Investigation of Aggregation in Solutions of C12E7 by the SANS Method

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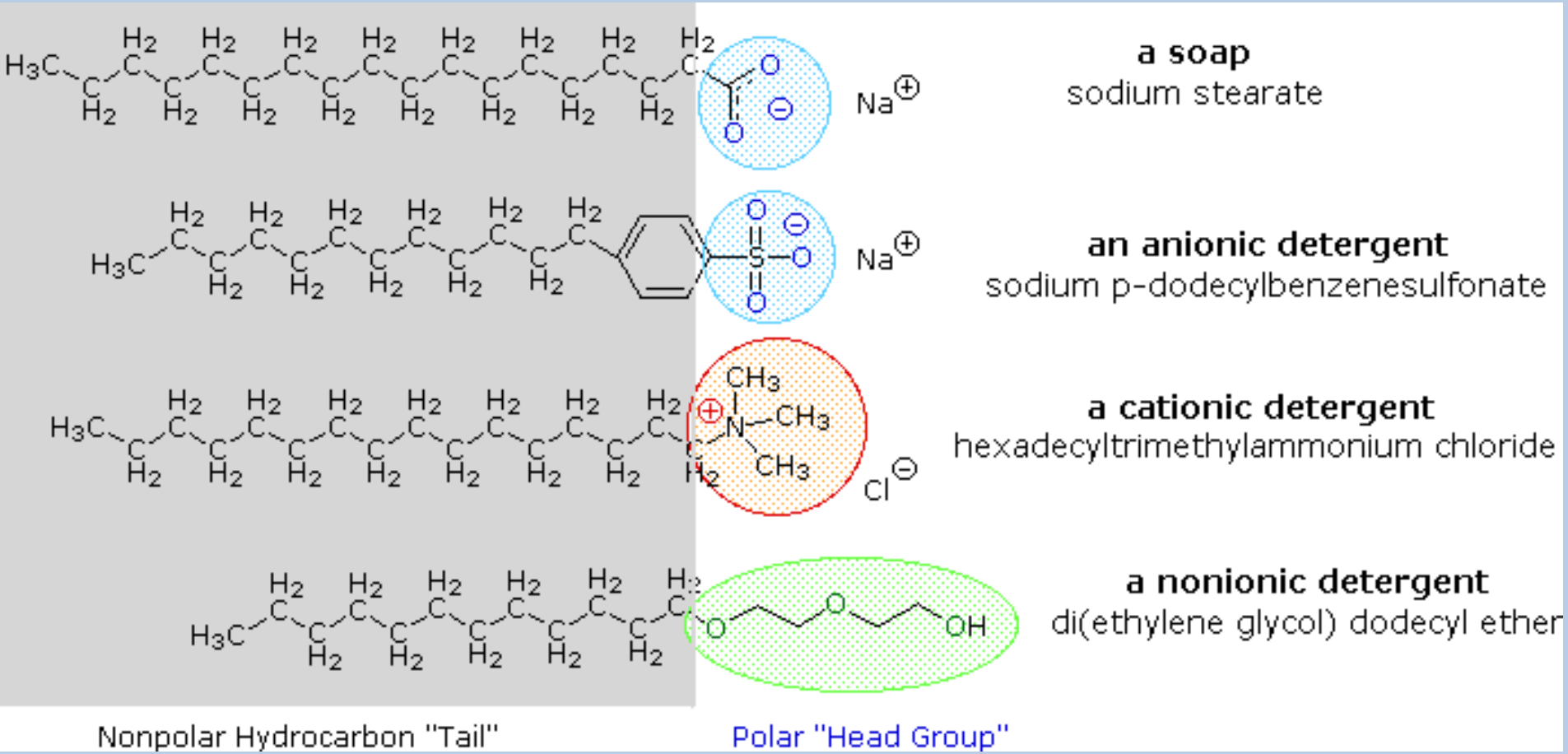
Purpose of the project

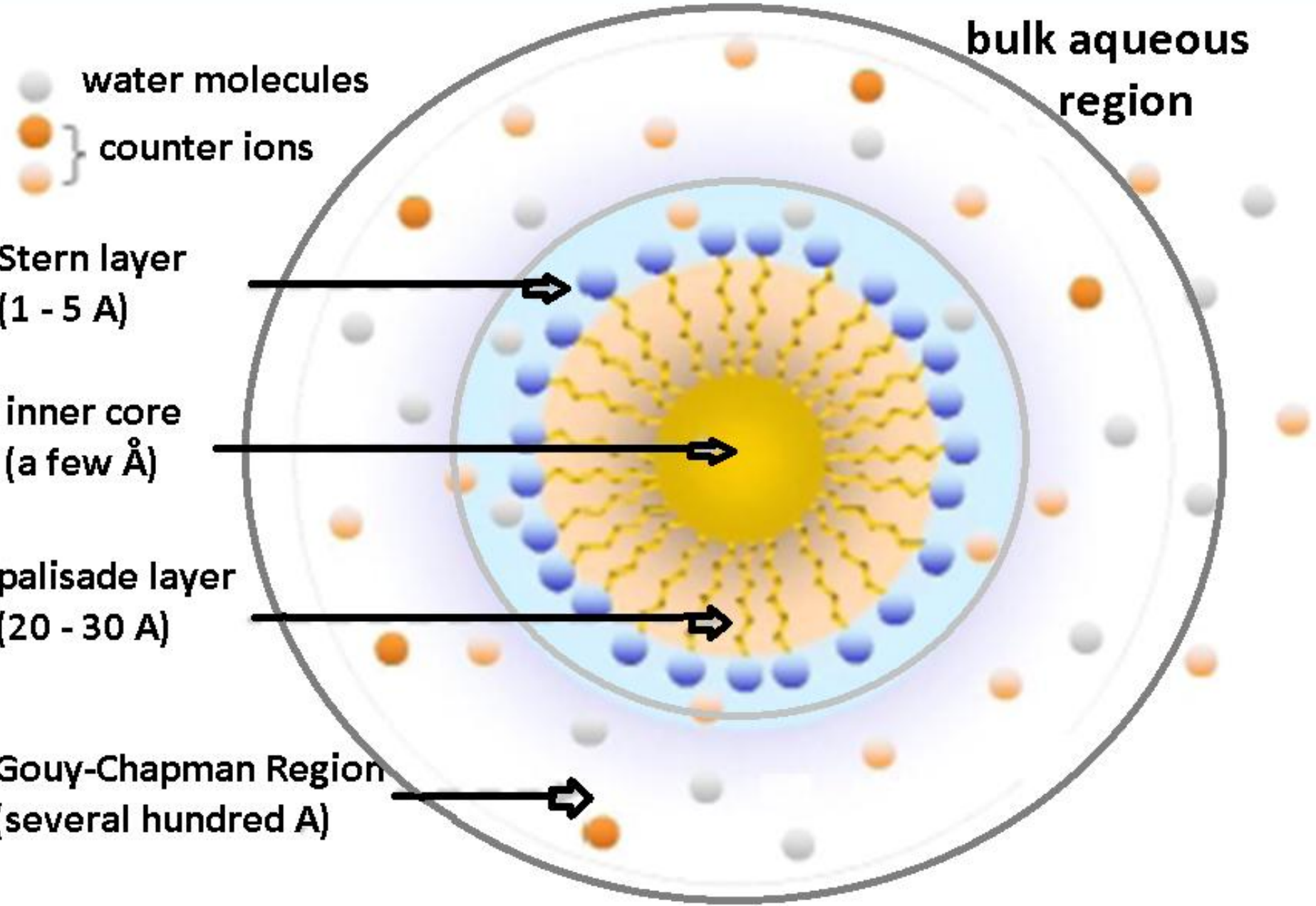
- Investigation of size and shape of micelles in **C12E7** solutions of different concentrations and at different temperatures.

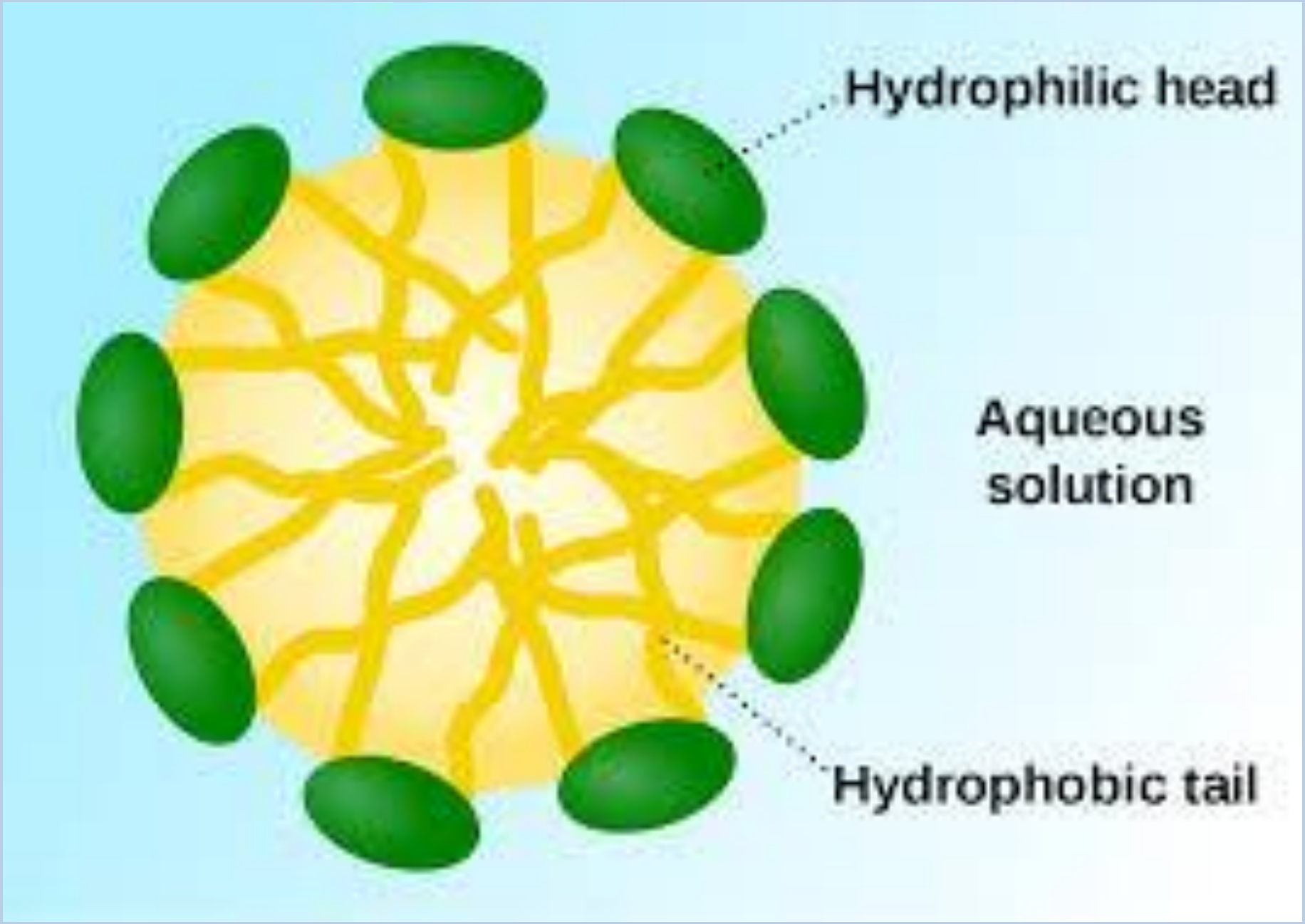
- Investigation of size and shape of micelles in mixture systems of **C12E7 and d-urea** solutions at different temperatures.

