

# Web Calculations for SANS

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NCNR Summer School

Neutron Small Angle Scattering and  
Reflectometry from Submicron Structures

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# Outline

- SLD Calculator
- Scattering Simulator
- Instrument Configurator  
(SASCALC)

# SLD Calculation

- Need all the information possible about the sample
- Stoichiometry
- Mass density (molecular volume)

hPEB	dPMB
$C_6H_{12}$	$C_5H_{4.5}D_{5.5}$
162 Å <sup>3</sup> /molecule	136 Å <sup>3</sup> /molecule
84 g/mol	75.5 g/mol
0.86 g/ml	0.92 g/ml

<http://www.ncnr.nist.gov/resources/sldcalc.html>

# SLD Results

hPEB

dPMB

Compound	C6H12
Density (g/cm <sup>3</sup> )	0.86
Wavelength (Å)	6
<input type="button" value="Calculate"/>	

Compound	C50H45D55
Density (g/cm <sup>3</sup> )	0.92
Wavelength (Å)	6
<input type="button" value="Calculate"/>	

Neutron SLD	-3.07E-7 (Å <sup>-2</sup> )
Cu Ka SLD	8.34E-6 + 9.36E-9i (Å <sup>-2</sup> );
Mo Ka SLD	8.33E-6 + 2.08E-9i (Å <sup>-2</sup> );
Neutron Inc. XS	5.93; 33.4 (cm <sup>-1</sup> )
Neutron Abs. XS	0.0823 (cm <sup>-1</sup> )
Neutron 1/e length	0.166 (cm)

Neutron SLD	3.89E-6 (Å <sup>-2</sup> )
Cu Ka SLD	8.27E-6 + 9.28E-9i (Å <sup>-2</sup> );
Mo Ka SLD	8.26E-6 + 2.06E-9i (Å <sup>-2</sup> );
Neutron Inc. XS	2.73; 31.3 (cm <sup>-1</sup> )
Neutron Abs. XS	0.037 (cm <sup>-1</sup> )
Neutron 1/e length	0.362 (cm)

$$b_1 = -4.99 \times 10^{-13} \text{ cm}$$

$$b_1 = 53.3 \times 10^{-13} \text{ cm}$$

$$\text{Contrast Factor} = (b_1/V_1 - b_2/V_2)^2 = 1.79 \times 10^{-11} \text{ \AA}^{-4}$$

# Calculate Scattering Pattern

- Estimate physical size and shape
- Pick an appropriate model
- Enter all known values
- Guess at the rest

\*Rules of Thumb \*

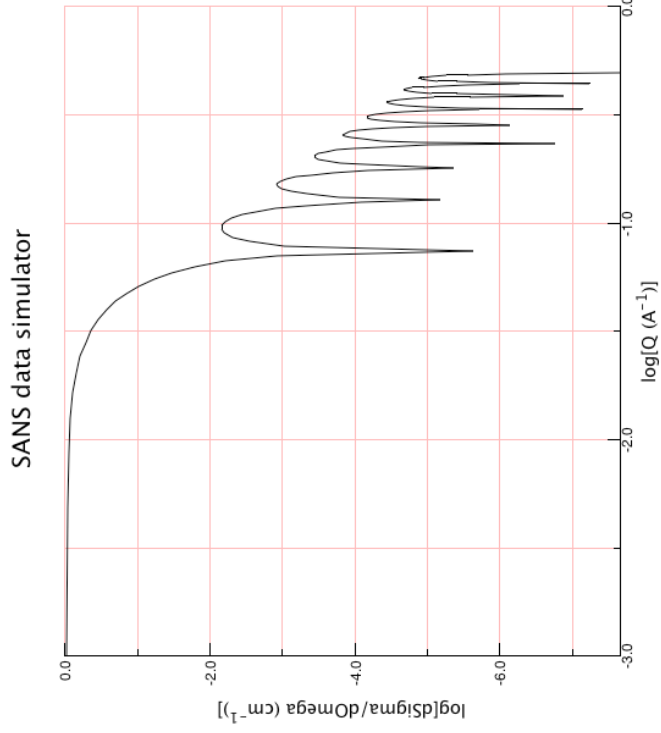
H<sub>2</sub>O T(1 mm) = 0.5,  $d\Sigma/d\Omega = 1 \text{ cm}^{-1}$

