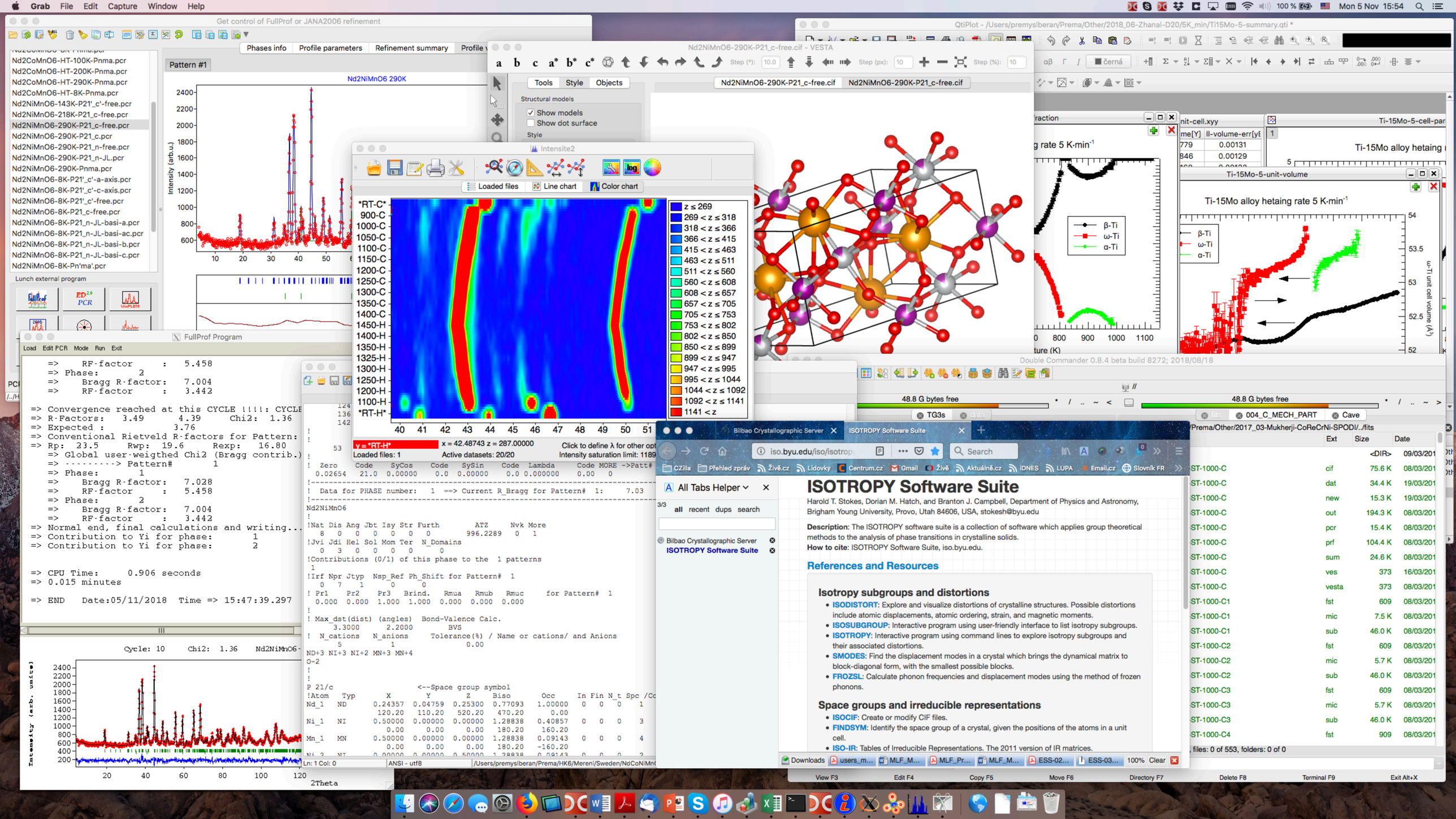
Data Reduction @ ESS

Gareth Murphy
Slides from: Andrew Jackson, Daniele Colognesi,
Tom Arnold, Premek Beran, Sebastian Jaksch …

the TOSCA team (ISIS, RAL, UK) kindly provided me with a picture
taken in the their cabin: the PC screen shows the MANTID software which is
used for the data reduction from
time-of-flight raw histograms to energy transfer spectra.


