INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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UNITED NATIONS INDUSTRIAL DEVELOPMENT ORGANIZATION

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SECOND SCHOOL ON THE USE OF SYNCHROTRON RADIATION IN SCIENCE AND TECHNOLOGY: *"JOHN FUGGLE MEMORIAL"*

25 October - 19 November 1993

Miramare - Trieste, Italy

Tutorial

"X-Ray Scattering Applied to Materials Science"

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(LNLS)
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II School on Use of Synchrotron Radiation in Science and Technology
Trieste 1993

Tutorial
"X-Ray Scattering Applied to Materials Science"

Aldo Craievich
LNLS, Campinas, Brazil

Content

1. <u>Generation of SAXS intensity functions produced by a set of spheres with a single-mode size distribution</u> (Guinier, Fournet, SAXS book)

This program provides the SAXS intensity function associated with a set of spherical particles forming a dilute system having a Gaussian size distribution:

$$I(q) = \sum_i g(R_i)\, \phi(qR_i) \quad ;$$

where $$g(R_i) = \frac{1}{w} e^{-\frac{\pi (R_i - \bar{R})^2}{w^2}}$$

and $$\phi(qR_i) = R_i^6 \left[3 \frac{sen\, qR_i - qR_i \cos qR_i}{(qR_i)^3} \right]^2$$

<u>Procedure</u>

- Run Sphere appl
- Enter Rav = 30
- Enter Width = 0
- Enter Rav = 30
- Enter Width = 15

- Enter Rav = 30
- Enter Width = 50
- Enter : "Name of output file"
- Plot Log I vs log q and discuss the differences between the three curves.
- Determine the slope in log I vs log q plots corresponding to Plot 3 in the Porod range.
- Plot 1 vs q focussing the oscilatory part. Verify the radius of the sphere corresponding to plot 1 (we have I(q) = 0 for qR = 4.52, 7.73, ...).
- Plot log I vs q^2 in the Guinier range. Determine the value of R_g and R ($R_G = \sqrt{\frac{5}{3}}\, R_g$) from the slope of the linear range.
- Comment on the value found for the Porod slope and on the R_G values corresponding to the different curves.

2. <u>Determination of the size distribution of a dilute system of particles assuming a log normal distribution</u> (Valter et al. J. Appl. Cryst. <u>18</u>, 205 (1985))

Single mode size distribution can often be approximated by a log-normal function:

g(R) =

where μ is the geometric overage radius and σ the geometrical standard deviation.

The SAXS curve yields:

I(0) (Guinier extrapolation) = 101.0

Slope (Guinier) = 800.0

K(lim Iq^4 ; q -> ∞ , Porod) = 29.5 . 10^{-4}

$Q_0 = \int_0^\infty I(q)\,dq = 5{,}223$

$Q_1 = \int_0^\infty q\,I(q)\,dq = 0{,}2631$

$Q_2 = \int_0^\infty q^2\,I(q)\,dq = 0{,}03391$

- Determine R_i ($i = d, \ell, f, v, G$)
- Plot R_i versus k
- Determine μ and σ
- Plot g(R)
- <u>Remark</u>: For the three last items use program "Lognormal"

3. <u>Determination of fractal parameters from SAXS measurements</u> (Craievich, J. de Physique, <u>2</u>, 801 (1992), Ramirez del Solar et al., J. Non-Cryst. Sol., <u>147</u>, 206 (1992))

- Data are in "Fractal data" file.
- Plot log I_1 and log I_2 vs q^2 (Guinier plot).
- Do a linear fitting on the linear part of the Guinier plots. Determine m0 and m_1 of the straight line for each curve.
- Plot log I_1 and log I_2 vs log q.
- Do a linear fitting of the central part of the SAXS curve. Determine the coefficients m_0 and m_1.
- Do a linear fitting of the Porod part of the SAXS curve. Determine m_0 and m_1.
- The program FRACTAL Appl determines R_g (Guinier radius of the aggregates), R_{C1} (radius of the aggregates calculated from $R_{C1} = 1/qC_1$, where q_{C1} is the low-q crossover) and R_{C2} (radius of the basic structural units calculated from $R_{C2} = 1/q_{C2}$, where q_{C2} is the high-q crossover).
- What you can say about the size of the basic structural unit and about the size of the fractal aggregates associated with SAXS curves 1 and 2?
- What you conclude about the fractal dimensionality and about the mechanism of aggregation?
- Use the data of the article (Ramirez del Solar et al.) and determine the time evolution of I(0) and R_G. These parameters are determined by applying Zimm equation (see the paper). The equation

$$I(0) \propto R_G^D$$

provides an alternative method to determine the fractal dimentionality of polymeric structures.

4. Validity of dynamical scaling theory in phase separation process

Data sheet "Data Phase Separ" corresponds to four SAXS curves associated with increasing demixion time: 10, 18, 24 and 32 min.

To demonstrate that dynamical scaling theory applies, the following equations should be verified:

i) $q_1 \propto t^{-a}$

ii) $I_{max} = t^{a'}$; $a' = 3a$

iii) $I(q/q_1, t)\, q_1^3 = F(q/q_1) \neq F(t)$

where $$q_1 = \frac{\int q\, I(q)\, dq}{\int I(q)\, dq}$$

- Plot I_1, I_2, I_3 and I_4 as function of q. Determine I_{max} for each curve.

