TABLE B.3

CUBIC SPLINE INTERPOLATING COEFFICIENTS FOR ARGON SCATTERING FACTORS (MO-KA RADIATION)

COHERENT

J	C(1,J)	C(2,J)	C(3,J)	C(4,J)
1	3.306E 02	0.0	-6.606E 03	1.014E 04
2	3.141E 02	-6.352E 02	-4.259E 03	2.665E 04
3	2.716E 02	-9.945E 02	-7.752E 02	1.637E 04
4	2.200E 02	-1.031E 03	1.399E 03	1.074E 04
5	1.719E 02	-8.644E 02	2.362E 03	-2.210E 03
6	1.346E 02	-6.337E 02	1.947E 03	-3.885E 03
7	1.078E 02	-4.487E 02	1.446E 03	-2.251E 03
8	8.898E 01	-3.097E 02	1.040E 03	-3.615E 03
9	7.610E 01	-2.148E 02	5.346E 02	-1.439E 03
10	5.997E 01	-1.222E 02	1.877E 02	-5.919E 02
11	4.962E 01	-9.061E 01	5.873E 01	-1.060E 02
12	4.115E 01	-7.992E 01	4.282E 01	5.290E 01
13	3.358E 01	-7.083E 01	4.949E 01	-3.910E 01
14	2.699E 01	-6.132E 01	4.482E 01	3.151E 01
15	2.131E 01	-5.204E 01	5.986E 01	8.738E 01
16	1.670E 01	-3.920E 01	3.054E 01	-4.679E 02
17	1.309E 01	-3.777E 01	1.049E 02	1.679E 03

INCOHERENT

J	C(1,J)	C(2,J)	C(3,J)	C(4,J)
1	0.0	0.0	2.400E 02	-2.006E 02
2	6.000E-03	2.395E 00	2.410E 02	6.008E 02
3	2.400E-02	4.820E 00	2.213E 02	-6.423E 02
4	5.709E-01	2.150E 01	1.236E 02	-9.276E 02
5	1.955E 00	3.153E 01	8.459E 00	-4.467E 02
6	3.552E 00	3.126E 01	-3.860E 01	-4.777E 01
7	5.019E 00	2.728E 01	-4.161E 01	1.761E 01
8	7.331E 00	1.914E 01	-3.457E 01	3.523E 01
9	8.899E 00	1.258E 01	-2.232E 01	5.202E 01
10	9.934E 00	8.631E 00	-9.758E 00	2.159E 01
11	1.070E 01	6.896E 00	-4.990E 00	4.505E 00
12	1.134E 01	5.943E 00	-4.080E 00	8.750E-02
13	1.189E 01	5.128E 00	-4.543E 00	-4.802E 00
14	1.236E 01	4.171E 00	-4.270E 00	1.233E 01

TABLE B.4

SCATTERING FACTORS FOR DATA ANALYSIS

MO-KA RADIATION

4*PI*SIN(θ)/λ	ARGON (COH)	ARGON (INC)	BE (COH)	BE (INC)
0.4629	321.46	0.32	14.68	0.32
0.5400	318.27	0.43	14.26	0.42
0.6171	314.65	0.55	13.80	0.53
0.6942	310.62	0.69	13.31	0.64
0.7713	306.19	0.84	12.79	0.76
0.8483	301.41	0.99	12.26	0.88
0.9254	296.31	1.16	11.71	0.99
1.0024	290.94	1.34	11.16	1.11
1.0794	285.32	1.52	10.62	1.22
1.1564	279.51	1.71	10.08	1.33
1.2334	273.52	1.90	9.56	1.43
1.3104	267.32	2.09	9.06	1.53
1.3873	261.11	2.29	8.58	1.61
1.4642	254.81	2.48	8.13	1.69
1.5411	248.46	2.68	7.71	1.76
1.6179	242.08	2.88	7.30	1.82
1.6947	235.69	3.07	6.93	1.88
1.7715	229.30	3.27	6.57	1.93
1.8482	222.96	3.46	6.24	1.98
1.9249	216.73	3.65	5.94	2.02
2.0016	210.51	3.84	5.66	2.05
2.0783	204.38	4.02	5.40	2.09
2.1549	198.36	4.21	5.16	2.12
2.2314	192.45	4.39	4.94	2.14
2.3079	186.68	4.56	4.74	2.17
2.3844	181.06	4.73	4.55	2.19
2.4608	175.60	4.90	4.38	2.21
2.5372	170.26	5.07	4.22	2.23
2.6135	165.16	5.23	4.08	2.25
2.6898	160.24	5.39	3.95	2.26
2.7660	155.50	5.55	3.83	2.28
2.8422	150.93	5.70	3.72	2.30
2.9183	146.53	5.85	3.63	2.31
2.9944	142.31	6.00	3.53	2.33
3.0704	138.24	6.14	3.45	2.35
3.1463	134.36	6.29	3.37	2.36
3.2222	130.62	6.42	3.30	2.37
3.2981	127.03	6.56	3.23	2.39
3.3738	123.59	6.69	3.17	2.40
3.4495	120.30	6.82	3.11	2.42

TABLE B.4 (cont.)

SCATTERING FACTORS FOR DATA ANALYSIS

MO-KA RADIATION

4*PI*SIN(θ)/λ	ARGON (COH)	ARGON (INC)	BE (COH)	BE (INC)
3.5252	117.14	6.94	3.06	2.43
3.6007	114.11	7.07	3.01	2.45
3.6762	111.22	7.19	2.96	2.46
3.7517	108.44	7.30	2.92	2.48
3.8270	105.79	7.42	2.87	2.49
3.9023	103.24	7.53	2.83	2.51
3.9775	100.80	7.64	2.80	2.52
4.0526	98.47	7.74	2.76	2.54
4.1277	96.24	7.85	2.72	2.55
4.2027	94.10	7.95	2.69	2.57
4.2776	92.07	8.04	2.65	2.58
4.3524	90.13	8.14	2.62	2.60
4.4271	88.27	8.23	2.59	2.61
4.5018	86.51	8.32	2.56	2.63
4.5764	84.82	8.41	2.53	2.64
4.6508	83.22	8.50	2.50	2.66
4.7252	81.68	8.58	2.47	2.68
4.7995	80.22	8.66	2.44	2.69
4.8737	78.81	8.74	2.41	2.71
4.9478	77.47	8.82	2.38	2.72
5.0219	76.17	8.89	2.35	2.74
5.0958	74.94	8.97	2.32	2.75
5.1696	73.74	9.04	2.29	2.77
5.2434	72.59	9.11	2.26	2.78
5.3170	71.48	9.18	2.23	2.80
5.3905	70.41	9.24	2.20	2.81
5.4639	69.38	9.31	2.17	2.83
5.5373	68.39	9.37	2.15	2.84
5.6105	67.44	9.43	2.12	2.86
5.6836	66.52	9.49	2.09	2.87
5.7566	65.63	9.55	2.06	2.89
5.8295	64.77	9.60	2.03	2.90
5.9023	63.94	9.66	2.01	2.91
5.9749	63.13	9.71	1.98	2.93
6.0475	62.36	9.77	1.95	2.94
6.1199	61.60	9.82	1.93	2.96
6.1923	60.86	9.87	1.90	2.97
6.2645	60.15	9.92	1.88	2.98
6.3365	59.46	9.97	1.85	2.99
6.4085	58.77	10.02	1.82	3.01

TABLE B.4 (cont.)

SCATTERING FACTORS FOR DATA ANALYSIS

MO-KA RADIATION

4*PI*SIN(θ)/λ	ARGON (COH)	ARGON (INC)	BE (COH)	BE (INC)
6.4804	58.11	10.07	1.80	3.02
6.5521	57.46	10.11	1.77	3.03
6.6237	56.83	10.16	1.75	3.05
6.6951	56.21	10.20	1.72	3.06
6.7665	55.60	10.25	1.70	3.07
6.8377	55.01	10.29	1.68	3.08
6.9088	54.43	10.34	1.65	3.09
6.9797	53.85	10.38	1.63	3.11
7.0506	53.29	10.42	1.60	3.12
7.1212	52.74	10.46	1.58	3.13
7.1918	52.20	10.50	1.56	3.14
7.2622	51.67	10.54	1.53	3.15
7.3325	51.14	10.58	1.51	3.16
7.4026	50.62	10.62	1.49	3.17
7.4726	50.11	10.66	1.46	3.18
7.5424	49.60	10.70	1.44	3.19
7.6122	49.10	10.74	1.42	3.20
7.6817	48.61	10.78	1.40	3.21
7.7511	48.12	10.81	1.37	3.22
7.8204	47.63	10.85	1.35	3.23
7.8895	47.15	10.89	1.33	3.24
7.9585	46.67	10.92	1.31	3.25
8.0273	46.20	10.96	1.29	3.26
8.0960	45.74	10.99	1.27	3.27
8.1645	45.27	11.03	1.24	3.28
8.2328	44.82	11.06	1.22	3.29
8.3010	44.36	11.10	1.20	3.29
8.3691	43.91	11.13	1.18	3.30
8.4370	43.47	11.17	1.16	3.31
8.5047	43.02	11.20	1.14	3.32
8.5722	42.58	11.23	1.12	3.33
8.6396	42.15	11.26	1.11	3.33
8.7069	41.72	11.30	1.09	3.34
8.7739	41.29	11.33	1.07	3.35
8.8408	40.87	11.36	1.05	3.36

APPENDIX C

ABSORPTION FACTORS

A. Introduction

In computing absorption factors that are required in the data analysis of x-ray diffraction data for fluids, the relative shape of the incident x-ray beam must be considered if the path length through the cell and sample is a function of incident beam position. Note that for a flat plate cell the path length is constant over the incident beam profile for a given scattering angle, but for a cylindrical cell the path length clearly is a function of the incident position.

In reality a flat beam profile is not obtainable for the size of samples that are irradiated and the beam profile actually appears Gaussian in shape. The following derivation indicates how an arbitrary beam profile may be incorporated in the absorption factor calculation. This procedure was used to compute the absorption factors used in this thesis.

B. Derivation

The scattered radiation from a differential volume element irradiated by a monochromatic x-ray source may be written as:

$$dI(2\theta) = k_s P(2\theta) R^{-2} J(2\theta) \exp\left[-\sum u_i l_i\right] I_o \rho_e dV \qquad (1)$$

where 2θ is the scattering angle, R is the distance from dV to the detector, $J(2\theta)$ is the intrinsic scattering power of the media per electron, k_s is a constant with units of length squared, I_o is the incident intensity, ρ_e is the electron density, u_i is the absorption coefficient over path l_i and $P(2\theta)$ is the polarization factor.

Integration of Eq. (1) yields:

$$I(2\theta) = k_s P(2\theta) J(2\theta) \int_V R^{-2} \rho_e I_o \exp\left[-\sum u_i l_i\right] dV \qquad (2)$$

If R and ρ_e are assumed constant over the volume of integration, Eq. (2) may be written as:

$$I(2\theta) = k_s P(2\theta) J(2\theta) \rho_e R^{-2} \int_V I_o \exp\left[-\sum u_i l_i\right] dV \qquad (3)$$

Now rewrite ρ_e as N_e/V where N_e is the total number of electrons in the sample and V is the volume of the sample:

$$I(2\theta) = k_s P(2\theta) J(2\theta) N_e R^{-2} \left\{ V^{-1} \int_V I_o \exp\left[-\sum u_i l_i\right] dV \right\} \qquad (4)$$

The quantity in the brackets in Eq. (4) is defined as the absorption factor.

Now define:

$$I_o = \bar{I}_o f(x,z,y=0) \qquad (5)$$

where $\bar{I}_o$ is the average incident intensity and a right hand cartesian coordinate frame is arbitrarily placed in space between the x-ray source and sample with the y-axis parallel to the incident beam. The function $f(x,z,y=0)$ is seen to be just a weighting function and is calculated from an experimentally measured incident beam profile by:

$$f(x,z,y=0) = I_o/\bar{I}_o \qquad (6)$$

Substitute Eq. (5) into Eq. (4) to obtain:

$$I(2\theta) = k_s P(2\theta) J(2\theta) N_e R^{-2} \bar{I}_o \left\{ V^{-1} \int_V f(x,z,y=0) \cdot \exp\left[-\sum u_i l_i\right] dV \right\} \qquad (7)$$

The absorption factor that appears in the brackets above does not depend on the magnitude of the incident intensity as it does in Eq. (4) and may be referred to as the absorption factor for unit incident intensity. Note that the f-function simply weights the scattering volume at (x,z,y) according to the incident intensity at (x,z,y=0).

The absorption factors referred to in the data analysis section are of the following form:

$$A(2\theta) = V^{-1} \int_V f(x,z,y=0)\exp\left[-\sum u_i l_i\right] dV \qquad (8)$$

It is to be noted that in an experiment where a sample is contained in a cylindrical cell that the f-function above is not necessarily the same for both the cell and the sample, as can be elucidated from the above equation.

In practice the beam profile for each experiment was measured as observed through the cell material. It is true that this distorted the incident beam profile somewhat, but note that all that was needed was a relative profile. It was assumed that the beryllium cell decreased the observed intensity uniformly since all of the main beam always went through the cell and beryllium is a weak absorber. Also it was highly impractical to move the cryostat once it was in position because of the alignment procedure.

Figure C.1 depicts the cell cross section relative to the incident beam with pertinent dimensions required in the computer program in Appendix H which was used to compute all absorption factors used in this thesis. The absorption factors for each experiment as identified by date are presented in Tables C.1 through C.12.

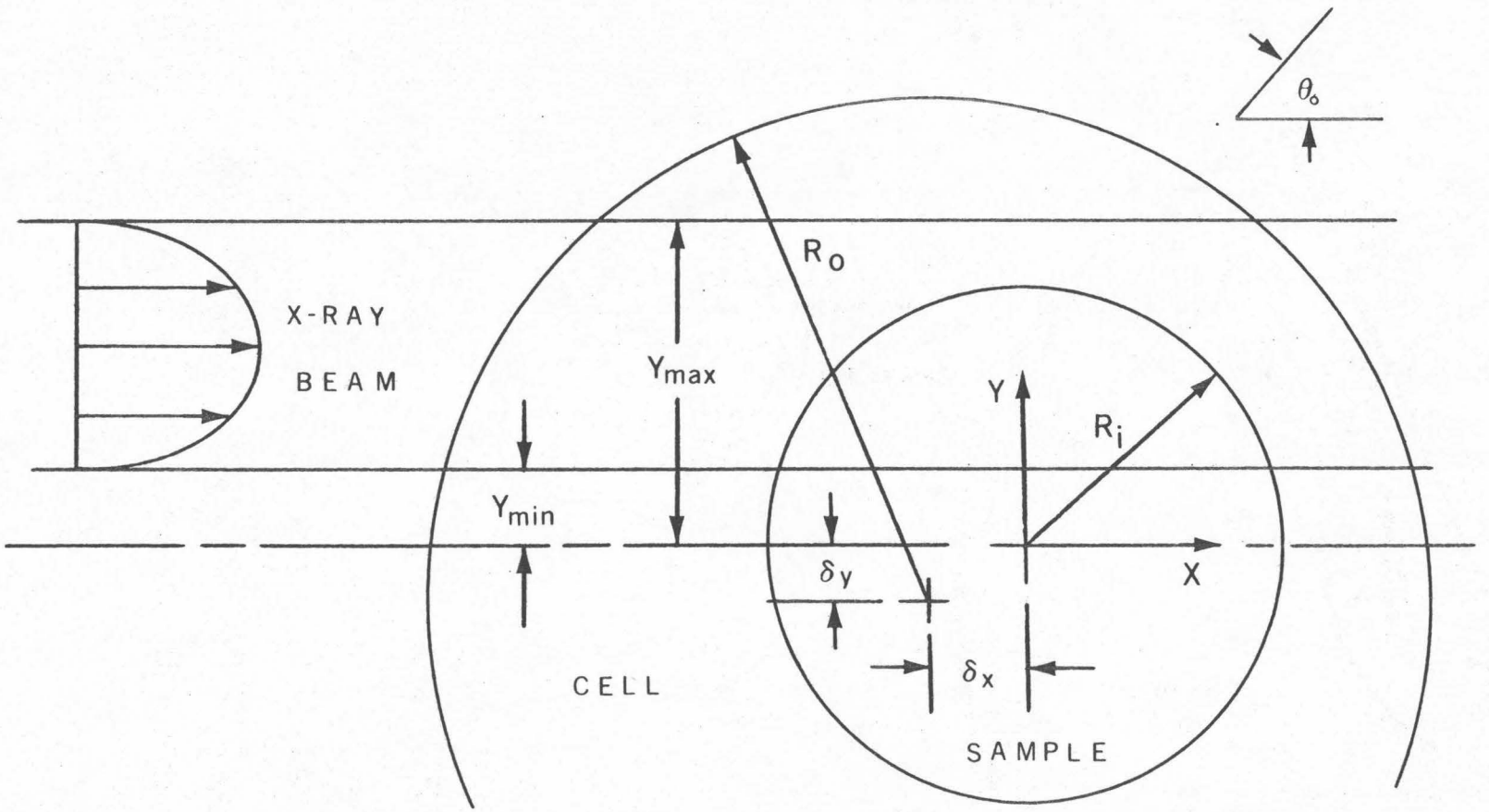

Figure C.1. Cross Section of Cell Relative to X-ray Beam Illustrating Dimensions Required to Compute Absorption Factors (See Appendix H)

TABLE C.1

ABSORPTION FACTORS
EXPERIMENT OF 2/23/71, T=143 DEG K, RHO=0.91 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
3.0	0.9070	0.4714	0.3649	0.9070	0.4713	0.3649
4.0	0.9067	0.4797	0.3670	0.9067	0.4797	0.3670
5.0	0.9065	0.4882	0.3691	0.9065	0.4881	0.3691
6.0	0.9062	0.4967	0.3713	0.9062	0.4966	0.3712
7.0	0.9060	0.5056	0.3734	0.9060	0.5055	0.3733
8.0	0.9057	0.5145	0.3755	0.9057	0.5143	0.3754
9.0	0.9055	0.5234	0.3777	0.9055	0.5232	0.3775
10.0	0.9052	0.5327	0.3798	0.9052	0.5325	0.3796
11.0	0.9050	0.5424	0.3819	0.9049	0.5421	0.3817
12.0	0.9047	0.5523	0.3841	0.9047	0.5520	0.3837
13.0	0.9045	0.5621	0.3862	0.9044	0.5618	0.3858
14.0	0.9042	0.5715	0.3883	0.9042	0.5712	0.3879
15.0	0.9040	0.5808	0.3905	0.9040	0.5804	0.3900
16.0	0.9039	0.5900	0.3926	0.9038	0.5896	0.3920
17.0	0.9037	0.5992	0.3947	0.9036	0.5987	0.3941
18.0	0.9036	0.6081	0.3968	0.9035	0.6076	0.3961
19.0	0.9034	0.6167	0.3989	0.9034	0.6163	0.3982
20.0	0.9034	0.6250	0.4010	0.9033	0.6245	0.4002
21.0	0.9033	0.6329	0.4031	0.9032	0.6324	0.4022
22.0	0.9033	0.6403	0.4052	0.9032	0.6398	0.4042
23.0	0.9033	0.6472	0.4073	0.9032	0.6467	0.4062
24.0	0.9033	0.6538	0.4094	0.9032	0.6533	0.4082
25.0	0.9034	0.6599	0.4114	0.9033	0.6594	0.4102
26.0	0.9035	0.6656	0.4135	0.9034	0.6651	0.4121
27.0	0.9037	0.6710	0.4155	0.9035	0.6704	0.4141
28.0	0.9038	0.6759	0.4175	0.9037	0.6754	0.4160
29.0	0.9040	0.6805	0.4196	0.9039	0.6799	0.4179
30.0	0.9042	0.6846	0.4215	0.9041	0.6841	0.4198
31.0	0.9044	0.6885	0.4235	0.9043	0.6879	0.4217
32.0	0.9047	0.6919	0.4255	0.9045	0.6914	0.4235
33.0	0.9050	0.6951	0.4274	0.9048	0.6946	0.4254
34.0	0.9053	0.6980	0.4293	0.9051	0.6975	0.4272
35.0	0.9055	0.7006	0.4312	0.9053	0.7001	0.4290
36.0	0.9059	0.7031	0.4331	0.9056	0.7026	0.4307
37.0	0.9062	0.7053	0.4350	0.9060	0.7048	0.4325
38.0	0.9065	0.7073	0.4368	0.9063	0.7069	0.4342
39.0	0.9068	0.7092	0.4386	0.9066	0.7087	0.4359
40.0	0.9072	0.7109	0.4404	0.9069	0.7104	0.4376
41.0	0.9075	0.7125	0.4422	0.9073	0.7120	0.4393
42.0	0.9079	0.7139	0.4439	0.9076	0.7134	0.4409
43.0	0.9082	0.7152	0.4457	0.9079	0.7147	0.4425

TABLE C.1 (cont.)

ABSORPTION FACTORS
EXPERIMENT OF 2/23/71, T=143 DEG K, RHO=0.91 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
44.0	0.9086	0.7164	0.4473	0.9083	0.7159	0.4441
45.0	0.9089	0.7175	0.4490	0.9086	0.7170	0.4456
46.0	0.9093	0.7184	0.4506	0.9090	0.7180	0.4471
47.0	0.9096	0.7193	0.4522	0.9093	0.7188	0.4486
48.0	0.9100	0.7201	0.4538	0.9097	0.7196	0.4501
49.0	0.9103	0.7208	0.4553	0.9100	0.7203	0.4515
50.0	0.9107	0.7214	0.4568	0.9104	0.7209	0.4529
51.0	0.9110	0.7220	0.4583	0.9107	0.7214	0.4543
52.0	0.9114	0.7224	0.4598	0.9110	0.7219	0.4556
53.0	0.9117	0.7228	0.4612	0.9114	0.7222	0.4569
54.0	0.9120	0.7231	0.4626	0.9117	0.7225	0.4582
55.0	0.9124	0.7232	0.4639	0.9120	0.7226	0.4594
56.0	0.9127	0.7232	0.4652	0.9123	0.7227	0.4606
57.0	0.9130	0.7232	0.4665	0.9127	0.7226	0.4617
58.0	0.9133	0.7233	0.4677	0.9130	0.7226	0.4629
59.0	0.9137	0.7233	0.4689	0.9133	0.7226	0.4640
60.0	0.9140	0.7232	0.4701	0.9136	0.7225	0.4650

TABLE C.2

ABSORPTION FACTORS
EXPERIMENT OF 6/16/71, T=143 DEG K, RHO=0.91 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
3.0	0.9190	0.5041	0.3659	0.9190	0.5041	0.3659
4.0	0.9188	0.5130	0.3681	0.9188	0.5129	0.3681
5.0	0.9185	0.5219	0.3703	0.9185	0.5218	0.3702
6.0	0.9183	0.5307	0.3725	0.9183	0.5306	0.3724
7.0	0.9180	0.5399	0.3748	0.9180	0.5398	0.3746
8.0	0.9178	0.5491	0.3770	0.9178	0.5490	0.3768
9.0	0.9176	0.5582	0.3792	0.9175	0.5581	0.3790
10.0	0.9174	0.5676	0.3814	0.9173	0.5675	0.3812
11.0	0.9172	0.5774	0.3836	0.9171	0.5773	0.3834
12.0	0.9169	0.5874	0.3859	0.9168	0.5872	0.3855
13.0	0.9167	0.5971	0.3881	0.9166	0.5969	0.3877
14.0	0.9165	0.6065	0.3903	0.9164	0.6062	0.3898
15.0	0.9163	0.6156	0.3925	0.9163	0.6153	0.3920
16.0	0.9162	0.6246	0.3947	0.9162	0.6242	0.3941
17.0	0.9161	0.6334	0.3969	0.9160	0.6330	0.3963
18.0	0.9160	0.6419	0.3991	0.9159	0.6415	0.3984
19.0	0.9159	0.6501	0.4012	0.9159	0.6496	0.4005
20.0	0.9159	0.6579	0.4034	0.9158	0.6574	0.4026
21.0	0.9159	0.6652	0.4055	0.9158	0.6647	0.4047
22.0	0.9159	0.6720	0.4077	0.9158	0.6716	0.4067
23.0	0.9160	0.6784	0.4098	0.9159	0.6779	0.4088
24.0	0.9161	0.6843	0.4119	0.9160	0.6839	0.4108
25.0	0.9162	0.6898	0.4140	0.9161	0.6894	0.4128
26.0	0.9164	0.6949	0.4161	0.9163	0.6945	0.4148
27.0	0.9166	0.6996	0.4182	0.9164	0.6992	0.4168
28.0	0.9168	0.7039	0.4202	0.9166	0.7034	0.4187
29.0	0.9170	0.7079	0.4223	0.9169	0.7074	0.4207
30.0	0.9173	0.7115	0.4243	0.9171	0.7110	0.4226
31.0	0.9176	0.7148	0.4263	0.9174	0.7143	0.4245
32.0	0.9178	0.7178	0.4283	0.9176	0.7173	0.4264
33.0	0.9181	0.7205	0.4302	0.9179	0.7201	0.4282
34.0	0.9184	0.7230	0.4322	0.9182	0.7226	0.4301
35.0	0.9187	0.7253	0.4341	0.9185	0.7249	0.4319
36.0	0.9190	0.7274	0.4360	0.9188	0.7270	0.4337
37.0	0.9194	0.7293	0.4379	0.9192	0.7289	0.4355
38.0	0.9198	0.7310	0.4397	0.9195	0.7306	0.4372
39.0	0.9201	0.7326	0.4415	0.9198	0.7322	0.4389
40.0	0.9205	0.7340	0.4433	0.9202	0.7336	0.4406
41.0	0.9209	0.7353	0.4451	0.9206	0.7349	0.4423
42.0	0.9212	0.7365	0.4468	0.9209	0.7361	0.4439
43.0	0.9216	0.7376	0.4485	0.9213	0.7372	0.4455

TABLE C.2 (cont.)