Grab File Edit Capture Window Help
Mon 5 Nov 15:54
Get control of FullProf or JANA2006 refinement
Phases info
Profile parameters
Refinement summary
Pattern #1
Nd2NiMnO6 290K
Nd2CoMnO6-HT-100K-Pnma.pcr
Nd2CoMnO6-HT-200K-Pnma.pcr
Nd2CoMnO6-HT-290K-Pnma.pcr
Nd2CoMnO6-HT-8K-Pnma.pcr
Nd2NiMnO6-143K-P21'_c'-free.pcr
Nd2NiMnO6-218K-P21_c-free.pcr
Nd2NiMnO6-290K-P21_c-free.pcr
Nd2NiMnO6-290K-P21_c.pcr
Nd2NiMnO6-290K-P21_n-free.pcr
Nd2NiMnO6-290K-P21_n-JL.pcr
Nd2NiMnO6-290K-Pnma.pcr
Nd2NiMnO6-8K-P21'_c'-a-axis.pcr
Nd2NiMnO6-8K-P21'_c'-c-axis.pcr
Nd2NiMnO6-8K-P21'_c'-free.pcr
Nd2NiMnO6-8K-P21_c-free.pcr
Nd2NiMnO6-8K-P21_n-JL-basi-a.pcr
Nd2NiMnO6-8K-P21_n-JL-basi-ac.pcr
Nd2NiMnO6-8K-P21_n-JL-basi-b.pcr
Nd2NiMnO6-8K-P21_n-JL-basi-c.pcr
Nd2NiMnO6-8K-Pn'ma'.pcr
Lunch external program
Nd2NiMnO6-290K-P21_c-free.cif - VESTA
Tools
Style
Objects
Structural models
Show models
Show dot surface
Style
Intensite2
Loaded files
Line chart
Color chart
RT-C
RT-H
z ≤ 269
269 < z ≤ 318
318 < z ≤ 366
366 < z ≤ 415
415 < z ≤ 463
463 < z ≤ 511
511 < z ≤ 560
560 < z ≤ 608
608 < z ≤ 657
657 < z ≤ 705
705 < z ≤ 753
753 < z ≤ 802
802 < z ≤ 850
850 < z ≤ 899
899 < z ≤ 947
947 < z ≤ 995
995 < z ≤ 1044
1044 < z ≤ 1092
1092 < z ≤ 1141
1141 < z
Loaded files: 1
Active datasets: 20/20
FullProf Program
Load
Edit PCR
Mode
Run
Exit
=> Convergence reached at this CYCLE !!!!: CYCLE
=> R-Factors: 3.49 4.39 Chi2: 1.36
=> Expected : 3.76
=> Conventional Rietveld R-factors for Pattern:
=> Rp: 23.5 Rwp: 19.6 Rexp: 16.80
=> Global user-weigthed Chi2 (Bragg contrib.)
=> Phase: 1
=> Bragg R-factor: 7.028
=> RF-factor : 5.458
=> Phase: 2
=> Bragg R-factor: 7.004
=> RF-factor : 3.442
=> Normal end, final calculations and writing...
=> Contribution to Yi for phase: 1
=> Contribution to Yi for phase: 2
=> CPU Time: 0.906 seconds
=> 0.015 minutes
=> END Date:05/11/2018 Time => 15:47:39.297
Cycle: 10 Chi2: 1.36 Nd2NiMnO6-
Intensity (arb. units)
2Theta
QtiPlot - /Users/premyslberan/Prema/Other/2018_06-Zhanal-D20/5K_min/Ti15Mo-5-summary.qti *
Ti-15Mo alloy hetaing rate 5 K·min-1
β-Ti
ω-Ti
α-Ti
Ti-15Mo-5-unit-volume
ω-Ti unit cell volume (Å3)
Double Commander 0.8.4 beta build 8272; 2018/08/18
48.8 G bytes free
TG3s
004_C_MECH_PART
Cave
Bilbao Crystallographic Server
ISOTROPY Software Suite
iso.byu.edu/iso/isotrop
All Tabs Helper
ISOTROPY Software Suite
Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, stokesh@byu.edu
Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.
How to cite: ISOTROPY Software Suite, iso.byu.edu.
References and Resources
Isotropy subgroups and distortions
ISODISTORT: Explore and visualize distortions of crystalline structures. Possible distortions include atomic displacements, atomic ordering, strain, and magnetic moments.
ISOSUBGROUP: Interactive program using user-friendly interface to list isotropy subgroups.
ISOTROPY: Interactive program using command lines to explore isotropy subgroups and their associated distortions.
SMODES: Find the displacement modes in a crystal which brings the dynamical matrix to block-diagonal form, with the smallest possible blocks.
FROZSL: Calculate phonon frequencies and displacement modes using the method of frozen phonons.
Space groups and irreducible representations
ISOCIF: Create or modify CIF files.
FINDSYM: Identify the space group of a crystal, given the positions of the atoms in a unit cell.
ISO-IR: Tables of Irreducible Representations. The 2011 version of IR matrices.
Prema/Other/2017_03-Mukherji-CoReCrNi-SPOD/../fits
Ext
Size
Date
files: 0 of 553, folders: 0 of 0

VS Reduction_Oct2018 - Igor Pro 7.08 64-bit

File Edit Data Analysis Statistics Macros Windows Panel Misc VSANS Help

WORK_SAM

Front Middle Back

sans19608.nxs.ngv

X 0.0745 qX +0.00000
Y 0.1212 qY +0.00000
q +0.00000
Counts 0

Front

File < File > Tab >

Isolate I vs. Q Annular Avg Spread Panels
Status isLog to WORK Restore Panels

sans19608.nxs.ngv

data;data#1;data#2;data#3;

Current data is from SAM
Description = C4S4 (T=30C) NG7 Trans MR
Wavelength is 6 A
SDD FL = 121.43 cm offset = -11 cm
SDD FR = 121.43 cm offset = 8.0008 cm
SDD FT = 162.43 cm offset = 15.498 cm
SDD FB = 162.43 cm offset = -15.796 cm

pixels

CAT - Sort ...

Filenames
Labels
Time

VSANS Reduction Controls

Pick Path File Catalog Help Feedback

Raw Data Reduction 1-D Ops 2-D Ops Misc Ops

Build Protocol

VSANS Reduction Protocol

Questions ?

Sample sans19521.nxs.ngv
file: sans19521.nxs.ngv,sans19534.nxs.ngv,

Background sans19514.nxs.
file: sans19485.nxs.ngv,

Empty Cell sans19513.nxs.
file: sans19520.nxs.ngv,

Sensitivity Plex_Oct_2018
file: Plex_Oct_2018_DIV,

Absolute
parameters: ask;TSTAND=1;

Mask AJJ2_antiflare_
file: AJJ2_antiflare_VSANS_M

Average
parameters: AVTYPE=Circula

Beg Trim: B=5;FT=3;FB=3;FL
End Trim: B=10;FT=5;FB=5;F

Save Protocol
Recall Protocol Exp
Delete Protocol Impo

V_TransmissionPanel

? Done

Open Beam sans19573.nxs.ngv
Label: Open beam NG7 2 inch BS NG7 Trans MR
XY Box: 5;13;54;67;
Panel: MR

Transmission sans19608.nxs.ngv
Label: C4S4 (T=30C) NG7 Trans MR
Group ID: 28

Sample sans19580.nxs.ngv
Label: C4S4 (T=30C) NG0 Scatt
Group ID: 28
Transmission: 0.612453
Error: 0.00126812

Calculate Calculate All In Popup

sans19593.nxs.nc	C4S2 (T=30C) NG0 Scatt	2018-10-19T01:15	Sample	SCATTERING	26	411	1.2	338.02	191	194	54.	230	0	0	6	0	3600	1
sans19578.nxs.nc	C4S2 (T=30C) NG0 Scatt	2018-10-18T18:47	Sample	SCATTERING	26	411	643	35.7644	191	226	12.	230	0	0	6	0	1800	1
sans19583.nxs.nc	C4S2 (T=30C) NG7 Scatt	2018-10-18T21:20	Sample	SCATTERING	26	121	738	41.0178	541	623	34.	230	0	0	6	7	1800	1
sans19598.nxs.nc	C4S2 (T=30C) NG7 Scatt	2018-10-19T05:18	Sample	SCATTERING	26	121	8.0	44573.8	541	7.4	412	230	0	0	6	7	1800	1
sans19588.nxs.nc	C4S2 (T=30C) NG7 Trans MR	2018-10-18T22:56	Sample	TRANSMISSION	26	121	405	40.54	541	344	34.	230	0	0	6	7	100	1
sans19606.nxs.nc	C4S2 (T=30C) NG7 Trans MR	2018-10-19T09:04	Sample	TRANSMISSION	26	121	153	153.45	541	389	389	230	0	0	6	7	100	1
sans19594.nxs.nc	C4S3 (T=30C) NG0 Scatt	2018-10-19T02:15	Sample	SCATTERING	27	411	1.2	352.04	191	207	57.	230	0	0	6	0	3600	1
sans19579.nxs.nc	C4S3 (T=30C) NG0 Scatt	2018-10-18T19:17	Sample	SCATTERING	27	411	623	34.6378	191	229	12.	230	0	0	6	0	1800	1
sans19599.nxs.nc	C4S3 (T=30C) NG7 Scatt	2018-10-19T05:49	Sample	SCATTERING	27	121	7.5	42070.1	541	8.2	456	230	0	0	6	7	1800	1