- Determine q_1 for each SAXS curve (use program "Phase separ").

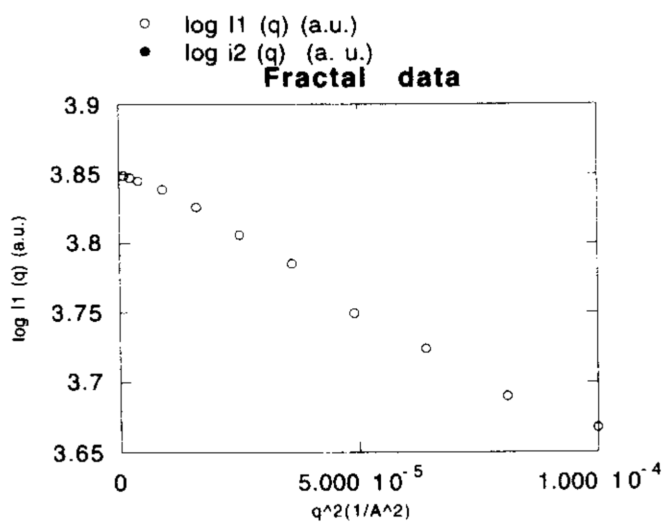
- Plot $I(q/q_1, t)\, q_1^3$ versus q/q_1 for every curve.

- Plot $q_1(t)$. Determine a.

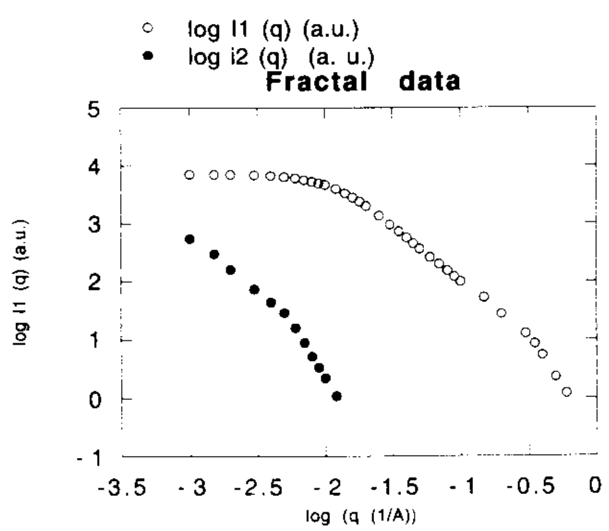
- Plot $q_{max}(t)$. Determine a'.

	q (1/A)	I1 (q) (a.u.)	I2 (q) (a. u.)	log (q (1/A))	log I1 (q) (a.u.)	log i2 (q) (a. u.)	q^2(1/A^2)
35	0.70000	0.62000			-0.20761		
36	0.80000	0.37000			-0.43180		
37	0.90000	0.27000			-0.56864		

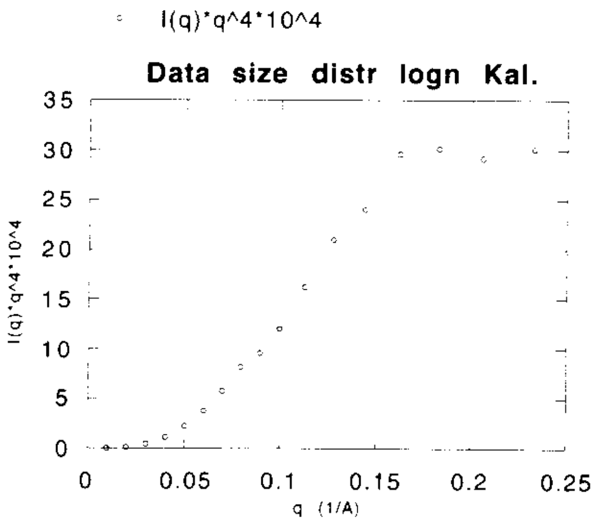
	q (1/A)	I1 (q) (a.u.)	I2 (q) (a. u.)	log (q (1/A))	log I1 (q) (a.u.)	log i2 (q) (a. u.)	q^2(1/A^2)
1	0.0010000	7060.0	550.00	-3.0000	3.8488	2.7404	1.0000e-06
2	0.0015000	7040.0	300.00	-2.8239	3.8476	2.4771	2.2500e-06
3	0.0020000	7000.0	160.00	-2.6990	3.8451	2.2041	4.0000e-06
4	0.0030000	6900.0	74.000	-2.5229	3.8388	1.8692	9.0000e-06
5	0.0040000	6700.0	44.000	-2.3979	3.8261	1.6435	1.6000e-05
6	0.0050000	6400.0	29.000	-2.3010	3.8062	1.4624	2.5000e-05
7	0.0060000	6100.0	16.000	-2.2218	3.7853	1.2041	3.6000e-05
8	0.0070000	5620.0	9.0000	-2.1549	3.7497	0.95424	4.9000e-05
9	0.0080000	5300.0	5.2000	-2.0969	3.7243	0.71600	6.4000e-05
10	0.0090000	4900.0	3.4000	-2.0458	3.6902	0.53148	8.1000e-05
11	0.0100000	4650.0	2.2000	-2.0000	3.6675	0.34242	1.0000e-04
12	0.012000	3950.0	1.0800	-1.9208	3.5966	0.033424	0.00014400
13	0.014000	3300.0		-1.8539	3.5185		0.00019600
14	0.016000	2800.0		-1.7959	3.4472		0.00025600
15	0.018000	2400.0		-1.7447	3.3802		0.00032400
16	0.020000	2000.0		-1.6990	3.3010		0.00040000
17	0.025000	1350.0		-1.6021	3.1303		0.00062500
18	0.030000	950.00		-1.5229	2.9777		0.00090000
19	0.035000	720.00		-1.4559	2.8573		0.0012250
20	0.040000	565.00		-1.3979	2.7520		0.0016000
21	0.045000	450.00		-1.3468	2.6532		0.0020250
22	0.050000	366.00		-1.3010	2.5635		0.0025000
23	0.060000	260.00		-1.2218	2.4150		0.0036000
24	0.070000	198.00		-1.1549	2.2967		0.0049000
25	0.080000	152.00		-1.0969	2.1818		0.0064000
26	0.090000	120.00		-1.0458	2.0792		0.0081000
27	0.10000	100.00		-1.0000	2.0000		0.010000
28	0.15000	54.000		-0.82391	1.7324		0.022500
29	0.20000	28.000		-0.69897	1.4472		0.040000
30	0.30000	13.000		-0.52288	1.1139		0.090000
31	0.35000	8.6000		-0.45593	0.93450		0.12250
32	0.40000	5.5000		-0.39794	0.74036		0.16000
33	0.50000	2.3000		-0.30103	0.36173		0.25000
34	0.60000	1.2000		-0.22185	0.079181		0.36000