D<sub>2</sub>O T(1 mm) = 0.9,  $d\Sigma/d\Omega = 0.06 \text{ cm}^{-1}$

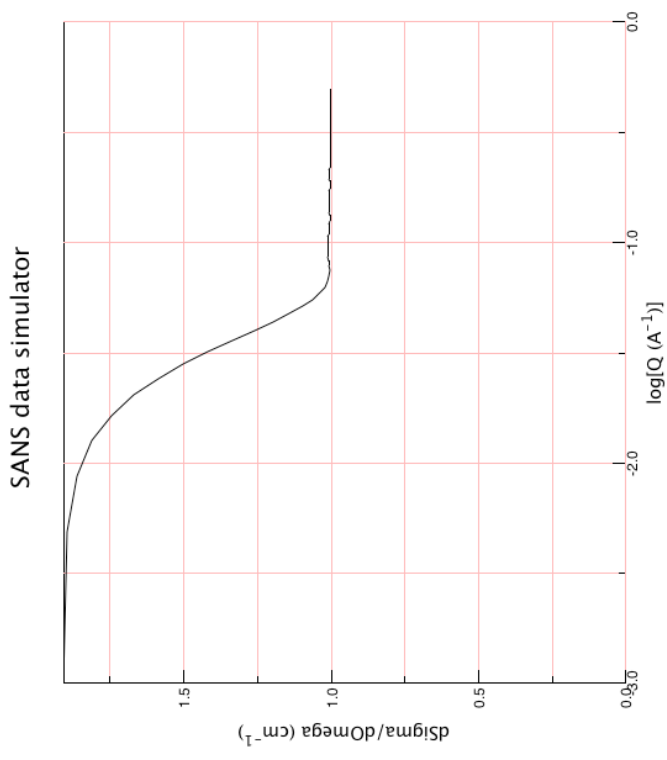
<http://www.ncnr.nist.gov/resources/simulator.html>

# Model Predictions - Simple Sphere

No background



Background =  $1 \text{ cm}^{-1}$



Show Data

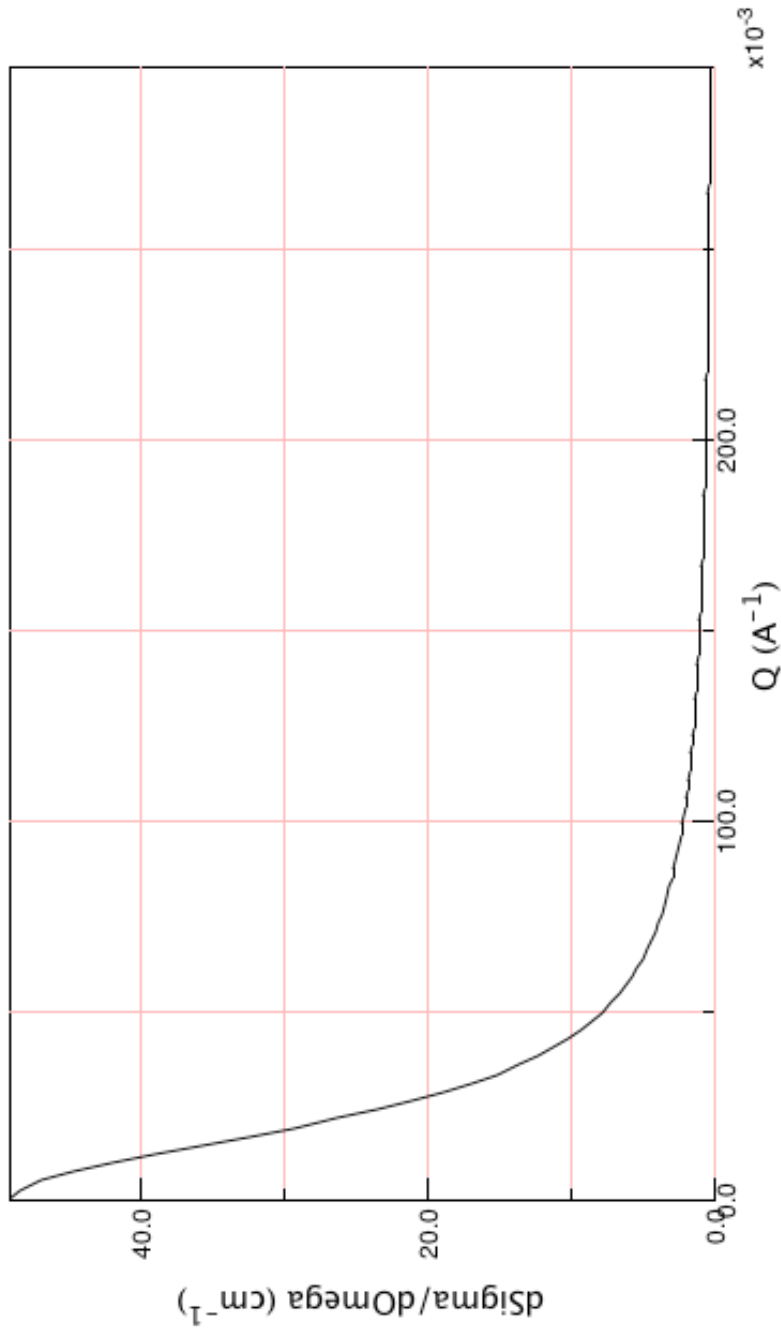
Sphere    Smear data?