ABSORPTION FACTORS
EXPERIMENT OF 6/16/71, T=143 DEG K, RHO=0.91 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
44.0	0.9219	0.7386	0.4502	0.9216	0.7381	0.4471
45.0	0.9223	0.7395	0.4518	0.9220	0.7390	0.4486
46.0	0.9227	0.7403	0.4534	0.9223	0.7398	0.4501
47.0	0.9231	0.7410	0.4550	0.9227	0.7404	0.4516
48.0	0.9234	0.7416	0.4565	0.9230	0.7410	0.4530
49.0	0.9238	0.7421	0.4580	0.9233	0.7416	0.4544
50.0	0.9241	0.7426	0.4595	0.9237	0.7421	0.4558
51.0	0.9244	0.7430	0.4609	0.9241	0.7426	0.4571
52.0	0.9247	0.7434	0.4623	0.9244	0.7430	0.4584
53.0	0.9250	0.7436	0.4637	0.9248	0.7432	0.4597
54.0	0.9253	0.7437	0.4651	0.9251	0.7433	0.4609
55.0	0.9257	0.7437	0.4664	0.9254	0.7432	0.4621
56.0	0.9261	0.7435	0.4677	0.9257	0.7429	0.4633
57.0	0.9264	0.7434	0.4689	0.9260	0.7428	0.4644
58.0	0.9267	0.7434	0.4701	0.9263	0.7428	0.4655
59.0	0.9270	0.7433	0.4713	0.9266	0.7426	0.4666
60.0	0.9273	0.7431	0.4724	0.9269	0.7424	0.4676

TABLE C.3

ABSORPTION FACTORS
EXPERIMENT OF 6/23/71, T=127 DEG K, RHO=1.116 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
3.0	0.9400	0.5002	0.3022	0.9400	0.5002	0.3022
4.0	0.9398	0.5105	0.3046	0.9398	0.5104	0.3045
5.0	0.9396	0.5207	0.3069	0.9396	0.5207	0.3069
6.0	0.9394	0.5308	0.3092	0.9394	0.5308	0.3092
7.0	0.9392	0.5412	0.3117	0.9391	0.5412	0.3115
8.0	0.9390	0.5515	0.3141	0.9389	0.5514	0.3139
9.0	0.9388	0.5617	0.3165	0.9388	0.5615	0.3162
10.0	0.9386	0.5721	0.3188	0.9386	0.5719	0.3186
11.0	0.9384	0.5829	0.3212	0.9384	0.5827	0.3209
12.0	0.9382	0.5939	0.3235	0.9382	0.5936	0.3233
13.0	0.9380	0.6045	0.3259	0.9380	0.6042	0.3255
14.0	0.9379	0.6147	0.3282	0.9379	0.6144	0.3278
15.0	0.9378	0.6245	0.3306	0.9378	0.6242	0.3301
16.0	0.9377	0.6341	0.3330	0.9377	0.6338	0.3324
17.0	0.9377	0.6434	0.3353	0.9377	0.6431	0.3347
18.0	0.9377	0.6525	0.3376	0.9376	0.6521	0.3370
19.0	0.9377	0.6611	0.3400	0.9376	0.6607	0.3392
20.0	0.9377	0.6692	0.3423	0.9376	0.6688	0.3415
21.0	0.9378	0.6768	0.3446	0.9377	0.6764	0.3437
22.0	0.9379	0.6838	0.3469	0.9377	0.6834	0.3460
23.0	0.9380	0.6903	0.3492	0.9379	0.6899	0.3482
24.0	0.9381	0.6963	0.3515	0.9380	0.6959	0.3503
25.0	0.9383	0.7018	0.3537	0.9382	0.7014	0.3525
26.0	0.9385	0.7069	0.3559	0.9384	0.7065	0.3546
27.0	0.9387	0.7115	0.3582	0.9387	0.7111	0.3568
28.0	0.9390	0.7158	0.3604	0.9389	0.7153	0.3589
29.0	0.9393	0.7197	0.3625	0.9392	0.7192	0.3609
30.0	0.9396	0.7232	0.3647	0.9395	0.7227	0.3630
31.0	0.9399	0.7264	0.3668	0.9398	0.7259	0.3650
32.0	0.9403	0.7294	0.3690	0.9401	0.7288	0.3671
33.0	0.9406	0.7320	0.3711	0.9404	0.7315	0.3691
34.0	0.9409	0.7344	0.3732	0.9408	0.7339	0.3711
35.0	0.9413	0.7366	0.3752	0.9411	0.7361	0.3730
36.0	0.9417	0.7386	0.3772	0.9414	0.7381	0.3749
37.0	0.9420	0.7404	0.3792	0.9418	0.7399	0.3768
38.0	0.9424	0.7420	0.3812	0.9421	0.7415	0.3787
39.0	0.9427	0.7435	0.3831	0.9424	0.7430	0.3805
40.0	0.9431	0.7448	0.3850	0.9428	0.7443	0.3823
41.0	0.9435	0.7460	0.3869	0.9432	0.7455	0.3841
42.0	0.9438	0.7471	0.3887	0.9436	0.7466	0.3858
43.0	0.9442	0.7481	0.3906	0.9439	0.7476	0.3876

TABLE C.3 (cont.)

ABSORPTION FACTORS
EXPERIMENT OF 6/23/71, T=127 DEG K, RHO=1.116 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
44.0	0.9445	0.7489	0.3924	0.9443	0.7485	0.3893
45.0	0.9449	0.7497	0.3941	0.9447	0.7492	0.3909
46.0	0.9453	0.7503	0.3958	0.9451	0.7498	0.3925
47.0	0.9456	0.7509	0.3975	0.9454	0.7504	0.3941
48.0	0.9460	0.7513	0.3991	0.9457	0.7508	0.3956
49.0	0.9463	0.7517	0.4007	0.9461	0.7512	0.3971
50.0	0.9467	0.7521	0.4023	0.9464	0.7516	0.3986
51.0	0.9471	0.7524	0.4039	0.9467	0.7519	0.4001
52.0	0.9474	0.7526	0.4054	0.9471	0.7522	0.4015
53.0	0.9478	0.7528	0.4069	0.9474	0.7523	0.4028
54.0	0.9481	0.7527	0.4083	0.9477	0.7522	0.4041
55.0	0.9484	0.7525	0.4096	0.9481	0.7519	0.4053
56.0	0.9487	0.7521	0.4109	0.9484	0.7514	0.4065
57.0	0.9490	0.7517	0.4122	0.9487	0.7511	0.4077
58.0	0.9493	0.7515	0.4135	0.9490	0.7508	0.4089
59.0	0.9496	0.7513	0.4147	0.9493	0.7506	0.4100
60.0	0.9499	0.7509	0.4159	0.9496	0.7501	0.4111

TABLE C.4

ABSORPTION FACTORS
EXPERIMENT OF 7/28/71, T=133 DEG K, RHC=1.054 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
3.0	0.9003	0.4741	0.3797	0.9003	0.4741	0.3797
4.0	0.9001	0.4832	0.3822	0.9001	0.4831	0.3821
5.0	0.8998	0.4928	0.3846	0.8998	0.4927	0.3845
6.0	0.8996	0.5022	0.3871	0.8996	0.5020	0.3869
7.0	0.8993	0.5118	0.3896	0.8993	0.5116	0.3894
8.0	0.8991	0.5220	0.3920	0.8991	0.5219	0.3918
9.0	0.8988	0.5330	0.3945	0.8988	0.5328	0.3943
10.0	0.8985	0.5439	0.3970	0.8985	0.5437	0.3967
11.0	0.8983	0.5544	0.3995	0.8983	0.5542	0.3992
12.0	0.8981	0.5644	0.4020	0.8981	0.5642	0.4017
13.0	0.8979	0.5741	0.4046	0.8979	0.5739	0.4041
14.0	0.8977	0.5837	0.4071	0.8978	0.5834	0.4066
15.0	0.8976	0.5931	0.4096	0.8976	0.5928	0.4090
16.0	0.8975	0.6024	0.4121	0.8975	0.6021	0.4114
17.0	0.8974	0.6116	0.4146	0.8974	0.6112	0.4139
18.0	0.8973	0.6205	0.4172	0.8973	0.6201	0.4163
19.0	0.8973	0.6289	0.4197	0.8972	0.6285	0.4188
20.0	0.8973	0.6368	0.4222	0.8972	0.6364	0.4212
21.0	0.8973	0.6440	0.4247	0.8972	0.6436	0.4236
22.0	0.8974	0.6507	0.4273	0.8973	0.6503	0.4261
23.0	0.8975	0.6567	0.4298	0.8974	0.6563	0.4285
24.0	0.8976	0.6622	0.4323	0.8975	0.6618	0.4309
25.0	0.8978	0.6673	0.4348	0.8977	0.6669	0.4333
26.0	0.8980	0.6720	0.4373	0.8979	0.6715	0.4357
27.0	0.8982	0.6762	0.4397	0.8981	0.6758	0.4380
28.0	0.8985	0.6802	0.4422	0.8983	0.6797	0.4404
29.0	0.8987	0.6838	0.4446	0.8985	0.6833	0.4427
30.0	0.8990	0.6871	0.4470	0.8988	0.6866	0.4450
31.0	0.8993	0.6902	0.4494	0.8991	0.6897	0.4473
32.0	0.8996	0.6930	0.4518	0.8994	0.6925	0.4496
33.0	0.8999	0.6956	0.4541	0.8997	0.6950	0.4518
34.0	0.9002	0.6979	0.4565	0.9000	0.6974	0.4540
35.0	0.9005	0.7000	0.4588	0.9003	0.6995	0.4562
36.0	0.9008	0.7019	0.4611	0.9006	0.7014	0.4584
37.0	0.9012	0.7036	0.4634	0.9010	0.7031	0.4605
38.0	0.9015	0.7051	0.4656	0.9013	0.7046	0.4626
39.0	0.9018	0.7065	0.4678	0.9017	0.7060	0.4647
40.0	0.9022	0.7078	0.4700	0.9020	0.7073	0.4667
41.0	0.9026	0.7090	0.4721	0.9023	0.7085	0.4687
42.0	0.9029	0.7101	0.4742	0.9027	0.7096	0.4707
43.0	0.9033	0.7111	0.4763	0.9030	0.7106	0.4727

TABLE C.4 (cont.)

ABSORPTION FACTORS
EXPERIMENT OF 7/28/71, T=133 DEG K, RHC=1.054 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
44.0	0.9036	0.7121	0.4783	0.9034	0.7115	0.4746
45.0	0.9040	0.7129	0.4803	0.9037	0.7124	0.4765
46.0	0.9043	0.7136	0.4823	0.9040	0.7132	0.4783
47.0	0.9047	0.7143	0.4842	0.9044	0.7139	0.4801
48.0	0.9050	0.7149	0.4861	0.9047	0.7144	0.4819
49.0	0.9053	0.7153	0.4880	0.9051	0.7149	0.4835
50.0	0.9057	0.7157	0.4898	0.9054	0.7153	0.4852
51.0	0.9061	0.7160	0.4915	0.9057	0.7156	0.4868
52.0	0.9064	0.7162	0.4932	0.9061	0.7157	0.4884
53.0	0.9068	0.7164	0.4949	0.9064	0.7159	0.4899
54.0	0.9071	0.7166	0.4965	0.9067	0.7160	0.4915
55.0	0.9074	0.7168	0.4982	0.9070	0.7162	0.4930
56.0	0.9077	0.7170	0.4998	0.9073	0.7164	0.4945
57.0	0.9080	0.7169	0.5013	0.9076	0.7163	0.4958
58.0	0.9083	0.7166	0.5027	0.9080	0.7160	0.4972
59.0	0.9086	0.7165	0.5042	0.9082	0.7158	0.4985
60.0	0.9089	0.7164	0.5056	0.9085	0.7157	0.4997

TABLE C.5

ABSORPTION FACTORS
EXPERIMENT OF 8/4/71, T=127 DEG K, RHO=1.116 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
3.0	0.9081	0.4312	0.3257	0.9081	0.4312	0.3256
4.0	0.9078	0.4404	0.3279	0.9078	0.4404	0.3278
5.0	0.9075	0.4502	0.3301	0.9075	0.4502	0.3300
6.0	0.9072	0.4599	0.3323	0.9072	0.4599	0.3322
7.0	0.9070	0.4699	0.3346	0.9070	0.4698	0.3344
8.0	0.9068	0.4807	0.3368	0.9068	0.4805	0.3366
9.0	0.9064	0.4921	0.3391	0.9064	0.4919	0.3388
10.0	0.9061	0.5037	0.3413	0.9061	0.5035	0.3410
11.0	0.9058	0.5149	0.3435	0.9058	0.5147	0.3432
12.0	0.9056	0.5258	0.3458	0.9055	0.5256	0.3454
13.0	0.9054	0.5364	0.3480	0.9053	0.5362	0.3476
14.0	0.9052	0.5469	0.3503	0.9051	0.5466	0.3498
15.0	0.9050	0.5573	0.3525	0.9049	0.5570	0.3520
16.0	0.9048	0.5678	0.3547	0.9047	0.5674	0.3542
17.0	0.9047	0.5781	0.3570	0.9046	0.5777	0.3564
18.0	0.9046	0.5882	0.3592	0.9045	0.5878	0.3586
19.0	0.9045	0.5979	0.3615	0.9044	0.5975	0.3607
20.0	0.9044	0.6070	0.3637	0.9043	0.6066	0.3629
21.0	0.9044	0.6154	0.3659	0.9043	0.6150	0.3650
22.0	0.9044	0.6232	0.3682	0.9043	0.6227	0.3672
23.0	0.9044	0.6303	0.3704	0.9043	0.6298	0.3693
24.0	0.9045	0.6369	0.3726	0.9044	0.6364	0.3714
25.0	0.9046	0.6429	0.3748	0.9045	0.6424	0.3735
26.0	0.9047	0.6485	0.3770	0.9046	0.6479	0.3756
27.0	0.9049	0.6536	0.3792	0.9048	0.6531	0.3777
28.0	0.9051	0.6583	0.3813	0.9050	0.6578	0.3797
29.0	0.9053	0.6626	0.3835	0.9053	0.6621	0.3818
30.0	0.9056	0.6666	0.3856	0.9055	0.6661	0.3838
31.0	0.9059	0.6703	0.3877	0.9058	0.6698	0.3858
32.0	0.9062	0.6737	0.3898	0.9060	0.6732	0.3878
33.0	0.9065	0.6768	0.3919	0.9063	0.6762	0.3897
34.0	0.9068	0.6796	0.3940	0.9066	0.6791	0.3917
35.0	0.9071	0.6821	0.3960	0.9069	0.6816	0.3936
36.0	0.9074	0.6844	0.3980	0.9072	0.6839	0.3955
37.0	0.9078	0.6864	0.4000	0.9075	0.6860	0.3974
38.0	0.9081	0.6883	0.4019	0.9078	0.6878	0.3992
39.0	0.9085	0.6899	0.4039	0.9082	0.6895	0.4011
40.0	0.9088	0.6915	0.4058	0.9085	0.6911	0.4029
41.0	0.9091	0.6930	0.4077	0.9088	0.6925	0.4047
42.0	0.9095	0.6943	0.4096	0.9092	0.6939	0.4065
43.0	0.9098	0.6956	0.4115	0.9095	0.6951	0.4082

TABLE C.5 (cont.)

ABSORPTION FACTORS
EXPERIMENT OF 8/4/71, T=127 DEG K, RHO=1.116 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
44.0	0.9102	0.6967	0.4133	0.9098	0.6963	0.4099
45.0	0.9105	0.6978	0.4151	0.9102	0.6973	0.4116
46.0	0.9109	0.6988	0.4169	0.9106	0.6982	0.4132
47.0	0.9112	0.6996	0.4186	0.9110	0.6991	0.4149
48.0	0.9116	0.7004	0.4203	0.9113	0.6998	0.4164
49.0	0.9119	0.7010	0.4220	0.9117	0.7005	0.4180
50.0	0.9123	0.7015	0.4236	0.9120	0.7010	0.4195
51.0	0.9127	0.7019	0.4252	0.9123	0.7014	0.4210
52.0	0.9130	0.7022	0.4268	0.9126	0.7018	0.4224
53.0	0.9134	0.7025	0.4283	0.9128	0.7021	0.4238
54.0	0.9137	0.7027	0.4298	0.9132	0.7023	0.4252
55.0	0.9140	0.7030	0.4312	0.9136	0.7025	0.4265
56.0	0.9143	0.7033	0.4326	0.9140	0.7027	0.4278
57.0	0.9147	0.7033	0.4340	0.9143	0.7027	0.4291
58.0	0.9150	0.7031	0.4354	0.9146	0.7025	0.4303
59.0	0.9153	0.7030	0.4367	0.9149	0.7024	0.4315
60.0	0.9156	0.7030	0.4380	0.9152	0.7023	0.4327

TABLE C.6

ABSORPTION FACTORS
EXPERIMENT OF 8/24/71, T=127 DEG K, RHO=1.098 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
3.0	0.9150	0.4671	0.3257	0.9150	0.4671	0.3257
4.0	0.9147	0.4765	0.3279	0.9147	0.4765	0.3279
5.0	0.9145	0.4865	0.3302	0.9144	0.4865	0.3301
6.0	0.9143	0.4962	0.3325	0.9141	0.4963	0.3323
7.0	0.9140	0.5062	0.3347	0.9139	0.5061	0.3346
8.0	0.9136	0.5169	0.3369	0.9137	0.5167	0.3368
9.0	0.9134	0.5282	0.3391	0.9134	0.5280	0.3390
10.0	0.9131	0.5396	0.3414	0.9131	0.5394	0.3412
11.0	0.9129	0.5505	0.3437	0.9129	0.5503	0.3434
12.0	0.9127	0.5610	0.3460	0.9127	0.5608	0.3456
13.0	0.9125	0.5712	0.3482	0.9125	0.5709	0.3478
14.0	0.9124	0.5811	0.3505	0.9124	0.5809	0.3500
15.0	0.9122	0.5910	0.3527	0.9122	0.5907	0.3522
16.0	0.9121	0.6008	0.3549	0.9121	0.6005	0.3544
17.0	0.9120	0.6105	0.3572	0.9120	0.6101	0.3566
18.0	0.9119	0.6198	0.3594	0.9119	0.6194	0.3587
19.0	0.9118	0.6287	0.3616	0.9118	0.6284	0.3609
20.0	0.9118	0.6371	0.3638	0.9118	0.6367	0.3630
21.0	0.9118	0.6448	0.3660	0.9118	0.6444	0.3651
22.0	0.9119	0.6518	0.3682	0.9119	0.6514	0.3672
23.0	0.9120	0.6582	0.3704	0.9119	0.6578	0.3693
24.0	0.9121	0.6641	0.3725	0.9121	0.6637	0.3714
25.0	0.9123	0.6695	0.3747	0.9122	0.6691	0.3735
26.0	0.9125	0.6744	0.3768	0.9124	0.6740	0.3756
27.0	0.9127	0.6790	0.3790	0.9126	0.6786	0.3776
28.0	0.9130	0.6832	0.3811	0.9128	0.6827	0.3796
29.0	0.9132	0.6870	0.3832	0.9130	0.6865	0.3816
30.0	0.9135	0.6905	0.3853	0.9133	0.6900	0.3836
31.0	0.9138	0.6937	0.3874	0.9136	0.6932	0.3856
32.0	0.9141	0.6967	0.3894	0.9139	0.6962	0.3875
33.0	0.9144	0.6994	0.3915	0.9142	0.6989	0.3894
34.0	0.9147	0.7019	0.3935	0.9145	0.7014	0.3913
35.0	0.9150	0.7041	0.3955	0.9148	0.7036	0.3932
36.0	0.9153	0.7061	0.3975	0.9151	0.7056	0.3951
37.0	0.9157	0.7079	0.3994	0.9155	0.7074	0.3969
38.0	0.9161	0.7095	0.4013	0.9158	0.7091	0.3987
39.0	0.9164	0.7109	0.4032	0.9161	0.7105	0.4005
40.0	0.9168	0.7123	0.4050	0.9165	0.7119	0.4023
41.0	0.9172	0.7136	0.4068	0.9169	0.7132	0.4040
42.0	0.9175	0.7147	0.4086	0.9172	0.7143	0.4057
43.0	0.9179	0.7158	0.4104	0.9176	0.7154	0.4074

TABLE C.6 (cont.)

ABSORPTION FACTORS
EXPERIMENT OF 8/24/71, T=127 DEG K, RHO=1.098 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
44.0	0.9182	0.7168	0.4122	0.9179	0.7163	0.4090
45.0	0.9186	0.7177	0.4139	0.9183	0.7172	0.4106
46.0	0.9190	0.7185	0.4156	0.9186	0.7180	0.4122
47.0	0.9194	0.7192	0.4173	0.9190	0.7187	0.4137
48.0	0.9197	0.7198	0.4189	0.9193	0.7193	0.4152
49.0	0.9201	0.7203	0.4205	0.9197	0.7198	0.4167
50.0	0.9204	0.7207	0.4220	0.9200	0.7202	0.4181
51.0	0.9207	0.7210	0.4235	0.9203	0.7205	0.4195
52.0	0.9210	0.7212	0.4249	0.9207	0.7208	0.4208
53.0	0.9212	0.7214	0.4263	0.9210	0.7210	0.4222
54.0	0.9216	0.7216	0.4277	0.9214	0.7212	0.4235
55.0	0.9220	0.7218	0.4292	0.9217	0.7213	0.4248
56.0	0.9224	0.7220	0.4306	0.9220	0.7214	0.4261
57.0	0.9227	0.7219	0.4319	0.9223	0.7213	0.4273
58.0	0.9230	0.7216	0.4332	0.9226	0.7210	0.4284
59.0	0.9233	0.7215	0.4344	0.9229	0.7208	0.4295
60.0	0.9236	0.7214	0.4356	0.9232	0.7206	0.4306

TABLE C.7

ABSORPTION FACTORS
EXPERIMENT OF 9/28/71(I), T=133 DEG K, RHO=1.054 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
3.0	0.9349	0.5275	0.3348	0.9349	0.5275	0.3347
4.0	0.9346	0.5372	0.3371	0.9346	0.5372	0.3370
5.0	0.9344	0.5475	0.3394	0.9344	0.5474	0.3393
6.0	0.9342	0.5574	0.3417	0.9342	0.5572	0.3415
7.0	0.9339	0.5673	0.3440	0.9339	0.5672	0.3438
8.0	0.9337	0.5779	0.3462	0.9337	0.5778	0.3461
9.0	0.9334	0.5891	0.3486	0.9334	0.5889	0.3484
10.0	0.9332	0.6002	0.3509	0.9332	0.6000	0.3506
11.0	0.9330	0.6108	0.3532	0.9330	0.6105	0.3529
12.0	0.9329	0.6208	0.3555	0.9329	0.6205	0.3552
13.0	0.9327	0.6304	0.3577	0.9327	0.6301	0.3574
14.0	0.9327	0.6397	0.3600	0.9326	0.6394	0.3596
15.0	0.9326	0.6488	0.3623	0.9325	0.6485	0.3618
16.0	0.9326	0.6578	0.3646	0.9324	0.6575	0.3640
17.0	0.9325	0.6665	0.3668	0.9324	0.6662	0.3662
18.0	0.9325	0.6748	0.3690	0.9324	0.6745	0.3684
19.0	0.9325	0.6827	0.3712	0.9324	0.6823	0.3705
20.0	0.9326	0.6900	0.3734	0.9325	0.6896	0.3727
21.0	0.9327	0.6966	0.3756	0.9326	0.6962	0.3748
22.0	0.9328	0.7025	0.3778	0.9327	0.7021	0.3769
23.0	0.9330	0.7079	0.3800	0.9329	0.7075	0.3790
24.0	0.9332	0.7128	0.3821	0.9331	0.7124	0.3811
25.0	0.9334	0.7172	0.3843	0.9333	0.7168	0.3831
26.0	0.9336	0.7212	0.3864	0.9335	0.7208	0.3851
27.0	0.9339	0.7249	0.3885	0.9338	0.7245	0.3872
28.0	0.9342	0.7283	0.3906	0.9340	0.7279	0.3892
29.0	0.9345	0.7314	0.3927	0.9343	0.7310	0.3911
30.0	0.9348	0.7343	0.3947	0.9346	0.7339	0.3931
31.0	0.9351	0.7369	0.3967	0.9349	0.7365	0.3950
32.0	0.9355	0.7394	0.3987	0.9352	0.7390	0.3969
33.0	0.9358	0.7416	0.4006	0.9356	0.7412	0.3988
34.0	0.9361	0.7436	0.4026	0.9359	0.7432	0.4007
35.0	0.9365	0.7454	0.4045	0.9363	0.7450	0.4025
36.0	0.9369	0.7470	0.4064	0.9367	0.7466	0.4043
37.0	0.9372	0.7484	0.4083	0.9370	0.7480	0.4061
38.0	0.9376	0.7497	0.4101	0.9374	0.7493	0.4078
39.0	0.9379	0.7508	0.4119	0.9377	0.7504	0.4095
40.0	0.9383	0.7519	0.4137	0.9381	0.7515	0.4112
41.0	0.9387	0.7529	0.4154	0.9385	0.7525	0.4128
42.0	0.9391	0.7538	0.4172	0.9388	0.7534	0.4145
43.0	0.9394	0.7547	0.4188	0.9392	0.7542	0.4160

TABLE C.7 (cont.)

ABSORPTION FACTORS
EXPERIMENT OF 9/28/71(I), T=133 DEG K, RHO=1.054 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
44.0	0.9398	0.7554	0.4205	0.9395	0.7549	0.4176
45.0	0.9402	0.7561	0.4221	0.9399	0.7556	0.4191
46.0	0.9406	0.7567	0.4237	0.9403	0.7562	0.4206
47.0	0.9409	0.7572	0.4252	0.9406	0.7567	0.4220
48.0	0.9413	0.7576	0.4268	0.9410	0.7571	0.4234
49.0	0.9416	0.7579	0.4282	0.9413	0.7574	0.4248
50.0	0.9420	0.7582	0.4297	0.9417	0.7577	0.4262
51.0	0.9424	0.7584	0.4311	0.9421	0.7579	0.4275
52.0	0.9427	0.7586	0.4325	0.9424	0.7581	0.4289
53.0	0.9431	0.7587	0.4339	0.9427	0.7582	0.4301
54.0	0.9434	0.7588	0.4352	0.9430	0.7582	0.4313
55.0	0.9437	0.7587	0.4364	0.9433	0.7581	0.4324
56.0	0.9440	0.7585	0.4376	0.9435	0.7579	0.4334
57.0	0.9442	0.7583	0.4387	0.9438	0.7576	0.4345
58.0	0.9446	0.7581	0.4399	0.9442	0.7574	0.4356
59.0	0.9449	0.7579	0.4411	0.9445	0.7572	0.4367
60.0	0.9452	0.7576	0.4421	0.9448	0.7569	0.4376

TABLE C.8

ABSORPTION FACTORS
EXPERIMENT OF 9/28/71(II), T=133 DEG K, RHO=1.054 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
3.0	0.9601	0.5962	0.3289	0.9601	0.5962	0.3288
4.0	0.9599	0.6062	0.3312	0.9599	0.6062	0.3312
5.0	0.9597	0.6167	0.3336	0.9597	0.6166	0.3336
6.0	0.9595	0.6266	0.3360	0.9595	0.6265	0.3359
7.0	0.9594	0.6366	0.3383	0.9594	0.6365	0.3382
8.0	0.9592	0.6470	0.3407	0.9592	0.6469	0.3406
9.0	0.9591	0.6578	0.3430	0.9590	0.6577	0.3429
10.0	0.9589	0.6685	0.3454	0.9588	0.6684	0.3452
11.0	0.9588	0.6785	0.3477	0.9587	0.6784	0.3475
12.0	0.9586	0.6879	0.3501	0.9586	0.6877	0.3498
13.0	0.9586	0.6968	0.3523	0.9586	0.6966	0.3520
14.0	0.9586	0.7053	0.3546	0.9586	0.7050	0.3543
15.0	0.9586	0.7135	0.3569	0.9586	0.7132	0.3565
16.0	0.9587	0.7214	0.3592	0.9586	0.7211	0.3587
17.0	0.9587	0.7290	0.3615	0.9587	0.7286	0.3609
18.0	0.9588	0.7361	0.3637	0.9588	0.7358	0.3631
19.0	0.9589	0.7427	0.3660	0.9589	0.7424	0.3652
20.0	0.9591	0.7488	0.3682	0.9590	0.7485	0.3674
21.0	0.9593	0.7542	0.3704	0.9592	0.7539	0.3695
22.0	0.9595	0.7591	0.3726	0.9594	0.7588	0.3717
23.0	0.9597	0.7634	0.3747	0.9596	0.7631	0.3738
24.0	0.9600	0.7673	0.3768	0.9599	0.7670	0.3758
25.0	0.9603	0.7708	0.3789	0.9602	0.7705	0.3779
26.0	0.9606	0.7740	0.3810	0.9605	0.7737	0.3799
27.0	0.9609	0.7769	0.3830	0.9608	0.7766	0.3819
28.0	0.9613	0.7796	0.3851	0.9611	0.7793	0.3839
29.0	0.9616	0.7821	0.3871	0.9615	0.7818	0.3858
30.0	0.9620	0.7843	0.3891	0.9618	0.7840	0.3877
31.0	0.9624	0.7864	0.3911	0.9621	0.7861	0.3896
32.0	0.9627	0.7883	0.3930	0.9625	0.7880	0.3914
33.0	0.9631	0.7900	0.3950	0.9629	0.7897	0.3932
34.0	0.9634	0.7915	0.3968	0.9632	0.7912	0.3950
35.0	0.9638	0.7929	0.3987	0.9636	0.7926	0.3968
36.0	0.9642	0.7941	0.4005	0.9640	0.7938	0.3985
37.0	0.9646	0.7952	0.4023	0.9644	0.7949	0.4002
38.0	0.9650	0.7962	0.4040	0.9647	0.7959	0.4019
39.0	0.9654	0.7970	0.4057	0.9651	0.7967	0.4035
40.0	0.9658	0.7978	0.4074	0.9655	0.7975	0.4051
41.0	0.9662	0.7985	0.4091	0.9659	0.7982	0.4067
42.0	0.9666	0.7992	0.4107	0.9663	0.7989	0.4082
43.0	0.9670	0.7998	0.4123	0.9667	0.7994	0.4097

TABLE C.8 (cont.)