Q (1/A)

```
groupName =   /entry/sample
S_HDF5ListGroup =   entry;
groupName =   /entry/sample
Done Processing Transmission List
```

Type here to search

8:31 PM
10/19/2018

	1:2:4 dChCl:hGlycerol:H2O/D2O + 20%hC12hTAB_SANS	2015-10-10T19:56:53	00:15:08	10.0046	Edler,Arnold,Jackson,Fernandez,Heenan
32381	HCHH Urea 50C 4h SANS	2015-10-10T20:13:08	00:15:08	10.0062	Edler,Arnold,Jackson,Fernandez,Heenan
32382	Actually HCHH_50C_SANS	2015-10-10T20:57:39	00:17:29	11.5630	Edler,Arnold,Jackson,Fernandez,Heenan
32383	1:2:4 dChCl:hGlycerol:H2O/D2Oc_SANS	2015-10-10T21:27:19	00:30:31	20.1903	Edler,Arnold,Jackson,Fernandez,Heenan
32384	1:2 h-ChCl:h-Urea + 0.1% d-SDS_SANS	2015-10-10T21:58:16	00:07:46	5.1232	Edler,Arnold,Jackson,Fernandez,Heenan
32385	1:2:4 dChCl:hGlycerol:H2O/D2Oa_SANS	2015-10-10T22:06:51	00:30:15	20.0051	Edler,Arnold,Jackson,Fernandez,Heenan
32386	1:2:4 dChCl:hGlycerol:H2O/D2Oc_SANS	2015-10-10T22:37:32	00:30:16	20.0110	Edler,Arnold,Jackson,Fernandez,Heenan
32387	1:2 h-ChCl:h-Urea + 0.1% d-SDS_SANS	2015-10-10T23:08:15	01:00:21	40.0024	Edler,Arnold,Jackson,Fernandez,Heenan
32388	1:2 h-ChCl:h-Urea + 0.2% d-SDS_SANS	2015-10-11T00:09:03	01:00:22	40.0062	Edler,Arnold,Jackson,Fernandez,Heenan
32389	1:2 h-ChCl:h-Urea + 0.5% d-SDS_SANS	2015-10-11T01:09:52	01:00:21	40.0013	Edler,Arnold,Jackson,Fernandez,Heenan
32390	1:2 h-ChCl:h-Urea + 1% d-SDS_SANS	2015-10-11T02:10:42	01:00:26	40.0045	Edler,Arnold,Jackson,Fernandez,Heenan
32391	1:2 h-ChCl:d-Urea + 0.1% h-SDS_SANS	2015-10-11T03:11:34	01:00:23	40.0079	Edler,Arnold,Jackson,Fernandez,Heenan
32392	1:2 h-ChCl:d-Urea + 0.2% h-SDS_SANS	2015-10-11T04:12:27	01:00:23	40.0081	Edler,Arnold,Jackson,Fernandez,Heenan
32393	1:2 h-ChCl:d-Urea + 0.5% h-SDS_SANS	2015-10-11T05:13:18	01:00:23	40.0048	Edler,Arnold,Jackson,Fernandez,Heenan
32394	1:2 h-ChCl:d-Urea + 1% h-SDS_SANS	2015-10-11T06:14:09	01:00:22	40.0101	Edler,Arnold,Jackson,Fernandez,Heenan
32395	1:2 h-ChCl:d-Urea + 0.1% d-SDS_SANS	2015-10-11T07:15:00	01:00:28	40.0037	Edler,Arnold,Jackson,Fernandez,Heenan
32396	1:2 h-ChCl:d-Urea + 0.2% d-SDS_SANS	2015-10-11T08:15:55	01:05:49	40.0067	Edler,Arnold,Jackson,Fernandez,Heenan
32397	1:2 h-ChCl:d-Urea + 0.5% d-SDS_SANS	2015-10-11T09:22:13	01:00:27	40.0094	Edler,Arnold,Jackson,Fernandez,Heenan
32398	1:2 h-ChCl:d-Urea + 1% d-SDS_SANS	2015-10-11T10:23:09	01:00:27	40.0081	Edler,Arnold,Jackson,Fernandez,Heenan
32399	H2O_SANS	2015-10-11T11:24:04	00:30:12	20.0079	Edler,Arnold,Jackson,Fernandez,Heenan
32400	D2O_SANS	2015-10-11T11:54:44	00:30:14	20.0078	Edler,Arnold,Jackson,Fernandez,Heenan
32401	H2O_TRANS	2015-10-11T12:25:32	00:12:04	8.0014	Edler,Arnold,Jackson,Fernandez,Heenan

in the case of SANS and Reflectometry, we use whatever software/ routines are used at the facility in question.
There is not a general "reduction of science data" approach.

For example for me for small angle scattering (just thinking recently):

At NIST, I use Igor Pro - I have a screenshot of that somewhere from a recent experiment that I'll dig out.
At ISIS, I use the ISIS Mantid interface
At SNS, I use the SNS Mantid interface
At ILL, I use GRASP (or historically LAMP) with the specific interface for the beamline I'm using
At Diamond, I use DAWN

At PSI I believe they use the BERSANS routines, which are also used at HZB (I think).

23-26/10/15

FIGARO EXPERIMENT Glycol/ChCl DES + SDS, CTAB DPPC, DMPC.

9-13-612

local contact: Richard Campbell.

Adrian Sanchez-Fernandez, Karen Edler, Tom Arnold.

trial of troughs Delrin - D_2O ok
Macor - D_2O curvature??

Delrin - hDES (ChCl:glycerol 1:2)
⇒ issues with beam hitting window?
add paper spacers 0.67 mm thick.
(7 sheets of paper)

Using trough sample changer "wrong way around" (PS@3022mm)

Direct Beam 1 #548799
θ = 0.623°
S2H = 0.40 S3H = 0.80
CHOP = 7% FOM = 30
S2W = 44 S3W = 32
ATW = 5.0
30 min @ 1329 c/s

Direct Beam 2 #548800
θ = 3.79°
S2H = 4.8 S3H = 1.6
CHOP = 7% FOM = 30
S2W = 44 S3W = 32
ATW = 0.40
20 min @ 7629 c/s

D_2O in Delrin trough P2 ~4.5ml
A1 6min #548802 (3211 c/s)
A2 45min #548803 (3401 c/s)

D_2O in Macor trough P3
A1 6min #548806 (3194 c/s)

ToF experiment SI 10546-1 26-Feb-3 March

Phospholipid behaviour in Deep Eutectic Solvents

Tom Arnold, Karen Edler, Adrian Sanchez-Fernandez, Andrew Jackson, Oliver Hammond

Local contact: Dr. Jonathan Rawle

Energy: 12.5 eV using DCD beam size ~60 μm

Pure water in the small trough.

