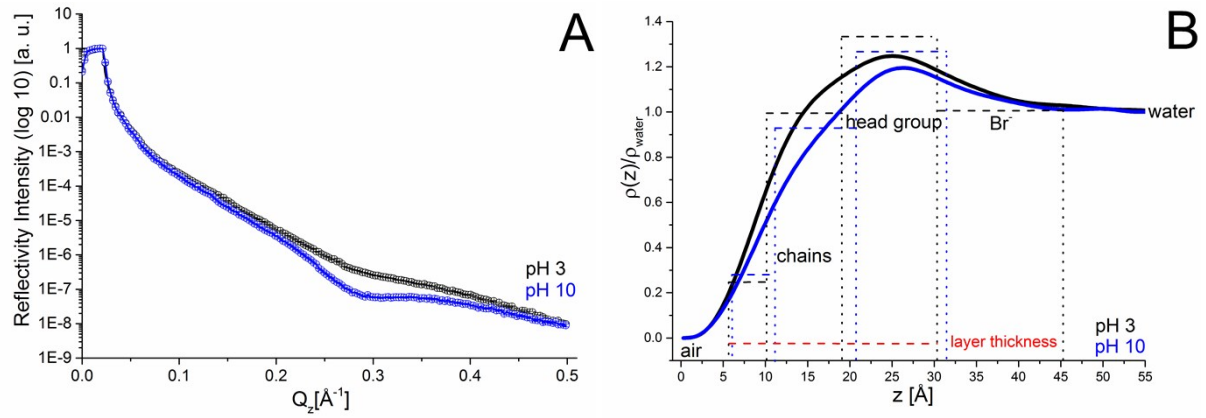

Figure S13: **A** X-ray reflectivity of **OO4** at 20 °C on HBr buffer at 30 mN·m^{-1}, **B** electron density normalized to that of water versus z. The box-model is shown.

Table S2: structural data obtained from fits of the specular X-ray reflectivity curves of OO4 on HBr buffer pH 3 and pH 10, 20 °C, 30 mN·m^{-1}.

	chain				head group				
	z [Å]	**ρ [e-/ Å^{-3}]**	**e$^-$ [e$^-$ / Å^{-2}]**	**theoretical number of electrons**	**z [Å]**	**ρ [e-/ Å^{-3}]**	**e$^-$ [e$^-$ / Å^{-2}]**	**theoretical number of electrons**	**measured numbers of electrons**
pH 3	13.492	1.24	3.421	286	11.267	1.332	5.029	194	413
pH 10	14.606	1.207	3.412	286	10.872	1.27	4.617	194	294

10 e$^-$ for H_2O; 36 e$^-$ for Br$^-$