ABSORPTION FACTORS
EXPERIMENT OF 9/28/71(II), T=133 DEG K, RHC=1.054 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
44.0	0.9673	0.8003	0.4139	0.9670	0.8000	0.4112
45.0	0.9677	0.8008	0.4154	0.9674	0.8004	0.4126
46.0	0.9681	0.8012	0.4169	0.9678	0.8008	0.4140
47.0	0.9684	0.8015	0.4183	0.9681	0.8011	0.4154
48.0	0.9688	0.8018	0.4197	0.9684	0.8013	0.4167
49.0	0.9691	0.8020	0.4211	0.9688	0.8015	0.4180
50.0	0.9695	0.8021	0.4224	0.9691	0.8016	0.4192
51.0	0.9699	0.8022	0.4237	0.9694	0.8017	0.4204
52.0	0.9702	0.8022	0.4249	0.9698	0.8017	0.4215
53.0	0.9705	0.8022	0.4262	0.9701	0.8016	0.4227
54.0	0.9708	0.8021	0.4274	0.9705	0.8015	0.4238
55.0	0.9711	0.8019	0.4285	0.9708	0.8013	0.4249
56.0	0.9713	0.8016	0.4296	0.9711	0.8010	0.4260
57.0	0.9716	0.8013	0.4307	0.9714	0.8006	0.4270
58.0	0.9720	0.8009	0.4317	0.9717	0.8002	0.4279
59.0	0.9723	0.8006	0.4327	0.9719	0.7998	0.4288
60.0	0.9726	0.8002	0.4337	0.9722	0.7994	0.4297

TABLE C.9

ABSORPTION FACTORS
EXPERIMENT OF 11/30/71, T=143 DEG K, RHO=0.91 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
3.0	0.8910	0.4494	0.4017	0.8910	0.4494	0.4016
4.0	0.8907	0.4572	0.4038	0.8907	0.4571	0.4038
5.0	0.8904	0.4656	0.4059	0.8904	0.4655	0.4059
6.0	0.8901	0.4740	0.4080	0.8901	0.4739	0.4081
7.0	0.8898	0.4828	0.4102	0.8898	0.4827	0.4102
8.0	0.8896	0.4923	0.4124	0.8896	0.4921	0.4122
9.0	0.8892	0.5024	0.4146	0.8892	0.5023	0.4143
10.0	0.8889	0.5128	0.4167	0.8889	0.5126	0.4164
11.0	0.8886	0.5230	0.4189	0.8886	0.5227	0.4185
12.0	0.8882	0.5329	0.4210	0.8883	0.5326	0.4206
13.0	0.8880	0.5427	0.4232	0.8880	0.5424	0.4228
14.0	0.8877	0.5523	0.4253	0.8877	0.5520	0.4249
15.0	0.8875	0.5620	0.4275	0.8874	0.5617	0.4270
16.0	0.8873	0.5717	0.4297	0.8872	0.5714	0.4291
17.0	0.8871	0.5814	0.4318	0.8869	0.5811	0.4312
18.0	0.8869	0.5909	0.4340	0.8868	0.5905	0.4333
19.0	0.8867	0.6000	0.4362	0.8866	0.5996	0.4353
20.0	0.8866	0.6086	0.4383	0.8865	0.6082	0.4374
21.0	0.8865	0.6166	0.4404	0.8864	0.6162	0.4394
22.0	0.8865	0.6240	0.4426	0.8864	0.6235	0.4415
23.0	0.8865	0.6308	0.4447	0.8864	0.6303	0.4435
24.0	0.8865	0.6371	0.4468	0.8864	0.6366	0.4455
25.0	0.8866	0.6429	0.4489	0.8865	0.6424	0.4475
26.0	0.8867	0.6483	0.4510	0.8866	0.6477	0.4495
27.0	0.8868	0.6532	0.4531	0.8867	0.6527	0.4515
28.0	0.8870	0.6577	0.4552	0.8868	0.6572	0.4535
29.0	0.8872	0.6619	0.4573	0.8870	0.6614	0.4555
30.0	0.8874	0.6658	0.4593	0.8872	0.6653	0.4574
31.0	0.8876	0.6694	0.4613	0.8874	0.6689	0.4593
32.0	0.8879	0.6727	0.4633	0.8877	0.6721	0.4612
33.0	0.8881	0.6757	0.4653	0.8879	0.6752	0.4631
34.0	0.8884	0.6784	0.4673	0.8882	0.6779	0.4650
35.0	0.8887	0.6809	0.4692	0.8885	0.6804	0.4668
36.0	0.8890	0.6831	0.4711	0.8888	0.6827	0.4686
37.0	0.8893	0.6852	0.4731	0.8891	0.6847	0.4704
38.0	0.8896	0.6870	0.4750	0.8894	0.6866	0.4722
39.0	0.8900	0.6887	0.4768	0.8898	0.6883	0.4740
40.0	0.8903	0.6903	0.4787	0.8901	0.6899	0.4757
41.0	0.8907	0.6918	0.4805	0.8904	0.6914	0.4774
42.0	0.8910	0.6931	0.4823	0.8908	0.6927	0.4791
43.0	0.8914	0.6944	0.4841	0.8911	0.6940	0.4808

TABLE C.9 (cont.)

ABSORPTION FACTORS
EXPERIMENT OF 11/30/71, T=143 DEG K, RHO=0.91 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
44.0	0.8917	0.6956	0.4859	0.8915	0.6951	0.4824
45.0	0.8921	0.6967	0.4876	0.8918	0.6962	0.4840
46.0	0.8925	0.6977	0.4893	0.8922	0.6972	0.4856
47.0	0.8928	0.6986	0.4910	0.8925	0.6981	0.4871
48.0	0.8931	0.6994	0.4926	0.8928	0.6989	0.4887
49.0	0.8935	0.7001	0.4942	0.8932	0.6996	0.4901
50.0	0.8938	0.7007	0.4958	0.8935	0.7002	0.4916
51.0	0.8941	0.7012	0.4973	0.8938	0.7007	0.4930
52.0	0.8944	0.7017	0.4988	0.8941	0.7012	0.4944
53.0	0.8948	0.7021	0.5002	0.8944	0.7016	0.4957
54.0	0.8951	0.7024	0.5017	0.8947	0.7019	0.4970
55.0	0.8955	0.7027	0.5031	0.8951	0.7022	0.4983
56.0	0.8959	0.7030	0.5045	0.8955	0.7024	0.4995
57.0	0.8962	0.7032	0.5059	0.8959	0.7026	0.5007
58.0	0.8965	0.7033	0.5071	0.8961	0.7027	0.5019
59.0	0.8968	0.7033	0.5084	0.8964	0.7027	0.5031
60.0	0.8971	0.7034	0.5096	0.8967	0.7028	0.5042

TABLE C.10

ABSORPTION FACTORS
EXPERIMENT OF 12/8/71, T=127 DEG K, RHO=1.098 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
3.0	0.9015	0.4164	0.3375	0.9015	0.4164	0.3374
4.0	0.9013	0.4253	0.3397	0.9013	0.4253	0.3396
5.0	0.9010	0.4349	0.3419	0.9010	0.4348	0.3419
6.0	0.9008	0.4445	0.3442	0.9008	0.4442	0.3441
7.0	0.9005	0.4544	0.3465	0.9005	0.4541	0.3463
8.0	0.9001	0.4651	0.3487	0.9001	0.4649	0.3485
9.0	0.8998	0.4765	0.3510	0.8997	0.4764	0.3508
10.0	0.8995	0.4882	0.3532	0.8994	0.4880	0.3530
11.0	0.8992	0.4996	0.3555	0.8991	0.4993	0.3552
12.0	0.8989	0.5106	0.3578	0.8988	0.5103	0.3574
13.0	0.8987	0.5214	0.3600	0.8986	0.5211	0.3596
14.0	0.8984	0.5320	0.3623	0.8983	0.5317	0.3619
15.0	0.8982	0.5427	0.3646	0.8981	0.5424	0.3641
16.0	0.8980	0.5534	0.3669	0.8979	0.5531	0.3663
17.0	0.8978	0.5641	0.3692	0.8977	0.5637	0.3685
18.0	0.8976	0.5745	0.3714	0.8975	0.5741	0.3707
19.0	0.8975	0.5845	0.3737	0.8974	0.5840	0.3729
20.0	0.8974	0.5939	0.3760	0.8973	0.5934	0.3751
21.0	0.8974	0.6026	0.3783	0.8973	0.6021	0.3773
22.0	0.8974	0.6106	0.3805	0.8973	0.6101	0.3794
23.0	0.8974	0.6180	0.3828	0.8973	0.6175	0.3816
24.0	0.8975	0.6248	0.3851	0.8974	0.6243	0.3838
25.0	0.8976	0.6310	0.3873	0.8975	0.6305	0.3859
26.0	0.8977	0.6367	0.3895	0.8976	0.6362	0.3880
27.0	0.8979	0.6420	0.3917	0.8978	0.6415	0.3901
28.0	0.8981	0.6469	0.3939	0.8979	0.6464	0.3922
29.0	0.8983	0.6514	0.3961	0.8981	0.6509	0.3943
30.0	0.8985	0.6555	0.3983	0.8983	0.6550	0.3964
31.0	0.8987	0.6593	0.4005	0.8985	0.6588	0.3985
32.0	0.8990	0.6628	0.4026	0.8988	0.6623	0.4005
33.0	0.8993	0.6660	0.4048	0.8991	0.6655	0.4025
34.0	0.8996	0.6689	0.4069	0.8994	0.6685	0.4045
35.0	0.8999	0.6715	0.4090	0.8997	0.6711	0.4065
36.0	0.9002	0.6739	0.4111	0.9000	0.6735	0.4085
37.0	0.9006	0.6760	0.4131	0.9003	0.6756	0.4104
38.0	0.9009	0.6780	0.4151	0.9007	0.6775	0.4123
39.0	0.9013	0.6798	0.4171	0.9010	0.6793	0.4142
40.0	0.9016	0.6814	0.4191	0.9013	0.6809	0.4161
41.0	0.9019	0.6829	0.4210	0.9016	0.6824	0.4179
42.0	0.9023	0.6843	0.4230	0.9020	0.6838	0.4198
43.0	0.9026	0.6856	0.4249	0.9023	0.6851	0.4215

TABLE C.10 (cont.)

ABSORPTION FACTORS
EXPERIMENT OF 12/8/71, T=127 DEG K, RHO=1.098 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
44.0	0.9030	0.6868	0.4268	0.9026	0.6863	0.4233
45.0	0.9033	0.6879	0.4286	0.9030	0.6874	0.4250
46.0	0.9037	0.6889	0.4304	0.9034	0.6884	0.4267
47.0	0.9040	0.6898	0.4322	0.9037	0.6893	0.4283
48.0	0.9044	0.6906	0.4340	0.9041	0.6901	0.4299
49.0	0.9047	0.6913	0.4357	0.9045	0.6908	0.4315
50.0	0.9051	0.6919	0.4374	0.9048	0.6914	0.4331
51.0	0.9055	0.6924	0.4391	0.9051	0.6919	0.4347
52.0	0.9058	0.6929	0.4407	0.9054	0.6923	0.4362
53.0	0.9062	0.6932	0.4423	0.9057	0.6926	0.4376
54.0	0.9065	0.6935	0.4438	0.9060	0.6929	0.4391
55.0	0.9068	0.6937	0.4453	0.9064	0.6931	0.4404
56.0	0.9071	0.6938	0.4467	0.9068	0.6933	0.4417
57.0	0.9074	0.6939	0.4482	0.9071	0.6934	0.4429
58.0	0.9078	0.6939	0.4496	0.9074	0.6933	0.4443
59.0	0.9081	0.6939	0.4509	0.9077	0.6932	0.4456
60.0	0.9084	0.6938	0.4523	0.9080	0.6932	0.4468

TABLE C.11

ABSORPTION FACTORS
EXPERIMENT OF 12/15/71, T=127 DEG K, RHO=1.135 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
3.0	0.9064	0.4186	0.3211	0.9064	0.4186	0.3211
4.0	0.9061	0.4277	0.3233	0.9061	0.4277	0.3233
5.0	0.9058	0.4375	0.3256	0.9058	0.4375	0.3255
6.0	0.9055	0.4473	0.3279	0.9055	0.4472	0.3277
7.0	0.9052	0.4574	0.3300	0.9052	0.4573	0.3299
8.0	0.9050	0.4683	0.3322	0.9050	0.4682	0.3321
9.0	0.9046	0.4800	0.3345	0.9046	0.4799	0.3343
10.0	0.9043	0.4919	0.3368	0.9043	0.4917	0.3365
11.0	0.9040	0.5034	0.3391	0.9040	0.5032	0.3387
12.0	0.9038	0.5145	0.3413	0.9037	0.5143	0.3409
13.0	0.9036	0.5254	0.3435	0.9035	0.5252	0.3431
14.0	0.9033	0.5362	0.3458	0.9033	0.5359	0.3453
15.0	0.9031	0.5470	0.3481	0.9031	0.5466	0.3475
16.0	0.9029	0.5578	0.3504	0.9029	0.5573	0.3497
17.0	0.9027	0.5684	0.3527	0.9028	0.5680	0.3519
18.0	0.9026	0.5788	0.3549	0.9026	0.5783	0.3541
19.0	0.9025	0.5888	0.3572	0.9025	0.5883	0.3563
20.0	0.9024	0.5982	0.3594	0.9024	0.5977	0.3585
21.0	0.9024	0.6069	0.3616	0.9024	0.6064	0.3607
22.0	0.9024	0.6148	0.3639	0.9024	0.6143	0.3628
23.0	0.9025	0.6222	0.3661	0.9024	0.6217	0.3650
24.0	0.9026	0.6289	0.3683	0.9025	0.6284	0.3671
25.0	0.9027	0.6351	0.3705	0.9026	0.6346	0.3692
26.0	0.9028	0.6408	0.3727	0.9027	0.6403	0.3713
27.0	0.9030	0.6461	0.3749	0.9029	0.6456	0.3734
28.0	0.9032	0.6509	0.3771	0.9031	0.6504	0.3755
29.0	0.9034	0.6554	0.3792	0.9033	0.6549	0.3775
30.0	0.9036	0.6595	0.3814	0.9035	0.6590	0.3796
31.0	0.9039	0.6633	0.3836	0.9037	0.6628	0.3816
32.0	0.9041	0.6667	0.3857	0.9040	0.6662	0.3837
33.0	0.9044	0.6699	0.3878	0.9043	0.6694	0.3857
34.0	0.9048	0.6728	0.3899	0.9046	0.6723	0.3876
35.0	0.9051	0.6754	0.3920	0.9049	0.6749	0.3896
36.0	0.9054	0.6778	0.3941	0.9052	0.6773	0.3915
37.0	0.9058	0.6799	0.3961	0.9055	0.6794	0.3934
38.0	0.9061	0.6818	0.3981	0.9058	0.6813	0.3953
39.0	0.9065	0.6836	0.4000	0.9062	0.6831	0.3972
40.0	0.9068	0.6852	0.4020	0.9065	0.6847	0.3990
41.0	0.9071	0.6867	0.4039	0.9068	0.6862	0.4008
42.0	0.9075	0.6881	0.4058	0.9072	0.6876	0.4026
43.0	0.9078	0.6894	0.4077	0.9075	0.6889	0.4044

TABLE C.11 (cont.)

ABSORPTION FACTORS
EXPERIMENT OF 12/15/71, T=127 DEG K, RHO=1.135 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
44.0	0.9081	0.6906	0.4096	0.9078	0.6901	0.4061
45.0	0.9085	0.6917	0.4114	0.9082	0.6912	0.4078
46.0	0.9089	0.6927	0.4132	0.9086	0.6922	0.4095
47.0	0.9092	0.6935	0.4149	0.9089	0.6930	0.4111
48.0	0.9096	0.6943	0.4167	0.9093	0.6938	0.4128
49.0	0.9100	0.6949	0.4183	0.9097	0.6944	0.4144
50.0	0.9103	0.6955	0.4200	0.9100	0.6950	0.4159
51.0	0.9106	0.6960	0.4216	0.9103	0.6955	0.4174
52.0	0.9110	0.6964	0.4232	0.9106	0.6959	0.4188
53.0	0.9113	0.6967	0.4248	0.9109	0.6962	0.4203
54.0	0.9116	0.6970	0.4263	0.9112	0.6965	0.4216
55.0	0.9120	0.6972	0.4278	0.9116	0.6966	0.4230
56.0	0.9124	0.6974	0.4292	0.9120	0.6967	0.4243
57.0	0.9127	0.6975	0.4306	0.9124	0.6967	0.4257
58.0	0.9130	0.6974	0.4320	0.9126	0.6967	0.4269
59.0	0.9133	0.6973	0.4334	0.9129	0.6966	0.4281
60.0	0.9136	0.6973	0.4347	0.9132	0.6966	0.4293

TABLE C.12

ABSORPTION FACTORS
EXPERIMENT OF 12/21/71, T=127 DEG K, RHO=1.135 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
3.0	0.9004	0.3741	0.3219	0.9004	0.3741	0.3219
4.0	0.9001	0.3821	0.3239	0.9001	0.3820	0.3239
5.0	0.8999	0.3907	0.3260	0.8999	0.3907	0.3259
6.0	0.8996	0.3994	0.3281	0.8996	0.3994	0.3279
7.0	0.8994	0.4085	0.3301	0.8994	0.4085	0.3300
8.0	0.8990	0.4185	0.3321	0.8990	0.4184	0.3320
9.0	0.8987	0.4293	0.3342	0.8987	0.4291	0.3340
10.0	0.8984	0.4404	0.3363	0.8984	0.4401	0.3360
11.0	0.8981	0.4513	0.3384	0.8981	0.4510	0.3380
12.0	0.8978	0.4620	0.3405	0.8978	0.4617	0.3401
13.0	0.8976	0.4726	0.3426	0.8976	0.4723	0.3421
14.0	0.8973	0.4833	0.3447	0.8973	0.4829	0.3442
15.0	0.8970	0.4941	0.3468	0.8970	0.4937	0.3463
16.0	0.8967	0.5051	0.3489	0.8967	0.5047	0.3484
17.0	0.8965	0.5162	0.3510	0.8965	0.5158	0.3504
18.0	0.8963	0.5272	0.3532	0.8963	0.5268	0.3524
19.0	0.8961	0.5380	0.3553	0.8961	0.5375	0.3545
20.0	0.8960	0.5484	0.3574	0.8959	0.5479	0.3565
21.0	0.8959	0.5582	0.3595	0.8958	0.5577	0.3585
22.0	0.8958	0.5675	0.3617	0.8956	0.5670	0.3605
23.0	0.8957	0.5763	0.3638	0.8956	0.5757	0.3626
24.0	0.8957	0.5845	0.3660	0.8955	0.5839	0.3646
25.0	0.8957	0.5922	0.3681	0.8955	0.5916	0.3666
26.0	0.8957	0.5994	0.3702	0.8955	0.5988	0.3686
27.0	0.8958	0.6060	0.3723	0.8956	0.6054	0.3706
28.0	0.8959	0.6122	0.3744	0.8957	0.6116	0.3726
29.0	0.8960	0.6180	0.3765	0.8958	0.6174	0.3746
30.0	0.8962	0.6233	0.3786	0.8960	0.6227	0.3766
31.0	0.8964	0.6282	0.3807	0.8962	0.6276	0.3786
32.0	0.8966	0.6327	0.3828	0.8964	0.6321	0.3806
33.0	0.8968	0.6369	0.3849	0.8966	0.6362	0.3825
34.0	0.8970	0.6406	0.3869	0.8968	0.6400	0.3845
35.0	0.8973	0.6441	0.3890	0.8971	0.6435	0.3864
36.0	0.8976	0.6472	0.3910	0.8974	0.6467	0.3883
37.0	0.8979	0.6501	0.3931	0.8977	0.6495	0.3902
38.0	0.8982	0.6527	0.3951	0.8980	0.6522	0.3920
39.0	0.8985	0.6551	0.3970	0.8983	0.6546	0.3939
40.0	0.8988	0.6573	0.3990	0.8986	0.6568	0.3957
41.0	0.8991	0.6594	0.4009	0.8989	0.6589	0.3975
42.0	0.8995	0.6613	0.4029	0.8992	0.6608	0.3993
43.0	0.8998	0.6631	0.4048	0.8995	0.6625	0.4011

TABLE C.12 (cont.)

ABSORPTION FACTORS
EXPERIMENT OF 12/21/71, T=127 DEG K, RHO=1.135 GM/CC

	COHERENT			INCOHERENT		
2θ	CELL	CELL/A	ARGON	CELL	CELL/A	ARGON
44.0	0.9002	0.6648	0.4066	0.8999	0.6642	0.4029
45.0	0.9005	0.6663	0.4085	0.9002	0.6657	0.4046
46.0	0.9008	0.6677	0.4104	0.9005	0.6671	0.4063
47.0	0.9012	0.6690	0.4122	0.9009	0.6684	0.4080
48.0	0.9015	0.6702	0.4140	0.9012	0.6696	0.4096
49.0	0.9019	0.6713	0.4158	0.9016	0.6707	0.4112
50.0	0.9022	0.6722	0.4175	0.9019	0.6716	0.4128
51.0	0.9026	0.6730	0.4192	0.9022	0.6724	0.4144
52.0	0.9029	0.6736	0.4208	0.9025	0.6731	0.4160
53.0	0.9033	0.6742	0.4225	0.9028	0.6737	0.4175
54.0	0.9036	0.6748	0.4241	0.9031	0.6743	0.4190
55.0	0.9039	0.6753	0.4257	0.9035	0.6747	0.4204
56.0	0.9042	0.6758	0.4273	0.9039	0.6751	0.4218
57.0	0.9045	0.6762	0.4289	0.9043	0.6754	0.4231
58.0	0.9049	0.6764	0.4303	0.9045	0.6757	0.4245
59.0	0.9052	0.6765	0.4318	0.9048	0.6758	0.4258
60.0	0.9055	0.6767	0.4332	0.9051	0.6760	0.4271

APPENDIX D

SPLINE DATA SMOOTHING

A. Introduction

In numerical analysis there is a need for a method to smooth data that will produce first derivatives of high quality. Data that are already quite smooth may be interpolated by the "spline fit" as described by Walsh,[1] et al, and presented in Appendix E. This interpolation procedure is analogous to the draftsman's spline and joins data by piecewise cubics and demands continuity at the junctions in the function value and the first and second derivatives. The resulting line and first derivative estimates are quite good.

The concept of the spline can be extended to smoothing, or line estimation, of data which are not smooth but contain scatter. Once again piecewise cubics are used but now with least squares criterion and the boundary points for the cubics must be chosen. At this point variations can be taken on the constraints joining the cubics. The method described by Klaus[2] demands continuity in the same manner as the interpolation and also treats the value of the function on the interval boundaries as unknowns. This particular method has been applied to thermodynamic data[2] which were relatively smooth. Because of the number of constraints and

constants in this procedure, the number of degrees of freedom can rapidly approach zero.

The method to be presented here demands only continuity in the function and its first derivative and does not treat the value of the function at the boundary points as unknowns. The release of some of the previous constraints increases the number of degrees of freedom.

The final choice of the smoothing procedure to be used in any particular case will be somewhat arbitrary since decisions must be made by the user. Therefore, experience with the data to be smoothed appears to be the final and best guide.

B. Derivation

Consider a third order polynomial of the form:

$$y = y(x) = a_{i1} + a_{i2}(x-x_i) + (x-x_i)^2\left[a_{i3} + a_{i4}(x-x_{i+1})\right] \quad (1)$$

$$\text{for } x_i \le x \le x_{i+1} \text{ and } i = 1,2,\ldots$$

Let the range of a set of data points be divided into N-1 intervals and in each interval minimize the error sum of squares which is:

$$\Phi_i = \sum_{j=1}^{N_i} (y_{ji}-y)^2 \quad (2)$$

where i identifies the interval, N_i is the number of observations in the i-th interval and y_{ji} is the j-th observation in the i-th interval.

Now demand continuity in y and y', the derivative, at all the mesh points x_i. Add these constraints to the error sum of squares for each interval using Lagrange multipliers.[3] Let λ_i be the multiplier for the y constraint and π_i be the multiplier for the y' constraint at x_i. Note that the end intervals will require special consideration and the following manipulations will be pertinent only to intervals which are not the first or the last.

