

# Structuring effect of some salts on glycerol carbonate: a near-infrared spectroscopy, small- and wide-angle X-ray scattering study

## Supplementary Material

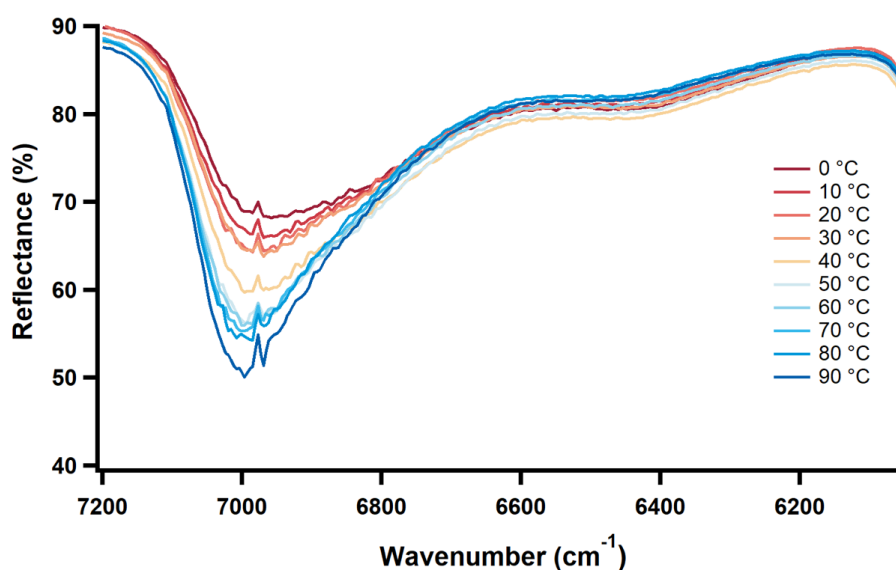
Duccio Tatini<sup>a</sup>, Ilaria Clemente<sup>a</sup>, Moira Ambrosi<sup>a</sup>, Sandra Ristori<sup>a</sup>,

Barry W. Ninham<sup>b</sup>, Pierandrea Lo Nostro<sup>a,c\*</sup>

a: Department of Chemistry "Ugo Schiff" and CSGI, University of Florence, 50019 Sesto Fiorentino (Firenze), Italy

b: Department of Applied Mathematics, Research School of Physical Sciences and Engineering, Australian National University, Canberra ACT 0200, Australia

c: Enzo Ferroni Foundation, 50019 Sesto Fiorentino (Firenze), Italy



**Figure S1.** NIR spectra of pure GC in the range 7200 – 6000 cm<sup>-1</sup> at 0, 10, 20, 30, 40, 50, 60, 70, 80 and 90 °C.