Scale 1	Qmin:	0.001
Radius (A)	Qmax:	0.5
Contrast (A-2)	# Points:	128
Background (cm-1)		

Vol Fraction (0-1) 0.01

# RPA Prediction

SANS data simulator



- Calculated using values in handout
- Background is not very significant

# Instrument Configuration

(SASCALC on the VAX)

- Estimate size
- Where in q-space is the scattering happening?

$$R_g = \sqrt{NI^2/6} \sim 100 \text{ \AA}$$

$$l \sim 6 \text{ \AA}$$

$$Q_{\min} < 1/R_g \sim 0.01 \text{ \AA}^{-1}$$

$$Q_{\max} > 1/l \sim 0.17 \text{ \AA}^{-1}$$

<http://www.ncnr.nist.gov/resources/sansplan.html>



# Instrument Configuration Simulation

## Instrument Configuration

NG1, 8M  NG3, 30M  NG7, 30M

Lambda (A):	6.0
dLam/Lam (FWHM):	0.15
Num guides:	4
Source Ap (cm):	5.0
Sample Position:	Chamber
Sample-Det (cm):	900
Sample Ap (cm):	1.27
Det offset (cm):	20
SamAp-Sam (cm):	10.0

This configuration for NG3, 30M yields:  
Lambda: 6.0 A dLam/Lam: 0.15 (FWHM)  
Number of guides: 4  
Intensity at sample: 9.7924E+005 Counts/sec  
Detector Offset: 20.00 cm  
Total Qmin: 0.0056 A<sup>-1</sup> Resolution: 29.208  
Total Qmax: 0.0709 A<sup>-1</sup> Resolution: 6.511  
Horizontal Qmax: 0.0604 A<sup>-1</sup>  
Vertical Qmax: 0.0372 A<sup>-1</sup>  
Beam diameter: 7.31 cm Umbra/Penumbra: 0.  
Beamstop diameter: 7.62 cm, (3.00 in)  
Source aperture diameter: 5.00 cm  
Sample Aperture diameter: 1.27 cm  
The sample chamber is set as the sample position  
Source aperture to sample aperture distance:  
1002.0 cm  
Sample aperture to sample distance:

# Other Tools on the NCNR Website

- Calculation tools <http://www.ncnr.nist.gov/resources/index.html>
- Nuclear properties <http://www.ncnr.nist.gov/resources/n-lengths/>
- Manuals <http://www.ncnr.nist.gov/programs/sans/manuals/index.html>
- Tutorials <http://www.ncnr.nist.gov/programs/sans/tutorials/index.html>
- Reduction and Analysis <http://www.ncnr.nist.gov/programs/sans/manuals/index.html>
- Instrument information [http://www.ncnr.nist.gov/programs/sans/sans\\_inst.html](http://www.ncnr.nist.gov/programs/sans/sans_inst.html)
- Available Equipment <http://www.ncnr.nist.gov/programs/sans/equipment/index.html>
- Access information! <http://www.ncnr.nist.gov/access.html>
- Proposal information <http://www.ncnr.nist.gov/beamtime.html>
- Monetary Assistance programs <http://www.ncnr.nist.gov/outreach.html>
- Summer School notices <http://www.ncnr.nist.gov/summerschool/index.html>