~~Effected SCAN~~

205591-92 Alignment

205594
1
597 XRR ⇒ a bit noisy + some meniscus effects? but almost fits (without normalisation)

205598
1
600 setting up slits etc. for GID

205601-02 Alignment

205603
1
606 repeat XRR but with Chiller turned off

205607
1
610 NORMALISATION SCANS
→ failed on final point. and was saturating diode for most of the early points.

205612
1 NORMALISATION REPEAT

205615
16
17 → stuck on last scan again (q=0.72)
Keeps sticking

- give up
- change to 1515 Trough 100×300mm

205618 alignment.

205619
1
622 - XRR test water, chiller pump = 5
data looks better but still has curved critical edge.

→ looked at GID but some artifact in the images. ⇒ related to small trough.

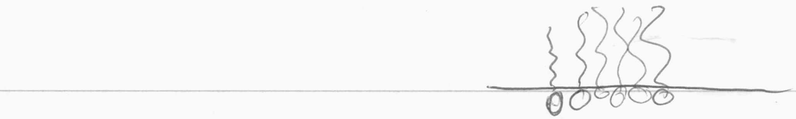
added DPPC

205623
24
25 Alignment

205626
1
629 XRR DPPC on water @ 20mN/m
hexlx = 0

DES 1:2 ChCl: Glycerol

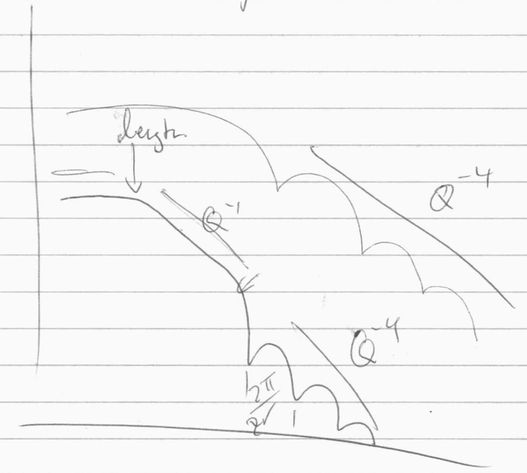
205630
31 Alignment.

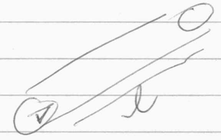


Exptcell from previously Ann

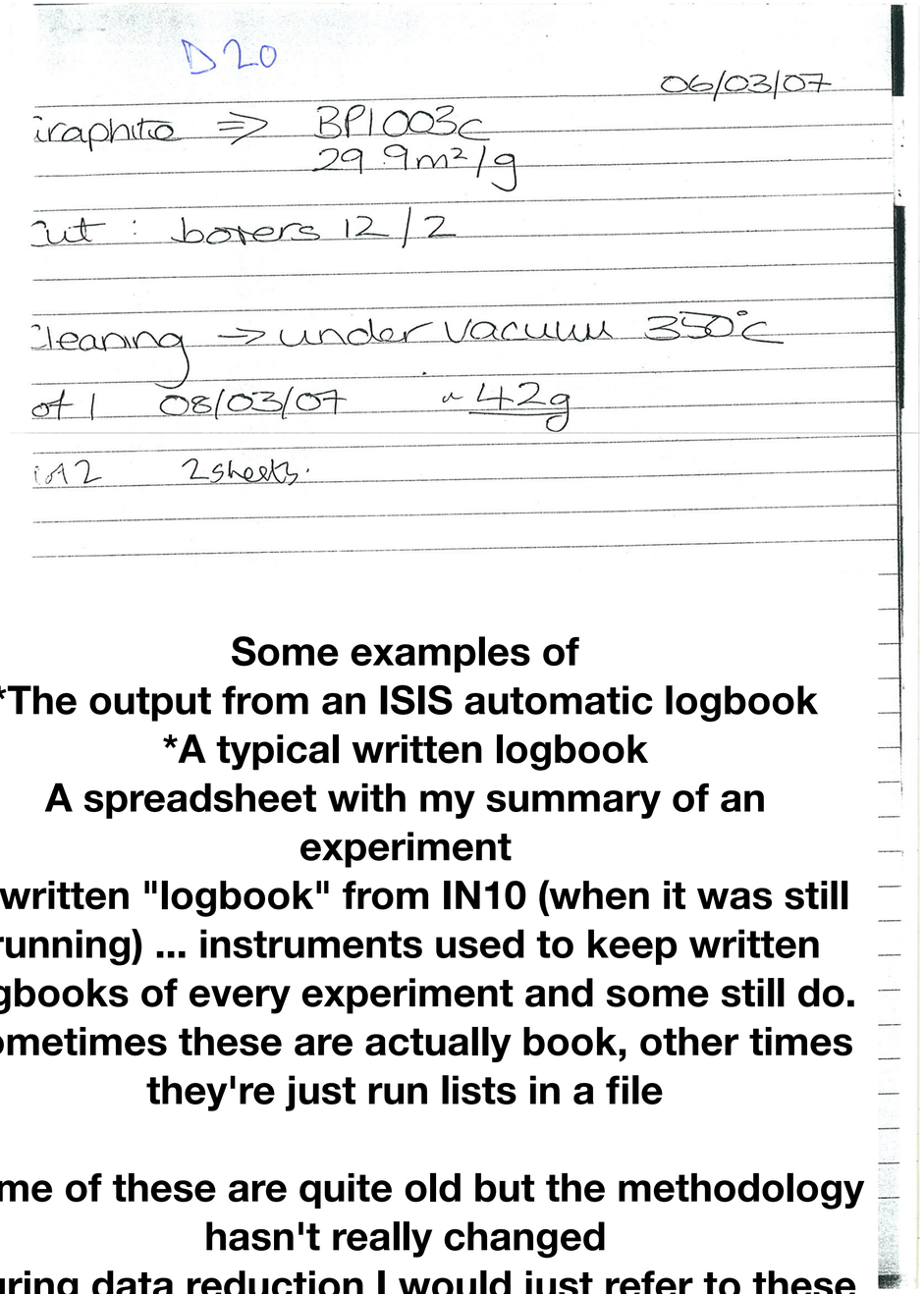
SANS = 83697
TRANS = 83689
DIRECT = 83698