The form of the constraints at x_i are, for continuity in y:

$$a_{i1}-a_{i-1,1}-a_{i-1,2}\,\Delta x_{i-1}-a_{i-1,3}\,\Delta x_{i-1}^2 = 0 \qquad (3)$$

and for continuity in y':

$$a_{i2}-a_{i-1,2}-2\,\Delta x_{i-1}a_{i-1,3}-a_{i-1,4}\,\Delta x_{i-1}^2 = 0 \qquad (4)$$

where $\Delta x_{i-1} = x_i - x_{i-1}$

The modified objective function for the i-th interval becomes:

$$\Phi_i = \sum_{j=1}^{N_i} \left[y_{ji} - a_{i1} - a_{i2}(x-x_i) - (x-x_i)^2 \left\{ a_{i3} + a_{i4}(x-x_{i+1}) \right\} \right]^2$$

$$+ \lambda_i \left[a_{i1} - a_{i-1,1} - a_{i-1,2} \Delta x_{i-1} - a_{i-1,3} \Delta x_{i-1}^2 \right]$$

$$+ \pi_i \left[a_{i2} - a_{i-1,2} - 2 \Delta x_{i-1} a_{i-1,3} - a_{i-1,4} \Delta x_{i-1}^2 \right] \qquad (5)$$

$$+ \lambda_{i+1} \left[a_{i+1,1} - a_{i1} - a_{i2} \Delta x_i - a_{i3} \Delta x_i^2 \right]$$

$$+ \pi_{i+1} \left[a_{i+1,2} - a_{i2} - 2 \Delta x_i a_{i3} - a_{i4} \Delta x_i^2 \right]$$

Now minimize Φ_i with respect to the coefficients a_{ij} for $j = 1,2,3,4$ and solve for the a_{ij} in terms of the Lagrange multipliers. Define the following to condense notation:

$$\Omega_{ji} = x_j - x_i \text{ where } y_{ji} = y(x_j) \qquad (6)$$

$$\Omega_i^m = \sum_{j=1}^{N_i} \Omega_{ji}^m \qquad (7)$$

$$(y\,\Omega_i^m) = \sum_{j=1}^{N_i} y_{ji}\,\Omega_{ji}^m \qquad (8)$$

$$\bar{a}_i = \begin{bmatrix} a_{i1} \\ a_{i2} \\ a_{i3} \\ a_{i4} \end{bmatrix} \qquad (9)$$

$$\bar{\bar{M}}_i = \begin{bmatrix} N_i & \Omega_i^1 & \Omega_i^2 & \Omega_i^2\Omega_{i+1}^1 \\ \Omega_i^1 & \Omega_i^2 & \Omega_i^3 & \Omega_i^3\Omega_{i+1}^1 \\ \Omega_i^2 & \Omega_i^3 & \Omega_i^4 & \Omega_i^4\Omega_{i+1}^1 \\ \Omega_i^2\Omega_{i+1}^1 & \Omega_i^3\Omega_{i+1}^1 & \Omega_i^4\Omega_{i+1}^1 & \Omega_i^4\Omega_{i+1}^2 \end{bmatrix} \tag{10}$$

$$\bar{B}_i = \begin{bmatrix} 2(y\Omega_i^0) - \lambda_i + \lambda_{i+1} \\ 2(y\Omega_i^1) - \pi_i + \Delta x_i\,\lambda_{i+1} + \pi_{i+1} \\ 2(y\Omega_i^2) + \lambda_{i+1}\Delta x_i^2 + 2\Delta x_i\,\pi_{i+1} \\ 2(y\Omega_i^2\Omega_{i+1}^1) + \pi_{i+1}\Delta x_i^2 \end{bmatrix} \tag{11}$$

The resulting system of equations for $\bar{a}_i$ in terms of the Lagrange multipliers is:

$$16\bar{\bar{M}}_i\bar{a}_i = \bar{B}_i \tag{12}$$

The above system of equations must now be solved for $\bar{a}_i$ in terms of $\bar{B}_i$ and the results substituted into the constraints to yield a system of equations for the

set of Lagrange multipliers. To that end let d^i_j be the j-th minor of the 4x4 system M_i divided by the determinant of M_i where the minors are numbered as follows:

$$\begin{matrix} d^i_1 & d^i_2 & d^i_3 & d^i_4 \\ d^i_5 & . & . & . \end{matrix} \qquad (13)$$

The general solution for a_{ij} is:

$$\begin{aligned} a_{ij} = (-1)^{j+1}\Big[\Big\{2(y\,\Omega^0_i) - \lambda_i + \lambda_{i+1}\Big\}d^i_j + \Big\{2(y\,\Omega^2_i) \\ + \Delta x_i^2\,\lambda_{i+1} + 2\,\Delta x_i\,\pi_{i+1}\Big\}d^i_{j+8}\Big] \\ + (-1)^j\Big[\Big\{2(y\,\Omega^1_i) - \pi_i + \Delta x_i\,\lambda_{i+1} + \pi_{i+1}\Big\}d^i_{j+4} \\ + \Big\{2(y\,\Omega^2_i\,\Omega^1_{i+1}) + \Delta x_i^2\,\pi_{i+1}\Big\}d_{j+12}\Big] \end{aligned} \qquad (14)$$

$$\text{for } j = 1,2,3,4$$

To condense notation rewrite a_{ij} as:

$$\begin{aligned} a_{ij} = w_{ij1} + w_{ij2}\,\lambda_i + w_{ij3}\,\lambda_{i+1} \\ + w_{ij4}\,\pi_i + w_{ij5}\,\pi_{i+1} \end{aligned} \qquad (15)$$

Upon substituting the a_{ij} into the two constraints at x_i, the following two equations are obtained,

for continuity in y:

$$(-w_{i-1,12} - \Delta x_{i-1} w_{i-1,22} - \Delta x_{i-1}^2 w_{i-1,32})\,\lambda_{i-1}$$

$$+(w_{i12} - w_{i-1,13} - \Delta x_{i-1} w_{i-1,23} - \Delta x_{i-1}^2 w_{i-1,33})\,\lambda_i$$

$$+ w_{i13}\,\lambda_{i+1}$$

$$+(-w_{i-1,14} - \Delta x_{i-1} w_{i-1,24} - \Delta x_{i-1}^2 w_{i-1,34})\,\pi_{i-1}$$

$$+(w_{i14} - w_{i-1,15} - \Delta x_{i-1} w_{i-1,25} - \Delta x_{i-1}^2 w_{i-1,35})\,\pi_i$$

$$+ w_{i15}\,\pi_{i+1}$$

$$= -w_{i11} + w_{i-1,11} + \Delta x_{i-1} w_{i-1,21} + \Delta x_{i-1}^2 w_{i-1,31} \qquad (16)$$

and for continuity in y':

$$(-w_{i-1,22} - 2\Delta x_{i-1} w_{i-1,32} - \Delta x_{i-1}^2 w_{i-1,42})\,\lambda_{i-1}$$

$$+(w_{i22} - w_{i-1,23} - 2\Delta x_{i-1} w_{i-1,33} - \Delta x_{i-1}^2 w_{i-1,43})\,\lambda_i$$

$$+ w_{i23}\,\lambda_{i+1}$$

$$+(-w_{i-1,24} - 2\Delta x_{i-1} w_{i-1,34} - \Delta x_{i-1}^2 w_{i-1,44})\,\pi_{i-1}$$

$$+(w_{i24}-w_{i-1,25}-2\Delta x_{i-1}w_{i-1,35}-\Delta x_{i-1}^2 w_{i-1,45})\pi_i$$

$$+w_{i25}\pi_{i+1}$$

$$= -w_{i21}+w_{i-1,21}+2\Delta x_{i-1}w_{i-1,31}+\Delta x_{i-1}^2 w_{i-1,41} \qquad (17)$$

To this point a system of equations for the Lagrange multipliers has been obtained. The range of the index on λ_i and π_i is from 2 to N-1 where there are N-1 intervals and N mesh points including the end points. Therefore, the index i on the set of equations defined by (16) and (17) ranges from 3 to N-2 since the indices in the equations range from i-1 to i+1. This yields 2(N-4) equations from which 2(N-2) unknowns must be determined which implies that four more equations are needed. Therefore, special consideration must be given to the form of the equations obtained from the first and last intervals because the general result does not apply to the mesh points x_2 and x_{N-1}. Four more equations can be generated from the two constraints at each of these two points.

Upon examining the form of the cubic in the first interval at $x = x_1$, it is determined that:

$$a_{11} = y(x_1) \qquad (18)$$

$$a_{12} = y'(x_1) \tag{19}$$

And hence a_{11} and a_{12} must be specified.

Carrying through the same minimization procedure as before yields the following for a_{13} and a_{14}:

$$\begin{bmatrix} T_1 & T_2 \\ T_3 & T_4 \end{bmatrix} \begin{bmatrix} a_{13} \\ a_{14} \end{bmatrix} = \begin{bmatrix} T_5 + \Delta x_1^2 \lambda_2 + 2\Delta x_1 \pi_2 \\ T_6 + \Delta x_1^2 \pi_2 \end{bmatrix} \tag{20}$$

where

$$T_1 = 2\Omega_1^4 \tag{21}$$

$$T_2 = 2\Omega_1^4 \Omega_2^1 \tag{22}$$

$$T_3 = T_2 \tag{23}$$

$$T_4 = 2\Omega_1^4 \Omega_2^2 \tag{24}$$

$$T_5 = 2\left[(y\Omega_1^2) - 2a_{11}\Omega_1^2 - 2a_{12}\Omega_1^3\right] \tag{25}$$

$$T_6 = 2\left[(y\Omega_1^2\Omega_2^1) - 2a_{11}\Omega_1^2\Omega_2^1 - 2a_{12}\Omega_1^3\Omega_2^1\right] \tag{26}$$

Solving for a_{13} and a_{14} in the form of Eq. (15) yields:

$$w_{131} = (2\Omega_1^4\Omega_2^2 T_5 - 2\Omega_1^4\Omega_2^1 T_6)/T \tag{27}$$

$$w_{132} = w_{134} = 0 \tag{28}$$

$$w_{133} = 2\Omega_1^4\Omega_2^2\Delta x_1^2/T \tag{29}$$

$$w_{135} = (4\Omega_1^4\Omega_2^2\Delta x_1 - 2\Omega_1^4\Omega_2^2\Delta x_1^2)/T \tag{30}$$

$$w_{141} = (2\Omega_1^4 T_5 - 2\Omega_1^4\Omega_2^1 T_6)/T \tag{31}$$

$$w_{142} = w_{144} = 0 \tag{32}$$

$$w_{143} = -2\Omega_1^4\Omega_2^1\Delta x_1^2/T \tag{33}$$

$$w_{145} = (2\Omega_1^4\Delta x_1^2 - 4\Omega_1^4\Omega_2^1\Delta x_1)/T \tag{34}$$

where T is the determinant of the T-matrix in Eq. (20).

Substituting these results into the constraint at x_2 yields, for continuity in y:

$$(w_{212} - 2\Delta x_1^2 w_{133})\lambda_2 + (w_{214} - \Delta x_1^2 w_{135})\pi_2 + w_{213}\lambda_3$$

$$+ w_{215}\pi_3 = -w_{211} + a_{11} + a_{12}\Delta x_1 + \Delta x_1^2 w_{131} \tag{35}$$

for continuity in y':

$$(w_{222}-2\Delta x_1 w_{133}-\Delta x_1^2 w_{143})\lambda_2$$

$$+(w_{224}-2\Delta x_1 w_{135}-\Delta x_1^2 w_{145})\pi_2+w_{223}\lambda_3+w_{225}\pi_3$$

$$= -w_{221}+a_{12}+2\Delta x_1 w_{131}+\Delta x_1^2 w_{141} \qquad (36)$$

Considering now the extreme right hand interval, once again $y(x_N)$ and $y'(x_N)$ are to be specified. This information is used to eliminate $a_{N-1,1}$ and $a_{N-1,4}$ as follows, letting M=N-1:

$$a_{M,1} = y(x_N)-a_{M,2}\Delta x_M-a_{M,3}\Delta x_M^2 \qquad (37)$$

$$a_{M,4} = (y'(x_N)-a_{M,2}-2\Delta x_M a_{M,3})\Delta x_M^{-2} \qquad (38)$$

Carrying through the same minimization procedure as before yields two equations in terms of the undetermined multipliers. The equation obtained from the continuity constraint in y is:

$$(-w_{N-2,12}-\Delta x_{N-2} w_{N-2,22}-\Delta x_{N-2}^2 w_{N-2,32})\lambda_{N-2}$$

$$+(w_{M,12}-w_{N-2,13}-\Delta x_{N-2} w_{N-2,23}-\Delta x_{N-2}^2 w_{N-2,33})\lambda_M$$

$$+(-w_{N-2,14}-\Delta x_{N-2} w_{N-2,24}-\Delta x_{N-2}^2 w_{N-2,34})\pi_{N-2}$$

$$+(w_{M,14}-w_{N-2,15}-\Delta x_{N-2}w_{N-2,25}-\Delta x_{N-2}^{2}w_{N-2,35})\,\pi_{M}$$

$$= -w_{M,11}+w_{N-2,11}+\Delta x_{N-2}w_{N-2,21}+\Delta x_{N-2}^{2}w_{N-2,31} \qquad (39)$$

And from the y' constraint at x_{N-1}:

$$(-w_{N-2,22}-2\,\Delta x_{N-2}w_{N-2,32}-\Delta x_{N-2}^{2}w_{N-2,42})\,\lambda_{N-2}$$

$$+(w_{M,22}-w_{N-2,23}-2\,\Delta x_{N-2}w_{N-2,33}-\Delta x_{N-2}^{2}w_{N-2,43})\,\lambda_{M}$$

$$+(-w_{N-2,24}-2\,\Delta x_{N-2}w_{N-2,34}-\Delta x_{N-2}^{2}w_{N-2,44})\,\pi_{N-2}$$

$$+(w_{M,24}-w_{N-2,25}-2\,\Delta x_{N-2}w_{N-2,35}-\Delta x_{N-2}^{2}w_{N-2,45})\,\pi_{M}$$

$$= -w_{M,21}+w_{N-2,21}+2\,\Delta x_{N-2}w_{N-2,31}+\Delta x_{N-2}^{2}w_{N-2,41} \qquad (40)$$

where the w_{ijk} are as follows:

$$w_{M,21} = \bar{\beta}_2\,\alpha_2' - \bar{\beta}_1\,\alpha_4' \qquad (41)$$

$$w_{M,22} = \Delta x_M(\alpha_4' - \Delta x_M\,\alpha_2') \qquad (42)$$

$$w_{M,23} = w_{M,25} = 0 \qquad (43)$$

$$w_{M,24} = -\alpha_4' \qquad (44)$$

$$w_{M,31} = \bar{\beta}_1 \alpha'_3 - \bar{\beta}_2 \alpha'_1 \tag{45}$$

$$w_{M,32} = \Delta x_M (\Delta x_M \alpha'_1 - \alpha'_3) \tag{46}$$

$$w_{M,33} = w_{M,35} = 0 \tag{47}$$

$$w_{M,34} = \alpha'_3 \tag{48}$$

The α and β terms are defined as follows:

$$\alpha_1 = 2 \sum_{j=1}^{N_M} (\Delta x_M - \Omega^1_{jM} + \Omega^2_{jM} \Omega^1_{jN} / \Delta x_M^2)^2 \tag{49}$$

$$\alpha_2 = 2 \sum_{j=1}^{N_M} (\Delta x_M^2 - \Omega^2_{jM} + 2 \Omega^2_{jM} \Omega^1_{jN} / \Delta x_M^2) \cdot$$

$$\cdot (\Delta x_M - \Omega^1_{jM} + \Omega^2_{jM} \Omega^1_{jN} / \Delta x_M^2) \tag{50}$$

$$\alpha_3 = \alpha_2 \tag{51}$$

$$\alpha_4 = 2 \sum_{j=1}^{N_M} (\Delta x_M - \Omega^2_{jM} + 2 \Omega^2_{jM} \Omega^1_{jN} / \Delta x_M)^2 \tag{52}$$

$$\beta_1 = \Delta x_M \lambda_M - \pi_M - 2 \sum_{j=1}^{N_M} (y_{jM} - y(x_N) - \Omega^2_{jM} \Omega^1_{jN} y'(x_N) / \Delta x_M^2) \cdot$$

$$\cdot (\Delta x_M - \Omega^1_{jM} + \Omega^2_{jM} \Omega^1_{jN} / \Delta x_M^2) \tag{53}$$

$$\beta_1 = \Delta x_M \lambda_M - \pi_M - \bar{\beta}_1 \quad \text{(identifies } \bar{\beta}_1\text{)} \tag{54}$$

$$\beta_2 = \lambda_M \Delta x_M^2 - 2 \sum_{j=1}^{N_M} (y_{jM} - y(x_N) - \Omega^2_{jM} \Omega^1_{jN} y'(x_N)/\Delta x_M^2).$$

$$(\Delta x_M^2 - \Omega^2_{jM} + 2 \Omega^2_{jM} \Omega^1_{jN}/\Delta x_M) \qquad (55)$$

$$\beta_2 = \lambda_M \Delta x_M - \bar{\beta}_2 \quad \text{(identifies } \bar{\beta}_2) \qquad (56)$$

$$a'_j = a_j/(a_1 a_4 - a_3 a_2) \quad \text{for } j = 1,2,3,4 \qquad (57)$$

For a set of data that have been divided into N-1 intervals with N mesh points, there are 2(N-2) unknowns in the form of the two Lagrange multipliers at each mesh point excluding the first and the last. Equations (16) and (17) provide a total of 2(N-4) equations involving the multipliers and (35), (36), (39) and (40) provide four more so that the number of unknowns equals the number of equations. These equations may be solved for the set of Lagrange multipliers and then the set of a_{ij} may be computed through the w_{ijk} coefficients.

Sufficient information has now been presented so that the equations can be programmed for a computer. Such a computer program has been written in FORTRAN IV for an IBM 370/155 system and is presented in the program listings in Appendix H.

C. Testing and Application

The question that arises is how does an individual derive and program the equations into a computer without making an error? There is no simple test problem such as there is in checking a Simpson's integration routine. However, the following was carried out to test the spline smoothing computer program.

A cubic test function of the form $y = 1+x(1+x(1+x))$ was used to generate 100 equi-spaced values of $y(x)$ to five significant digits between $x = 0$ and $x = 2$ inclusive. These "exact" data were then smoothed using six equi-spaced mesh points in the stated range. Analytic values for the derivatives at the end points were used. Values of the smoothed data were then generated from the resulting five cubics. The smoothed values differed from the exact values by at most one unit in the fifth digit. The smoothed results were then plotted in the form of a line and also eleven exact values as designated by x were also plotted. This plot is presented in Figure D.1 and shows the relative agreement, which is judged satisfactory.

An application arises for a smoothing routine in nuclear magnetic resonance (NMR) work. The ultimate desire in certain aspects of NMR is to obtain the real term of the Fourier transform of a time varying voltage signal. The data inherently have noise and are available

in digital form. A smoothing technique such as the one presented here may be used to put a line estimate through the data and the resulting smooth curve Fourier transformed. A sample of such data from a multiple pulsed NMR experiment[4] with the resulting smoothed line estimate is presented in Figure D.2. The computation of the Fourier transform of this signal is presented in Appendix F.

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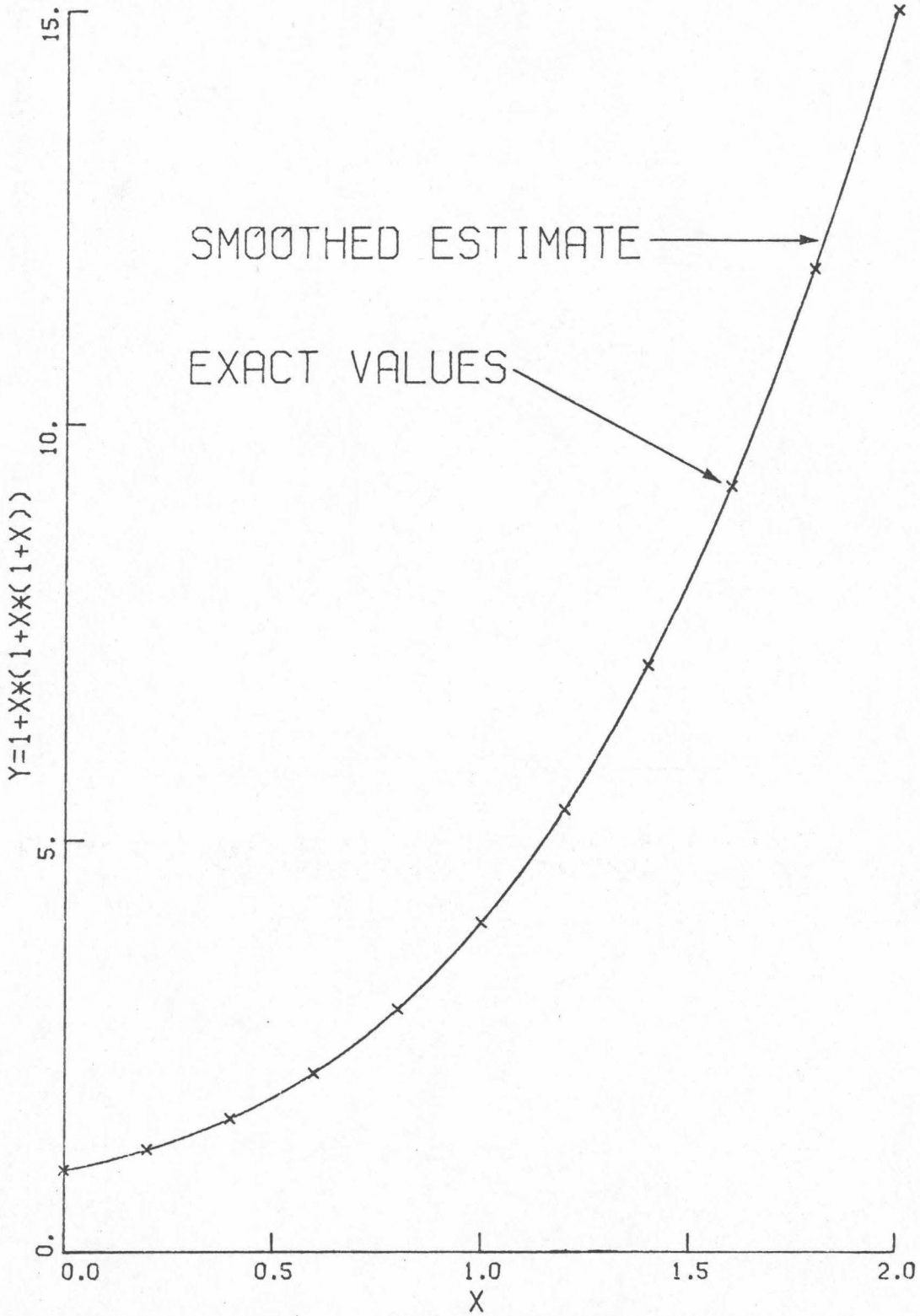

Figure D.1. Results of Numerical Test of Spline Smoothing Computer Program

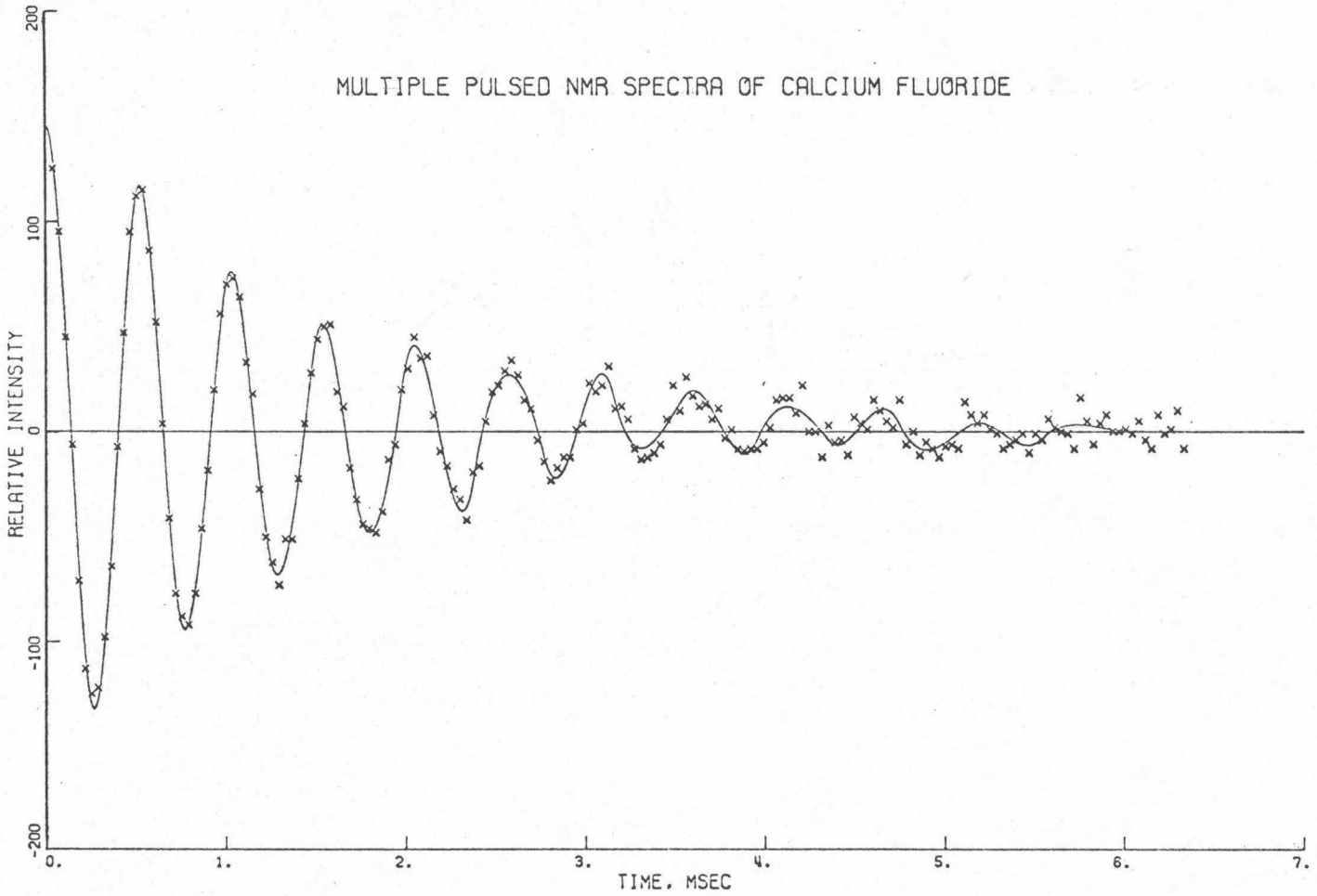

Figure D.2. Example of Spline Smoothing Applied to NMR Data[4]

APPENDIX E

INTERPOLATION BY CUBIC SPLINE[1]

The concept behind the spline fit is the following. Suppose the range $a \leq x \leq b$ is divided into N intervals and the value of a function $y(x)$ is given at the N+1 mesh points, x_i, that divide the intervals. Join the mesh points by piecewise cubics and demand that the first and second derivatives be continuous. These cubics can then be used to estimate $y(x)$ between the mesh points. The best approximation properties of the spline fit are presented in the literature.[1] The derivation follows:

Consider a polynomial interpolate of the form:

$$y(x) = A_{i0}+A_{i1}(x-x_{i-1})+(x-x_{i-1})^2 \cdot \left[A_{i2}+A_{i3}(x-x_i)\right] \qquad (1)$$

$$\text{for } x_{i-1} \leq x \leq x_i$$

Taking the derivative twice yields:

$$y'(x) = A_{i1}+2(x-x_{i-1})\left[A_{i2}+A_{i3}(x-x_i)\right] +(x-x_{i-1})^2 A_{i3} \qquad (2)$$

$$y''(x) = 2(x-x_{i-1})A_{i3}+2\left[A_{i2}+A_{i3}(x-x_i)\right]$$

$$+2(x-x_{i-1})A_{i3} \qquad (3)$$

Evaluate $y(x)$ at x_{i-1} and x_i to obtain:

$$y(x_{i-1}) = A_{i0} \qquad (4)$$

$$y(x_i) = A_{i0}+A_{i1}\Delta x_i+A_{i2}\Delta x_i^2 \qquad (5)$$

and

$$\Delta x_i = x_i-x_{i-1} \qquad (6)$$

Evaluate $y'(x)$ at x_{i-1} and x_i to obtain:

$$y'(x_{i-1}) = A_{i1} \qquad (7)$$

$$y'(x_i) = A_{i1}+2A_{i2}\Delta x_i+A_{i3}\Delta x_i^2 \qquad (8)$$

To here A_{i0} and A_{i1} are determined. Now solve for A_{i2} from $y(x_i)$:

$$A_{i2} = \left[y(x_i)-y(x_{i-1})-y'(x_{i-1})\Delta x_i\right]/\Delta x_i^2 \qquad (9)$$

Substitute the above result in $y'(x_i)$ and solve for A_{i3}:

$$A_{i3} = \left[y'(x_i)-y'(x_{i-1})\right]/\Delta x_i^2 - 2\left[\Delta y_i/\Delta x_i^2 - y'(x_{i-1})/\Delta x_i\right]/\Delta x_i \qquad (10)$$

and

$$\Delta y_i = y_i - y_{i-1} \qquad (11)$$

Now equate $y''(x)$ from adjacent intervals at the point x_i, rearrange and multiply by $\Delta x_i \Delta x_{i+1}/2$ to obtain:

$$\Delta x_{i+1}y'(x_{i-1})+2(\Delta x_{i+1}+\Delta x_i)y'(x_i)+\Delta x_i y'(x_{i+1}) = 3(\Delta x_{i+1}\Delta y_i/\Delta x_i+\Delta x_i\Delta y_{i+1}/\Delta x_{i+1}) \qquad (12)$$

The above equation is valid for i = 3, . . . , N-1.
For i = 2, one has:

$$2(\Delta x_3+\Delta x_2)y'(x_2)+\Delta x_2 y'(x_3) = 3(\Delta x_3\Delta y_2/\Delta x_2+\Delta x_2\Delta y_3/\Delta x_3)-\Delta x_3 y'(x_1) \qquad (13)$$

and for i = N, where M = N+1:

$$\Delta x_M y'(x_{N-1}) + 2(\Delta x_M + \Delta x_N) y'(x_N)$$

$$= 3(\Delta x_M \Delta y_N / \Delta x_N + \Delta x_N \Delta y_M / \Delta x_M) - \Delta x_N y'(x_M) \qquad (14)$$

Therefore, in order to solve for the derivatives at the mesh points, from which all the a_{ij} can be calculated, the derivatives must be known or estimated at x_1 and x_M. Note that the resulting system of equations is diagonally dominant and a solution may always be obtained (use Gershgorin's theorem[2]).