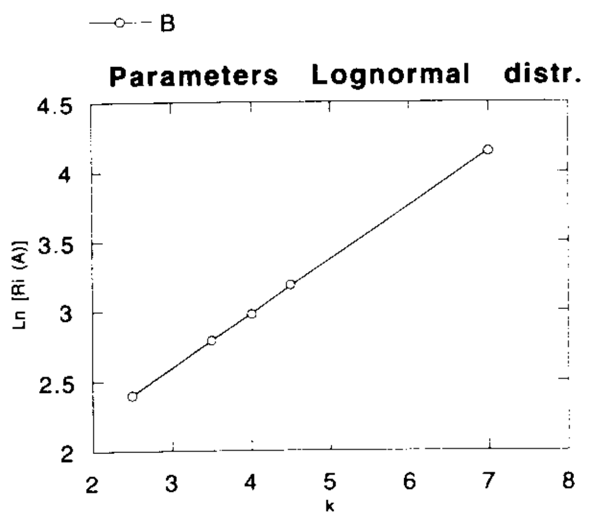
log I1 (q) (a.u.)
log i2 (q) (a. u.)
Fractal data
3.9
3.85
3.8
3.75
3.7
3.65
log I1 (q) (a.u.)
0
5.000 10^-5
1.000 10^-4
q^2(1/A^2)

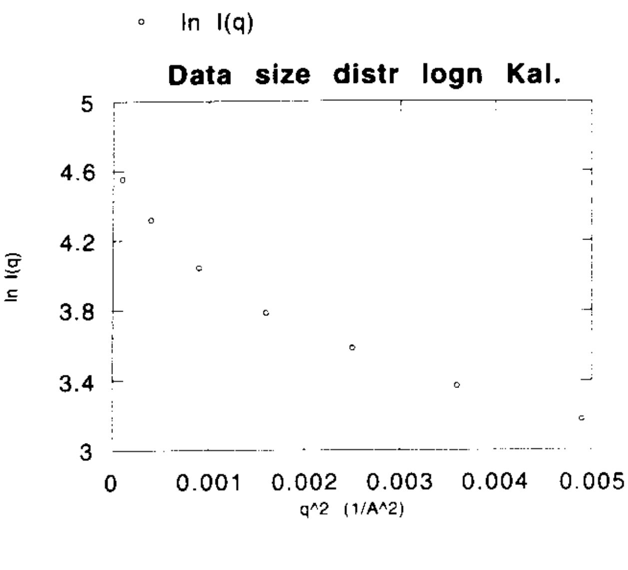


log I1 (q) (a.u.)
log i2 (q) (a. u.)
Fractal data
5
4
3
2
1
0
- 1
log I1 (q) (a.u.)
-3.5
- 3
-2.5
- 2
-1.5
- 1
-0.5
0
log (q (1/A))