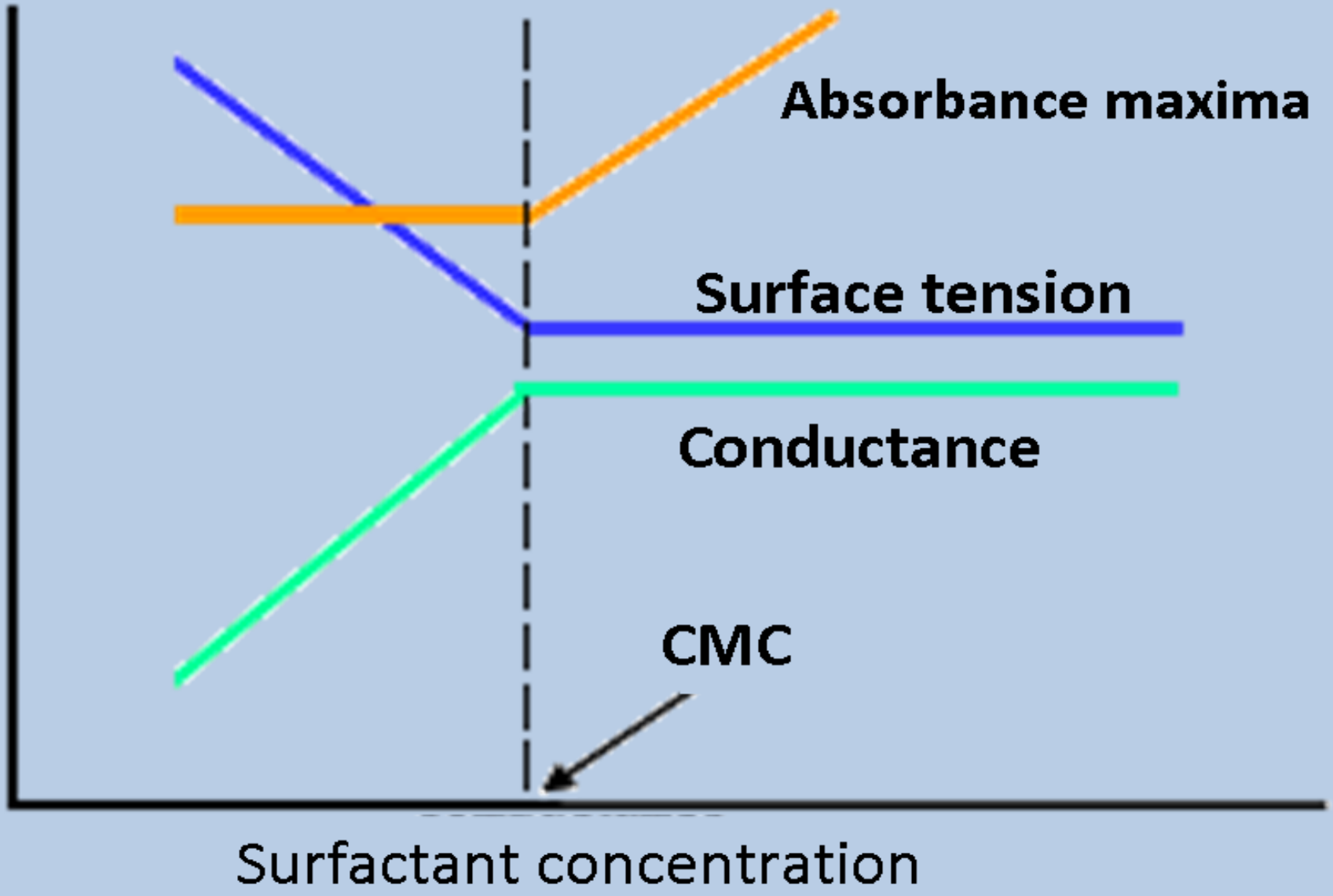
Surfactants



Micelles – structure of aggregations




Hydrophilic head
Aqueous solution
Hydrophobic tail


Absorbance maxima
Surface tension
Conductance
CMC
Surfactant concentration

NONIONIC SURFACTANTS type CiEj

In the conventional notation CiEj,

”C” and ”E” refer to alkyl (CH)x and ethoxylate (CH2CH2O) units.

NONIONIC SURFACTANTS

•Nonionic surfactants such as oligo(oxyyethylene)-n-alkyl ether (abbreviated as CiEj) show a rich phase behaviour in aqueous mixtures.

•At very low surfactant concentrations, the surfactant dissolves to unimers.

•With an increase in the surfactant concentration, the temperature dependent **critical micelle concentration (CMC)** is passed and the surfactant molecules form micelles, mostly globular, at least at low temperatures.

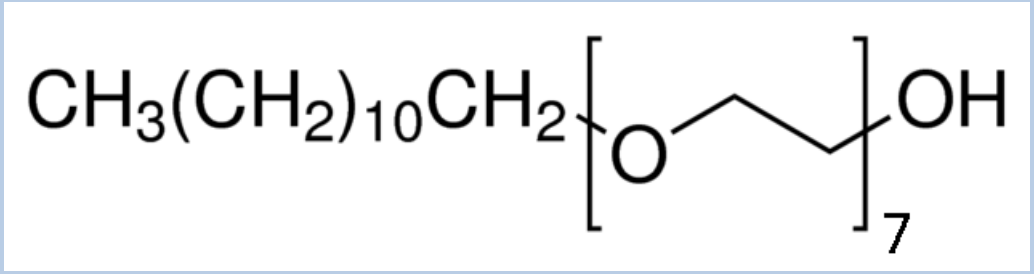
•Above the so-called **cloud curve**, the solutions first become very turbid and then the phases separate into two micellar solutions of extremely different surfactant contents.

•The position of the critical point depends on the overall chain length of the amphiphile and the hydrophilic-lipophilic balance.

•The understanding of the binary phase behaviour and structural properties is central for understanding of ternary mixtures with oil (microemulsions).

Heptaethylene Glycol Monododecyl Ether (C12E7)

- Synonym: $C_{12}E_7$, Dodecylheptaglycol, Polyoxyethylene (7) lauryl ether
- Classification: nonionic detergent
- Molecular Formula: $C_{26}H_{54}O_8$
- CAS Number: 3055-97-8
  Formula Weight: 494.70
  pH: 3-8 (1% solution in water)



Application

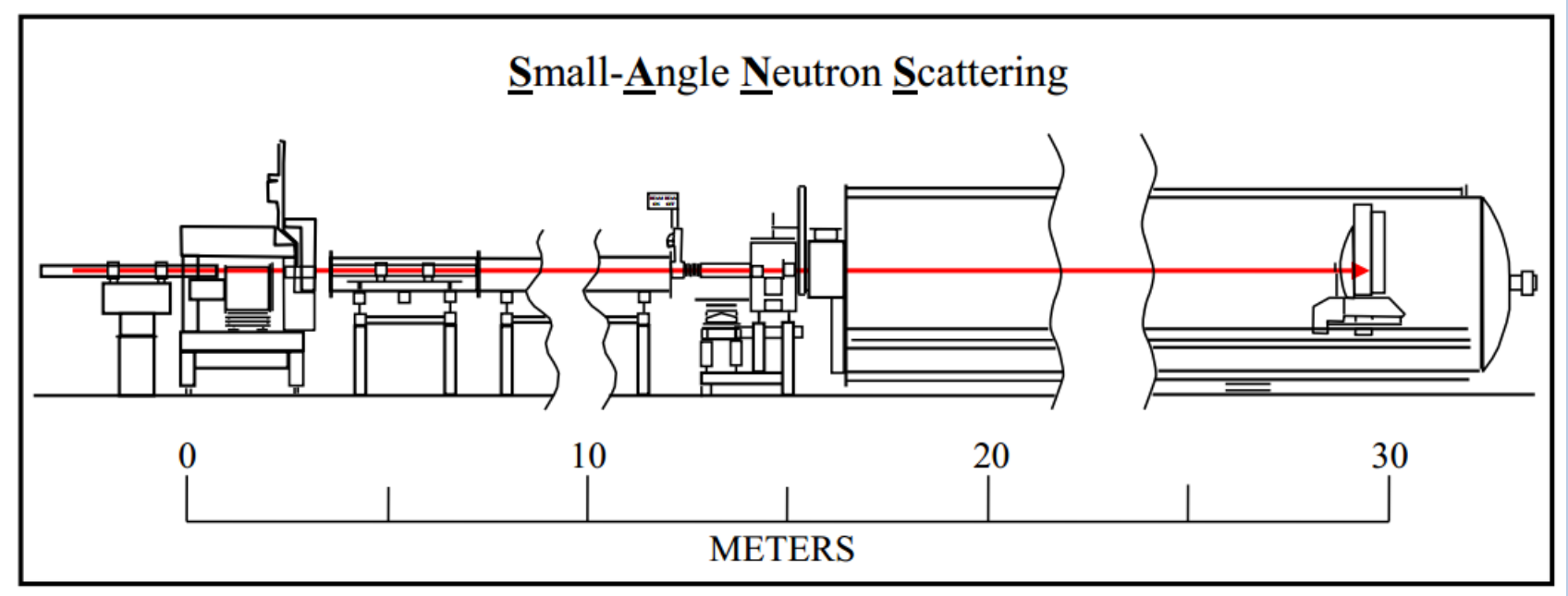
- Heptaethylene glycol monododecyl ether is a kind of non-ionic detergent which can be utilized as a source of carbon and energy by an organism isolated from activated sludge.