REFERENCES FOR APPENDIX E

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APPENDIX F

FOURIER TRANSFORM CALCULATION

All the Fourier transforms in this work were evaluated by integrating the spline cubic approximate to the data, either as obtained from interpolation[1] or smoothing.[2] In the calculation of a Fourier transform, the integrals of interest are:

$$F_s(\xi) = \int_0^\infty f(x)\sin(\xi x)dx \qquad (1)$$

$$F_c(\xi) = \int_0^\infty f(x)\cos(\xi x)dx \qquad (2)$$

In the study of liquid structure using diffraction data, Eq. (1) is of interest and in the NMR work described in Appendix D, Eq. (2) is of interest.

The function to be transformed is considered to be available in the spline cubic form as:

$$f(x) = C_{i1}+C_{i2}(x-x_{i-1})+(x-x_{i-1})^2\cdot$$

$$\cdot\left[C_{i3}+C_{i4}(x-x_i)\right] \qquad (3)$$

$$\text{for } x_{i-1} \le x \le x_i$$

This form is converted to the following:

$$f(x) = A_{i1}+A_{i2}x+A_{i3}x^2+A_{i4}x^3 \qquad (4)$$

$$\text{for } x_{i-1} \leq x \leq x_i$$

where

$$A_{i1} = C_{i1}-C_{i2}x_{i-1}+C_{i3}x_{i-1}^2-C_{i4}x_{i-1}^2x_i \qquad (5)$$

$$A_{i2} = C_{i2}-2C_{i3}x_{i-1}+C_{i4}x_{i-1}(x_{i-1}+2x_i) \qquad (6)$$

$$A_{i3} = C_{i3}-C_{i4}(2x_{i-1}+x_i) \qquad (7)$$

$$A_{i4} = C_{i4} \qquad (8)$$

Hence, the cubic approximate is integrated over each interval for a value of the transform variable, ξ, and the results summed over all intervals. The integrals to be evaluated are of the form:[3]

$$\int x^n \sin(\xi x)dx \qquad (9)$$

$$\int x^n \cos(\xi x)dx \qquad (10)$$

Given the cubic approximate to f(x) to a sufficiently large value of x so that $f(x_g) \approx 0$ for all $x \geq x_g$, the transform is:

$$F_s(\xi) = \sum_{i=1}^{m} \left\{ (A_{i1}/\xi)\cos(u)+(A_{i2}/\xi^2)\left[\sin(u)-u*\cos(u)\right] \right.$$
$$+(A_{i3}/\xi^3)\left[2u*\sin(u)-(u^2-2)\cos(u)\right]$$
$$\left. +(A_{i4}/\xi^4)\left[3(u^2-2)\sin(u)-u(u^2-6)\cos(u)\right] \right\}_{u_i}^{u_{i+1}} \qquad (11)$$

and

$$F_c(\xi) = \sum_{i=1}^{m} \left\{ (A_{i1}/\xi)\sin(u)+(A_{i2}/\xi^2)\left[\cos(u)+u*\sin(u)\right] \right.$$
$$+(A_{i3}/\xi^3)\left[2u*\cos(u)+(u^2-2)\sin(u)\right]$$
$$\left. +(A_{i4}/\xi^4)\left[3(u^2-2)\cos(u)+u(u^2-6)\sin(u)\right] \right\}_{u_i}^{u_{i+1}} \qquad (12)$$

where $u_i = \xi x_i$ and there are m+1 mesh points.

This technique was tested on such functions as exp(-x), x*exp(-x) and x*exp(-x)*cos(kx) and the results were satisfactory.

An application of this technique to NMR is the Fourier transform of the smoothed data that were presented in Appendix D. The full Fourier transform is presented

in Figures F.1 and F.2. Of particular interest[4] is the width of the peak at half height in the cosine transform, which is about 210 Hertz in this case.

The computer program used to compute the Fourier transforms in the work is presented in Appendix H.

REFERENCES FOR APPENDIX F

1. J. L. Walsh, J. H. Ahlberg and E. N. Nilson, Journal of Math. & Mech. 11, 225(1962), Also see Appendix E.

2. B. E. Kirstein, Appendix D.

3. H. B. Dwight, Tables of Integrals and Other Mathematical Data, Macmillan Co., N. Y.(1961).

4. R. W. Vaughan, personal communication.

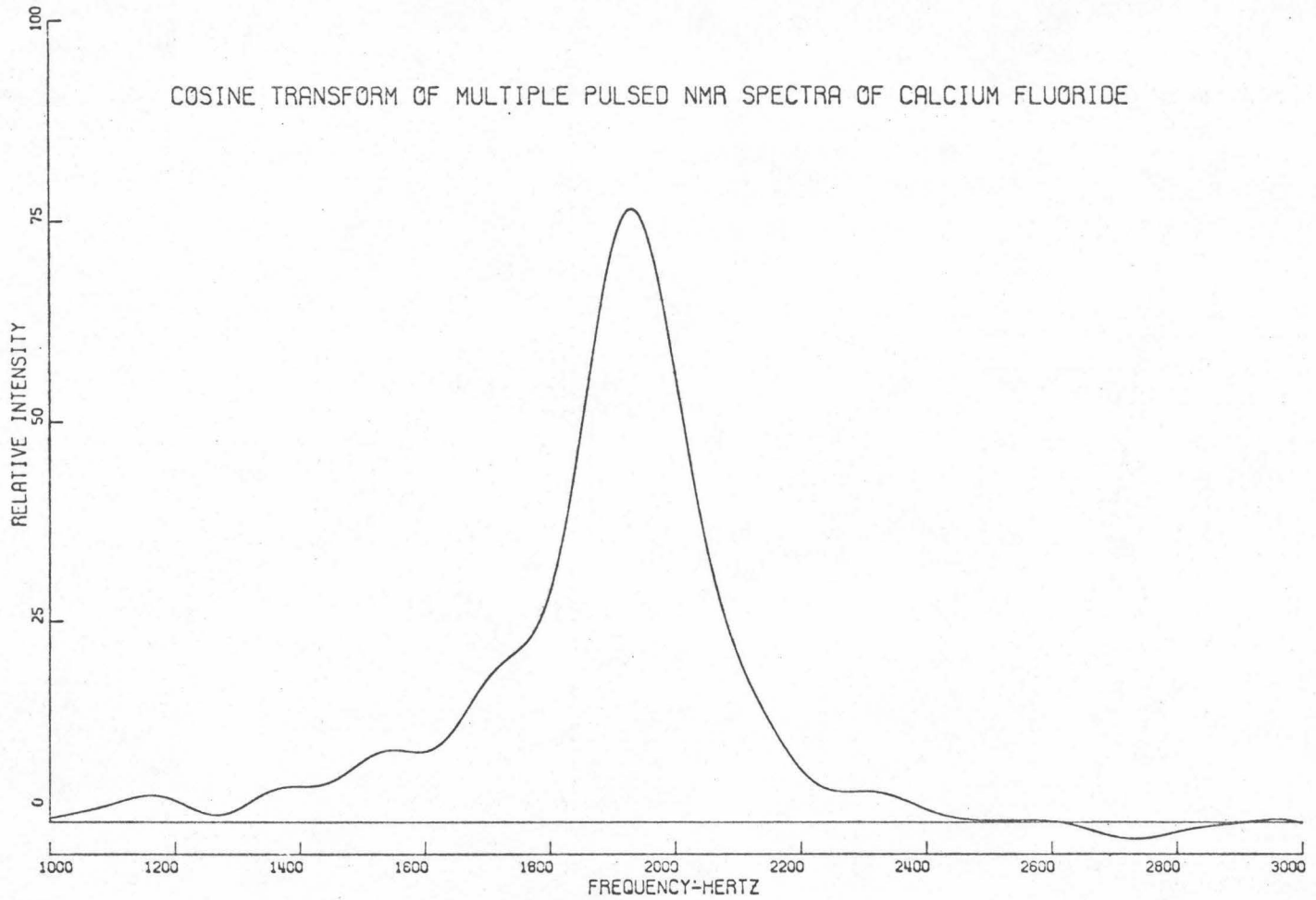

Figure F.1. Results of Example Calculation

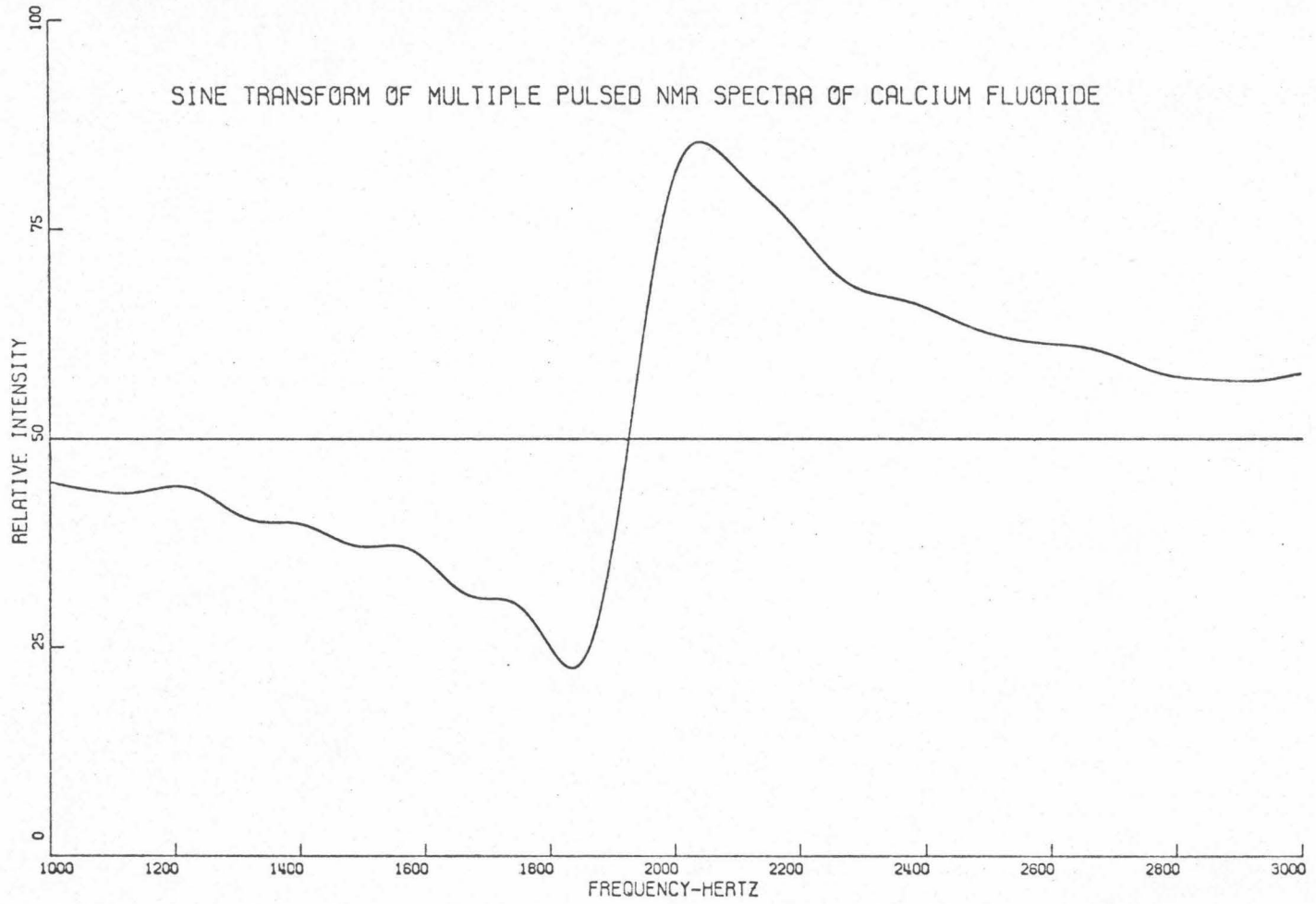

Figure F.2. Results of Example Calculation

APPENDIX G

DISTORTION CORRECTION

A. Introduction

The collimation of x-rays in diffraction studies of fluids which are contained in a cylindrical cell usually consists of vertical sollers and a small divergent slit on a "line" x-ray source and of horizontal sollers and a wide divergent slit on the detector assembly. This system gives rise to distortion which is an averaging of the scattered radiation over the scattering angles accepted by the detector. With the recent development of the smoothing technique as presented in Appendix D, it is now possible to present a correction procedure for this type of distortion. The desired and net result of this presentation is a calculation of the undistorted intensity at all detector angles.

The distortion problem is cast in the form of an idealized single dimension x-ray source, sample and detector as depicted in Figures G.1 and G.2. In this model the line source, sample and detector are parallel and of equal length. Distortion resulting from other forms of divergence in the laboratory is assumed small. A perfect line source is assumed because the incident x-ray beam was collimated with vertical sollers. An interpretation of the perfect source is that one point

on the source irradiates only one point on the sample and the line that connects these two points is perpendicular to both the line source and sample.

B. Derivation

Writing an equation for the differential "intensity" observed at a detector position y scattered from a sample position x, assuming a uniform x-ray source, yields:

$$dI(\theta_o) = k_s P(\theta) R^{-2}(\theta) \rho_e J(\theta) I_o dxdy \qquad (1)$$

where ρ_e is the electron density with units of electrons/length, k_s is a constant with units of length squared, I_o is the incident intensity with units of energy/length/time, θ is the scattering angle, θ_o is the detector position, $P(\theta)$ is the polarization factor, $J(\theta)$ is the intrinsic scattering power of the media per electron and R is the distance to the detector. The correction for the scattered ray entering the detector at an oblique rather than a 90^o angle is neglected and in reality is small.

A check on units then gives the dimensions on $I(\theta_o)$ as energy/time which is not an intensity. This quantity must be normalized by the length of the detector to become an intensity, but is the observed laboratory quantity. Note that absorption factors have been

neglected and that $P(\theta)$ and $R^{-2}(\theta)$ depend on θ. In order to integrate Eq. (1), the previous quantities are taken out of the integration and assigned values at θ_o since they are essentially constant over the range of integration. Hence:

$$I(\theta_o) = k_s I_o \, e P(\theta_o) R^{-2}(\theta_o) \iint J(\theta) dx dy \qquad (2)$$

Now adopt the coordinate system for the line sample and detector such that $x = 0$ is the midpoint of the sample and $y = 0$ is the midpoint of the detector and the positive direction for both x and y is to the right as viewed from the x-ray source. This then gives θ, the scattering angle, for a photon scattered from x to y with the detector at θ_o, as derived in Section E, as:

$$\theta = \sin^{-1}\left\{\left[\frac{R^2 \sin^2\theta_o + (x-y)^2}{R^2 + (x-y)^2}\right]^{\frac{1}{2}}\right\} \qquad (3)$$

Now digress a moment and examine in Table G.1 the maximum divergence angle relative to the detector position for the x-ray system used in this thesis. The sample length essentially equaled the detector length and was about 3/8 inch. The distance to the detector from the sample was about 6-3/4 inches. The maximum

divergence occurred when x-y = L, where L designates the length of the sample, which is the case of scattering from one end of the sample to the other end of the detector. Note that only two points on the sample could scatter this way.

One can now make an important observation. The quantity $\theta - \theta_o$ was relatively small compared to the fluctuations in the scattered intensity due to a fluid sample. In other words, $\theta - \theta_o$ never spanned more than a fraction of one peak.

Since the detector accepted a relatively small range of scattering angles at all θ_o, assume that $J(\theta)$ may be represented as a truncated Taylor's series expanded about any detector position θ_o:

$$J(\theta) = J(\theta_o) + J'(\theta_o)(\theta - \theta_o) + \tfrac{1}{2}J''(\theta_o)(\theta - \theta_o)^2 \qquad (4)$$

where a prime denotes a derivative. Also demand that all derivatives greater than order two be equal to zero. Notationally lump together $k_s I_o \rho_e P(\theta_o)/R^2(\theta_o)$ and call this product K and then substitute $J(\theta)$ into Eq. (2) to obtain:

$$I(\theta_o)/K = J(\theta_o)\iint dxdy + J'(\theta_o)\iint(\theta - \theta_o)dxdy$$

$$+ \tfrac{1}{2}J''(\theta_o)\iint(\theta-\theta_o)^2 dxdy \qquad (5)$$

The limits of integration are fixed by the lengths of the detector and sample and do not depend on θ.

The object now is to determine $J(\theta_o)\iint dxdy$. Note that from the spline smoothing technique one has a piecewise cubic representation of $I(\theta_o)$. This implies that derivatives of $I(\theta_o)$ through order three can be generated, with some caution of course. Therefore differentiate Eq. (5) with respect to θ_o only twice and examine. For notational convenience define $\int f(x,y)dA$ as $\iint f(x,y)dxdy$ from now on. Differentiating Eq. (5):

$$I'(\theta_o)/K = J'(\theta_o)\int(d\theta/d\theta_o)dA$$

$$+ J''(\theta_o)\int(\theta-\theta_o)(d\theta/d\theta_o)dA \qquad (6)$$

Taking the derivative one more time yields:

$$I''(\theta_o)/K = J'(\theta_o)\int(d^2\theta/d\theta_o^2)dA$$

$$+ J''(\theta_o)\int\left[(\theta-\theta_o)(d^2\theta/d\theta_o^2)+(d\theta/d\theta_o)^2\right]dA \qquad (7)$$

To here, the three equations as defined by (5),

(6) and (7) contain three unknowns, namely: $J(\theta_o)$, $J'(\theta_o)$ and $J''(\theta_o)$. Multiply Eq. (5), (6) and (7) by K and rearrange to obtain:

$$\overline{\overline{\triangle}} \begin{bmatrix} KJ(\theta_o)\int dA \\ KJ'(\theta_o) \\ KJ''(\theta_o) \end{bmatrix} = \begin{bmatrix} I(\theta_o) \\ I'(\theta_o) \\ I''(\theta_o) \end{bmatrix} \qquad (8)$$

The 3x3 matrix $\overline{\overline{\triangle}}$ is:

$$\overline{\overline{\triangle}} \equiv$$

$$\begin{bmatrix} 1 & \int(\theta-\theta_o)dA & \frac{1}{2}\int(\theta-\theta_o)^2 dA \\ 0 & \int(d\theta/d\theta_o)dA & \int(\theta-\theta_o)(d\theta/d\theta_o)dA \\ 0 & \int(d^2\theta/d\theta_o^2)dA & \int\left[(\theta-\theta_o)(d^2\theta/d\theta_o^2)+(d\theta/d\theta_o)^2\right]dA \end{bmatrix} \qquad (9)$$

Therefore, solve for the undistorted intensity at θ_o which is $KJ(\theta_o)\int dA$. In the x-ray experiment on fluids the data are taken on a relative basis and later scaled to match an atomic scattering curve at high θ_o so there is no need to worry about K at the present time.

Consider a special case for a scattering curve that is constant, in other words, $I(\theta_o) = C$ for all θ_o.

This will then give from Eq. (8) the result $KJ(\theta_o)\int dA$ and $I(\theta_o)$ are equal, which is what is expected.

The slopes of $I(\theta_o)$ may be obtained from the spline smoothing technique derived from the cubic spline interpolation concept as presented in Appendix D. The integrals in the matrix $\overline{\overline{\triangle}}$ are two dimensional, but may be reduced to a one dimension integral by the coordinate transform indicated in Section F.

It is to be noted that Eq. (8) is general with respect to the θ function and θ depends on the particular laboratory scattering geometry.

C. Test Case

A way to test the correction scheme is to assume $J(\theta)$ is a quadratic. Since the assumed Taylor's series includes the quadratic term, the correction scheme should be exact in this case.

To that end, assume:

$$J(\theta) = b+a\theta^2 \tag{10}$$

where b and a are constants. The undistorted or true intensity at the detector angle θ_o will be:

$$I^*(\theta_o) = KJ(\theta_o)\int dA = KL^2(b+a\theta_o^2) \tag{11}$$

where the sample and detector are of length L. The

observed intensity in the laboratory will be:

$$I(\theta_o) = K\int(b+a\theta^2)dA \tag{12}$$

The variable θ now is defined by some arbitrary function $\theta(x,y,\theta_o)$ which depends on the particular geometry. Integration of Eq. (12) yields:

$$I(\theta_o) = KbL^2+aK\int\theta^2 dA \tag{13}$$

From $I(\theta_o)$ above generate $I'(\theta_o)$ and $I''(\theta_o)$ and assume that these quantities may be measured exactly in the laboratory. Using Leibnitz's rule:[1]

$$I'(\theta_o) = 2aK\int\theta(d\theta/d\theta_o)dA \tag{14}$$

$$I''(\theta_o) = 2aK\int\left[(d\theta/d\theta_o)^2+\theta(d^2\theta/d\theta_o^2)\right]dA \tag{15}$$

Now solve Eq. (8) to obtain the undistorted intensity which should be the same as Eq. (11).

The determinant of $\overline{\overline{\triangle}}$ in Eq. (9) is:

$$|\overline{\overline{\triangle}}| = (d\theta/d\theta_o)^3 \tag{16}$$

To obtain the true intensity using Cramer's Rule, replace column one of $\overline{\overline{\triangle}}$ by the $I(\theta_o)$ column vector in Eq. (8),

call this new matrix the augmented matrix, $\overline{\overline{\triangle}}_a$, evaluate the determinant and divide by $|\overline{\overline{\triangle}}|$. Evaluating $|\overline{\overline{\triangle}}_a|$ results in:

$$|\overline{\overline{\triangle}}_a| = \left[KbL^2+aK\int\theta^2 dA-Ka\int(\theta^2-\theta_o^2)dA\right](d\theta/d\theta_o)^3 \qquad (17)$$

Therefore, the final result:

$$I^*(\theta_o) = |\overline{\overline{\triangle}}_a|/|\overline{\overline{\triangle}}| = KL^2(b+a\theta_o^2) \qquad (18)$$

This result for $I^*(\theta_o)$ is the same as Eq. (11) and the procedure is exact for $J(\theta)$ of order θ^2. The computation for $J(\theta)$ of order one follows through also.

D. Numerical Test

Consider the following numerical example to illustrate the correction procedure. Suppose the true scattering curve goes as $\cos(20*\theta_o)+1$. The distorted curve relative to the true curve is obtained by evaluating

$$I(\theta_o) = \int\left[\cos(20*\theta)+1\right]dA/\int dA \qquad (19)$$

where θ is now given by Eq. (3).

The above integration was carried out for 101 evenly spaced values of θ_o between zero and 30° inclusive using Simpson's Rule. The integration limits used

approximated laboratory conditions and were for a sample-detector distance of 6-3/4 inches and a sample length of 3/4 inches. These 101 values of the distorted intensity were interpolated by the cubic spline technique[1] to obtain the first and second derivatives of $I(\theta_o)$.

Eleven values of the undistorted intensity were then recovered and the results are presented in Table C.2. In most cases the agreement between the exact value and recovered value is seen to be good to three decimal places.

E. Determination of Scattering Angle

The scattering angle for a photon scattered from point x on the sample to point y on the detector as depicted in Figure G.2 may be determined as follows. Referring to Figure G.3, where the positive direction is to the right, the ray R1 has a length $\left[R^2+(x-y)^2\right]^{\frac{1}{2}}$. The radius of the base of the scattering cone which contains R1 is $\left[R^2\sin^2\theta_o+(x-y)^2\right]^{\frac{1}{2}}$. Hence the result:

$$\theta = \sin^{-1}\left\{\left[\frac{R^2\sin^2\theta_o+(x-y)^2}{R^2+(x-y)^2}\right]^{\frac{1}{2}}\right\} \qquad (3)$$

F. Discussion of Integrals

The integrals involved in the description of the distortion problem for the source, sample and detector geometry used in this work are of the type:

$$2\int_{-L}^{L}\int_{0}^{L} f(x,y)\,dx\,dy \tag{20}$$

where the sample and detector are of length 2L. Because of the form of θ as derived in Section E, f(x,y) is a function of x-y.

This combination of the independent variables suggests a change of variables, namely:

$$x = \tfrac{1}{2}(u+v) \tag{21}$$

$$y = \tfrac{1}{2}(u-v) \tag{22}$$

Subtracting yields:

$$v = x-y \tag{23}$$

The Jacobian[2] of this transformation is:

$$\left|\frac{\partial(x,y)}{\partial(u,v)}\right| = \tfrac{1}{2} \tag{24}$$

Therefore the integrals may be transformed as:

$$\iint f(x-y)\,dx\,dy = \tfrac{1}{2}\iint f(v)\,du\,dv \tag{25}$$

The limits of integration transform as:

$$y = -L = \tfrac{1}{2}(u-v) \quad \text{or} \quad u = v-2L \tag{26}$$

$$y = +L = \tfrac{1}{2}(u-v) \quad \text{or} \quad u = v+2L \tag{27}$$

$$x = 0 = \tfrac{1}{2}(u+v) \quad \text{or} \quad u = -v \tag{28}$$

$$x = +L = \tfrac{1}{2}(u+v) \quad \text{or} \quad u = 2L-v \tag{29}$$

Figure G.4 indicates how these limits transform to the (u,v) plane. From Eq. (26) through (29) and Figure G.4, the integral in Eq. (20), after integrating out u, the free variable, becomes:

$$2\int_{-L}^{L}\int_{0}^{L} f(x,y)\,dx\,dy = L\int_{-L}^{L} f(v)\,dv + \int_{-L}^{0} vf(v)\,dv + \int_{L}^{2L} (2L-v)f(v)\,dv \tag{30}$$

Therefore the two dimension integral of Eq. (20) is reduced to a one dimension integral and a substantial savings in computer time has been realized by using this transformation in the evaluation of integrals of this type.

G. Conclusion

Under the assumptions of the derivation, the distortion correction provides a means to obtain the true or undistorted intensity of an x-ray experiment. The procedure is exact for true scattering functions, $J(\theta)$, of order θ^2.