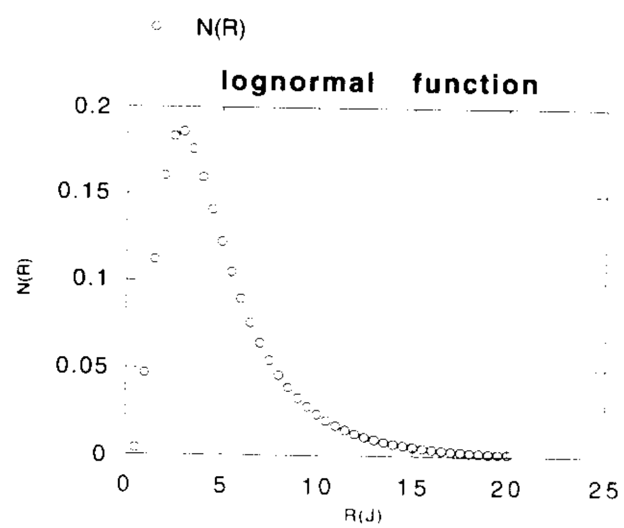


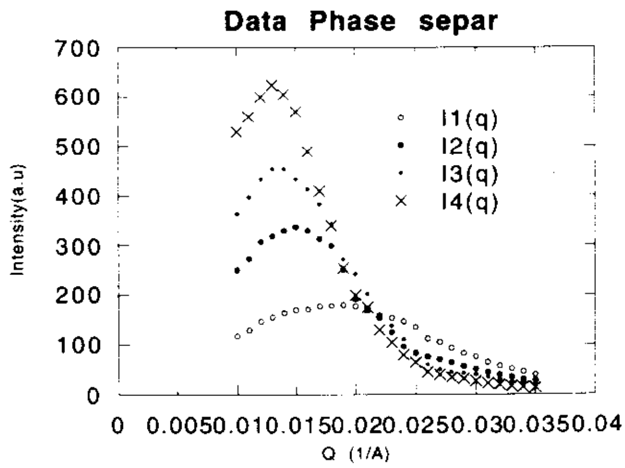
	q (1/A)	I(q)	I(q)*q	I(q)*q^2	ln I(q)	q^2 (1/A^2)	q^4*10^4	I(q)*q^4*10^4
1	0.0100000	95.000	0.95000	0.0095000	4.5539	1.0000e-04	1.0000e-04	0.0095000
2	0.020000	75.000	1.5000	0.030000	4.3175	0.00040000	0.0016000	0.12000
3	0.030000	57.000	1.7100	0.051300	4.0431	0.00090000	0.0081000	0.46170
4	0.040000	44.000	1.7600	0.070400	3.7842	0.0016000	0.025600	1.1264
5	0.050000	36.000	1.8000	0.090000	3.5835	0.0025000	0.062500	2.2500
6	0.060000	29.000	1.7400	0.10440	3.3673	0.0036000	0.12960	3.7584
7	0.070000	24.000	1.6800	0.11760	3.1781	0.0049000	0.24010	5.7624
8	0.080000	20.000	1.6000	0.12800	2.9957	0.0064000	0.40960	8.1920
9	0.090000	14.610	1.3149	0.11834	2.6817	0.0081000	0.65610	9.5856
10	0.10000	11.980	1.1980	0.11980	2.4832	0.0100000	1.0000	11.980
11	0.11280	10.000	1.1280	0.12724	2.3026	0.012724	1.6190	16.190
12	0.12730	7.9800	1.0159	0.12932	2.0769	0.016205	2.6261	20.956
13	0.14360	5.6500	0.81134	0.11651	1.7317	0.020621	4.2522	24.025
14	0.16200	4.3000	0.69660	0.11285	1.4586	0.026244	6.8875	29.616
15	0.18280	2.7000	0.49356	0.090223	0.99325	0.033416	11.166	30.149
16	0.20600	1.6200	0.33372	0.068746	0.48243	0.042436	18.008	29.173
17	0.23250	1.0300	0.23947	0.055678	0.029559	0.054056	29.221	30.097


B
Parameters Lognormal distr.
Ln [Ri (A)]
4.5
4
3.5
3
2.5
2
2
3
4
5
6
7
8
k

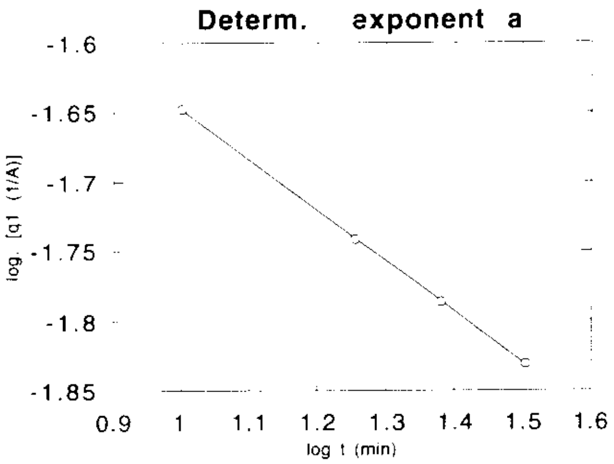

ln I(q)
Data size distr logn Kal.
ln I(q)
5
4.6
4.2
3.8
3.4
3
0
0.001
0.002
0.003
0.004
0.005
q^2 (1/A^2)