- It can facilitate degradation of waste hydrocarbons such as crude oil and vegetable oil

C12E8
(Octaethylene glycol monododecyl)

- Detergent used for the study of membrane proteins in a native-like state, e.g. ATPase. Used in the mixed micellar assay for lipoxygenase activity at neutral pH and for functional reconstitution of influenza virus envelopes.
- Octaethylene glycol monododecyl ether has been used in research on the intestinal sodium transport mechanisms. It has also been used in a study to investigate interactions between dyes and surfactants in inkjet ink used for textiles.

SANS theoretical background (Small-angle neutron scattering)



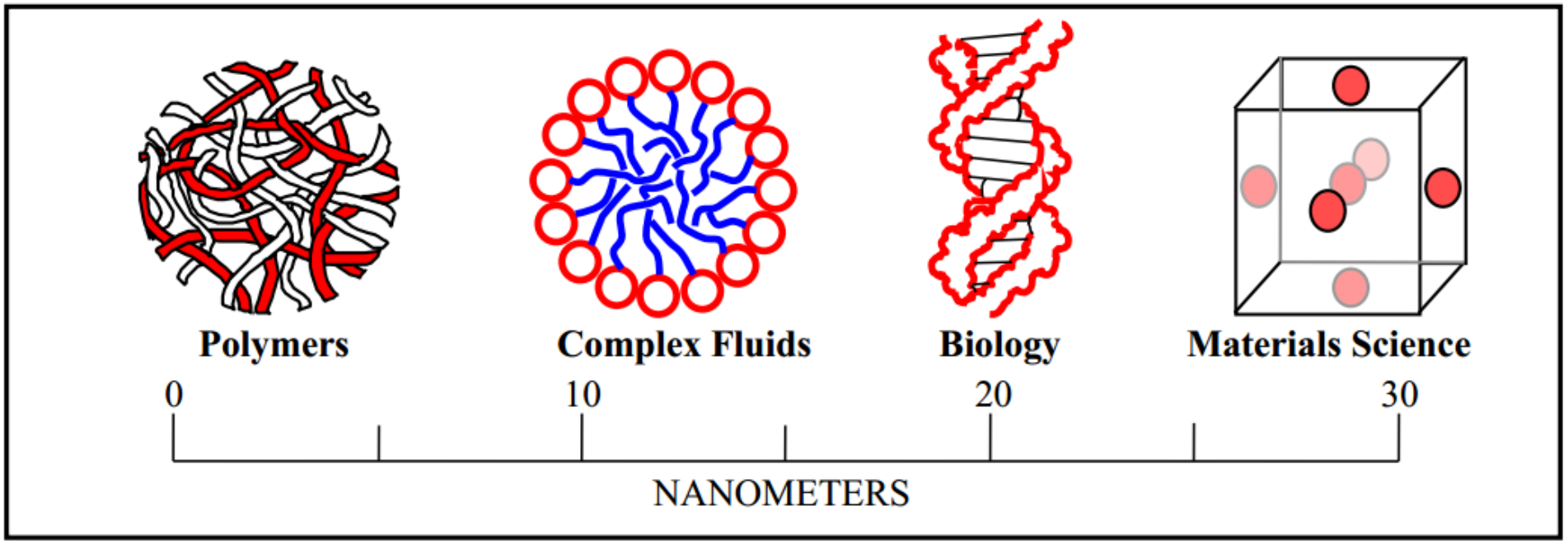
Information from SANS

- Size
- Shape
- Molecular weight
- Interaction distance
- Self-Assembly

0.008˚ - 8˚

SANS yields information on the spatial arrangement of heterogeneities of 1 to 300nm (20,000nm for USANS)

Range of SANS



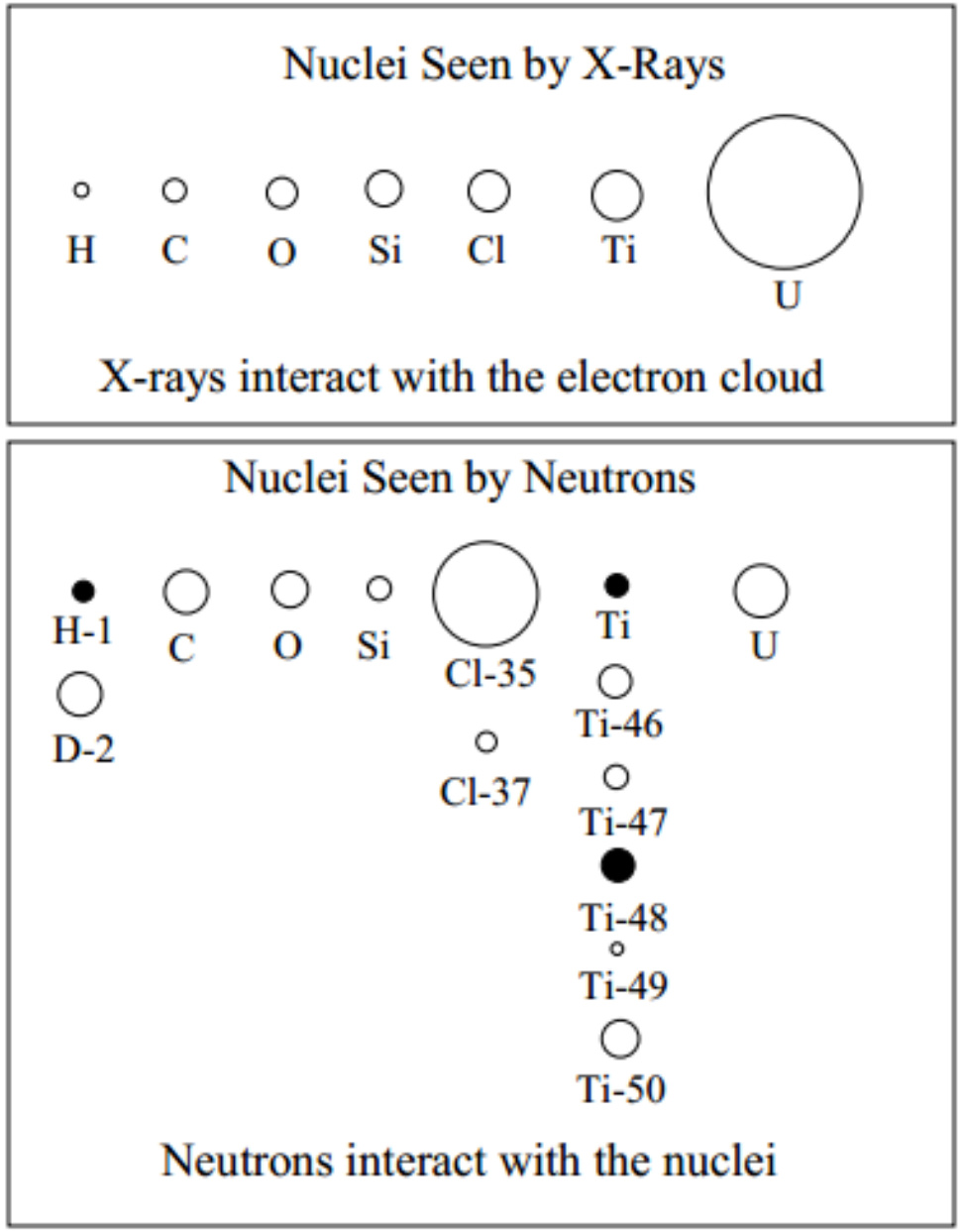
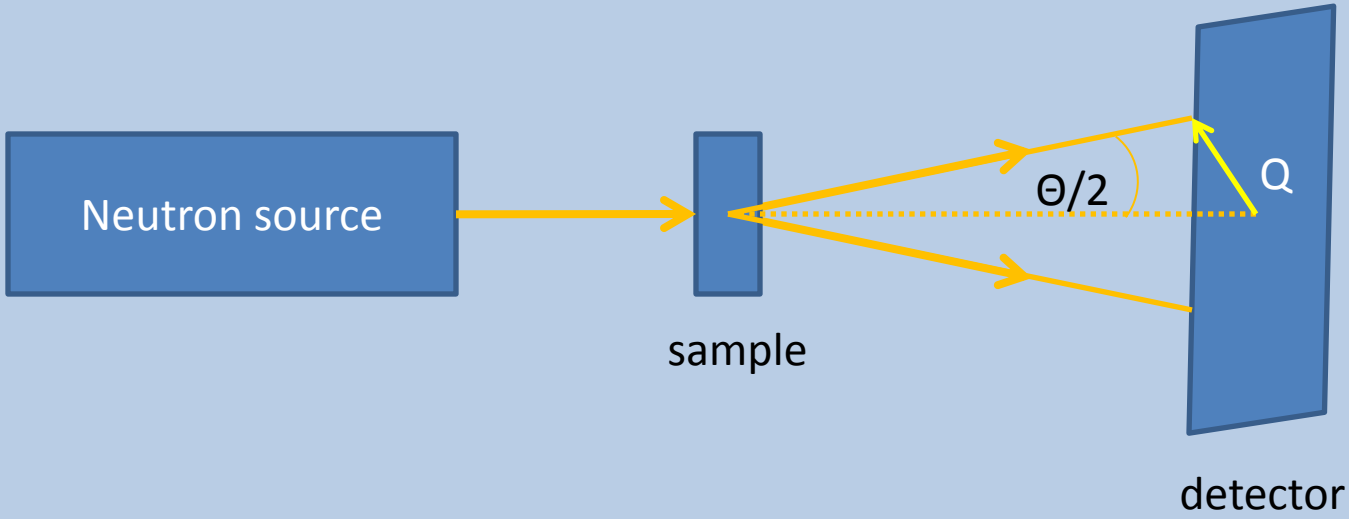


Figure 1: Neutrons are scattered from nuclei while x-rays are scattered from electrons. Scattering lengths for a few elements are compared. Negative neutron scattering lengths are represented by dark circles.