All the data in this thesis were corrected for distortion according to this procedure and the computer program used to do this is presented in Appendix H. Also the computer program to perform the distortion, such as that in the numerical example, is presented in Appendix H.

REFERENCES FOR APPENDIX G

1. J. L. Walsh, J. H. Ahlberg and E. N. Nilson, Journal of Math. & Mech. 11, 225(1962).

2. F. B. Hildebrand, Advanced Calculus for Application, Prentice-Hall, Inc., Englewood Cliffs, N. J. (1962).

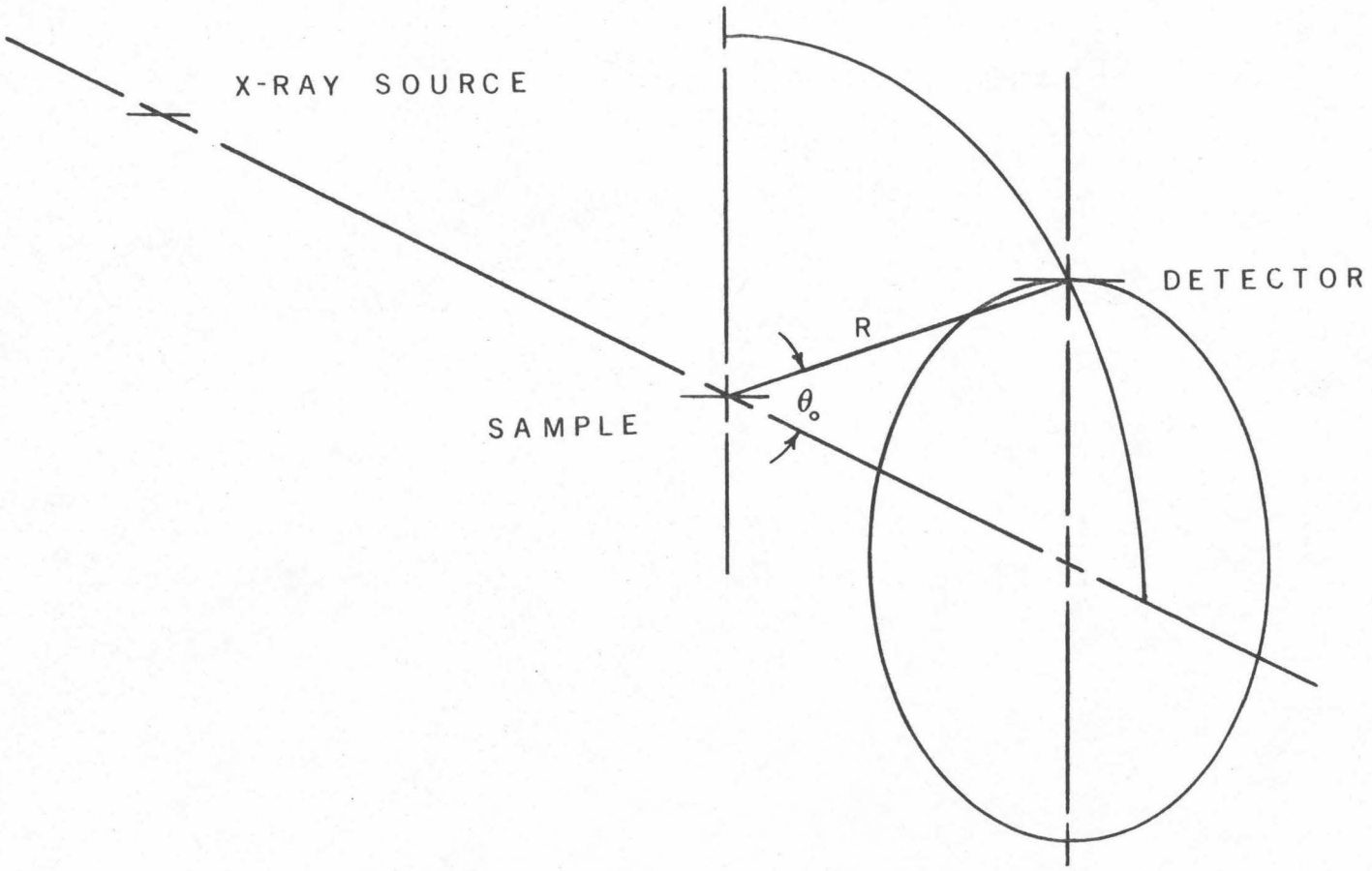

Figure G.1. Illustration of Scattering at θ_o

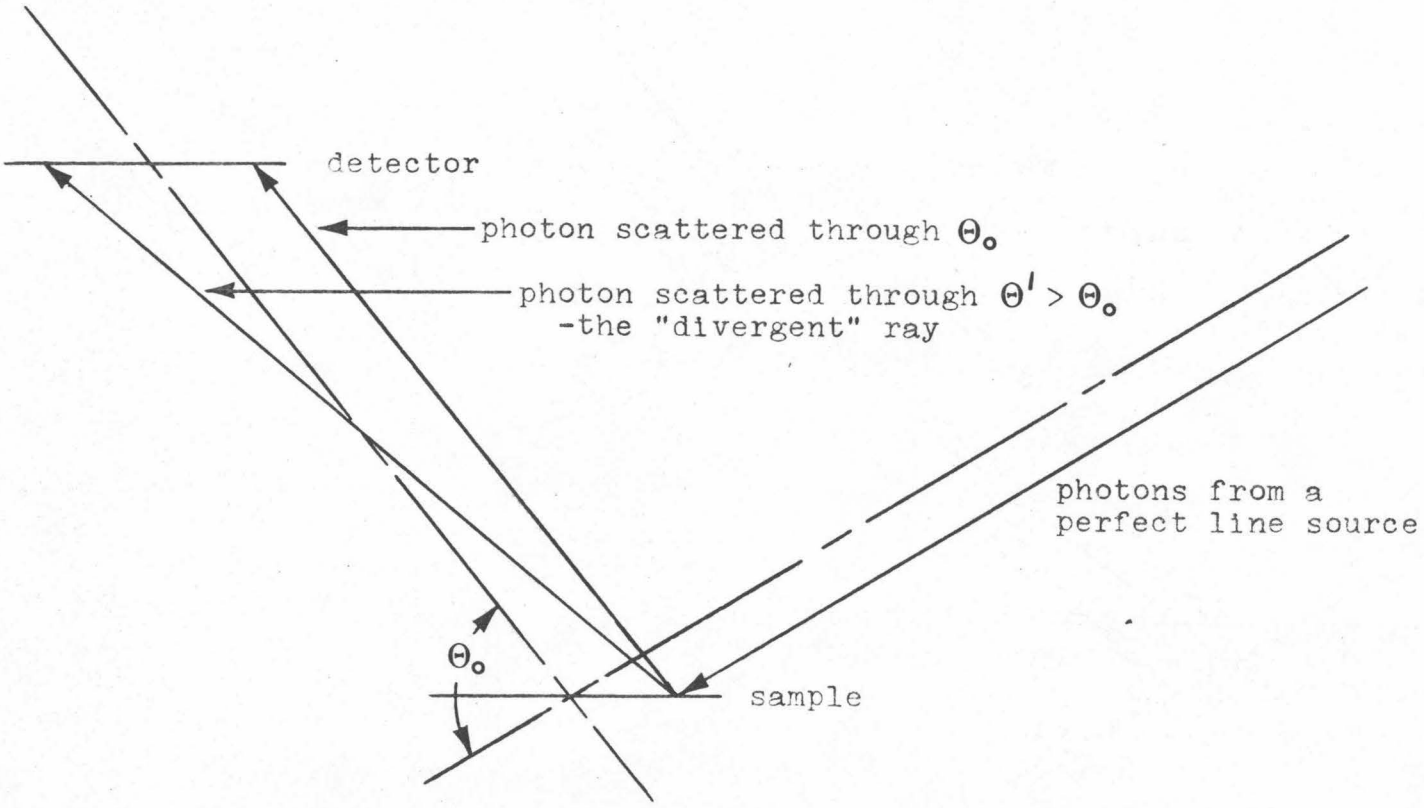

Figure G.2. Illustration of Divergent Scattering at θ_o

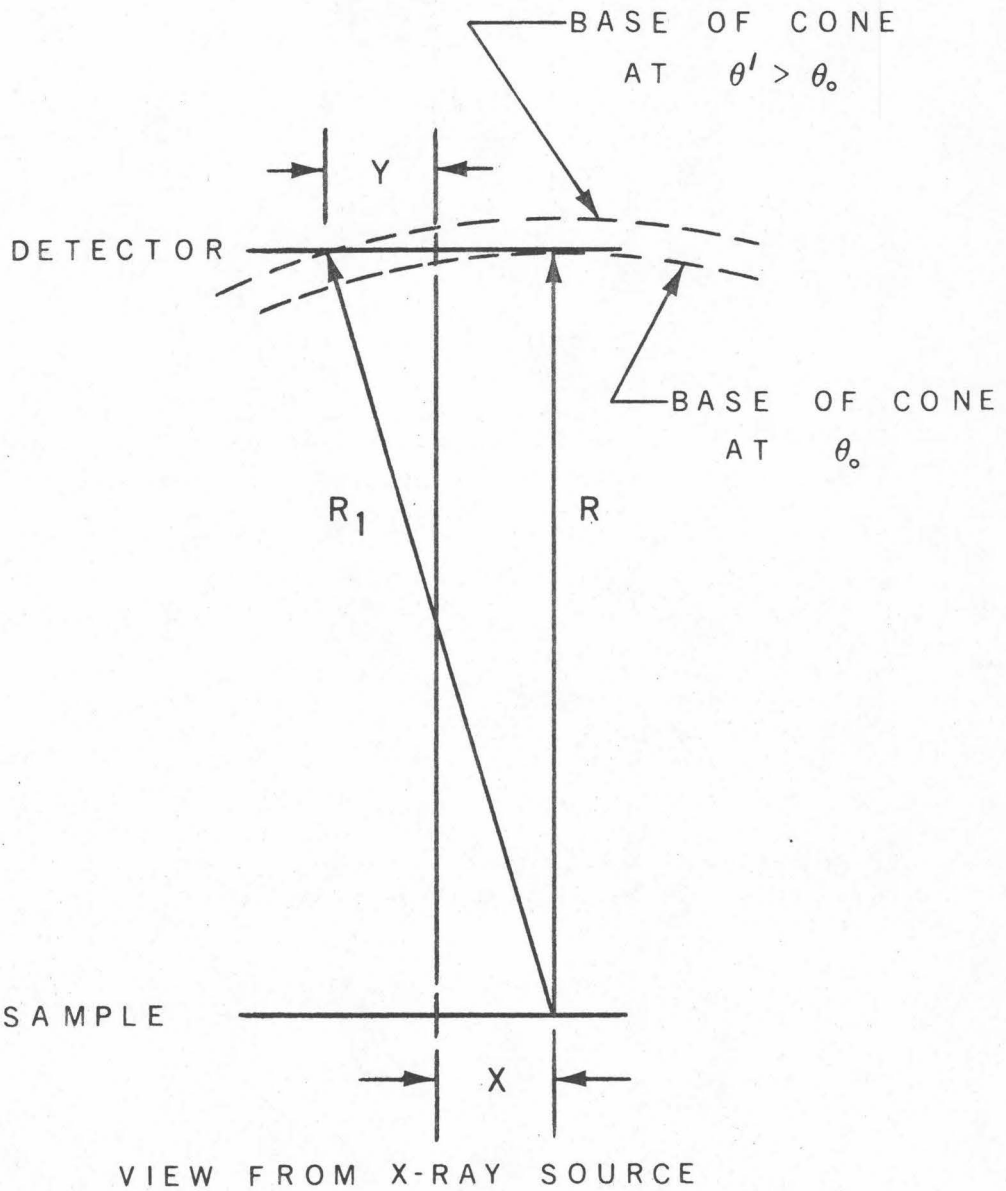

Figure G.3. Illustration of Divergent Scattering at θ_o Viewed from X-ray Source

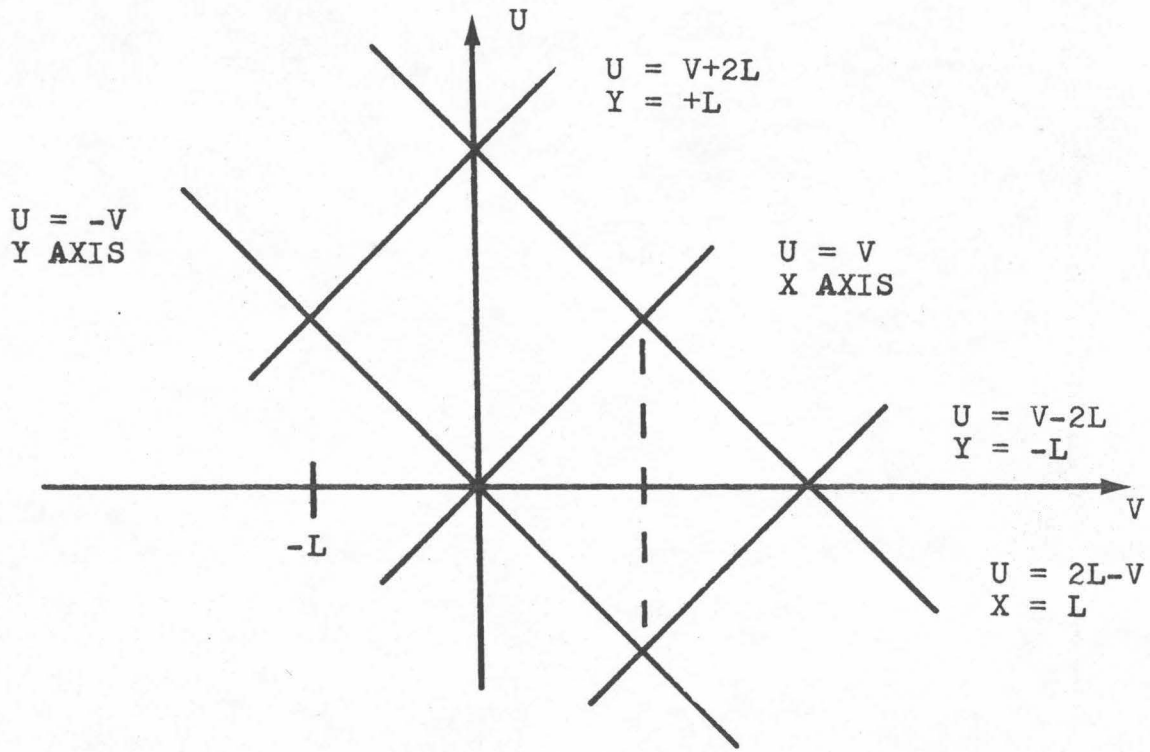

Figure G.4. Transformation of Limits of Integration Used in Distortion Correction

TABLE G.1

Maximum Divergence for Sample-Detector Distance of 6-3/4 Inches and Sample Length of 3/8 Inch

θ_o (Degrees)	Maximum $\theta - \theta_o$ (Degrees)
0	3.2
1	2.35
2	1.77
3	1.38
4	1.12
5	0.94
10	0.49
15	0.33
20	0.24
30	0.15
40	0.11
50	0.08
60	0.05
70	0.03
80	0.02
90	0.

θ_o = detector position

θ = scattering angle of divergent ray

TABLE G.2

Results of Distortion Correction for Numerical Example

θ_o (Deg.)	Distorted Value	Exact Value	Recovered Value
1.2	1.5716	1.9135	1.9177
2.7	1.2884	1.5877	1.5883
4.2	0.8729	1.1045	1.1044
5.7	0.4435	0.5932	0.5931
8.7	1.13E-2	5.48E-3	5.52E-3
11.7	0.4968	0.4121	0.4122
14.7	1.4744	1.4066	1.4066
17.7	1.9963	1.9945	1.9945
20.7	1.5418	1.5878	1.5878
23.7	0.5515	0.5933	0.5933
26.7	3.20E-3	5.49E-3	5.49E-3

APPENDIX H

COMPUTER PROGRAM LISTINGS

A. Introduction

Some of the more important computer programs used in this thesis are presented in Tables H.1 through H.5 since the calculations they represent are directly responsible for the conclusions drawn and to rewrite these programs would require a fair amount of labor. There are five program listings presented and they are the data smoothing routine as derived in Appendix D, the Fourier transform calculation as derived in Appendix F, the absorption factor calculation as derived in Appendix C, the distortion correction as derived in Appendix G, and the distortion-only integration also derived in Appendix G.

The input description that follows describes only the data necessary to get the particular program to execute and no attempt is made here to describe the Job Control Language (JCL) or the use of the peripheral save data devices.

B. Input Description for Data Smoothing with Spline

Input Sequence	Format	Variables or Information
1	I5	Number of input data sets to be smoothed which is the number of times cards 2 - 8 are to appear.
2	20A4	Any alphanumeric information the user desires as an identification to be printed on page 1 of the output.
3	3I5	ND, NI, NWT; The number of observations, the number of intervals and the number of observations to weight.
4	20A4	FMT, the input format to be used to read in the raw data, the parentheses must be included.
5	FMT	The observations (x,y).
6	8F10.0	XI, the mesh points of which there are NI+1.
7	4F10.0	YA, YB, YAP, YBP; The value of the function at the left extreme of the independent variable, the value of the function at the right extreme, the derivatives at the left and right extremes respectively.
8	16I5	Here NWT ordered pairs of numbers, (i,j), are to appear, denoting that the i-th observation in the input stream is to be weighted k times.

Note that the user may alter the subroutine OUTPUT in Table H.1 to give any additional output as desired.

C. Input Description for Fourier Transform Calculation Using a Spline Line Estimate

Input Sequence	Format	Variables or Information
1	2F10.0,I10	RMIN,RMAX,NR; The minimum value of the transform variable, the maximum value and the number of values of the transform to be computed, evenly spaced between RMIN and RMAX as given by RSTEP=(RMAX-RMIN)/(NR-1)

The user must supply two subroutines, GIVEIN and FINAL as described in the comments listed in these subroutines.

D. Input Description for Absorption Factor Calculation (See Figure C.1, Appendix C)

Input Sequence	Format	Variables or Information
1	2I5	NANG,NWD; The number of angles to perform the calculation for and if NWD=1, punch the results.
2	7F10.0,2I5	DX,DY,RI,RO,WAVE,BE,AR,NTH, NR1; The δ_x and δ_y offset of the outside diameter axis from the inside diameter axis, the inner radius, the outer radius all in centimeters, the wavelength of the incident radiation in angstroms, the density of the beryllium and argon in gm/cc and the two integration control parameters for the r and θ integrations using the fourth Newton-Coates formula which denote the number of (32,12, 32,14) groupings to use in the integration.
3	4F10.0,2I5	YMIN,YMID,YMAX,S1,NCELL,NBEAM; The position of the lower edge of the beam relative to the sample x-axis, the position of the upper sample-cell wall, the position of the upper edge of the beam all in centimeters, the step size of 0.01^{o} 2θ as observed on the cell in centimeters, the number of points to be read in to describe the main beam profile over the sample space and likewise for the cell, these last two numbers must be odd.
4	8F10.0	NANG angles at which to perform the absorption factor calculation.

D. Input Description for Absorption Factor Calculation (Continued)

Input Sequence	Format	Variables or Information
5	F10.0	NBEAM numbers that describe the main beam profile as observed beginning with the lowest observation angle.

E. Input Description for Distortion Correction and Distortion Calculation

The input descriptions may be adequately obtained by reading the comment cards in the program listings and noting in which FORMAT a particular variable is written on the output stream.

```
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 MX
      REAL*4 FMT(20),IDENT(20)
      DIMENSION ARRAY(26,27),WW(300),ZZ(300),X(10,80),Y(10,80),DX(10),XI
     1(11),MX(4,4),D(17),T(6),W(10,4,5),DX2(10),ALP(4),A(10,4),BX(26)
      DIMENSION N(10),NW(2,10)
      DATA W(1,3,2),W(1,3,4),W(1,4,2),W(1,4,4)/0.D0,0.D0,0.D0,0.D0/
      DATA LBIG1,LBIG2,LBIG3/10,80,300/
C
C     SORTING THE RAW DATE INTO X(K,J) AND Y(K,J); K=INTERVAL, J=OBSERVATION,
C     IN OTHER WORDS, THE J-TH OBSERVATION IN THE K-TH INTERVAL.
C     ND=TOTAL NUMBER OF OBSERVATIONS.
C     XI(K) STORES LOCATIONS OF MESH POINTS IN ORDER.
C     N(J) STORES NUMBER OF OBSERVATIONS IN EACH INTERVAL.
C     NI=NUMBER OF INTERVALS.
C     ARRAY IS SYSTEM OF EQUATIONS.
C     WW(J) IS RAW X, ZZ(J) IS RAW Z.
C     X(J,I) STORES THE I-TH DATA POINT IN INTERVAL J, LIKEWISE FOR Y(J,I).
C     DX(J) STORES DELTA X, THE J-TH INTERVAL WIDTH.
C
      READ (5,100) NJOB
      DO 7900 NTIME=1,NJOB
      DO 25 K=1,5
      DO 25 J=1,2
25    W(1,J,K)=0.D0
      WRITE (6,10) NTIME
10    FORMAT(1H1,10X,'SPLINE-LEAST SQUARE FIT USING CUBICS, RUN NUMBER',
     1I2)
      DO 125 K=1,30
      DO 125 J=1,31
      ARRAY(K,J)=0.D0
125   CONTINUE
      READ (5,101) IDENT
```


TABLE H.1

```
      READ (5,100) ND,NI,NWT
100   FORMAT(3I5)
      IF(NI.GT.LBIG1.OR.ND.GT.LBIG3) GO TO 710
      IF(NI.LT.4) GO TO 715
      READ (5,101) FMT
101   FORMAT(20A4)
      READ (5,FMT) ((WW(K),ZZ(K)),K=1,ND)
      NL=NI+1
      READ (5,102) (XI(J),J=1,NL)
102   FORMAT(8F10.0)
      READ (5,120) YA,YB,YAP,YBP
120   FORMAT(4F10.0)
      WRITE (6,15) IDENT
15    FORMAT(/,10X,'CARD INPUT IDENTIFICATION:',20A4)
      WRITE (6,115) FMT
115   FORMAT(//,10X,'RAW DATA READ IN CN ',20A4)
      WRITE (6,11) ND
11    FORMAT(//,10X,'TOTAL OBSERVATIONS = ',I6)
      WRITE (6,12) YA,YB,YAP,YBP
12    FORMAT(//,10X,'Y(A) = ',1PD11.4,', Y(B) = ',1PD11.4,', DY(A)/DX =
     1',1PD11.4,', DY(B)/DX = ',1PD11.4)
      NW(1,1)=999
      IF(NWT.EQ.0) GO TO 16
      WRITE (6,17) NWT
17    FORMAT(/,10X,'EXPECT TO WEIGHT ',I3,' POINTS.')
      READ (5,18) ((NW(K,J),K=1,2),J=1,NWT)
18    FORMAT(16I5)
      WRITE (6,19)
19    FORMAT(/,10X,'INPUT #      WEIGHT-1',/)
      DO 21 J=1,NWT
      WRITE (6,20) (NW(K,J),K=1,2)
20    FORMAT(11X,I3,11X,I3)
21    CONTINUE
```

```
16    J=2
      I=0
      LN=1
      DO 475 K=1,ND
      IF(WW(K).LT.XI(J)) GO TO 468
      N(J-1)=I
      I=0
      J=J+1
468   I=I+1
      IF(I.GT.LBIG2) GO TO 700
      IF(K.NE.NW(1,LN)) GO TO 57
      NPIG=NW(2,LN)
      DO 29 NTW=1,NPIG
      Y(J-1,I)=ZZ(K)
      X(J-1,I)=WW(K)
29    I=I+1
      LN=LN+1
57    X(J-1,I)=WW(K)
      Y(J-1,I)=ZZ(K)
475   CONTINUE
      N(J-1)=I
      WRITE (6,501)
501   FORMAT(//,10X,'ECHO CHECK OF INPUT ACCORDING TO INTERVALS.')
      NDATA=0
      DO 525 J=1,NI
      DX(J)=XI(J+1)-XI(J)
      DX2(J)=DX(J)*DX(J)
      WRITE (6,526) J,N(J),DX(J)
526   FORMAT(//,10X,'INTERVAL NUMBER ',I3,' WITH ',I3,' OBSERVATIONS AND
     1 DELTA-X = ',1PD11.4)
      WRITE (6,527)
527   FORMAT(//,10X,'OBSERVATION       X(I)           Y(I)',/)
      NDATA=NDATA+N(J)
```

TABLE H.1 (cont.)

```
      NTOAD=N(J)
      DO 529 K=1,NTOAD
      WRITE (6,528) K,X(J,K),Y(J,K)
528   FORMAT(14X,I2,9X,1PD11.4,4X,1PD11.4)
529   CONTINUE
525   CONTINUE
      WRITE (6,876) NDATA
876   FORMAT(/,10X,'TOTAL OBSERVATIONS PROCESSED ',I5)
      WRITE (6,13)
13    FORMAT(/,10X,'MESH POINTS,     J      X(J)',/)
      WRITE (6,14) ((K,XI(K)),K=1,NL)
14    FORMAT(26X,I2,2X,1PD11.4)
      NIN=NI-1
      DO 1000 J=2,NIN
      DO 850 K1=1,4
      T(K1)=0.D0
      DO 850 K2=1,4
850   MX(K1,K2)=0.D0
      NTOAD=N(J)
      DO 880 K=1,NTOAD
      RX1=X(J,K)-XI(J)
      RX2=X(J,K)-XI(J+1)
      RXS1=RX1*RX1
      RXS2=RX2*RX2
      RXC1=RXS1*RX1
      RXP4=RXS1*RXS1
      MX(1,2)=MX(1,2)+RX1
      MX(1,3)=MX(1,3)+RXS1
      MX(1,4)=MX(1,4)+RXS1*RX2
      MX(2,3)=MX(2,3)+RXC1
      MX(2,4)=MX(2,4)+RXC1*RX2
      MX(3,3)=MX(3,3)+RXP4
      MX(3,4)=MX(3,4)+RXP4*RX2
```

TABLE H.1 (cont.)

```
      MX(4,4)=MX(4,4)+RXP4*RXS2
      T(1)=T(1)+Y(J,K)
      T(2)=T(2)+Y(J,K)*RX1
      T(3)=T(3)+Y(J,K)*RXS1
      T(4)=T(4)+Y(J,K)*RXS1*RX2
880   CONTINUE
      DO 881 K=1,4
881   T(K)=2.D0*T(K)
      MX(1,1)=N(J)
      MX(2,2)=MX(1,3)
      DO 846 K1=1,3
      J1=K1+1
      DO 845 K2=J1,4
845   MX(K2,K1)=MX(K1,K2)
846   CONTINUE
      CALL DET(MX,D)
      DO 925 K=1,4
      SIGN=(-1)**(K+1)
      W(J,K,1)=SIGN*(T(1)*D(K)+T(3)*D(K+8)-T(2)*D(K+4)-T(4)*D(K+12))
      W(J,K,2)=-SIGN*D(K)
      W(J,K,3)=SIGN*(D(K)+DX2(J)*D(K+8)-DX(J)*D(K+4))
      W(J,K,4)=SIGN*D(K+4)
      W(J,K,5)=SIGN*(2.D0*DX(J)*D(K+8)-DX2(J)*D(K+12)-D(K+4))
925   CONTINUE
1000  CONTINUE
C
C     BEGIN FILLING MATRIX TO BE REDUCED.
C     E X C E P T   THE LAST AND FIRST TWO ROWS.
C
C     K=ROW INDEX, M=COLUMN INDEX.
C     IB= COLUMN INDEX OF THE B VECTOR IN THE MATRIX EQN AX=B.
C     MSIZE=MATRIX SIZE.
C     SOLVING FOR 2*(NI-1) UNKNOWNS.
```