	Q (1/A)	I1(q)	I2(q)	I3(q)	I4(q)	I1(q)*q	I2(q)*q	I3(q)*q	I4(q)*q	q/q1(1)	I1*q1^3	q/q1(2)	I2*q1^3	q/q1(3)
1	0.0100000	118.08	250.80	363.60	530.00	1.1808	2.5080	3.6360	5.3000	0.44444	0.0013450	0.55127	0.0014971	0.61162
2	0.011000	129.60	273.60	397.94	560.00	1.4256	3.0096	4.3773	6.1600	0.48889	0.0014762	0.60639	0.0016332	0.67278
3	0.012000	146.88	307.80	434.30	600.00	1.7626	3.6936	5.2116	7.2000	0.53333	0.0016731	0.66152	0.0018373	0.73395
4	0.013000	155.52	319.20	454.50	624.00	2.0218	4.1496	5.9085	8.1120	0.57778	0.0017715	0.71665	0.0019053	0.79511
5	0.014000	164.16	330.60	454.50	605.00	2.2982	4.6284	6.3630	8.4700	0.62222	0.0018699	0.77178	0.0019734	0.85627
6	0.015000	169.92	337.44	434.30	570.00	2.5488	5.0616	6.5145	8.5500	0.66667	0.0019355	0.82690	0.0020142	0.91743
7	0.016000	171.36	330.60	414.10	490.00	2.7418	5.2896	6.6256	7.8400	0.71111	0.0019519	0.88203	0.0019734	0.97859
8	0.017000	177.12	313.50	383.80	410.00	3.0110	5.3295	6.5246	6.9700	0.75556	0.0020175	0.93716	0.0018713	1.0398
9	0.018000	178.56	299.82	343.40	340.00	3.2141	5.3968	6.1812	6.1200	0.80000	0.0020339	0.99228	0.0017897	1.1009
10	0.019000	180.00	250.80	272.70	255.00	3.4200	4.7652	5.1813	4.8450	0.84444	0.0020503	1.0474	0.0014971	1.1621
11	0.020000	177.12	191.52	242.40	200.00	3.5424	3.8304	4.8480	4.0000	0.88889	0.0020175	1.1025	0.0011432	1.2232
12	0.021000	172.80	168.72	202.00	175.00	3.6288	3.5431	4.2420	3.6750	0.93333	0.0019683	1.1577	0.0010071	1.2844
13	0.022000	158.40	153.90	156.55	130.00	3.4848	3.3858	3.4441	2.8600	0.97778	0.0018043	1.2128	0.00091865	1.3456
14	0.023000	154.08	125.40	138.37	105.00	3.5438	2.8842	3.1825	2.4150	1.0222	0.0017551	1.2679	0.00074853	1.4067
15	0.024000	146.88	96.900	111.10	80.000	3.5251	2.3256	2.6664	1.9200	1.0667	0.0016731	1.3230	0.00057841	1.4679
16	0.025000	135.36	83.220	86.860	65.000	3.3840	2.0805	2.1715	1.6250	1.1111	0.0015418	1.3782	0.00049675	1.5291
17	0.026000	112.32	76.380	60.600	46.000	2.9203	1.9859	1.5756	1.1960	1.1556	0.0012794	1.4333	0.00045592	1.5902
18	0.027000	105.12	70.680	50.500	40.000	2.8382	1.9084	1.3635	1.0800	1.2000	0.0011974	1.4884	0.00042190	1.6514
19	0.028000	93.600	64.980	45.450	35.000	2.6208	1.8194	1.2726	0.98000	1.2444	0.0010662	1.5436	0.00038787	1.7125
20	0.029000	83.520	57.000	43.430	32.000	2.4221	1.6530	1.2595	0.92800	1.2889	0.00095135	1.5987	0.00034024	1.7737
21	0.030000	76.320	51.300	40.400	28.000	2.2896	1.5390	1.2120	0.84000	1.3333	0.00086933	1.6538	0.00030622	1.8349
22	0.031000	64.800	45.600	35.350	23.000	2.0088	1.4136	1.0958	0.71300	1.3778	0.00073811	1.7089	0.00027219	1.8960
23	0.032000	57.600	39.900	30.300	20.000	1.8432	1.2768	0.96960	0.64000	1.4222	0.00065610	1.7641	0.00023817	1.9572
24	0.033000	51.840	35.340	26.260	17.000	1.7107	1.1662	0.86658	0.56100	1.4667	0.00059049	1.8192	0.00021095	2.0183
25	0.034000	46.080	30.780	23.230	15.000	1.5667	1.0465	0.78982	0.51000	1.5111	0.00052488	1.8743	0.00018373	2.0795
26	0.035000	40.320	28.500	20.200	14.000	1.4112	0.99750	0.70700	0.49000	1.5556	0.00045927	1.9294	0.00017012	2.1407