SANS fundamentals



$$I(Q) = A \times P(Q) \times S(Q)$$

$$P(Q) = \left| \int \rho(r) e^{-iQr} dr^3 \right|^2 \Big/ \left| \int \rho(r) dr^3 \right|^2$$

$$A = n v^2 \Delta\rho^2$$

I(Q) – intensity
A – const.
P(Q) – normalized form factor
S(Q) – structure factor
(for dilute solutions S=1)
n – number of density
v – volume of particle
Δρ – difference of length density scattering (contrast)
Q – scattering vector

Atomic nucleus	b [fm]	Molar weight [g/mol]
^{1}H	- 3.741	1
^{2}H	+ 6.674	2
C	+ 6.646	12
N	+ 9.362	14
O	+ 5.805	16
Br	+ 6.795	173

Scattering length density

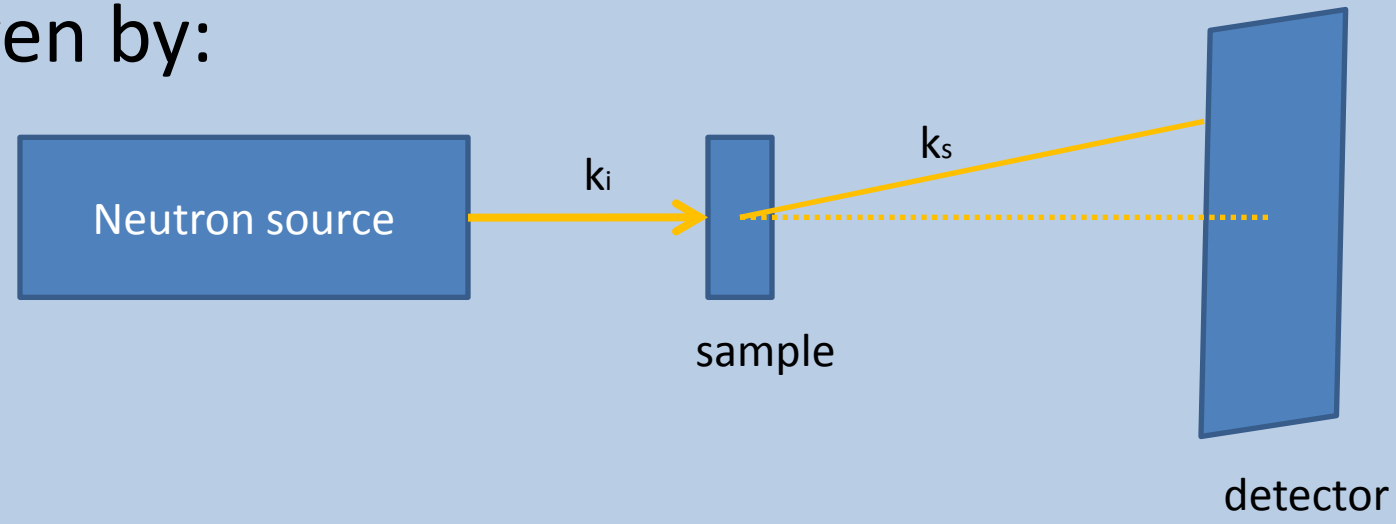
- Define a "Scattering Length Density"

$$\rho(\vec{\mathbf{r}}) = b_i \, \delta(\vec{\mathbf{r}} - \vec{\mathbf{r}}_i) \qquad \text{or} \qquad \rho = \frac{\sum_i^n b_i}{\overline{V}}$$

$\overline{V}$ is the volume containing the n atoms

The scattering vector

The modulus of the resultant between the incident, k_i, and scattered, k_s, wavevectors, given by:



$$Q = |Q| = |k_s - k_i| = \frac{4\pi n}{\lambda}\sin(\Theta/2)$$

Differential cross–section

Contains all the information on the shape, size and interactions of the scattering bodies in the sample.

$$\frac{\delta\Sigma}{\delta\Omega}(Q) = N_p V_p^2 (\Delta\sigma)^2 P(Q) S(Q) + B_{inc}$$

N_p – number concentration of scattering bodies

V_p^2 – square of the volume of scattering body

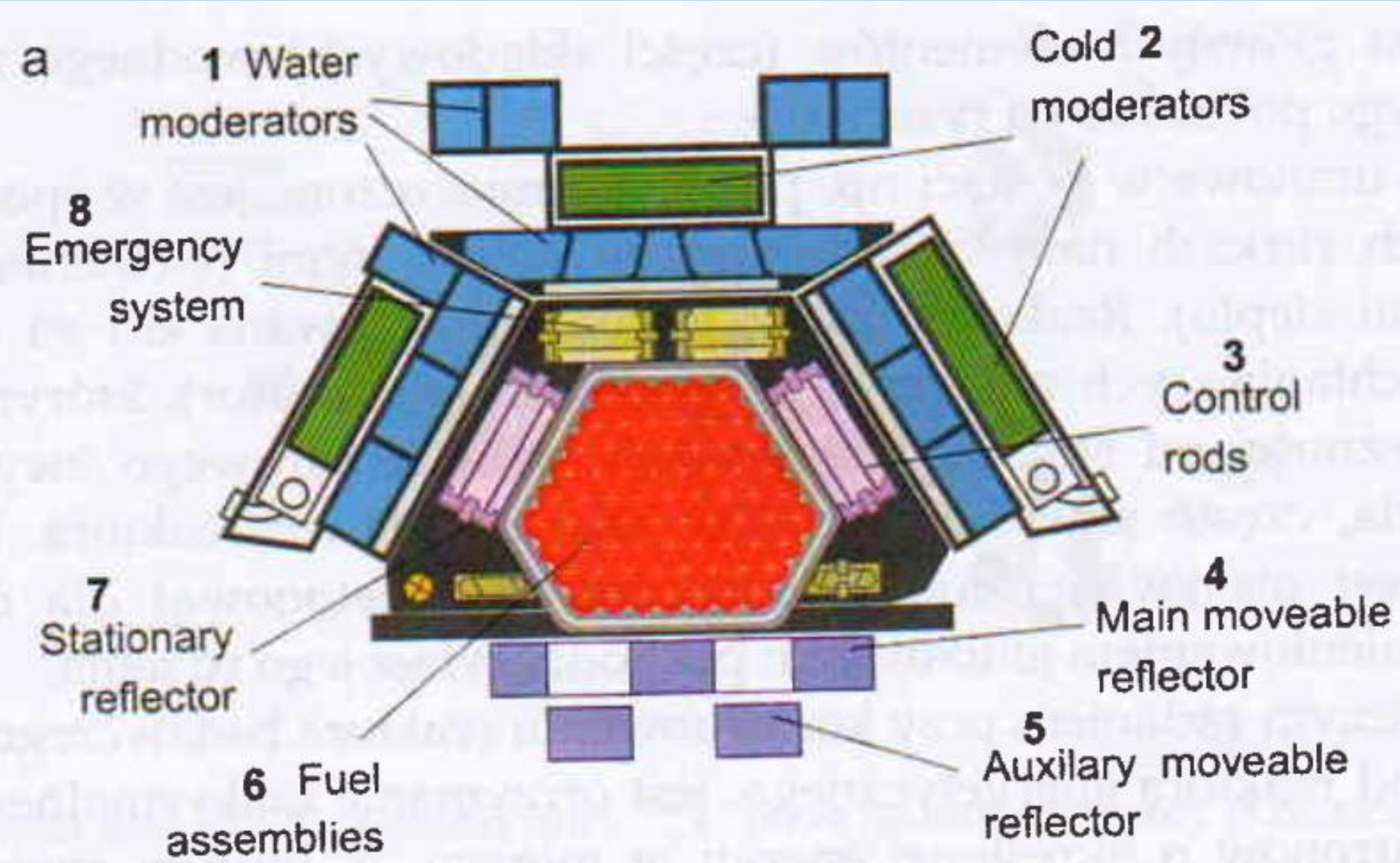
$\Delta\sigma^2$ – square of the difference in neutron scattering length densities

