

Summer School 2014
NG3 Instructions Sheet

SANS RUN NUMBERS

	1m trans	1m scatt	4m trans	4m scatt	13m trans	13 m scat
--	----------	----------	----------	----------	-----------	-----------

Trans empty beam	2		6		12	
------------------	---	--	---	--	----	--

Empty cell		3	7	9	-	13
Blocked beam		4	-	10	-	14
5% sds/d2o 10c		5	8	11	-	15
5% sds/d2o 20c		17	18	19	-	20
5% sds/d2o 30c		22	23	24	-	25
5% sds/d2o 40c		27	28	29	-	30
5% sds/d2o 50c		32	33	34	-	35
5% sds/d2o 60c		37	38	39	-	40
5% sds/d2o 70c		42	43	44	-	45
5% sds/d2o 80c		47	48	49	-	50
5% sds/d2o 90c		52	53	54	-	55
5% sds/d2o 26c		57	58	59	-	60

SANS DATA REDUCTION

In your folder, you'll find all the raw data files as well as the reduced files (for example named 5%_sds_d2o_10c.abs for the 10 °C temperature and so on). An Igor experiment mar14.pxp contains the protocols used to reduce the data. Please open the mar14.pxp file and familiarize yourself with the three main steps needed to reduce data

Step 1. Calculate the transmissions. Use the following tabs: Raw Data, Transmission, List Files. Please familiarize yourself with how the various files are linked.

Step 2. Reduce the data sets corresponding to the three measured configurations for the 10 °C temperature. Use the following tabs: Reduction, Reduce Multiple Files, Reduce All Files in Popup. Reduce the data sets for the 1 m, 4 m and 13 m data sets.

Step 3. Splice the data sets for the different configurations into one data file. The SANS run numbers table will be needed here. Use the following tabs. 1-D Ops, Sort, then plot the 13 m (top), 4 m (middle) and 1 m (bottom), click Auto Scale than Write Combined File to a name like 5%_sds_d2o_10c.abs.

Plot the reduced data files for a few temperatures. Use the following tabs. 1-D Ops, Plot in order to observe the data trends when temperature is increased.

You can notice that data sets for temperatures higher than 50 °C have abnormally high low-Q. **What could be the cause?** Display the culprit data sets; i.e, taken at 13 m for these temperatures. Use the following tabs. Raw Data, Display Raw Data, then pick out file 35, 40, 45, 50, or 55. **What do you notice in the raw data image? What could cause such a flare close to the beamstop?**

SANS DATA ANALYSIS

Inspect the data trends shown in Figure 1 of the handout. **What are the main features? What can you infer?**

Familiarize yourself with the model described in the “Scattering Model” section of the handout.

With the Igor experiment mar14.pxp open, use the following tabs. Macros, Load NCNR Analysis Macros. Choose the Uniform Ellipsoid_Sq.ipf model from the Procedure_List. Load 1D Data (5%_sds_d2o_10c.abs), then Plot 1D Function (SmearredEllipsoid_SC), then Append 1D. When you have the reduced data set and the model fit on the same plot, Use Cursors (place them at $Q_{\min} = 0.01 \text{ \AA}^{-1}$ and $Q_{\max} = 0.4 \text{ \AA}^{-1}$), adjust the various parameters by hand to get the two curves close. In order to help the fit adjust parameters close to $R_a=15 \text{ \AA}$, $R_b=24 \text{ \AA}$, and fix SLD solvent = 6.4 E-6 (for d-water), monovalent salt = 0 (for no salt), Temperature = 283 K and dielectric const = 83.52 (from Table 1 in handout), then Do 1D Fit. The fit result can be found in file smared_ellipsoid_sc_fit_10c.pxp.