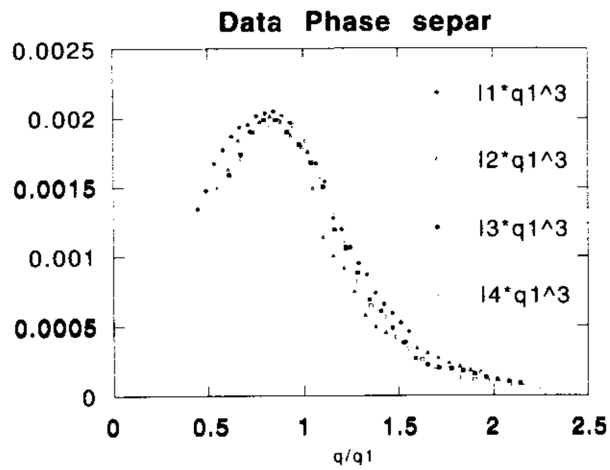


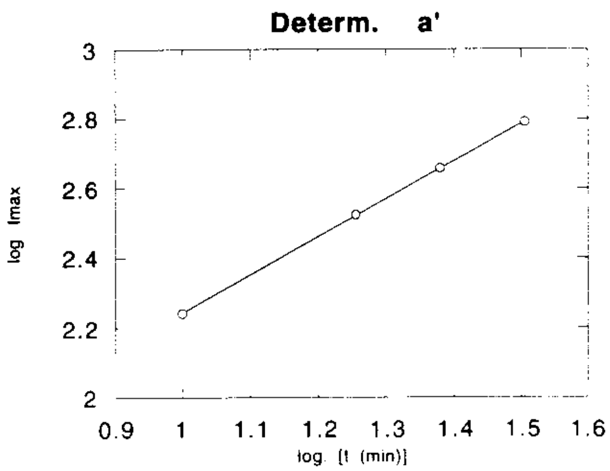


	I3*q1^3	q/q1(4)	I4*q1^3
1	0.0015892	0.67751	0.0017043
2	0.0017393	0.74526	0.0018007
3	0.0018982	0.81301	0.0019293
4	0.0019865	0.88076	0.0020065
5	0.0019865	0.94851	0.0019454
6	0.0018982	1.0163	0.0018329
7	0.0018099	1.0840	0.0015756
8	0.0016775	1.1518	0.0013184
9	0.0015009	1.2195	0.0010933
10	0.0011919	1.2873	0.00081997
11	0.0010595	1.3550	0.00064312
12	0.00088289	1.4228	0.00056273
13	0.00068424	1.4905	0.00041803
14	0.00060478	1.5583	0.00033764
15	0.00048559	1.6260	0.00025725
16	0.00037964	1.6938	0.00020901
17	0.00026487	1.7615	0.00014792
18	0.00022072	1.8293	0.00012862
19	0.00019865	1.8970	0.00011255
20	0.00018982	1.9648	0.00010290
21	0.00017658	2.0325	9.0036e-05
22	0.00015451	2.1003	7.3958e-05
23	0.00013243	2.1680	6.4312e-05
24	0.00011478	2.2358	5.4665e-05
25	0.00010153	2.3035	4.8234e-05
26	8.8289e-05	2.3713	4.5018e-05



	t (min)	Imax (t)	Q1(t) (1/A)	log t [(min)]	log Imax	log [q1(1/A)]
1	10.000	174.20	0.022500	1.0000	2.2410	-1.6478
2	18.000	334.00	0.018140	1.2553	2.5237	-1.7414
3	24.000	454.00	0.016350	1.3802	2.6571	-1.7865
4	32.000	618.00	0.014760	1.5051	2.7910	-1.8309

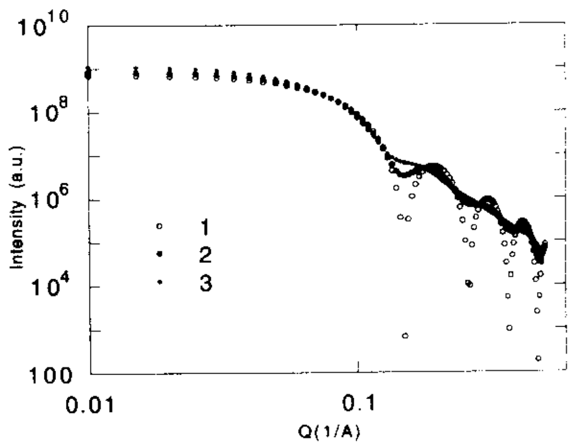

Data Phase separ
0.0025
0.002
0.0015
0.001
0.0005
0
0.5
1
1.5
2
2.5
q/q1
I1*q1^3
I2*q1^3
I3*q1^3
I4*q1^3


Determ. a'
3
2.8
2.6
2.4
2.2
2
0.9
1
1.1
1.2
1.3
1.4
1.5
1.6
log Imax
log [t (min)]