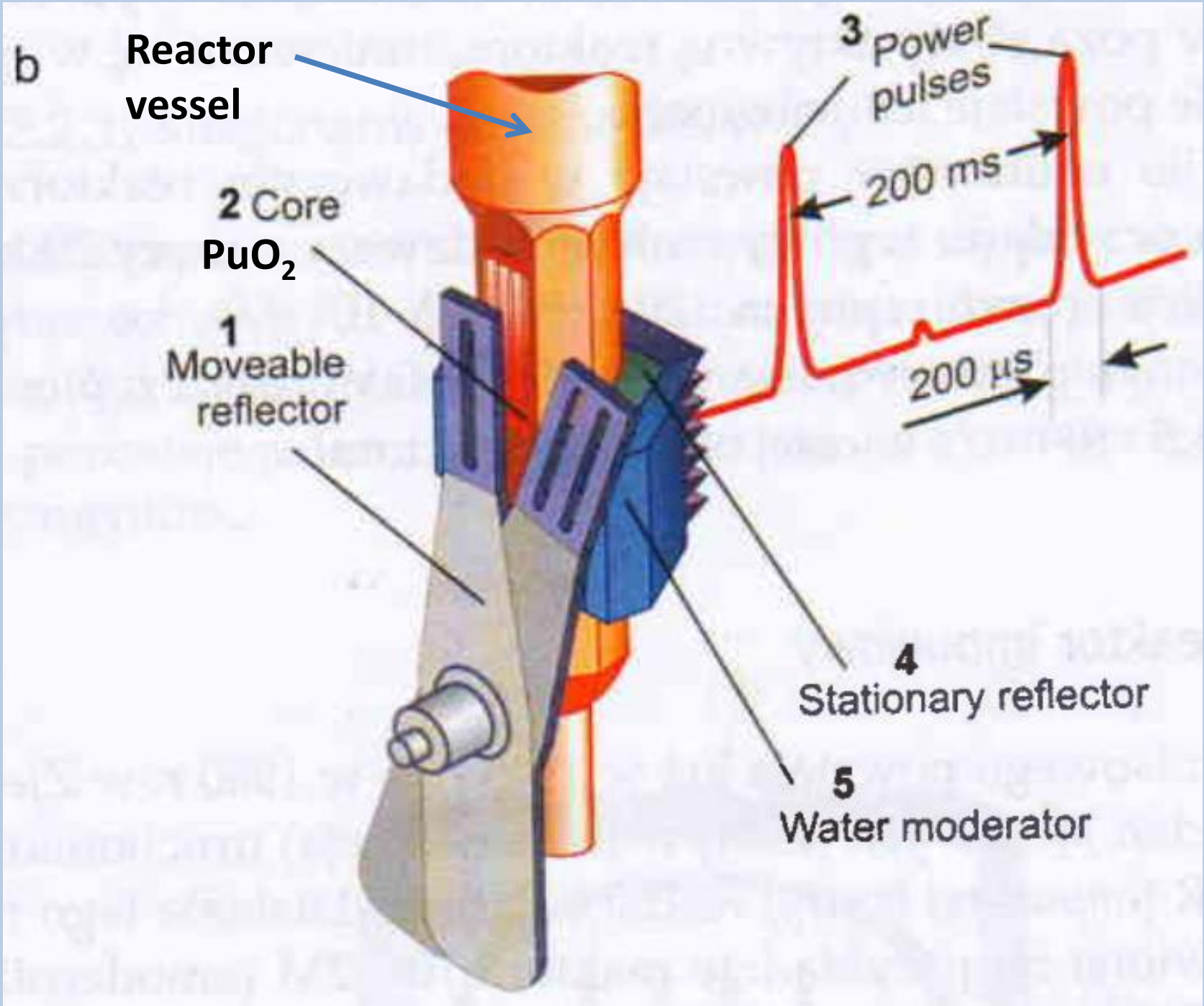
Q – the modulus of the scattering vector

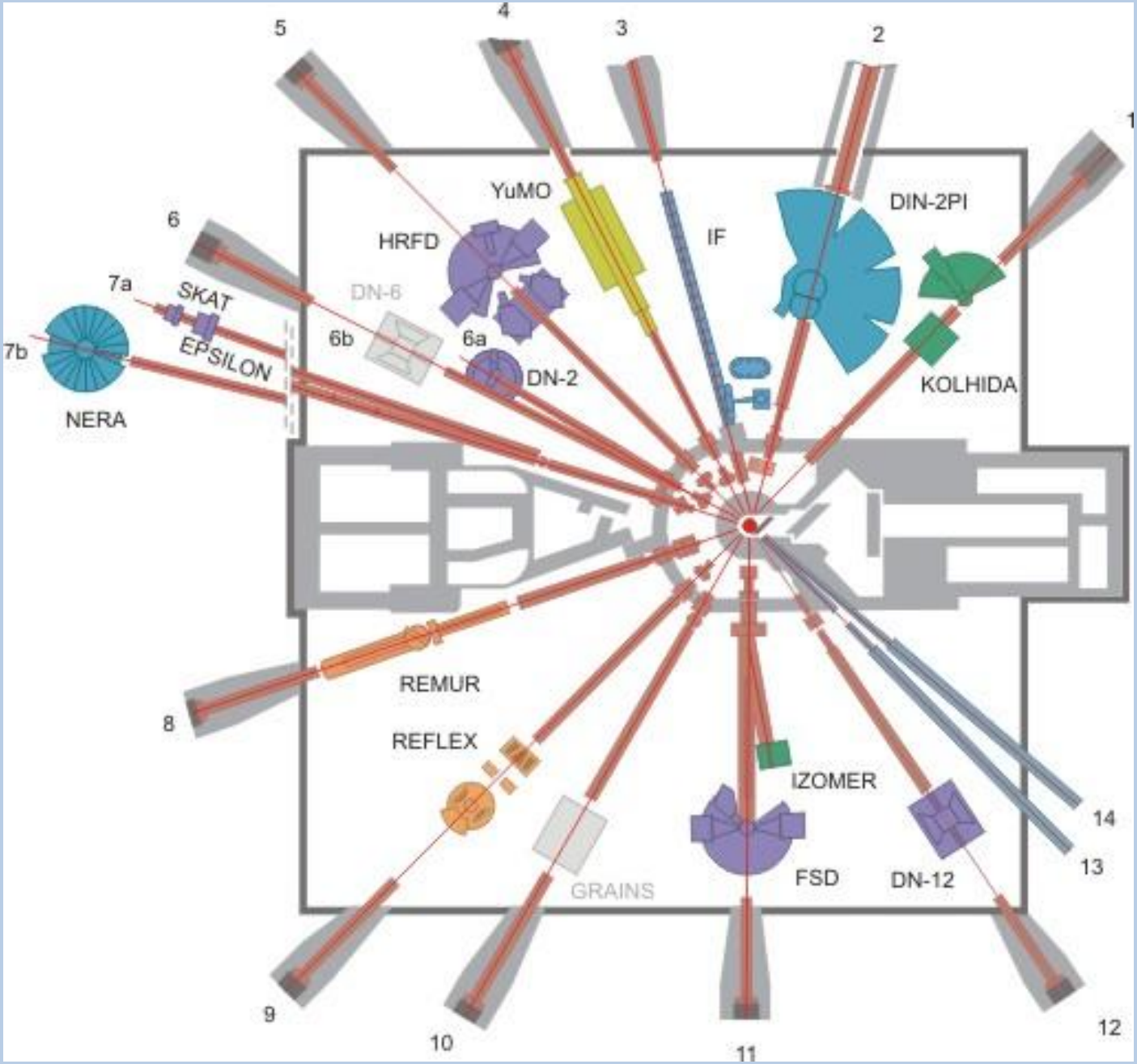
B_{inc} – the isotropic incoherent background signal

Equipment

Fast Pulsed Reactor IBR -2M

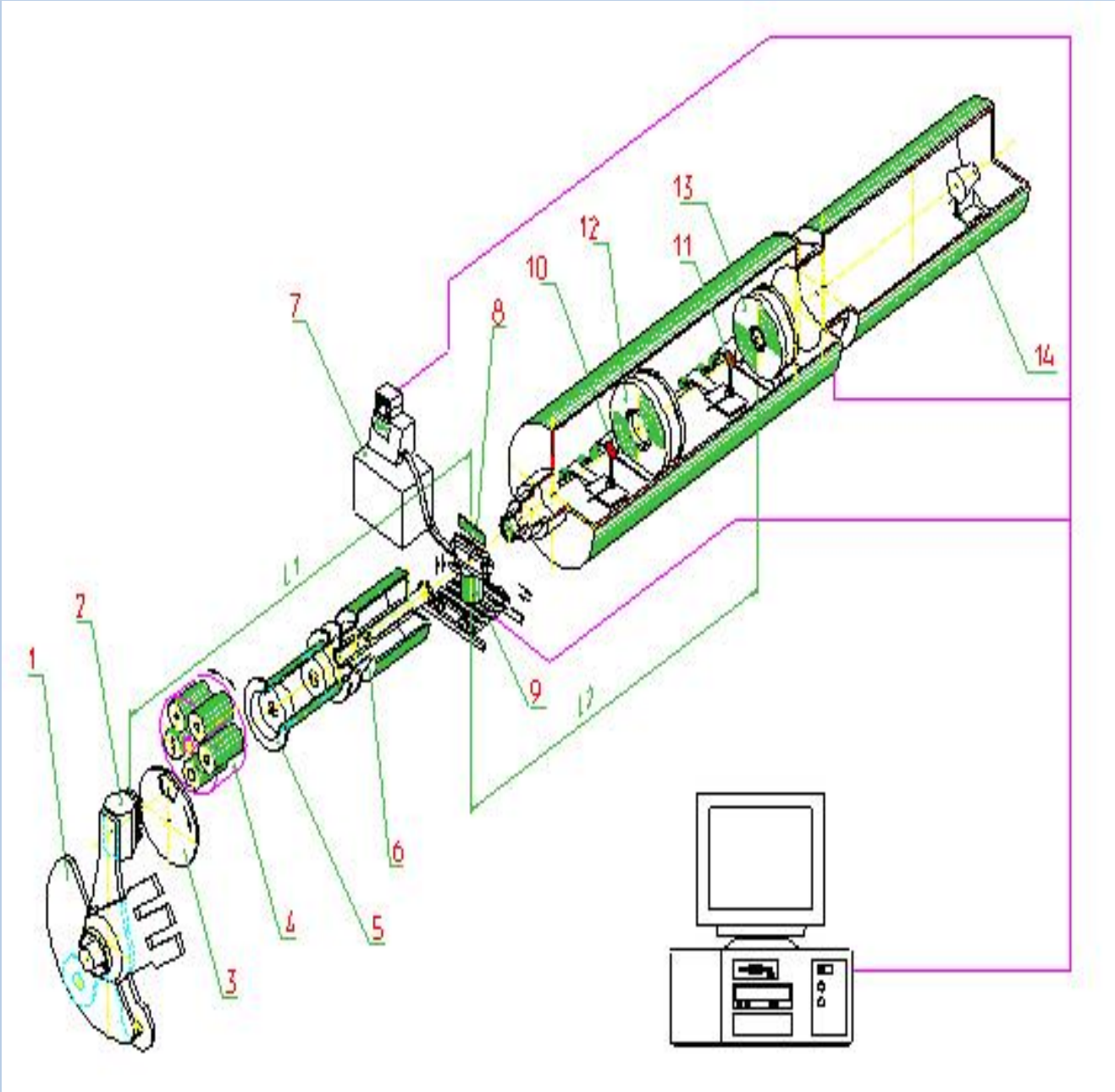



b
Reactor vessel
3 Power pulses
200 ms
2 Core PuO_2
1 Moveable reflector
200 μs
4 Stationary reflector
5 Water moderator