## Definition two power law from SASView online manual

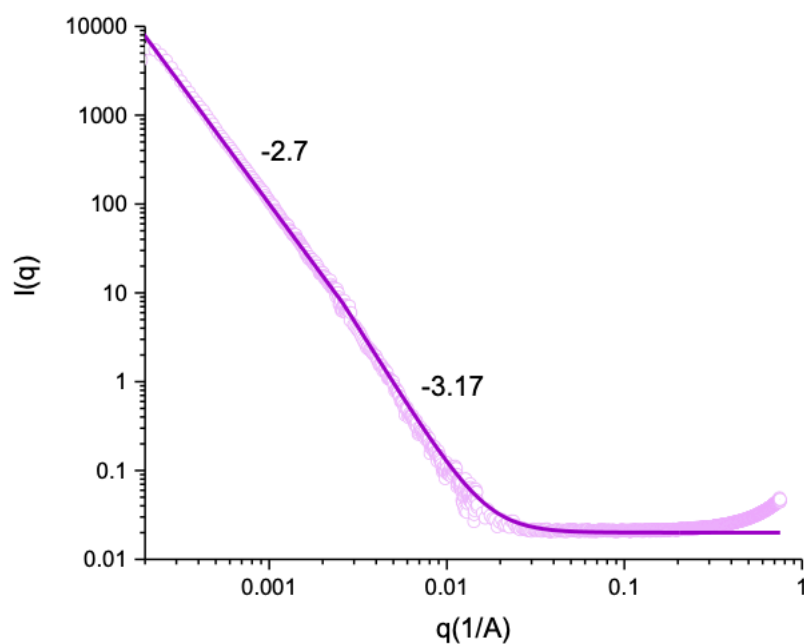
The scattering intensity  $I(q)$

is calculated as

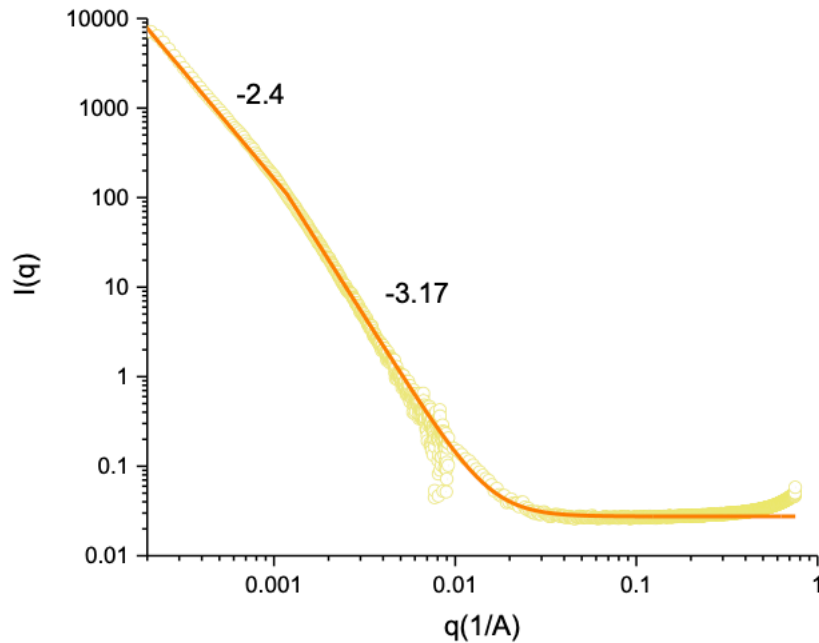
$$I(q) = \begin{cases} Aq^{-m_1} + bkg & q \leq q_c \\ Cq^{-m_2} + bkg & q > q_c \end{cases}$$

where  $q_c$  is the location of the crossover from one slope to the other,  $A$  is the scaling coefficient that sets the overall intensity of the lower  $q$  power law region,  $m_1$  is the power law exponent at low  $q$ ,  $m_2$  is the power law exponent at high  $q$  and  $bkg$  is the background. The scaling of the second power law region (coefficient  $C$ ) is then automatically scaled to match the first by the following formula:

$$C = \frac{Aq_c^{m_2}}{q_c^{m_1}}$$



**Figure S2.** Pure GC 1D SAXS intensity spectrum (pink dots) and two power law model fit (solid line).



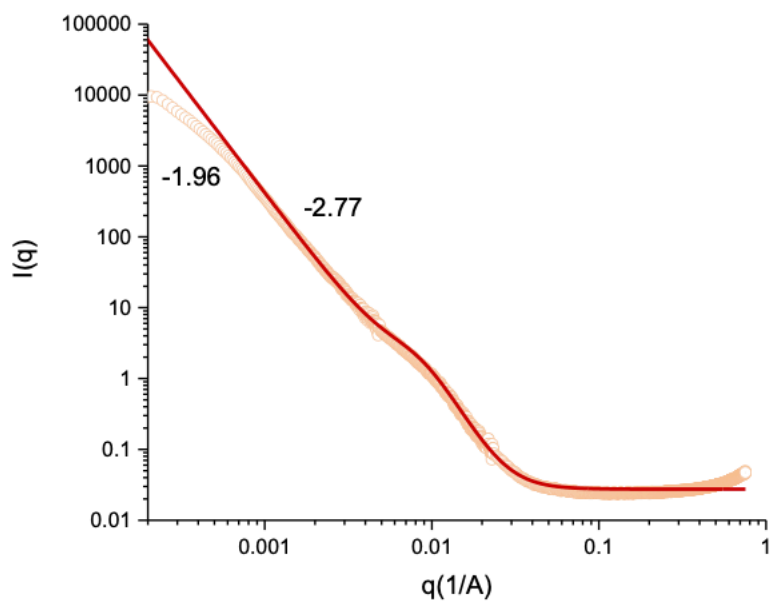
**Figure S3.** 1D SAXS intensity spectrum (yellow dots) and two power law model fit (solid line) of saturated  $\text{K}_3\text{PO}_4$  solution in GC.