Mask100-MAN-135 - Hollamby-Nomal-8mm.txt





P # 3
Q # 11
R # 16


D2O

06/03/07

graphite ⇒ BP1003C
29.9 m²/g

cut : boters 12/2

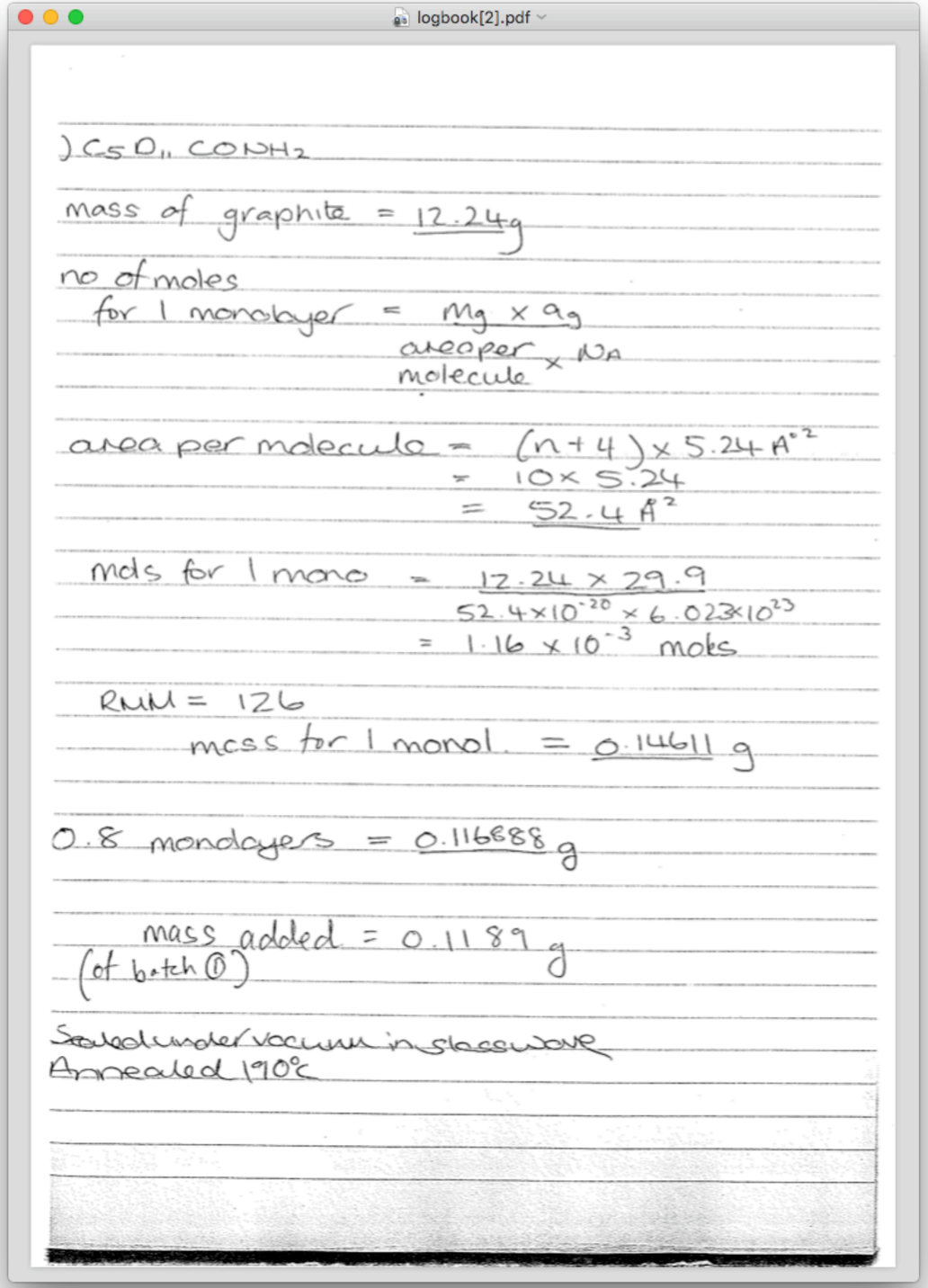
cleaning ⇒ under vacuum 350°C

of 1 08/03/07 ~42g

in 2 2 sheets.

Some examples of
***The output from an ISIS automatic logbook**
***A typical written logbook**
A spreadsheet with my summary of an experiment
A written "logbook" from IN10 (when it was still running) ... instruments used to keep written logbooks of every experiment and some still do.
Sometimes these are actually book, other times they're just run lists in a file

Some of these are quite old but the methodology hasn't really changed
During data reduction I would just refer to these and enter the relevant runs into the software.


logbook[2].pdf

) $C_5O_{11}CONH_2$

mass of graphite = 12.24g

no of moles for 1 monolayer = $\frac{Mg \times 9g}{\text{area per molecule} \times N_A}$

area per molecule = $(n+4) \times 5.24\,A^{\circ 2}$
= 10×5.24
= $52.4\,A^2$

mols for 1 mono = $\frac{12.24 \times 29.9}{52.4 \times 10^{-20} \times 6.023 \times 10^{23}}$
= 1.16×10^{-3} mols

RMM = 126
mass for 1 monol. = 0.14611 g

0.8 mondayers = 0.116888 g

mass added = 0.1189 g
(of batch ①)