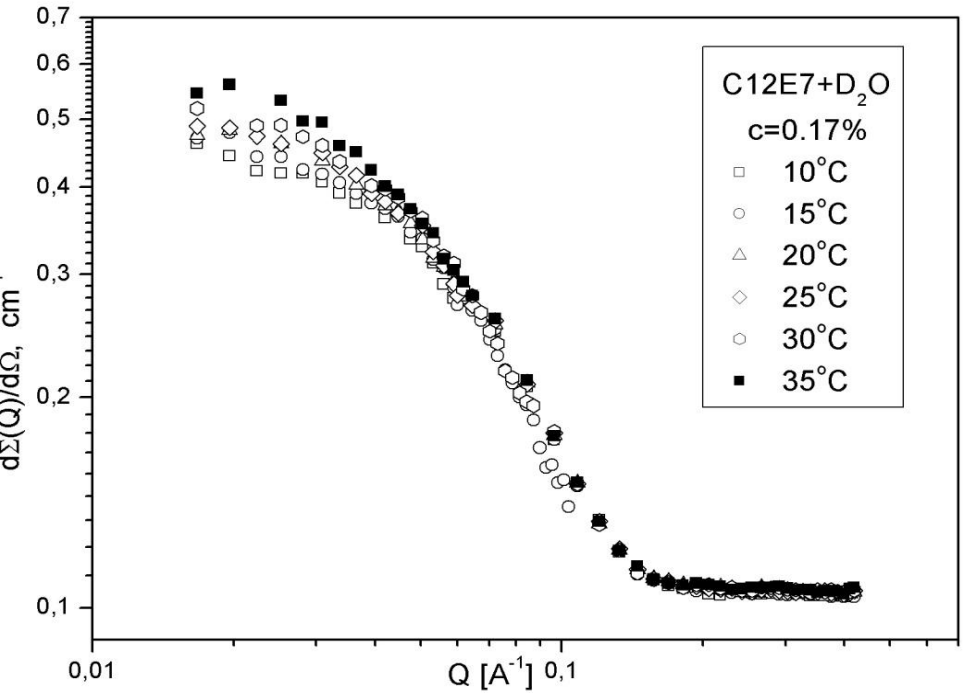

5
4
3
2
1
6
7a
7b
SKAT
EPSILON
NERA
DN-6
6b
6a
DN-2
YuMO
HRFD
IF
DIN-2PI
KOLHIDA
REMUR
8
REFLEX
IZOMER
14
13
GRAINS
FSD
DN-12
9
10
11
12

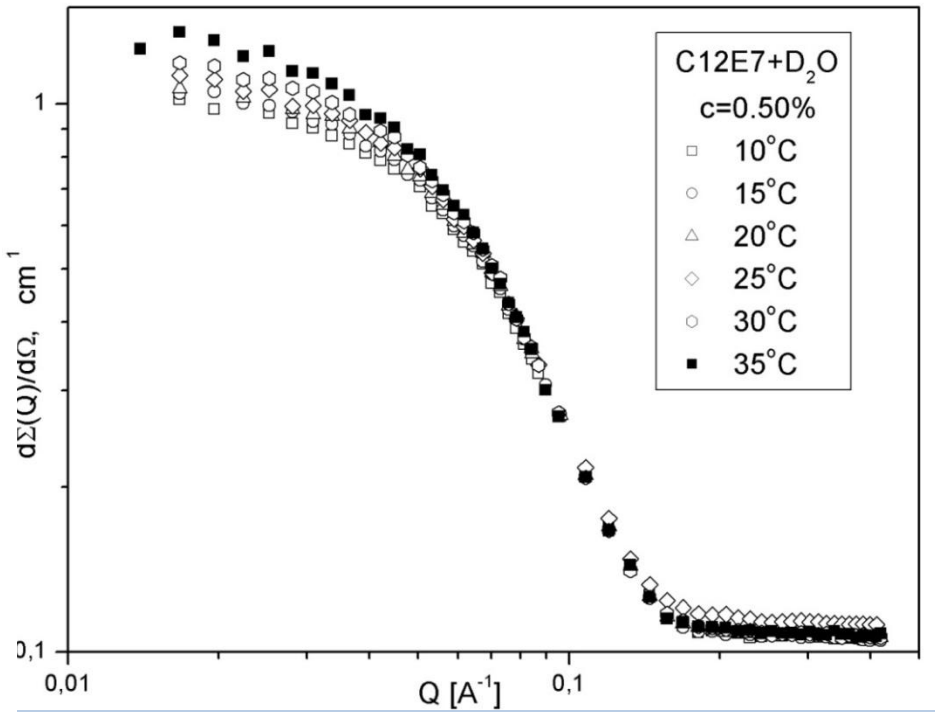
Spectrometer YuMO

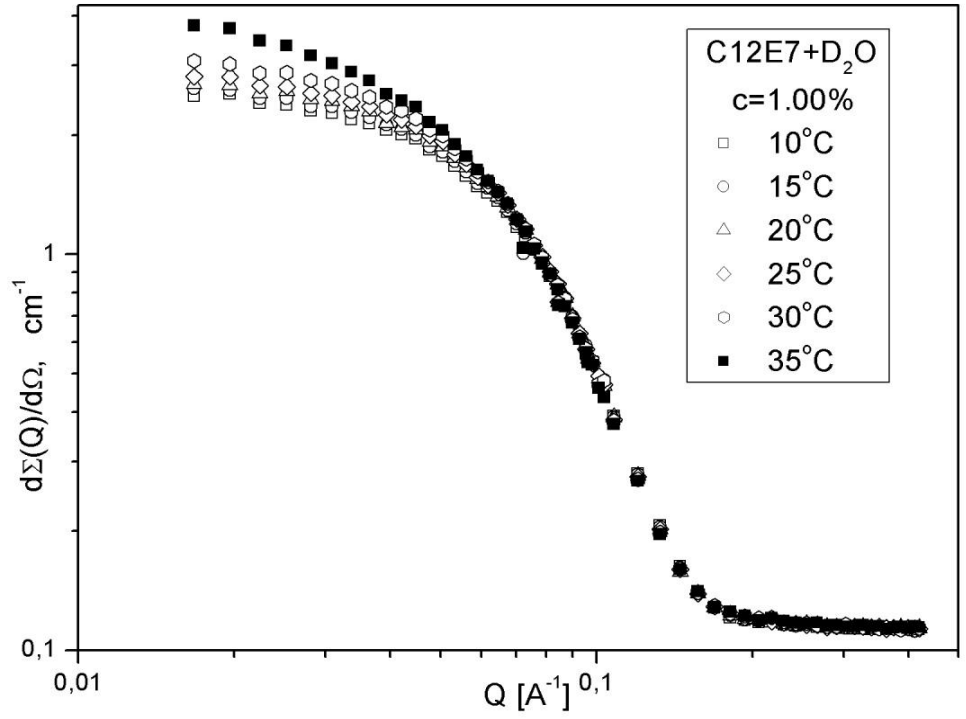
1 – two reflectors
2 – zone of reactor
with moderator
3 – chopper
4 – first collimator
5 – vacuum tube
6 – second collimator
7 – thermostate
8 – sample table
and sample holder
9 – goniometer
10 – V-standard
11 – V-standard
12- ring-wire detector
13 – position-sensitive
detector “Volga”
14 – direct beam
detector