### Definition correlation length from SASView online manual

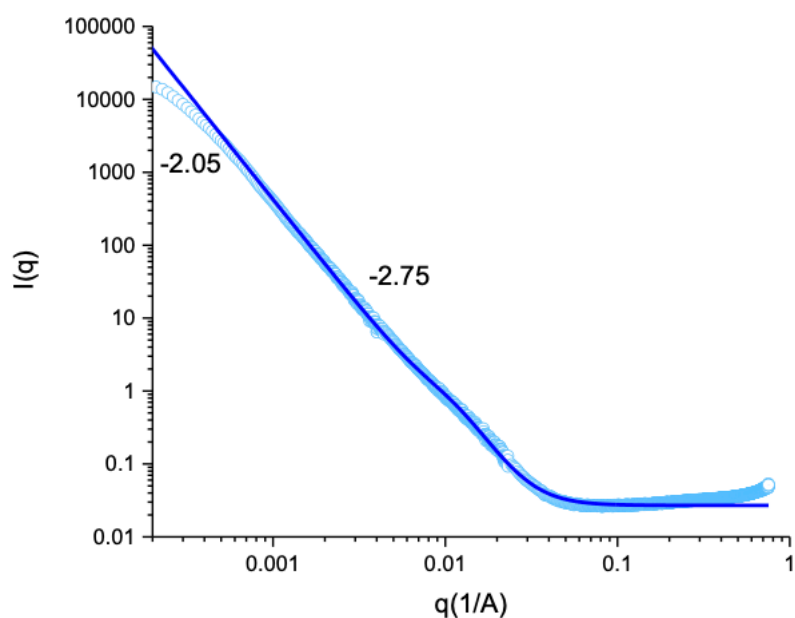
The scattering intensity  $I(q)$  is calculated as:

$$I(q) = \frac{A}{q^n} + \frac{C}{1 + (q\xi)^m} + bkg$$

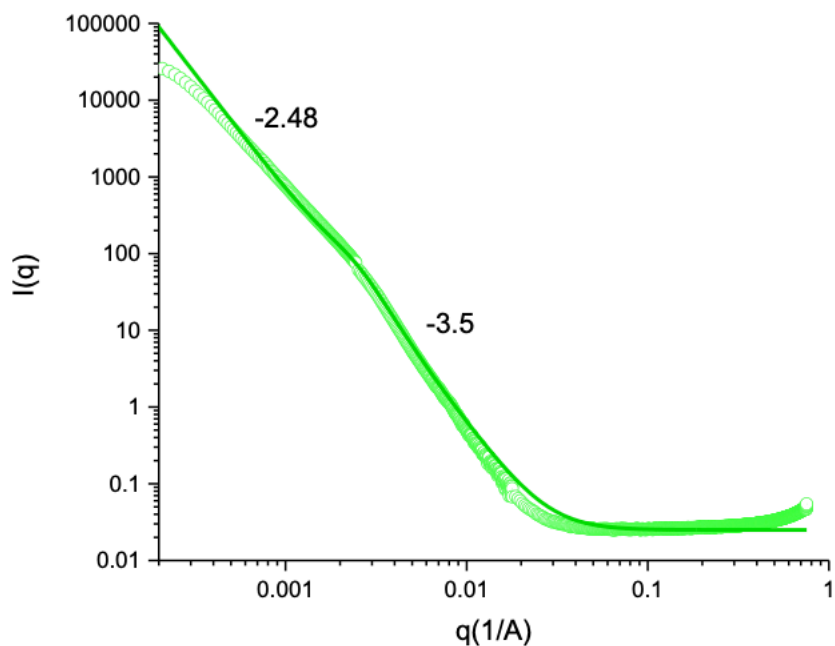
The first term is due to the Porod scattering from the clusters (exponent  $n$ ) and the second term is a Lorentzian function describing the scattering from a ribbon structure (exponent  $m$ ). This second term reflects the ribbon/solvent interactions and therefore the thermodynamics. The two factors  $A$  and  $C$ , and the two exponents  $n$  and  $m$  are used as fitting parameters. (Respectively *porod\_scale*, *lorentz\_scale*, *porod\_exp* and *lorentz\_exp* in the program parameter list.) The remaining parameter  $\xi$  (*cor\_length* in the parameter list) is a correlation length for the ribbons. Note that when  $m = 2$  this functional form becomes the familiar Lorentzian function. Some interpretations of the values of  $A$  and  $C$  are possible depending on the values of  $m$  and  $n$ .