Sealed under vacuum in glass wave
Annealed 190°C

SAXS I22 23rd January 2015

Run #	Sample #	Code	Description	Temp
197353	1	100	1:2 ChCl:Urea	30
197389	2	101	1.6e-4 SDS in 1:2 ChCl:Urea	30
197352	3	102	9.8e-4 SDS in 1:2 ChCl:Urea	30
197351	4	103	1.2e-3 SDS in 1:2 ChCl:Urea	30
197388	5	104	1.7e-3 SDS in 1:2 ChCl:Urea	30
197387	6	105	3.8e-3 SDS in 1:2 ChCl:Urea	30
197386	7	106	6.1e-3 SDS in 1:2 ChCl:Urea	30
197385	8	107	1.5e-2 SDS in 1:2 ChCl:Urea	30
197384	9	108	3.2e-2 SDS in 1:2 ChCl:Urea	30
197383	10	119	2.4e-2 SDS in 1:2 ChCl:Urea	30
197382	11	109	3.6e-4 SDS in 1:2 ChCl:Urea	30
197381	12	W100	1:2 ChCl:Urea+5wt% water	30
197380	13	W101	1.6e-4 SDS in 1:2 ChCl:Urea+5wt% water	30
197379	14	W102	9.8e-4 SDS in 1:2 ChCl:Urea+5wt% water	30
197378	15	W103	1.2e-4 SDS in 1:2 ChCl:Urea+5wt% water	30
197377	16	W104	1.7e-3 SDS in 1:2 ChCl:Urea+5wt% water	30
197376	17	W105	3.8e-3 SDS in 1:2 ChCl:Urea+5wt% water	30
197375	18	W106	6.1e-3 SDS in 1:2 ChCl:Urea+5wt% water	30
197374	19	W107	1.5e-2 SDS in 1:2 ChCl:Urea+5wt% water	30
197373	20	W108	3.2e-2 SDS in 1:2 ChCl:Urea+5wt% water	30
197372	21	W119	2.4e-2 SDS in 1:2 ChCl:Urea+5wt% water	30
197371	22	W109	3.6e-4 SDS in 1:2 ChCl:Urea+5wt% water	30
197412	23	100	1:2 ChCl:Urea	50
197411	24	101	1.5e-4 SDS in 1:2 ChCl:Urea	50
197410	25	102	9.8e-4 SDS in 1:2 ChCl:Urea	50
197409	26	103	1.2e-4 SDS in 1:2 ChCl:Urea	50
197408	27	104	1.7e-3 SDS in 1:2 ChCl:Urea	50
197407	28	105	3.8e-3 SDS in 1:2 ChCl:Urea	50
197406	29	106	6.1e-3 SDS in 1:2 ChCl:Urea	50
197405	30	107	1.5e-2 SDS in 1:2 ChCl:Urea	50
197404	31	108	3.2e-2 SDS in 1:2 ChCl:Urea	50
197403	32	119	2.4e-2 SDS in 1:2 ChCl:Urea	50
197402	33	109	3.6e-4 SDS in 1:2 ChCl:Urea	50
197203	34	500	1:2 ChCl:Glycerol	30
197271	35	501	1.5e-4 SDS in 1:2 ChCl:Glycerol	30
197272	36	502	3.7e-4 SDS in 1:2 ChCl:Glycerol	30
197273	37	503	8.0e-4 SDS in 1:2 ChCl:Glycerol	30
197274	38	504	1.9e-3 SDS in 1:2 ChCl:Glycerol	30
197275	39	505	3.7e-3 SDS in 1:2 ChCl:Glycerol	30
197276	40	506	7.6e-3 SDS in 1:2 ChCl:Glycerol	30
197277	41	507	1.9e-2 SDS in 1:2 ChCl:Glycerol	30
197278	42	508	4.0e-2 SDS in 1:2 ChCl:Glycerol	30
197279	43	519	3.0e-2 SDS in 1:2 ChCl:Glycerol	30
197202	44	541	1.5e-4 C12TAB in 1:2 ChCl:Glycerol	30

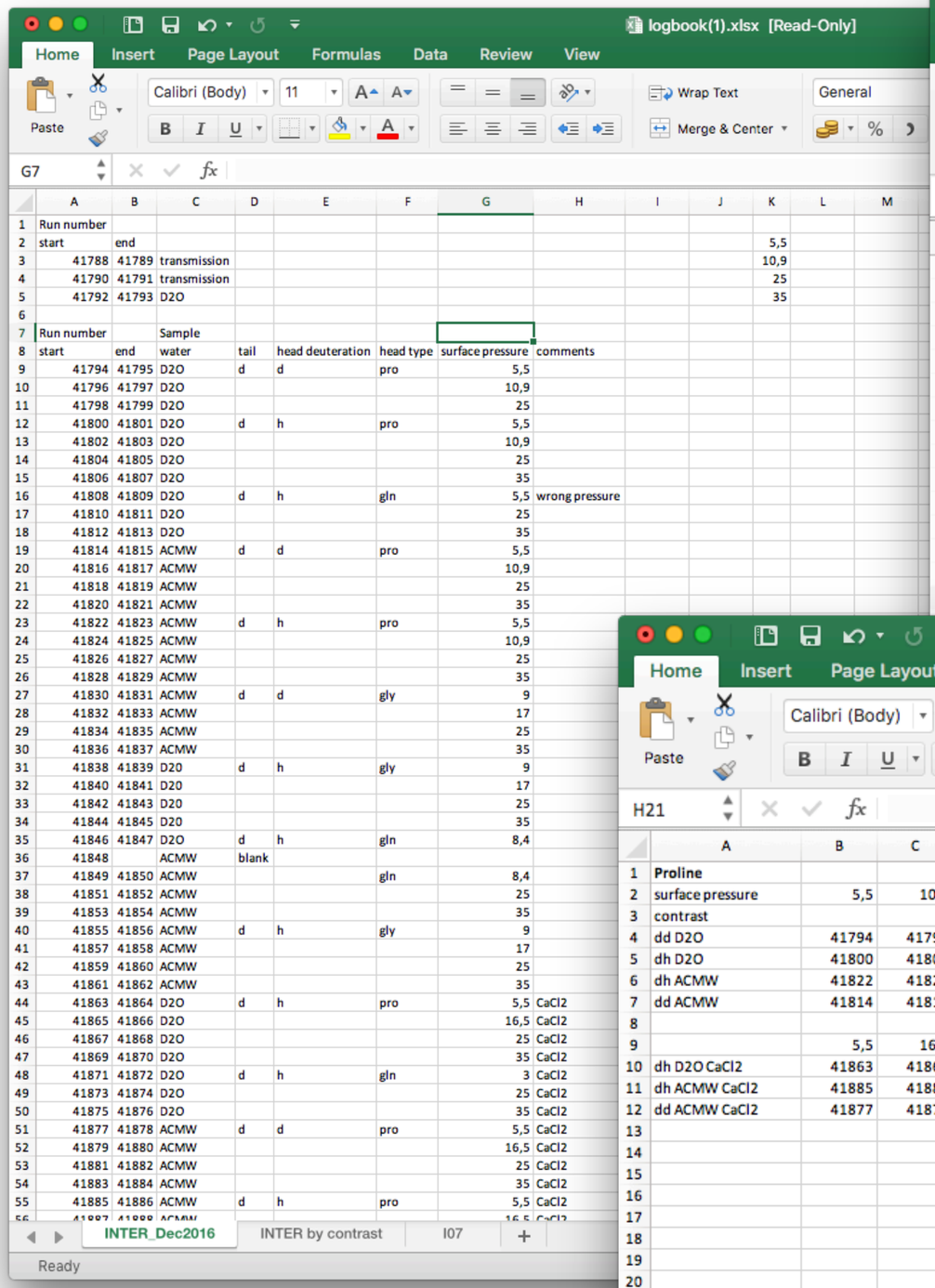
IN10 Logsheet form **Team:** R. Cook, T. Arnold, S. Larese, T. Seydel **Monochromator:** Si 111 vmp. **Sample environment:** cryostat + cryofurnace