TABLE H.1 (cont.)

```
C
      MSIZE=2*NIN
      IB=MSIZE+1
      M=1
      N3=NI-3
      DO 3000 J=1,N3
      J1=J+1
      J2=J+2
      K=2*J+1
      K1=K+1
      ARRAY(K,M)=-W(J1,1,2)-DX(J1)*W(J1,2,2)-DX2(J1)*W(J1,3,2)
      ARRAY(K,M+1)=-W(J1,1,4)-DX(J1)*W(J1,2,4)-DX2(J1)*W(J1,3,4)
      ARRAY(K,M+2)=W(J2,1,2)-W(J1,1,3)-DX(J1)*W(J1,2,3)-DX2(J1)*W(J1,3,3
     1)
      ARRAY(K,M+3)=W(J2,1,4)-W(J1,1,5)-DX(J1)*W(J1,2,5)-DX2(J1)*W(J1,3,5
     1)
      ARRAY(K,M+4)=W(J2,1,3)
      ARRAY(K,M+5)=W(J2,1,5)
      ARRAY(K,IB)=W(J1,1,1)+DX(J1)*W(J1,2,1)+DX2(J1)*W(J1,3,1)-W(J2,1,1)
      ARRAY(K1,M)=-W(J1,2,2)-2.D0*DX(J1)*W(J1,3,2)-DX2(J1)*W(J1,4,2)
      ARRAY(K1,M+1)=-W(J1,2,4)-2.D0*DX(J1)*W(J1,3,4)-DX2(J1)*W(J1,4,4)
      ARRAY(K1,M+2)=W(J2,2,2)-W(J1,2,3)-2.D0*DX(J1)*W(J1,3,3)-DX2(J1)*W(
     1J1,4,3)
      ARRAY(K1,M+3)=W(J2,2,4)-W(J1,2,5)-2.D0*DX(J1)*W(J1,3,5)-DX2(J1)*W(
     1J1,4,5)
      ARRAY(K1,M+4)=W(J2,2,3)
      ARRAY(K1,M+5)=W(J2,2,5)
      ARRAY(K1,IB)=W(J1,2,1)+2.D0*DX(J1)*W(J1,3,1)+DX2(J1)*W(J1,4,1)-W(J
     12,2,1)
      M=M+2
3000  CONTINUE
C
C     FIRST INTERVAL
```

TABLE H.1 (cont.)

```
C
      A(1,1)=YA
      A(1,2)=YAP
      DO 600 K=1,6
600   T(K)=0.DO
      NTOAD=N(1)
      DO 603 K=1,NTOAD
      RX1=X(1,K)-XI(1)
      RX2=RX1*RX1
      RX3=RX2*RX1
      RX4=RX3*RX1
      RZ1=X(1,K)-XI(2)
      RZ2=RZ1*RZ1
      T(1)=T(1)+RX4
      T(2)=T(2)+RX4*RZ1
      T(4)=T(4)+RX4*RZ2
      TEMP=RX2*(Y(1,K)-A(1,1)-RX1*A(1,2))
      T(5)=T(5)+TEMP
      T(6)=T(6)+TEMP*RZ1
603   CONTINUE
      T(3)=T(2)
      T(5)=2.DO*T(5)
      T(6)=2.DO*T(6)
      DM=2.DO*(T(1)*T(4)-T(3)*T(2))
      W(1,3,1)=(T(4)*T(5)-T(2)*T(6))/DM
      W(1,3,3)=DX2(1)*T(4)/DM
      W(1,3,5)=(2.DO*DX(1)*T(4)-DX2(1)*T(2))/DM
      W(1,4,1)=(T(1)*T(6)-T(2)*T(5))/DM
      W(1,4,3)=-DX2(1)*T(2)/DM
      W(1,4,5)=(DX2(1)*T(1)-2.DO*DX(1)*T(2))/DM
      ARRAY(1,1)=W(2,1,2)-DX2(1)*W(1,3,3)
      ARRAY(1,2)=W(2,1,4)-DX2(1)*W(1,3,5)
      ARRAY(1,3)=W(2,1,3)
```


TABLE H.1 (cont.)

```
      ARRAY(1,4)=W(2,1,5)
      ARRAY(1,IB)=A(1,1)+A(1,2)*DX(1)+DX2(1)*W(1,3,1)-W(2,1,1)
      ARRAY(2,1)=W(2,2,2)-2.D0*DX(1)*W(1,3,3)-DX2(1)*W(1,4,3)
      ARRAY(2,2)=W(2,2,4)-2.D0*DX(1)*W(1,3,5)-DX2(1)*W(1,4,5)
      ARRAY(2,3)=W(2,2,3)
      ARRAY(2,4)=W(2,2,5)
      ARRAY(2,IB)=A(1,2)+2.D0*DX(1)*W(1,3,1)+DX2(1)*W(1,4,1)-W(2,2,1)
C
C     LAST INTERVAL
C
      DO 651 K=1,4
651   ALP(K)=0.D0
      B1=0.D0
      B2=0.D0
      NTOAD=N(NI)
      DO 655 K=1,NTOAD
      RX1=X(NI,K)-XI(NI)
      RX2=X(NI,K)-XI(NL)
      TEMP1=DX(NI)+RX1*(RX1*RX2/DX2(NI)-1.D0)
      TEMP2=DX2(NI)+RX1*RX1*(2.D0*RX2/DX(NI)-1.D0)
      ALP(1)=ALP(1)+TEMP1*TEMP1
      ALP(2)=ALP(2)+TEMP1*TEMP2
      ALP(4)=ALP(4)+TEMP2*TEMP2
      TEMP3=Y(NI,K)-YB-RX1*RX1*RX2*YBP/DX2(NI)
      B1=B1+TEMP3*TEMP1
      B2=B2+TEMP3*TEMP2
655   CONTINUE
      ALP(3)=ALP(2)
      DO 657 K=1,4
657   ALP(K)=2.D0*ALP(K)
      B1=2.D0*B1
      B2=2.D0*B2
      DETA=ALP(1)*ALP(4)-ALP(2)*ALP(2)
```

TABLE H.1 (cont.)

```
      DO 656 K=1,4
656   ALP(K)=ALP(K)/DETA
      W(NI,1,1)=YB-DX(NI)*(B2*ALP(2)-B1*ALP(4))-DX2(NI)*(B1*ALP(3)-B2*AL
     1P(1))
      W(NI,1,2)=-DX2(NI)*(ALP(4)-DX(NI)*ALP(2)+DX(NI)*(DX(NI)*ALP(1)-ALP
     1(3)))
      W(NI,1,4)=DX(NI)*(ALP(4)-DX(NI)*ALP(3))
      W(NI,4,1)=(YBP-B2*ALP(2)+B1*ALP(4)-2.D0*DX(NI)*(B1*ALP(3)-B2*ALP(1
     1)))/DX2(NI)
      W(NI,4,2)=(DX2(NI)*ALP(2)-DX(NI)*ALP(4)-2.D0*DX(NI)*(DX2(NI)*ALP(1
     1)-DX(NI)*ALP(3)))/DX2(NI)
      W(NI,4,4)=(ALP(4)-2.D0*DX(NI)*ALP(3))/DX2(NI)
      W(NI,2,1)=B2*ALP(2)-B1*ALP(4)
      W(NI,2,2)=DX(NI)*ALP(4)-DX2(NI)*ALP(2)
      W(NI,2,4)=-ALP(4)
      W(NI,3,1)=B1*ALP(3)-B2*ALP(1)
      W(NI,3,2)=DX2(NI)*ALP(1)-DX(NI)*ALP(3)
      W(NI,3,4)=ALP(3)
      J=IB-2
      K=IB-4
      N2=NI-1
      ARRAY(J,K)=-W(N2,1,2)-DX(N2)*W(N2,2,2)-DX2(N2)*W(N2,3,2)
      ARRAY(J,K+1)=-W(N2,1,4)-DX(N2)*W(N2,2,4)-DX2(N2)*W(N2,3,4)
      ARRAY(J,K+2)=W(NI,1,2)-W(N2,1,3)-DX(N2)*W(N2,2,3)-DX2(N2)*W(N2,3,3
     1)
      ARRAY(J,K+3)=W(NI,1,4)-W(N2,1,5)-DX(N2)*W(N2,2,5)-DX2(N2)*W(N2,3,5
     1)
      ARRAY(J,IB)=W(N2,1,1)+DX(N2)*W(N2,2,1)+DX2(N2)*W(N2,3,1)-W(NI,1,1)
      J=J+1
      ARRAY(J,K)=-W(N2,2,2)-2.D0*DX(N2)*W(N2,3,2)-DX2(N2)*W(N2,4,2)
      ARRAY(J,K+1)=-W(N2,2,4)-2.D0*DX(N2)*W(N2,3,4)-DX2(N2)*W(N2,4,4)
      ARRAY(J,K+2)=W(NI,2,2)-W(N2,2,3)-2.D0*DX(N2)*W(N2,3,3)-DX2(N2)*W(N
     12,4,3)
```

TABLE H.1 (cont.)

```
      ARRAY(J,K+3)=W(NI,2,4)-W(N2,2,5)-2.D0*DX(N2)*W(N2,3,5)-DX2(N2)*W(N
     12,4,5)
      ARRAY(J,IB)=W(N2,2,1)+2.D0*DX(N2)*W(N2,3,1)+DX2(N2)*W(N2,4,1)-W(NI
     1,2,1)
      DO 682 K=1,4
      W(NI,K,3)=0.D0
      W(NI,K,5)=0.D0
682   CONTINUE
      CALL SSAUG(ARRAY,BX,MSIZE,IERR)
      GO TO (81,82), IERR
82    WRITE (6,83)
83    FORMAT(///,10X,'***   REDUCTION ERROR   ***')
      GO TO 7900
81    WRITE (6,900)
900   FORMAT(//,10X,'THE UNDETERMINED MULTIPLIER VECTOR,     J
     1 X(J)',/)
      DO 902 J=1,MSIZE
      WRITE (6,901) J,BX(J)
901   FORMAT(48X,I2,4X,1PD11.4)
902   CONTINUE
      J1=1
      DO 5500 J=2,NIN
      J2=J1+1
      J3=J1+2
      J4=J1+3
      DO 5499 K=1,4
      A(J,K)=W(J,K,1)+W(J,K,2)*BX(J1)+W(J,K,3)*BX(J3)+W(J,K,4)*BX(J2)+W(
     1J,K,5)*BX(J4)
5499  CONTINUE
      J1=J1+2
5500  CONTINUE
      A(1,3)=W(1,3,1)+W(1,3,3)*BX(1)+W(1,3,5)*BX(2)
      A(1,4)=W(1,4,1)+W(1,4,3)*BX(1)+W(1,4,5)*BX(2)
```

TABLE H.1 (cont.)

```
      DO 5322 J=1,4
      A(NI,J)=W(NI,J,1)+W(NI,J,2)*BX(MSIZE-1)+W(NI,J,4)*BX(MSIZE)
5322  CONTINUE
      WRITE (6,84)
84    FORMAT(//,10X,'COEFFICIENTS FOR EACH INTERVAL.')
      WRITE (6,85)
85    FORMAT(//,7X,'INTERVAL       A(J,1)          A(J,2)          A(J,3
     1)          A(J,4)',/)
      DO 90 J=1,NI
      WRITE (6,91) J,(A(J,K),K=1,4)
91    FORMAT(9X,I3,2X,5(5X,1PD11.4))
90    CONTINUE
      CALL OUTPUT(A,XI,WW,ZZ,ND,NI)
7900  CONTINUE
      GO TO 699
700   WRITE (6,701) J
701   FORMAT(///,10X,'********** STORAGE EXCEEDED IN INTERVAL ',I3,'-1,
     1 JOB TERMINATED.')
      GO TO 699
710   WRITE (6,711) LBIG1,LBIG3
711   FORMAT(///,10X,'**********  TOO MUCH DATA INPUT, NO MORE THAN ',I
     14,' INTERVALS OR ',I4,' DATA POINTS IS EXPECTED.')
      GO TO 699
715   WRITE (6,716)
716   FORMAT(///,10X,'********** NUMBER OF INTERVAL CANNOT BE LESS THAN
     14, JOB TERMINATED.')
699   WRITE (6,92)
92    FORMAT(///,10X,'END OF MAIN ROUTINE.')
      CALL EXIT
      END
      SUBROUTINE SSAUG(A,X,N,IERR)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(26,27),X(1)
```

TABLE H.1 (cont.)

```
      DATA ERROR/1.D-25/
C
C     THIS GAUSSIAN ELIMINATION ROUTINE IS PARTICULAR TO SLFIT ONLY,
C
      IERR=1
      NM=N-1
      NN=N+1
      DO 500 I=1,NM
      II=I+1
      TEMP=0.DO
      MBIG=0
      DO 100 K=I,N
      IF(DABS(A(K,I)).LT.DABS(TEMP)) GO TO 100
      MBIG=K
      TEMP=A(K,I)
100   CONTINUE
      IF(DABS(TEMP).GT.ERROR) GO TO 101
      IERR=2
      GO TO 999
101   IF(MBIG.EQ.I) GO TO 105
      DO 103 IC=I,NN
      CHAN=A(I,IC)
      A(I,IC)=A(MBIG,IC)
      A(MBIG,IC)=CHAN
103   CONTINUE
105   NI=I+3
      IF(NI.GT.N) NI=N
      DO 110 M=II,NI
      AM=A(M,I)/A(I,I)
      DO 109 J=II,NN
      A(M,J)=A(M,J)-AM*A(I,J)
109   CONTINUE
110   CONTINUE
```

TABLE H.1 (cont.)

```
500   CONTINUE
      X(N)=A(N,NN)/A(N,N)
      DO 800 ND=1,NM
      IX=N-ND
      IY=IX+1
      SUM=0.DO
      NI=IX+5
      IF(NI.GT.N) NI=N
      DO 700 J=IY,NI
      SUM=SUM+A(IX,J)*X(J)
700   CONTINUE
      X(IX)=(A(IX,NN)-SUM)/A(IX,IX)
800   CONTINUE
999   CONTINUE
      RETURN
      END
      SUBROUTINE DET(A,D)
      REAL*8 A(4,4),D(17),T(14)
      T(1)=A(3,3)*A(4,4)-A(4,3)*A(4,3)
      T(2)=A(3,2)*A(4,4)-A(4,3)*A(4,2)
      T(3)=A(3,2)*A(4,3)-A(3,3)*A(4,2)
      T(4)=A(2,2)*A(4,4)-A(4,2)*A(4,2)
      T(5)=A(2,2)*A(4,3)-A(3,2)*A(4,2)
      T(6)=A(2,2)*A(3,3)-A(3,2)*A(3,2)
      T(7)=A(3,1)*A(4,4)-A(4,3)*A(4,1)
      T(8)=A(3,1)*A(4,3)-A(3,3)*A(4,1)
      T(9)=A(2,1)*A(4,4)-A(4,2)*A(4,1)
      T(10)=A(2,1)*A(4,3)-A(3,2)*A(4,1)
      T(11)=A(2,1)*A(4,3)-A(4,2)*A(3,1)
      T(12)=A(2,1)*A(3,3)-A(3,2)*A(3,1)
      T(13)=A(2,1)*A(4,2)-A(2,2)*A(4,1)
      T(14)=A(2,1)*A(3,2)-A(2,2)*A(3,1)
      D(1)=A(2,2)*T(1)-A(3,2)*T(2)+A(4,2)*T(3)
```

TABLE H.1 (cont.)

```
      D(2)=A(2,1)*T(1)-A(3,1)*T(2)+A(4,1)*T(3)
      D(3)=A(2,1)*T(2)-A(3,1)*T(4)+A(4,1)*T(5)
      D(4)=A(2,1)*T(3)-A(3,1)*T(5)+A(4,1)*T(6)
      D(6)=A(1,1)*T(1)-A(3,1)*T(7)+A(4,1)*T(8)
      D(7)=A(1,1)*T(2)-A(3,1)*T(9)+A(4,1)*T(10)
      D(8)=A(1,1)*T(3)-A(3,1)*T(11)+A(4,1)*T(12)
      D(11)=A(1,1)*T(4)-A(2,1)*T(9)+A(4,1)*T(13)
      D(12)=A(1,1)*T(5)-A(2,1)*T(11)+A(4,1)*T(14)
      D(16)=A(1,1)*T(6)-A(2,1)*T(12)+A(3,1)*T(14)
      D(5)=D(2)
      D(9)=D(3)
      D(13)=D(4)
      D(10)=D(7)
      D(14)=D(8)
      D(15)=D(12)
      D(17)=A(1,1)*D(1)-A(1,2)*D(2)+A(1,3)*D(3)-A(1,4)*D(4)
      DO 100 K=1,16
100   D(K)=0.5D0*D(K)/D(17)
      RETURN
      END
      SUBROUTINE OUTPUT(A,XI,W,Z,ND,NI)
      REAL*8 A(10,4),XI(1),W(1),Z(1)
C
C     THE USER SUPPLIES WHATEVER SPECIAL OUTPUT HE DESIRES IN THIS SUB-
C     ROUTINE, SUCH AS PLOTS.
C     A STORES THE CUBIC COEFFICIENTS.
C     XI STORES THE MESH POINTS.
C     W,Z STORES THE RAW X,Y DATA.
C     ND IS THE NUMBER OF DATA POINTS AND NI IS THE NUMBER OF INTERVALS.
C
      RETURN
      END
```

TABLE H.1 (cont.)

```
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION XI(200),UI(200),YS(200),YC(200),X(200),A(4,200)
      CALL GIVEIN(XI,A,NI)
      READ (5,100) RMIN,RMAX,NR
100   FORMAT(2F10.0,I10)
      NR1=NR-1
      RSTEP=(RMAX-RMIN)/NR1
      NIMAX=NI+1
      DO 10000 N=1,NR
      R=(N-1)*RSTEP+RMIN
      YC(N)=0.D0
      YS(N)=0.D0
      X(N)=R
      DO 500 L=1,NIMAX
500   UI(L)=R*XI(L)
      C2=DCOS(UI(1))
      S2=DSIN(UI(1))
      DO 700 L=1,NI
      C1=C2
      S1=S2
      C2=DCOS(UI(L+1))
      S2=DSIN(UI(L+1))
      R2=R*R
      R3=R*R2
      R4=R*R3
      T1=A(1,L)*(C1-C2)/R
      Q1=A(1,L)*(S2-S1)/R
      TEMP=UI(L+1)*C2-UI(L)*C1
      TROT=UI(L+1)*S2-UI(L)*S1
      T2=A(2,L)*(S2-S1-TEMP)/R2
      Q2=A(2,L)*(C2-C1+TROT)/R2
      U22=UI(L+1)*UI(L+1)
      U12=UI(L)*UI(L)
```

```
      TEMP=UI(L+1)*S2-UI(L)*S1
      TROT=UI(L+1)*C2-UI(L)*C1
      T3=A(3,L)*(2.D0*TEMP-(U22-2.D0)*C2+(U12-2.D0)*C1)/R3
      Q3=A(3,L)*(2.D0*TROT+(U22-2.D0)*S2-(U12-2.D0)*S1)/R3
      T4=A(4,L)*(3.D0*((U22-2.D0)*S2-(U12-2.D0)*S1)-UI(L+1)*(U22-6.D0)*C
     12+UI(L)*(U12-6.D0)*C1)/R4
      Q4=A(4,L)*(3.D0*((U22-2.D0)*C2-(U12-2.D0)*C1)+UI(L+1)*(U22-6.D0)*S
     12-UI(L)*(U12-6.D0)*S1)/R4
      YS(N)=YS(N)+T1+T2+T3+T4
      YC(N)=YC(N)+Q1+Q2+Q3+Q4
700   CONTINUE
10000 CONTINUE
      CALL FINAL(X,YS,YC,NR,NI)
      STOP
      END
      SUBROUTINE FINAL(W,ZS,ZC,NR,NI)
      REAL*8 W(1),ZS(1),ZC(1)
C
C     THE USER WRITES THIS SUBROUTINE TO OUTPUT THE RESULTS, SUCH AS
C     PRINT, ETC.
C     W(J) STORES THE INDEPENDENT VARIABLE IN THE TRANSFORM DOMAIN.
C     ZS(J) STORES THE SIN TRANSFORM.
C     ZC(J) STORES THE COS TRANSFORM.
C     NR = MAX VALUE OF J.
C     NI = NUMBER OF INTERVALS USED BY SPLINE.
C     THERE IS NO LEAD CONSTANT ON THE INTEGRAL(S).
C
      RETURN
      END
      SUBROUITNE GIVEIN(X,A,NI)
      REAL*8 A(4,1),X(1)
C
C     THE USER READS OR GENERATES THE INPUT CUBIC COEFFICIENTS AND THE
```

TABLE H.2 (cont.)

```
C     MESH POINTS.
C     NI = NUMBER OF INTERVALS.
C     A(4,J) STORES THE COEFFICIENTS OF Y(X) = A1 + X*(A2 + X*(A3 + X*A4))
C     X(J) STORES THE MESH POINTS.
C
      RETURN
      END
```

TABLE H.2 (cont.)

```
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 M,M2,ML
      REAL*4 ABSC(6),PSTORE(120),ABSINC(120,2)
      COMMON /TOAD/ STEPB,NSW,NBEAM
      DIMENSION Q(6,120),P(6,120)
      DATA SCALE,PIE,F/57.2957795,3.1415927,0.444444444444444D-1/
      DATA T1,T2,T3,T4,T5,T6/0.,0.,0.,0.,0.,0./
      ROOTP(A,B,C)=(DSQRT(B*B-4.D0*A*C)-B)/(2.D0*A)
      F1(Z)=(((-0.00213D0*Z+0.365D0)*Z-0.029D0)*Z+0.057D0)*Z+0.1415D0
      F2(Z)=(((-4.18D0*Z+40.D0)*Z-0.029D0)*Z+0.058D0)*Z+0.1437D0
      ASEG(X,R)=P2*R*R-X*DSQRT(R*R-X*X)-R*R*DARSIN(X/R)
      P2=PIE/2.D0
C
C     NANG=NUMBER OF ANGLES TO DO CALCULATION AT.
C     NWD=PUNCH CONTROL, IF NWD=1, PUNCH RESULTS.
C
      READ (5,100) NANG,NWD
100   FORMAT(2I5)
      READ (5,101) DX,DY,RI,RO,WAVE,BE,AR,NTH,NR1
101   FORMAT(7F10.0,2I5)
      READ (5,103) YMIN,YMID,YMAX,S1,NCELL,NBEAM
103   FORMAT(4F10.0,2I5)
        STEPB=S1
      READ (5,102) (PSTORE(J),J=1,NANG)
102   FORMAT(8F10.0)
      RO2=RO*RO
      RI2=RI*RI
      DX2=DX*DX
      DY2=DY*DY
      C1=DX2+DY2-RO2
      UBC=F1(WAVE)
      UAC=F2(WAVE)
      UBC=-UBC*BE
```


TABLE H.3

```
      UAC=-UAC*AR
      NR=4*NR1+5
      NA=4*NTH+5
      STEPA=PIE/(NA-1)
C
C     NFT=PRINT CONTROL ON IRRADIATED AREAS (VOLUMES).
C     BS MEANS BEAM-SHAPE DESCRIPTION.
C     YMIN IS THE LOWER EDGE OF THE BEAM.
C     YMAX IS THE UPPER EDGE OF THE BEAM.
C     NBEAM=NUMBER OF BEAM VALUES TO BE READ IN.
C
      NFT=1
      WRITE (6,800)
800   FORMAT(1H1,9X,'ABSORPTION COEFFICIENT CALCULATION.')
      WRITE (6,801) RI,RO
801   FORMAT(/,10X,'INNER RADIUS = ',1PD11.4,', OUTER = ',1PD11.4,' CM.'
     1)
      WRITE (6,802) DX,DY
802   FORMAT(/,10X,'INNER CIRCLE IS AT ORIGIN, OUTER IS AT DX = ',1PD11.
     14,', DY = ',1PD11.4,' CM.')
      WRITE (6,803) WAVE
803   FORMAT(/,10X,'WAVE LENGTH = ',1PD11.4,' ANGSTROM.')
      WRITE (6,804) BE,AR
804   FORMAT(/,10X,'DENSITY OF BE = ',1PD11.4,', ARGON = ',1PD11.4,' GM/
     1CC.')
      WRITE (6,805) NTH,NR1
805   FORMAT(/,10X,'STEP SIZE CONTROL FOR NEWTON-COATES INTEGRATION, NTH
     1=',I5,', NRI=',I5)
      T1=-UAC
      T2=-UBC
      WRITE (6,807) T1,T2
807   FORMAT(/,10X,'COHERENT ABSORPTION COEFFICIENT FOR ARGON = ',1PD11.
     14,', FOR BE = ',1PD11.4,' RECIPROCAL CM.')
```

TABLE H.3 (cont.)

```
      WRITE (6,104) YMIN,YMAX
104   FORMAT(/,10X,'LOWER EDGE OF BEAM AT Y = ',1PD11.4,', UPPER AT = ',
     11PD11.4,' CM.')
      WRITE (6,108) YMID,NCELL
108   FORMAT(/,10X,'UPPER SAMPLE WALL IS AT ',1PD11.4,', CM AND THERE AR
     1E ',I3,' POINTS FROM YMIN TO THE UPPER WALL.')
      WRITE (6,105) NBEAM
105   FORMAT(/,10X,'READ ',I5,' POINTS TO DESCRIBE THE BEAM.')
      WRITE (6,109) S1
109   FORMAT(/,10X,'1/100 DEGREE TWOTHETA CORRESPONDS TO ',1PD11.4,' CM.
     1')
      WRITE (6,106) NWD
106   FORMAT(/,10X,'PUNCH CONTROL, NWD=',I2,', IF 1 PUNCH RESULTS.')
      CALL BDES(YMIN,YMID,YMAX,S1,NCELL,NBEAM)
      DO 10000 NTIME=1,NANG
      PHI=PSTORE(NTIME)
      PHI=PHI/SCALE
      WAV=WAVE+0.0243D0*(1.D0-DCOS(PHI))
      M=DTAN(PHI)
      M2=M*M
      ML=1.D0+M2
      UBI=F1(WAV)
      UAI=F2(WAV)
      UAI=-UAI*AR
      UBI=-UBI*BE
      T1=-UAI
      T2=-UBI
      ABSINC(NTIME,1)=T1
      ABSINC(NTIME,2)=T2
      ANGLE=0.D0
      DO 400 KA=1,NA
      CA=DCOS(ANGLE)
      SA=DSIN(ANGLE)
```