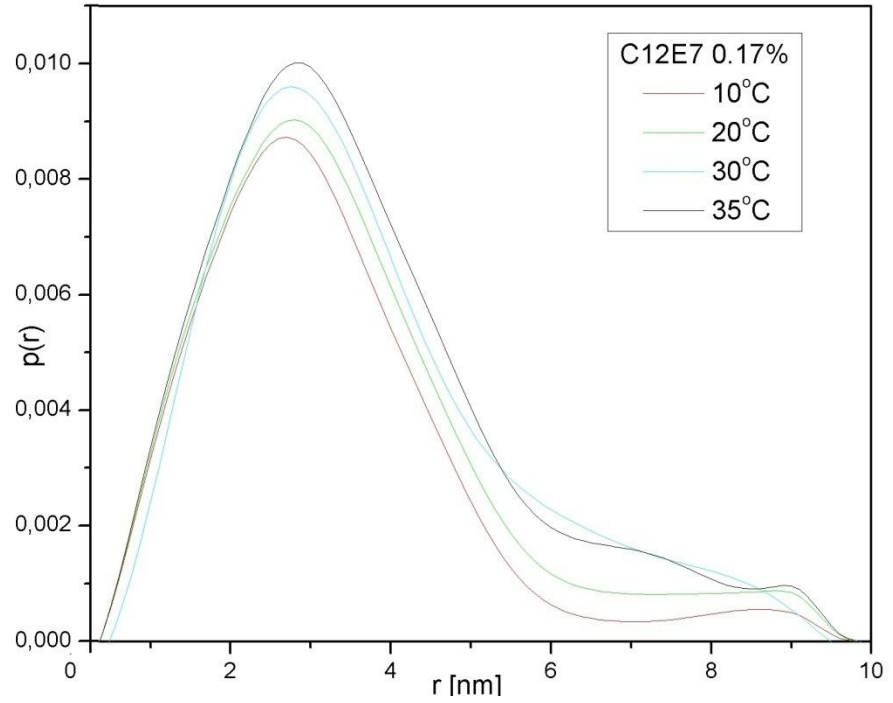


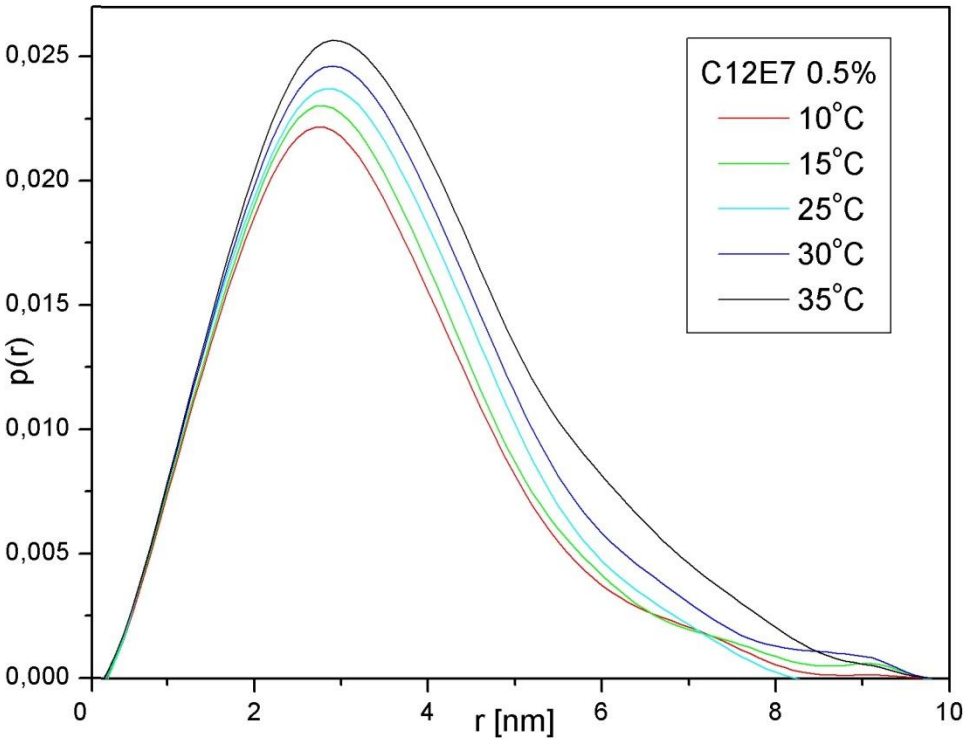
Experimental results

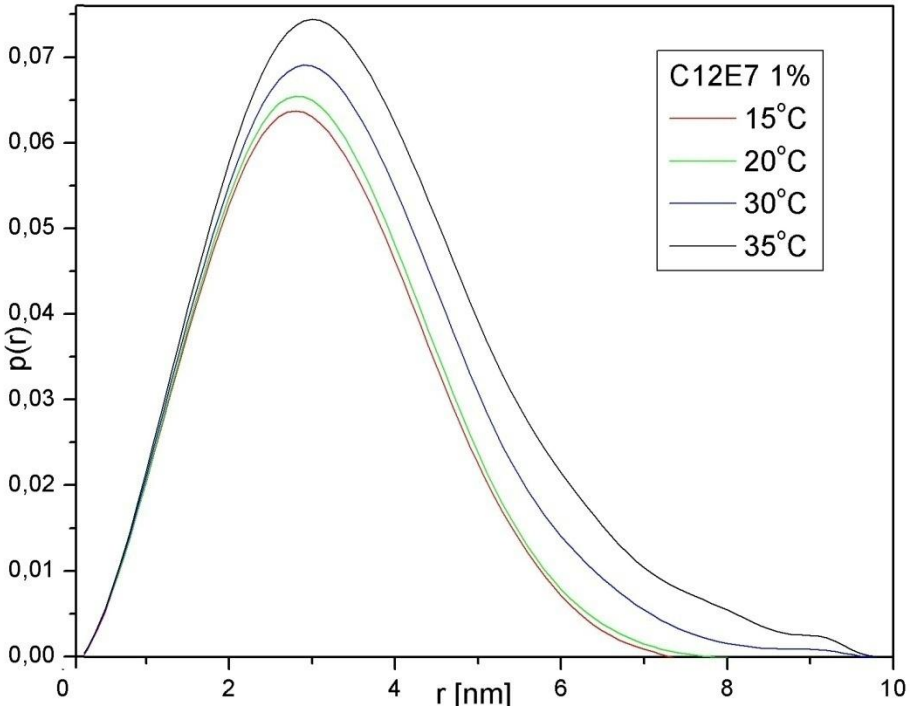

C12E7+D2O
c=0.17%
10°C
15°C
20°C
25°C
30°C
35°C
dΣ(Q)/dΩ, cm-1
Q [A-1]
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0,01
0,1


C12E7+D2O
c=0.50%
10°C
15°C
20°C
25°C
30°C
35°C
dΣ(Q)/dΩ, cm-1
Q [A-1]
1
0,1
0,01
0,1


C12E7+D2O
c=1.00%
10°C
15°C
20°C
25°C
30°C
35°C
dΣ(Q)/dΩ, cm-1
Q [A-1]
1
0,1
0,01
0,1


C12E7 0.17%
10°C
20°C
30°C
35°C
p(r)
r [nm]
0,000
0,002
0,004
0,006
0,008
0,010
0
2
4
6
8
10


C12E7 0.5%
10°C
15°C
25°C
30°C
35°C
p(r)
r [nm]
0,000
0,005
0,010
0,015
0,020
0,025
0
2
4
6
8
10


C12E7 1%
15°C
20°C
30°C
35°C
p(r)
r [nm]
0,00
0,01
0,02
0,03
0,04
0,05
0,06
0,07
0
2
4
6
8
10