Date	Sample	Run number from	Run number to	Acc.	Run time	Tset (K)	Treg (K)	Tsam (K)	Doppler f(Hz) or Mono temp.	Monitor flux (n/s)	Comments (Slits wide open; no Bragg peaks shielded; cylindrical sample containers)
22/3/07	pure MgO	22875		—	300s/step	↓ → 370		not connected	—	230	batch 207E in Ø48mm cryofurnace
23/3/07	Vanadium foil in Al cyl.	22876		—	〃	40	131 ↘ 117		—	220	mass 13.126g foil thickness 0.2mm 2.5 turns height 50mm in Ø70mm cryostat
〃	pure MgO	22877		—	〃	*	140 ↘ ↗	〃	—	220	batch 207D in Ø70 mm cryostat
〃	Butane on MgO	22878		—	〃			〃	—		207E in 48mm cryofurnace
24/3/07	1 mono Ethane on MgO	22879		—	〃			〃	—		batch 207D in Ø70mm cryostat
〃		22880		—					—		
〃	1 mono. Butane on MgO	22881		—	〃				—		batch 207E in 48mm cryofurnace
〃	〃	22882		—					—		
〃		22883		—					—		BEAM CLOSED
〃	3 mono. Ethane	22884		—	〃				—		batch 207D in 70mm cryostat
〃	〃	22885		—	〃				—		
26/3/07	2 mono Butane	22886		—					—	230	207E in 48mm cryofurnace
〃		22887		—					—		stopped
〃	pure MgO	22888		—					—		207G in 48mm cryofurnace
〃	2 mono Butane	22889		—					—		207E in 48mm cryofurnace
〃	5 mono Ethane	22890		—					—		207D in Ø70mm cryostat
〃	〃	22891		—					—		
〃	1 mono Pentane	22892		—					—		207G in 48mm cryofurnace

note: partly wrong run titles in data files; refer to logbook and these logsheets.

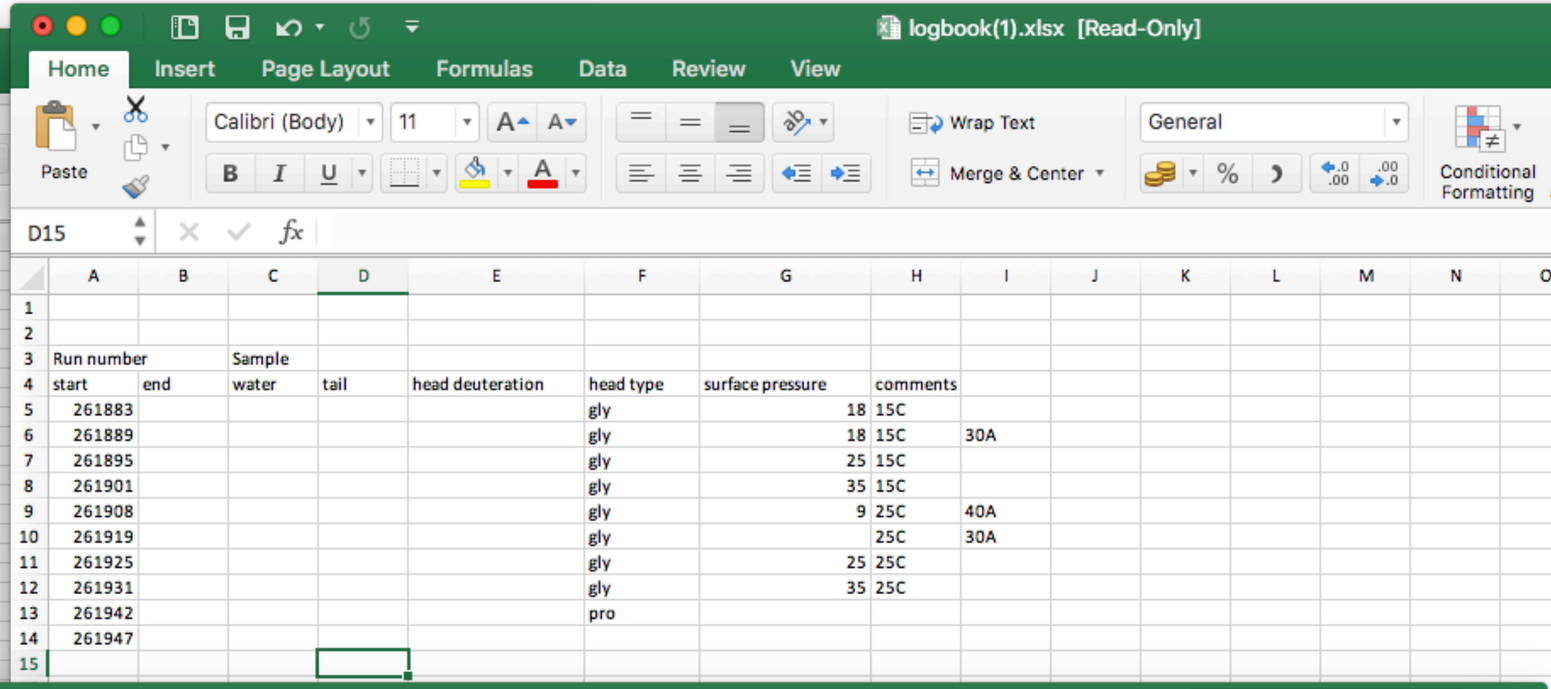
reactor cycle: 2007-1 experiment: 7-05-28

A written "logbook" from IN10 (when it was still running)