	Q(1/A)	1	2	3	q^2 (1/A^2)
35	0.17500	3.9430e+06	4.7946e+06	5.0253e+06	0.030625
36	0.18000	4.6680e+06	4.8578e+06	4.6068e+06	0.032400
37	0.18500	5.1577e+06	4.7662e+06	4.1700e+06	0.034225
38	0.19000	5.3910e+06	4.5374e+06	3.7350e+06	0.036100
39	0.19500	5.3735e+06	4.2002e+06	3.3188e+06	0.038025
40	0.20000	5.1310e+06	3.7885e+06	2.9344e+06	0.040000
41	0.20500	4.7039e+06	3.3369e+06	2.5899e+06	0.042025
42	0.21000	4.1416e+06	2.8772e+06	2.2888e+06	0.044100
43	0.21500	3.4963e+06	2.4359e+06	2.0309e+06	0.046225
44	0.22000	2.8197e+06	2.0330e+06	1.8133e+06	0.048400
45	0.22500	2.1581e+06	1.6818e+06	1.6311e+06	0.050625
46	0.23000	1.5505e+06	1.3893e+06	1.4790e+06	0.052900
47	0.23500	1.0266e+06	1.1564e+06	1.3512e+06	0.055225
48	0.24000	6.0577e+05	9.8016e+05	1.2425e+06	0.057600
49	0.24500	2.9750e+05	8.5400e+05	1.1486e+06	0.060025
50	0.25000	1.0180e+05	7.6958e+05	1.0657e+06	0.062500
51	0.25500	10650	7.1775e+05	9.9121e+05	0.065025
52	0.26000	9722.8	6.8942e+05	9.2311e+05	0.067600
53	0.26500	80277	6.7636e+05	8.6014e+05	0.070225
54	0.27000	2.0115e+05	6.7155e+05	8.0150e+05	0.072900
55	0.27500	3.5065e+05	6.6944e+05	7.4675e+05	0.075625
56	0.28000	5.0824e+05	6.6601e+05	6.9567e+05	0.078400
57	0.28500	6.5591e+05	6.5860e+05	6.4814e+05	0.081225
58	0.29000	7.7919e+05	6.4576e+05	6.0407e+05	0.084100
59	0.29500	8.6776e+05	6.2699e+05	5.6338e+05	0.087025
60	0.30000	9.1570e+05	6.0246e+05	5.2594e+05	0.090000
61	0.30500	9.2136e+05	5.7284e+05	4.9160e+05	0.093025
62	0.31000	8.8694e+05	5.3902e+05	4.6015e+05	0.096100
63	0.31500	8.1780e+05	5.0206e+05	4.3135e+05	0.099225
64	0.32000	7.2163e+05	4.6302e+05	4.0494e+05	0.10240
65	0.32500	6.0759e+05	4.2296e+05	3.8065e+05	0.10562
66	0.33000	4.8535e+05	3.8291e+05	3.5822e+05	0.10890
67	0.33500	3.6428e+05	3.4383e+05	3.3739e+05	0.11223
68	0.34000	2.5268e+05	3.0666e+05	3.1794e+05	0.11560

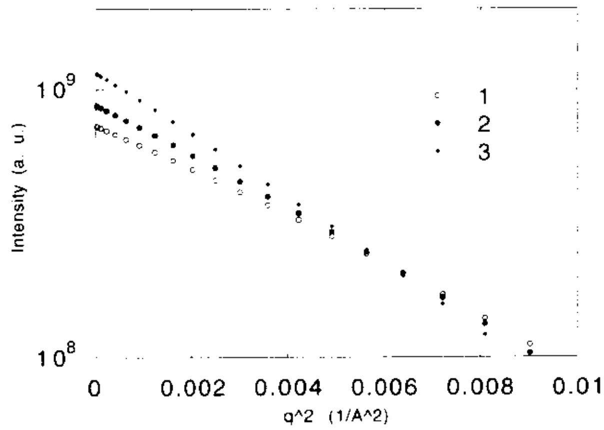
	Q(1/A)	1	2	3	q^2 (1/A^2)
1	0.0050000	7.2571e+08	8.6769e+08	1.1474e+09	2.5000e-05
2	0.0100000	7.1598e+08	8.5420e+08	1.1254e+09	1.0000e-04
3	0.015000	6.9998e+08	8.3212e+08	1.0897e+09	0.00022500
4	0.020000	6.7810e+08	8.0205e+08	1.0415e+09	0.00040000
5	0.025000	6.5083e+08	7.6481e+08	9.8240e+08	0.00062500
6	0.030000	6.1878e+08	7.2140e+08	9.1440e+08	0.00090000
7	0.035000	5.8265e+08	6.7292e+08	8.3968e+08	0.0012250
8	0.040000	5.4320e+08	6.2060e+08	7.6053e+08	0.0016000
9	0.045000	5.0127e+08	5.6570e+08	6.7922e+08	0.0020250
10	0.050000	4.5768e+08	5.0947e+08	5.9792e+08	0.0025000
11	0.055000	4.1327e+08	4.5312e+08	5.1863e+08	0.0030250
12	0.060000	3.6886e+08	3.9778e+08	4.4304e+08	0.0036000
13	0.065000	3.2521e+08	3.4446e+08	3.7256e+08	0.0042250
14	0.070000	2.8300e+08	2.9402e+08	3.0822e+08	0.0049000
15	0.075000	2.4285e+08	2.4717e+08	2.5073e+08	0.0056250
16	0.080000	2.0527e+08	2.0444e+08	2.0043e+08	0.0064000
17	0.085000	1.7067e+08	1.6616e+08	1.5736e+08	0.0072250
18	0.090000	1.3933e+08	1.3252e+08	1.2129e+08	0.0081000
19	0.095000	1.1146e+08	1.0355e+08	9.1781e+07	0.0090250
20	0.100000	8.7110e+07	7.9108e+07	6.8217e+07	0.0100000
21	0.10500	6.6279e+07	5.8961e+07	4.9889e+07	0.011025
22	0.11000	4.8851e+07	4.2771e+07	3.6035e+07	0.012100
23	0.11500	3.4639e+07	3.0131e+07	2.5885e+07	0.013225
24	0.12000	2.3392e+07	2.0589e+07	1.8706e+07	0.014400
25	0.12500	1.4811e+07	1.3677e+07	1.3825e+07	0.015625
26	0.13000	8.5660e+06	8.9262e+06	1.0654e+07	0.016900
27	0.13500	4.3080e+06	5.8909e+06	8.6941e+06	0.018225
28	0.14000	1.6856e+06	4.1603e+06	7.5443e+06	0.019600
29	0.14500	3.5686e+05	3.3702e+06	6.8940e+06	0.021025
30	0.15000	662.06	3.2095e+06	6.5158e+06	0.022500
31	0.15500	3.2545e+05	3.4232e+06	6.2542e+06	0.024025
32	0.16000	1.0758e+06	3.8121e+06	6.0115e+06	0.025600
33	0.16500	2.0369e+06	4.2297e+06	5.7355e+06	0.027225
34	0.17000	3.0360e+06	4.5767e+06	5.4062e+06	0.028900