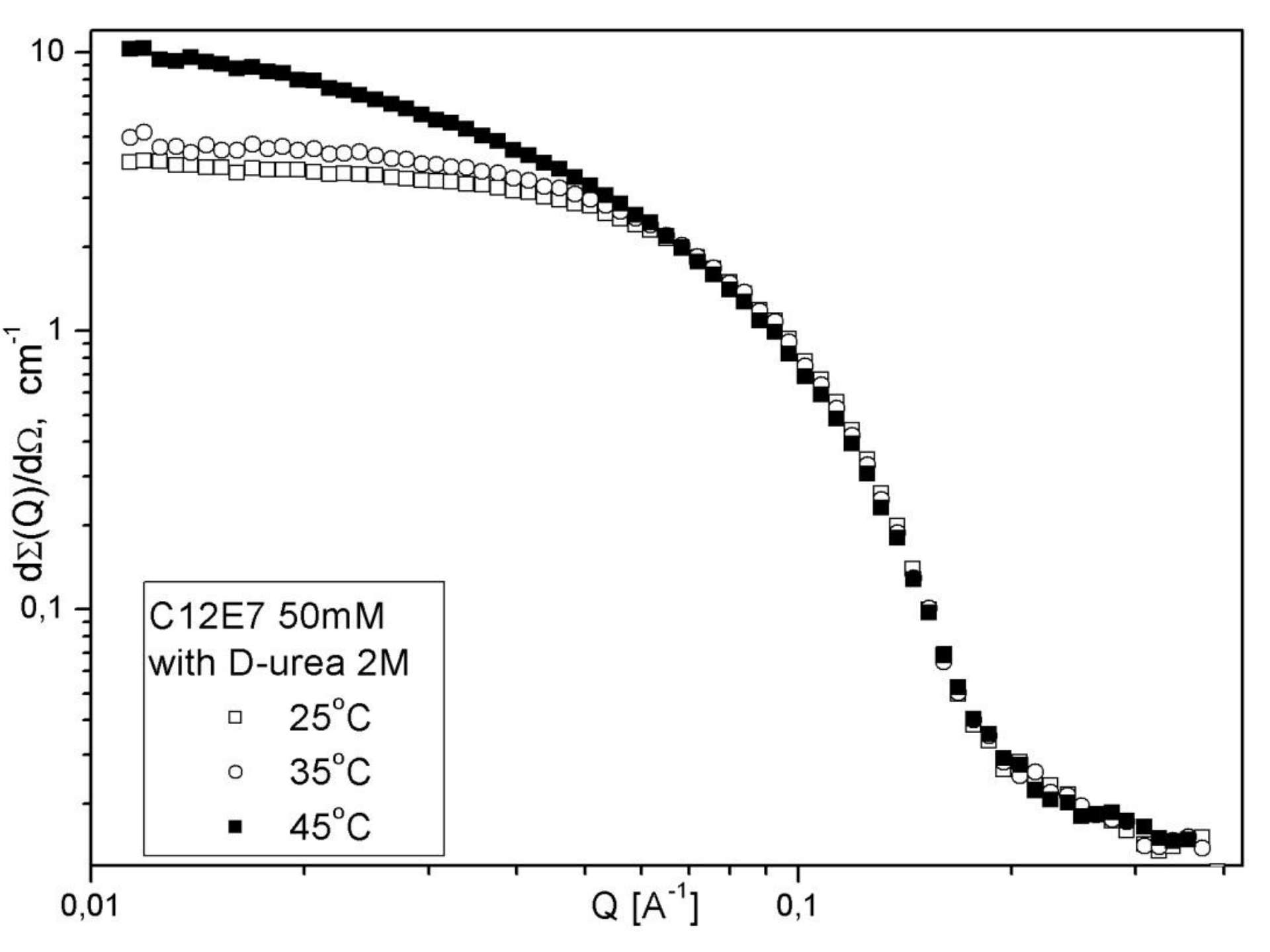
Fitter
Model: Ball

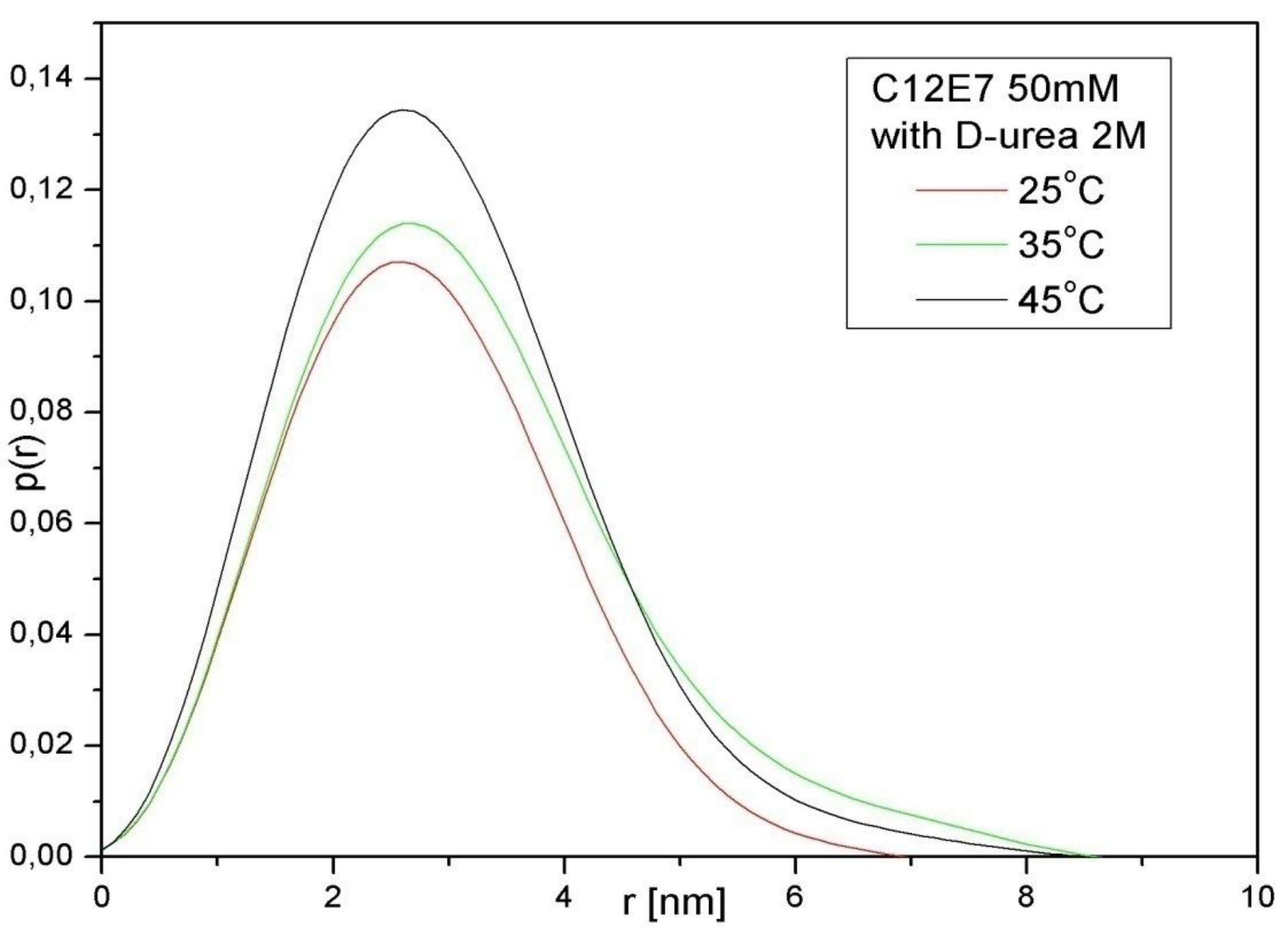
Concentration: 0.17%

Temp [^{0}C]	Radius [A]	+/- [A]
10	26.3	0.2
15	26.8	0.2
20	27.0	0.2
30	27.3	0.2

Concentration: 0.50%

Temp [^{0}C]	Radius [A]	+/- [A]
10	26.9	0.1
15	27.2	0.1
20	27.3	0.1
35	28.2	0.1

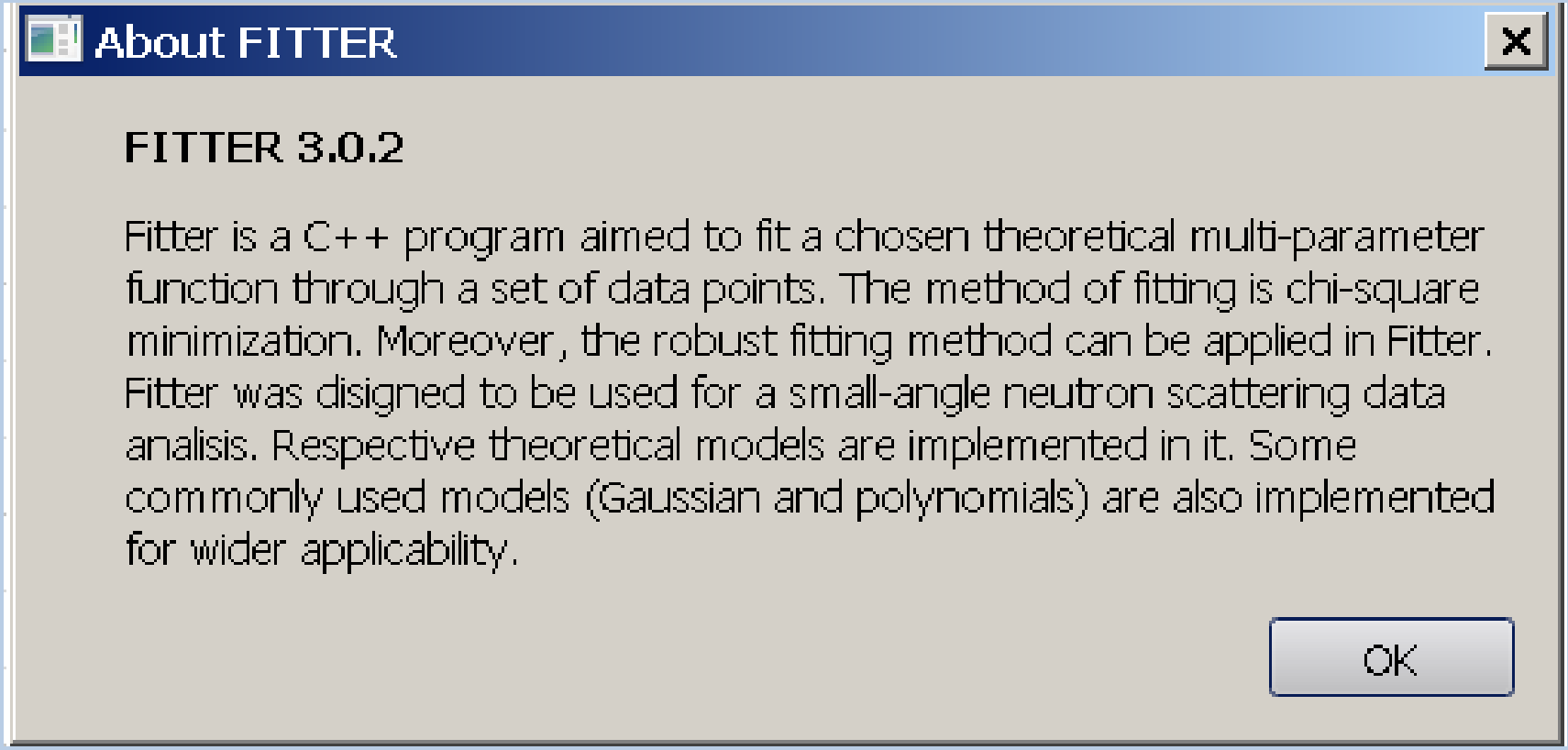

10
1
0,1
dΣ(Q)/dΩ, cm-1
C12E7 50mM
with D-urea 2M
25°C
35°C
45°C
0,01
Q [A-1]
0,1


C12E7 50mM
with D-urea 2M
25°C
35°C
45°C
p(r)
r [nm]
0,00
0,02
0,04
0,06
0,08
0,10
0,12
0,14
0
2
4
6
8
10

Conclusions

- In all cases, micelles appeared to be spherical
- In all cases, with increasing temperature the radius of spheres increased. The concentration of micelles in the solution also increased.
- With increasing surfactant concentration, the concentration of micelles in the solution also increased, but the radius of micelles reamained nearly the same
- After adding d-urea, micelles became more spherically symmetric
- Increasing the d-urea concentration had no influence on the radius and concentration of the micelles in the solution (results for concentrations of 4M and 8M were analogical as in case of 2M)

Software


About FITTER
FITTER 3.0.2
Fitter is a C++ program aimed to fit a chosen theoretical multi-parameter function through a set of data points. The method of fitting is chi-square minimization. Moreover, the robust fitting method can be applied in Fitter. Fitter was disigned to be used for a small-angle neutron scattering data analisis. Respective theoretical models are implemented in it. Some commonly used models (Gaussian and polynomials) are also implemented for wider applicability.
OK


About GIFT
Generalized Indirect Fourier Transformation
Version 02-2005
GIFT
PCh-Graz
© O.Glatter, J.Brunner-Popela, B.Weyerich,
G.Fritz, A.Bergmann, Th. Frühwirth, J.Innerlohinger
Support: otto.glatter@kfunigraz.ac.at


About Origin
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Tel: (413) 586-2013
Fax: (413) 585-0126

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Internet resources 13.07.2017

- http://www.sigmaaldrich.com/catalog/product/sigma/p8800?lang=en&region=RU
- https://pubchem.ncbi.nlm.nih.gov/compound/76459#section=Top
- https://www.scbt.com/scbt/product/heptaethylene-glycol-monododecyl-ether-3055-97-8
- https://cfpub.epa.gov/ncer_abstracts/index.cfm/fuseaction/display.highlight/abstract/515/report/F