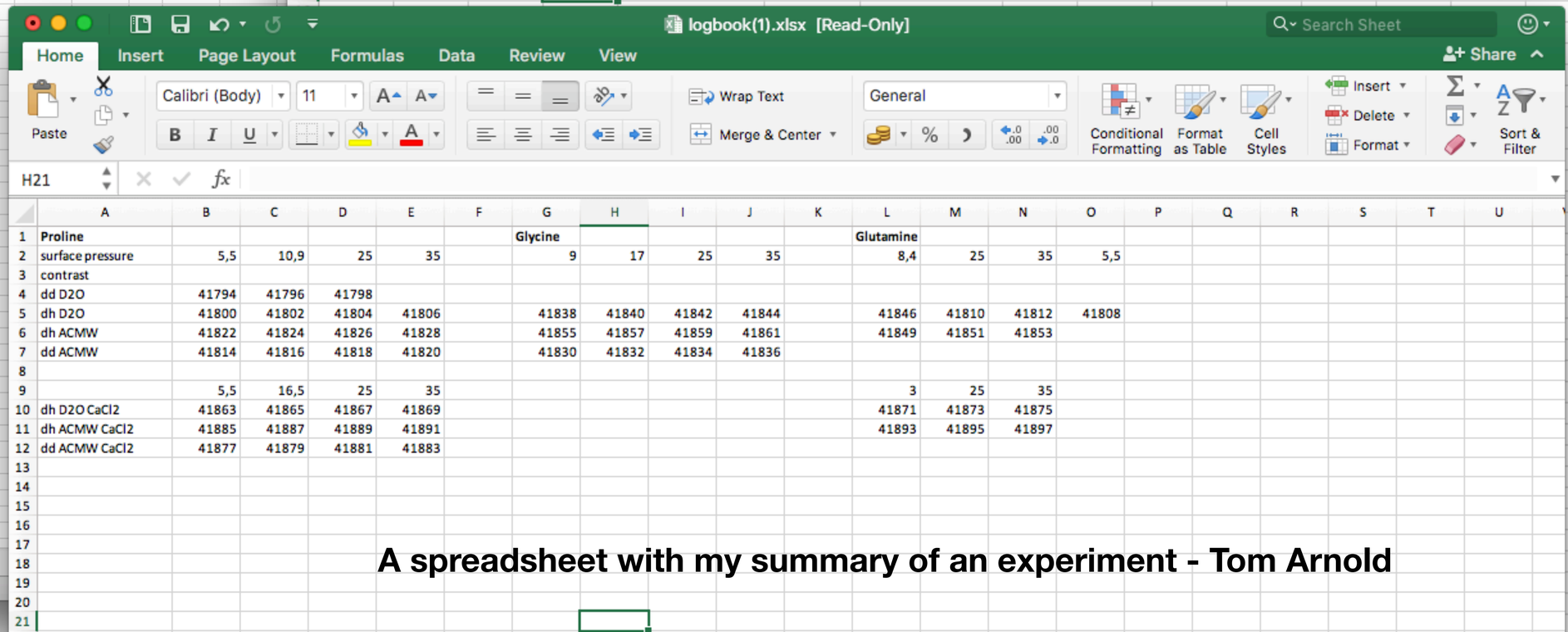
logbook(1).xlsx [Read-Only]

	A	B	C	D	E	F	G	H
1	Run number							
2	start	end						
3	41788	41789	transmission					
4	41790	41791	transmission					
5	41792	41793	D2O					
6								
7	Run number		Sample					
8	start	end	water	tail	head deuteration	head type	surface pressure	comments
9	41794	41795	D2O	d	d	pro	5,5	
10	41796	41797	D2O				10,9	
11	41798	41799	D2O				25	
12	41800	41801	D2O	d	h	pro	5,5	
13	41802	41803	D2O				10,9	
14	41804	41805	D2O				25	
15	41806	41807	D2O				35	
16	41808	41809	D2O	d	h	gln	5,5	wrong pressure
17	41810	41811	D2O				25	
18	41812	41813	D2O				35	
19	41814	41815	ACMW	d	d	pro	5,5	
20	41816	41817	ACMW				10,9	
21	41818	41819	ACMW				25	
22	41820	41821	ACMW				35	
23	41822	41823	ACMW	d	h	pro	5,5	
24	41824	41825	ACMW				10,9	
25	41826	41827	ACMW				25	
26	41828	41829	ACMW				35	
27	41830	41831	ACMW	d	d	gly	9	
28	41832	41833	ACMW				17	
29	41834	41835	ACMW				25	
30	41836	41837	ACMW				35	
31	41838	41839	D20	d	h	gly	9	
32	41840	41841	D20				17	
33	41842	41843	D20				25	
34	41844	41845	D20				35	
35	41846	41847	D2O	d	h	gln	8,4	
36	41848		ACMW	blank				
37	41849	41850	ACMW			gln	8,4	
38	41851	41852	ACMW				25	
39	41853	41854	ACMW				35	
40	41855	41856	ACMW	d	h	gly	9	
41	41857	41858	ACMW				17	
42	41859	41860	ACMW				25	
43	41861	41862	ACMW				35	
44	41863	41864	D2O	d	h	pro	5,5	CaCl2
45	41865	41866	D2O				16,5	CaCl2
46	41867	41868	D2O				25	CaCl2
47	41869	41870	D2O				35	CaCl2
48	41871	41872	D2O	d	h	gln	3	CaCl2
49	41873	41874	D2O				25	CaCl2
50	41875	41876	D2O				35	CaCl2
51	41877	41878	ACMW	d	d	pro	5,5	CaCl2
52	41879	41880	ACMW				16,5	CaCl2
53	41881	41882	ACMW				25	CaCl2
54	41883	41884	ACMW				35	CaCl2
55	41885	41886	ACMW	d	h	pro	5,5	CaCl2



logbook(1).xlsx [Read-Only]

	A	B	C	D	E	F	G	H	I
1									
2									
3	Run number		Sample						
4	start	end	water	tail	head deuteration	head type	surface pressure	comments	
5	261883					gly	18	15C	
6	261889					gly	18	15C	30A
7	261895					gly	25	15C	
8	261901					gly	35	15C	
9	261908					gly	9	25C	40A
10	261919					gly		25C	30A
11	261925					gly	25	25C	
12	261931					gly	35	25C	
13	261942					pro			
14	261947								
15									



logbook(1).xlsx [Read-Only]

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	Proline						Glycine					Glutamine			
2	surface pressure	5,5	10,9	25	35		9	17	25	35		8,4	25	35	5,5
3	contrast														
4	dd D2O	41794	41796	41798											
5	dh D2O	41800	41802	41804	41806		41838	41840	41842	41844		41846	41810	41812	41808
6	dh ACMW	41822	41824	41826	41828		41855	41857	41859	41861		41849	41851	41853	
7	dd ACMW	41814	41816	41818	41820		41830	41832	41834	41836					
8															
9		5,5	16,5	25	35							3	25	35	
10	dh D2O CaCl2	41863	41865	41867	41869							41871	41873	41875	
11	dh ACMW CaCl2	41885	41887	41889	41891							41893	41895	41897	
12	dd ACMW CaCl2	41877	41879	41881	41883										

A spreadsheet with my summary of an experiment - Tom Arnold

Where do we go from here?

- Are there any problems with the current system(s)?
- Can we extend web solutions to include all scientists’ metadata needs?
- Would scientists use such an interface or previous way is still preferable?