**Figure S4.** 1D SAXS intensity spectrum (orange dots) and correlation length model fit (solid line) of KF 0.21M solution in GC.



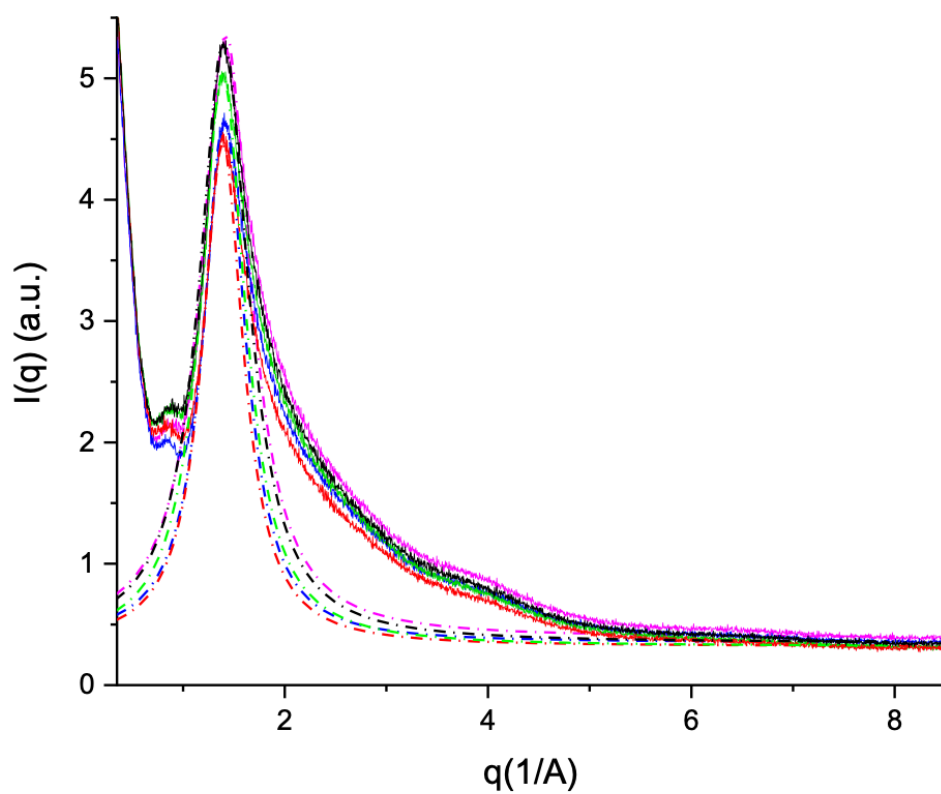
**Figure S5.** 1D SAXS intensity spectrum (light blue dots) and correlation length model fit (solid line) of saturated KF solution in GC.



**Figure S6.** 1D SAXS intensity spectrum (green dots) and correlation length model fit (solid line) of saturated  $\text{K}_2\text{CO}_3$  solution in GC.

**Table S1.** Fitting parameters extracted from the SAXS data analysis.

Sample	Power 1	Power 2	Crossover ( $\text{\AA}^{-1}$ )	Porod exp	Lorentz exp	Correlation length ( $\text{\AA}$ )
Pure GC	2.7	3.17	0.0026	-	-	-
KF 0.21 M	-	-	-	3.08	4.35	113
Saturated KF	-	-	-	2.95	4	88
Saturated $\text{K}_2\text{CO}_3$	-	-	-	3.05	5.3	400
Saturated $\text{K}_3\text{PO}_4$	2.4	3.2	0.00118	-	-	-



**Figure S7.** Peak fitting for the different samples (experimental values in solid lines, fitting curves in dashed lines): pure GC (pink), GC in the presence of saturated  $\text{K}_3\text{PO}_4$  (blue),  $\text{K}_2\text{CO}_3$  (green), KF (red) and 0.21 M KF (black).