Spheres: Rm=30 A   Wi=0, 15, 50 A



	Q(1/A)	1	2	3	q^2 (1/A^2)
69	0.34500	1.5728e+05	2.7228e+05	2.9967e+05	0.11902
70	0.35000	82841	2.4148e+05	2.8243e+05	0.12250
71	0.35500	31975	2.1498e+05	2.6610e+05	0.12602
72	0.36000	5166.3	1.9330e+05	2.5064e+05	0.12960
73	0.36500	951.85	1.7680e+05	2.3602e+05	0.13323
74	0.37000	16238	1.6558e+05	2.2230e+05	0.13690
75	0.37500	46716	1.5943e+05	2.0954e+05	0.14063
76	0.38000	87328	1.5786e+05	1.9783e+05	0.14440
77	0.38500	1.3275e+05	1.6010e+05	1.8726e+05	0.14822
78	0.39000	1.7786e+05	1.6509e+05	1.7790e+05	0.15210
79	0.39500	2.1809e+05	1.7162e+05	1.6977e+05	0.15603
80	0.40000	2.4982e+05	1.7836e+05	1.6284e+05	0.16000
81	0.40500	2.7049e+05	1.8399e+05	1.5698e+05	0.16402
82	0.41000	2.7875e+05	1.8733e+05	1.5199e+05	0.16810
83	0.41500	2.7448e+05	1.8740e+05	1.4761e+05	0.17222
84	0.42000	2.5863e+05	1.8358e+05	1.4349e+05	0.17640
85	0.42500	2.3305e+05	1.7558e+05	1.3926e+05	0.18063
86	0.43000	2.0030e+05	1.6357e+05	1.3457e+05	0.18490
87	0.43500	1.6332e+05	1.4808e+05	1.2911e+05	0.18923
88	0.44000	1.2516e+05	1.3003e+05	1.2268e+05	0.19360
89	0.44500	88750	1.1058e+05	1.1521e+05	0.19802
90	0.45000	56619	91060	1.0677e+05	0.20250
91	0.45500	30753	72817	97632	0.20703
92	0.46000	12459	57110	88200	0.21160
93	0.46500	2317.0	44973	79008	0.21622
94	0.47000	188.66	37116	70651	0.22090
95	0.47500	5289.2	33864	63719	0.22562
96	0.48000	16304	35119	58723	0.23040
97	0.48500	31539	40378	56013	0.23523
98	0.49000	49096	48783	55723	0.24010
99	0.49500	67042	59204	57732	0.24503
100	0.50000	83576	70357	61651	0.25000

Sphere data



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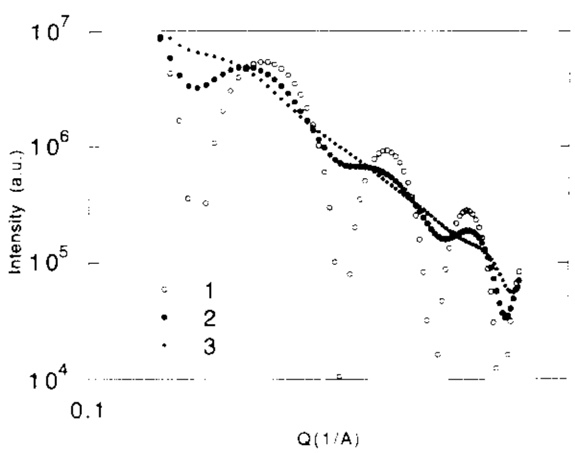

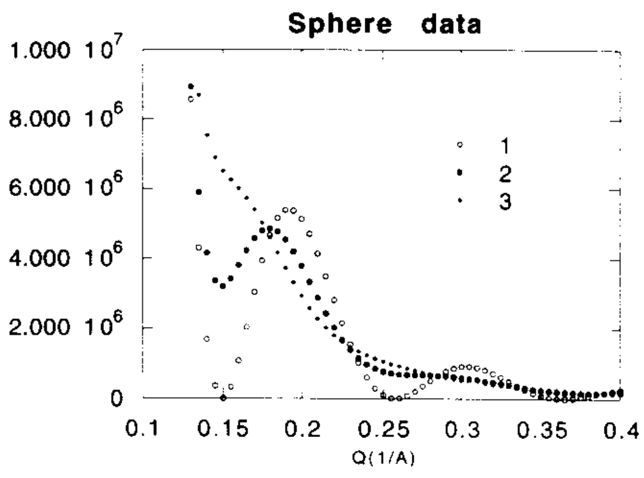
Sphere data
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6.000 10^6
4.000 10^6
2.000 10^6
0
0.1
0.15
0.2
0.25
0.3
0.35
0.4
Q(1/A)
1
2
3