TABLE H.3 (cont.)

```
      A=1.D0
      B=-2.D0*(DX*CA+DY*SA)
C
C     R IS THE DISTANCE FROM 0,0 TO THE OUTER CIRCLE AT ANGLE.
C
      R=ROOTP(A,B,C1)
      STEPR=(R-RI)/(NR-1)
      H1=STEPR
C
C     NSW=1, CALCULATE 4 CELL COEFFICIENTS.
C     NSW=2, CALCULATE 2 SAMPLE COEFFICIENTS.
C
      NSW=1
434   DO 300 KR=1,NR
C
C     CALCULATE COORDINATES OF SCATTERED-RAY INTERSECTION WITH OUTER WALL.
C     FOR BOTH CELL AND SAMPLE SCATTERING,
C     DEXIT=DISTANCE-EXIT THRU CELL WALL FROM X-Y,
C     DINCLL=DISTANCE-INCIDENT THRU CELL WALL TO X-Y,
C     DSAMPI=DISTANCE-INCIDENT THRU SAMPLE TO X-Y,
C     DSAMPE=DISTANCE-EXIT THRU SAMPLE FROM X-Y.
C
      X=R*CA
      Y=R*SA
      BFACT=R*BEAM(Y)
      IF(BFACT.EQ.0.D0) GO TO 351
      Y2=Y*Y
      B1=Y-M*X
      B12=B1*B1
      B=-2.D0*(B1+M*DX+M2*DY)
      C=B12+2.D0*B1*M*DX+M2*C1
      TEST=B*B-4.D0*ML*C
      IF(TEST.LE.0.D0) GO TO 250
```

TABLE H.3 (cont.)

```
      YE=ROOTP(ML,B,C)
      GO TO 251
250   YE=Y
251   XE=(YE-B1)/M
      DEXIT=DSQRT((X-XE)**2+(Y-YE)**2)
C
C     CALCULATE COORDINATES OF INCIDENT RAY INTERSECTION WITH OUTER WALL.
C
      XN=DX-DSQRT(RO2-(Y-DY)**2)
      GO TO (70,71),NSW
70    IF(Y.GT.RI) GO TO 275
      IF(ANGLE.GT.P2) GO TO 375
      X2=DSQRT(RI2-Y2)
      DSAMPI=2.D0*X2
      DINCLL=X-DSAMPI-XN
      DSAMPE=0.D0
      GO TO 290
375   TEST=M2*B12-ML*(B12-RI2)
C
C     CHECK FOR SCATTERED RAY GOING THRU SAMPLE SPACE.
C
      IF(TEST.GT.0.D0) GO TO 377
C
C     SCATTERED RAY DOES NOT GO THRU SAMPLE SPACE.
C
275   DINCLL=X-XN
      DSAMPI=0.D0
      DSAMPE=0.D0
      GO TO 290
C
C     SCATTERED RAY GOES THRU SAMPLE SPACE.
C
377   T2=-M*B1
```

TABLE H.3 (cont.)

```
      T3=DSQRT(TEST)
      X1=(T2-T3)/ML
      X2=(T2+T3)/ML
      Y1=X1*M+B1
      Y3=X2*M+B1
      DSAMPE=DSQRT((X1-X2)**2+(Y1-Y3)**2)
      DEXIT=DEXIT-DSAMPE
      DSAMPI=0.D0
      DINCLL=X-XN
290   T1=UBC*DINCLL
      T2=T1+UAC*DSAMPI
      T3=UBC*DEXIT
      T4=UBI*DEXIT
      T5=T3+UAC*DSAMPE
      T6=T4+UAI*DSAMPE
C
C     Q1=CELL SCATTERING, COHERENT, EMPTY.
C     Q2=CELL SCATTERING, INCOHERENT, EMPTY.
C     Q3=CELL SCATTERING, COHERENT, WITH SAMPLE.
C     Q4=CELL SCATTERING, INCOHERENT, WITH SAMPLE.
C
355   Q(1,KR)=DEXP(T1+T3)*BFACT
      Q(2,KR)=DEXP(T1+T4)*BFACT
      Q(3,KR)=DEXP(T2+T5)*BFACT
      Q(4,KR)=DEXP(T2+T6)*BFACT
      GO TO 300
351   GO TO (355,360),NSW
71    XIN=-DSQRT(RI2-Y2)
      DSAMPI=X-XIN
      DINCLL=XIN-XN
      B=2.D0*M*B1
      C=B12-RI2
      X1=ROOTP(ML,B,C)
```


TABLE H.3 (cont.)

```
      Y1=M*X1+B1
      DSAMPE=DSQRT((X-X1)**2+(Y-Y1)**2)
      DEXIT=DEXIT-DSAMPE
      T1=UBC*DINCLL+UAC*DSAMPI
      T2=T1+UAC*DSAMPE+DEXIT*UBC
      T3=T1+UAI*DSAMPE+DEXIT*UBI
C
C     Q5=SAMPLE SCATTERING, COHERENT.
C     Q6=SAMPLE SCATTERING, INCOHERENT.
C
      Q(5,KR)=DEXP(T2)*BFACT
      Q(6,KR)=DEXP(T3)*BFACT
      GO TO 300
360   Q(5,KR)=0.D0
      Q(6,KR)=0.D0
300   R=R-STEPR
      IF(NSW.EQ.2) GO TO 444
      NSW=2
      R=RI
      STEPR=R/(NR-1)
      H2=STEPR
      GO TO 434
444   SC=H1*F
      DO 311 L=1,4
      CALL COATES(Q,YNT,SC,L,NR,NR1)
      P(L,KA)=YNT
311   CONTINUE
      SC=H2*F
      L=5
      CALL COATES(Q,YNT,SC,L,NR,NR1)
      P(L,KA)=YNT
      L=6
      CALL COATES(Q,YNT,SC,L,NR,NR1)
```

```
      P(L,KA)=YNT
      ANGLE=ANGLE+STEPA
400   CONTINUE
C
C     COMPUTE IRRADIATED AREAS OF THE CELL AND SAMPLE.
C     NOTE OUTER WALL CENTER NOT AT ORIGIN.
C
      IF(NFT.EQ.2) GO TO 854
      NFT=2
      RBIG=RO+DY
      YTP1=YMIN-DY
      YTP2=YMAX-DY
      IF(YMAX.GE.RBIG) GO TO 535
      IF(YMAX.GE.RI) GO TO 534
      VSAMPL=ASEG(YMIN,RI)-ASEG(YMAX,RI)
      VCELL=ASEG(YTP1,RO)-ASEG(YTP2,RO)-VSAMPL
      GO TO 536
534   VSAMPL=ASEG(YMIN,RI)
      VCELL=ASEG(YTP1,RO)-ASEG(YTP2,RO)-VSAMPL
      GO TO 536
535   VSAMPL=ASEG(YMIN,RI)
      VCELL=ASEG(YTP1,RO)-VSAMPL
536   WRITE (6,821) VSAMPL,VCELL
821   FORMAT(/,10X,'VOLUME OF SAMPLE = ',1PD13.6,', CELL = ',1PD13.6)
      WRITE (6,667)
667   FORMAT(//,10X,'TWOTHETA     COH-CELL     INC-CELL     COH-CELL/SAMP
     1LE     INC-CELL/SAMPLE     COH-SAMPLE     INC-SAMPLE',/)
854   SC=STEPA*F
      DO 500 L=1,6
      CALL COATES(P,YNT,SC,L,NA,NTH)
      ABSC(L)=YNT
500   CONTINUE
      DO 925 L=1,4
```

TABLE H.3 (cont.)

```
      ABSC(L)=ABSC(L)/VCELL
925   CONTINUE
      ABSC(5)=ABSC(5)/VSAMPL
      ABSC(6)=ABSC(6)/VSAMPL
      WRITE (6,665) PSTORE(NTIME),ABSC
665   FORMAT(/,11X,F6.2,4X,1PE11.4,2X,1PE11.4,5X,1PE11.4,9X,1PE11.4,6X,1
     1PE11.4,6X,1PE11.4)
      IF(NWD.EQ.1) PUNCH 19, ABSC,PSTORE(NTIME)
19    FORMAT(6(2X,F6.4),5X,F6.2)
C
C     END OF CALCULATION AT ONE ANGLE.
C
10000 CONTINUE
      WRITE (6,676)
676   FORMAT(/,10X,'INCOHERENT ABSORPTION COEFFICIENTS IN RECIPROCAL CM.
     1')
      WRITE (6,675)
675   FORMAT(/,10X,'TWOTHETA        ARGON-INC-ABSC        BERY-INC-ABSC',/
     1)
      DO 679 K=1,NANG
      WRITE (6,678) PSTORE(K),(ABSINC(K,J),J=1,2)
678   FORMAT(11X,F6.2,7X,1PE11.4,10X,1PE11.4)
679   CONTINUE
      CALL EXIT
      END
      SUBROUTINE BDES(YMIN,YMID,YMAX,SC,NCELL,NBEAM)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /SHAPE/ B(100,2)
      DIMENSION BEAM(100),H(100)
      READ (5,100) (BEAM(J),J=1,NBEAM)
100   FORMAT(F10.0)
      CALL SIMPLE(BEAM,YNT,SC,NCELL)
      YL=YNT
```

TABLE H.3 (cont.)

```
      CALL SIMPLE(BEAM,YNT,SC,NBEAM)
      TOTAL=YNT
      NX=NBEAM-NCELL+1
      L=1
      DO 101 K=NCELL,NBEAM
      H(L)=BEAM(K)
101   L=L+1
      CALL SIMPLE(H,YNT,SC,NX)
      WRITE (6,102)
102   FORMAT(//,10X,'BEAM DESCRIPTION PARAMETERS')
      WRITE (6,95)
95    FORMAT(//,10X,'ECHO CHECK OF BEAM INPUT:  K   BEAM-COUNTS',/)
      DO 98 K=1,NBEAM
      WRITE (6,97) K,BEAM(K)
97    FORMAT(35X,I3,3X,F10.0)
98    CONTINUE
      WRITE (6,103) YL,YNT,TOTAL
103   FORMAT(/,10X,'LOWER AREA = ',1PD11.4,', UPPER = ',1PD11.4,', TOTAL
     1 = ',1PD11.4)
      YL=YL/(YMID-YMIN)
      TOTAL=TOTAL/(YMAX-YMIN)
      WRITE (6,104) YL,TOTAL
104   FORMAT(/,10X,'AVERAGE SAMPLE INTENSITY = ',1PD11.4,', CELL = ',1PD
     111.4)
      DO 105 K=1,NBEAM
      B(K,1)=0.D0
105   B(K,2)=0.D0
      DO 106 K=1,NBEAM
106   B(K,1)=BEAM(K)/TOTAL
      DO 107 K=1,NCELL
107   B(K,2)=BEAM(K)/YL
      WRITE (6,108)
108   FORMAT(/,10X,'FINAL F-PARAMETERS FOR BEAM DESCRIPTIONS.')
```

TABLE H.3 (cont.)

```
      WRITE (6,109)
109   FORMAT(/,20X,'CELL          SAMPLE',/)
      DO 111 K=1,NBEAM
      WRITE (6,110) K,B(K,1),B(K,2)
110   FORMAT(5X,I3,9X,1PD11.4,3X,1PD11.4)
111   CONTINUE
      RETURN
      END
      SUBROUTINE SIMPLE(H,YNT,SC,M)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION H(1)
C
C     M=TOTAL NUMBER OF POINTS AND IS ODD.
C     SC=STEP SIZE AND THIS CORRESPONDS TO 1/100 DEGREE TWOTHETA.
C
      NDEX=(M-3)/2
      J=2
      YNT=0.
      DO 100 K=1,NDEX
      YNT=YNT+4.0*H(J)+2.0*H(J+1)
100   J=J+2
      YNT=SC*(YNT+H(1)+H(M)+4.0*H(M-1))/3.0
      RETURN
      END
      SUBROUTINE COATES(H,YNT,SC,L,NR,NR1)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION H(6,1)
      YNT=0.DO
      J=4
      DO 100 K=1,NR1
      YNT=YNT+32.DO*(H(L,J)+H(L,J+2))+14.DO*H(L,J+1)+12.DO*H(L,J+3)
100   J=J+4
      YNT=SC*(YNT+7.DO*(H(L,1)+H(L,NR))+32.DO*(H(L,2)+H(L,NR-1))+12.DO*H
```

TABLE H.3 (cont.)

```
     1(L,3))
      RETURN
      END
      DOUBLE PRECISION FUNCTION BEAM(Y)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /SHAPE/ B(100,2)
      COMMON /TOAD/ STEPB,NSW,NBEAM
      A=Y/STEPB
      N1=A
      DELTA=A-N1
      N1=N1+1
      N2=N1+1
      IF(N2.GT.NBEAM) GO TO 40
      BEAM=B(N1,NSW)*(1.-DELTA)+B(N2,NSW)*DELTA
      GO TO 50
40    BEAM=0.D0
50    RETURN
      END
```

TABLE H.3 (cont.)

```
      REAL*4 LENGTH,MATRIX(3,7)
      COMMON /P/ R2,C1,C2,C3,THETA
      DIMENSION Y(3,40,6),X(3,40),S(4,6),H(3),SAVE(5,120),TRUE(2,200),
     1FMT(20),ECHO(20),B(116,14)
      DATA L3,N/3,10/
C
C     COMMUNICATING WITH 3 DISKPAKS.
C     READ SMOOTHED DATA - DERIVATIVES FROM FT19F001,
C     DSN=BXK.SMOOTH.SCRATCH.PATCH
C
C     READ B(J,K), ALL OF THE BIG ARGON ARRAY VIA FT11F001.
C
C     WRITE ARGON INTENSITY ON LAB REFERENCE CORRECTED FOR DISTORTION ON
C     FT17F001, DSN=BXK.DISTORT
C
C     NPOINT=NUMBER OF POINTS TO UNDISTORT.
C     SAVE(1,K) STORES TWOTHETA IN DEGREES.
C     SAVE(2,K) STORES OBSERVED SMOOTHED INTENSITY.
C     SAVE(3,K) STORES THE FIRST DERIVATIVE OF THE INTENSITY.
C     SAVE(4,K) STORES THE SECOND DERIVATIVE OF THE INTENSITY.
C     SAVE(5,K) STORES S=4*PIE*SIN()/LAMBDA.
C     Y(3,40,6), X(3,40), S(4,6), H(3), ARE USED DURING INTEGRATION.
C     X1(200), Y1(200), DD(3), ARE USED IN PLOTTING.
C     R IS THE DISTANCE FROM SAMPLE TO DETECTOR.
C     LENGTH = DETECTOR SIZE = SAMPLE SIZE.
C     THETA IS GONIOMETER 2THETA.
C     INDEX NOTATION ON Y(J,K,L) - VALUE OF FUNCTION(S).
C     THERE ARE THREE CONTRIBUTIONS TO THE INTEGRALS DENOTED BY J.
C     K INDEXES THE INDEPENDENT VARIABLE LOCATION X(J,K).
C     L DENOTES L-TH INTEGRAL.
C     N+1 MUST BE ODD, THIS IS THE NUMBER OF POINTS FOR THE SIMPSONS.
C
      READ (5,20) NPOINT
```

```
20    FORMAT(I5)
      WRITE (6,31) NPOINT
31    FORMAT(1H1,10X,'UN-DISTORT ',I5,'  DATA POINTS.')
      READ (5,44) ECHO
44    FORMAT(20A4)
      WRITE (6,46) ECHO
46    FORMAT(/,10X,'CARD INPUT IDENTIFICATION: ',20A4)
      READ (5,32) R,LENGTH
32    FORMAT(2F10.0)
      WRITE (6,33) R,LENGTH
33    FORMAT(/,10X,'SAMPLE-DETECTOR DISTANCE = ',F10.2,', DETECTOR AND S
     1AMPLE LENGTH = ',F10.3,' IN CONSISTENT UNITS.')
      LENGTH=LENGTH/2.
C
C     INPUT DATA TO SAVE(J,K) HERE.
C
      READ (19) SAVE
C
C     THIS DOLOOP CHANGES DERIVATIVES WRT S=4*PIE*SIN()/LAMBDA TO DERIVATIVES
C     WRT TWOTHETA.  NOTE THE SMOOTHING WAS DONE OVER S SPACE.
C
      DO 113 K=1,NPOINT
      TEMP=SAVE(1,K)/114.59
      COZ=COS(TEMP)
      SAVE(4,K)=79.1604*COZ*COZ*SAVE(4,K)-4.4204*SIN(TEMP)*SAVE(3,K)
      SAVE(3,K)=8.8408*SAVE(3,K)*COZ
113   CONTINUE
      R2=R*R
      N1=N+1
      H1=LENGTH/N
      H2=2*H1
      DO 100 K=1,N1
      K1=K-1
```

TABLE H.4 (cont.)

```
      X(1,K)=H2*K1-LENGTH
      X(2,K)=H1*K1-LENGTH
100   X(3,K)=H1*K1+LENGTH
      H(1)=H2/3
      H(2)=H1/3
      H(3)=H(2)
      WRITE (6,515)
515   FORMAT(/,10X,'TWOTHETA          F(X)          DF(X)/DX       DDF(
     1X)/DDX     4*PIE*SIN()/W    REAL F(X)    REAL DF(X)/DX',/)
C
C     USING N=10, DOING 11 POINT SIMPSONS.
C     -L<X(1,K)<L
C     -L<X(2,K)<0
C     L<X(3,K)<2L
C     THE THREE ROWS OF Y CONTAIN THE FUNCTION CONTRIBUTION TO EACH INTEGRAL
C     IN U-V SPACE AS INDICATED BY THE THREE ROWS OF THE X ARRAY.
C     S2THETA IS THE SCATTERED 2THETA, 2THETA IS THE DETECTOR POSITION.
C     DERVIATIVES OF S2THETA ARE D(S2THETA) AND WRT 2THETA.
C     F1(X) IS S2THETA-2THETA
C     F2(X) IS THE FIRST DERIVATIVE OF S2THETA
C     F3(X) IS THE SECOND DERIVATIVE OF S2THETA
C     Y(J,K,1) IS S2THETA-2THETA                                          (1,2)
C     Y(J,K,2) IS (S2THETA-2THETA)**2                                     (1,3)
C     Y(J,K,3) IS D(S2THETA)                                              (2,2)
C     Y(J,K,4) IS D(S2THETA)*(S2THETA-2THETA)                             (2,3)
C     Y(J,K,5) IS DD(S2THETA)                                             (3,2)
C     Y(J,K,6) IS (S2THETA-2THETA)*DD(S2THETA) + D(S2THETA)**2            (3,3)
C
      DO 1000 NP=1,NPOINT
      THETA=SAVE(1,NP)/57.295
      SN=SIN(THETA)
      C1=R2*SN*SN
      C2=R*SN
```

TABLE H.4 (cont.)

```
      C3=R*COS(THETA)
      DO 150 J=1,3
      DO 150 K=1,6
150   S(J,K)=0.
      DO 300 K=1,N1
      A1=F1(X(1,K))
      A2=F1(X(2,K))
      A3=F1(X(3,K))
      D=2*LENGTH-X(3,K)
      Y(1,K,1)=A1
      Y(2,K,1)=X(2,K)*A2
      Y(3,K,1)=D*A3
      Y(1,K,2)=A1*A1
      Y(2,K,2)=Y(2,K,1)*A2
      Y(3,K,2)=Y(3,K,1)*A3
      B1=F2(X(1,K))
      B2=F2(X(2,K))
      B3=F2(X(3,K))
      Y(1,K,3)=B1
      Y(2,K,3)=X(2,K)*B2
      Y(3,K,3)=D*B3
      Y(1,K,4)=A1*B1
      Y(2,K,4)=X(2,K)*A2*B2
      Y(3,K,4)=D*A3*B3
      C11=F3(X(1,K))
      C12=F3(X(2,K))
      C13=F3(X(3,K))
      Y(1,K,5)=C11
      Y(2,K,5)=X(2,K)*C12
      Y(3,K,5)=D*C13
      Y(1,K,6)=A1*C11+B1*B1
      Y(2,K,6)=X(2,K)*(A2*C12+B2*B2)
      Y(3,K,6)=D*(A3*C13+B3*B3)
```


TABLE H.4 (cont.)

```
300   CONTINUE
C
C     BEGIN EVALUATING THREE PARTS TO INTEGRAL I.
C     NX IS THE LAST POSITION OF THE 4,2 PAIRS DESIGNATING THE 4 POSITION.
C
      NX=N-2
      DO 500 I=1,6
      DO 400 K=2,NX,2
      DO 389 J=1,3
389   S(J,I)=S(J,I)+4*Y(J,K,I)+2*Y(J,K+1,I)
400   CONTINUE
C
C     FINISH UP INTEGRAL I.
C
      DO 399 J=1,3
399   S(J,I)=H(J)*(S(J,I)+Y(J,1,I)+Y(J,N1,I)+4*Y(J,N,I))
500   CONTINUE
C
C     ADD UP THE 3 CONTRIBUTIONS TO INTEGRAL I.
C
      DO 502 J=1,6
502   S(1,J)=LENGTH*S(1,J)
      DO 505 J=1,6
505   S(4,J)=S(1,J)+S(2,J)+S(3,J)
      MATRIX(1,1)=1.
      MATRIX(2,1)=0.
      MATRIX(3,1)=0.
      MATRIX(1,2)=S(4,1)*2
      MATRIX(1,3)=S(4,2)
      MATRIX(2,2)=S(4,3)*2
      MATRIX(2,3)=S(4,4)*2
      MATRIX(3,2)=S(4,5)*2
      MATRIX(3,3)=S(4,6)*2
```

TABLE H.4 (cont.)

```
      MATRIX(1,4)=SAVE(2,NP)
      MATRIX(2,4)=SAVE(3,NP)
      MATRIX(3,4)=SAVE(4,NP)
      CALL FCCLEM(L3,MATRIX)
      TRUE(1,NP)=MATRIX(1,4)
      TRUE(2,NP)=MATRIX(2,4)
1000  CONTINUE
      DO 499 K=1,NPOINT
      WRITE (6,501) K,(SAVE(J,K),J=1,5),TRUE(1,K),TRUE(2,K)
501   FORMAT(1X,I3,7(5X,1PE11.4))
499   CONTINUE
      CALL DISTUT(TRUE,SAVE,NPOINT)
      WRITE (6,705)
705   FORMAT(1H1,10X,'CALCULATE NORMALIZATION COEFFICIENT FOR EACH POINT
     1, SMOOTHED AND CORRECTED FOR DISTORTION.')
      WRITE (6,256)
256   FORMAT(/,9X,'POINT          NORMALIZATION',/)
      READ (11) B
      DO 700 K=1,NPOINT
      SCALE=(B(K,14)*(B(K,12)*B(K,8)+B(K,13)*B(K,9)))/TRUE(1,K)
      WRITE (6,701) K,SCALE
701   FORMAT(10X,I3,10X,1PE11.4)
700   CONTINUE
      WRITE (17) TRUE
      STOP
      END
      FUNCTION F1(B)
      COMMON /P/ R2,C1,C2,C3,THETA
      X=B*B
      F1=ARSIN(SQRT((C1+X)/(R2+X)))-THETA
      RETURN
      END
      FUNCTION F2(X)
```

```
      COMMON /P/ R2,C1,C2,C3,THETA
      F2=C2/SQRT(C1+X*X)
      RETURN
      END
      FUNCTION F3(B)
      COMMON /P/ R2,C1,C2,C3,THETA
      X=C1+B*B
      F3=C3*(1.-C1/X)/SQRT(X)
      RETURN
      END
      SUBROUTINE FOOLEM(L,ARRY)
      DIMENSION ARRY(3,7)
      NL=L+1
      DO 59 N=1,L
      TEMP=0.
      DO 62 M=N,L
      IF(ABS(ARRY(M,N))-ABS(TEMP)) 62,62,61
61    TEMP=ARRY(M,N)
      MBIG=M
62    CONTINUE
      DO 63 J=1,NL
      CHAN=ARRY(MBIG,J)
      ARRY(MBIG,J)=ARRY(N,J)
      ARRY(N,J)=CHAN
63    CONTINUE
      BOS=ARRY(N,N)
      DO 64 J=1,NL
64    ARRY(N,J)=ARRY(N,J)/BOS
      DO 68 J=1,L
      IF(N-J) 65,68,65
65    DO 67 K=1,NL
      IF(K-N) 66,67,66
66    ARRY(J,K)=ARRY(J,K)-ARRY(J,N)*ARRY(N,K)
```


TABLE H.4 (cont.)

```
67      CONTINUE
68      CONTINUE
59      CONTINUE
        RETURN
        END
```


TABLE H.4 (cont.)

```
      SUBROUTINE SMEAR
      REAL*4 L,L2
      INTEGER PCODE
      DIMENSION T(2,200),RESULT(2,200),V(40),U(40),TWOT(40),Z1(11),
     1Z2(11),C(40),ECHO(20),TITLE(4),X1(150),Y1(150),DD(3)
      DATA RESULT,DD(1),NL,NI/400*1.,0.,31,11/
C
C     L IS ONE-HALF THE SAMPLE LENGTH IN INCHES.
C     ********* BUT, ENTER L AS THE ACTUAL SAMPLE LENGTH BECAUSE A /2 OCCURS.
C     R IS THE SAMPLE-DETECTOR DISTANCE IN INCHES.
C     DO EVERYTHING IN RADIANS.
C
      READ (18) T
      READ (5,10) R,L,TWOTHE,DELTA,NP,NMAX,PCODE
10    FORMAT(4F10.0,3I5)
      READ (5,16) ECHO
16    FORMAT(20A4)
      DELTA=DELTA/57.295
      TWOTHE=TWOTHE/57.295
      T(2,1)=TWOTHE
      Y1(1)=T(1,1)
      X1(1)=17.86*SIN(T(2,1)/2.)
      DO 50 K=2,NP
      T(2,K)=T(2,K-1)+DELTA
      X1(K)=17.86*SIN(T(2,K)/2.)
      Y1(K)=T(1,K)
50    CONTINUE
      WRITE (6,15)
15    FORMAT(1H1,9X,'THIS PROGRAM DISTORTS DATA TO A SPECIFIED SAMPLE-DE
     1TECTOR DISTANCE.')
      WRITE (6,171)
171   FORMAT(/,10X,'**** WARNING: THIS SMEARING ROUTINE IS ONLY VALID IF
     1 THE INPUT DATA IS CORRECTED TO A SAMPLE-DETECTOR DISTANCE OF INFI
```

```
     2NITY.')
      WRITE (6,17) ECHO
17    FORMAT(/,10X,'CARD INPUT ID: ',20A4)
      WRITE (6,180) R,L
180   FORMAT(/,10X,'SAMPLE-DETECTOR DISTANCE = ',F6.2,', SAMPLE LENGTH =
     1 ',F5.3,', IN CONSISTENT UNITS.')
      WRITE (6,181) NMAX
181   FORMAT(/,10X,'SMEARING THE INPUT DATA UP TO THE ',I3,'-TH POINT, D
     1ISTORTED = UNDISTORTED AFTERWARDS.',/)
      WRITE (6,99)
99    FORMAT(14X,'TWOTHETA   UNDISTORTED      DISTORTED      MAX-ANGLE
     1  RATIO',/)
C
C     GENERATE VALUES OF V, X, INTENSITY AND THEN INTEGRATE.
C
      L=L/2.
      L2=2.*L
      FOURL2=4.*L*L
      DELTAV=L/10.
      V(1)=-L
      U(1)=V(1)*V(1)
      DO 444 K=2,NL
      V(K)=V(K-1)+DELTAV
      U(K)=V(K)*V(K)
444   CONTINUE
      R2=R*R
C
C     INTEGRATE FOR DISTORTED INTENSITY USING 11 POINT SIMPSONS ON EACH
C     OF THE THREE REGIONS IN U-V SPACE.
C
C      1  2  3  4  5  6  7  8  9 10 11      V*F(V)          Z1(K)    -L<V<0
C     11 12 13 14 15 16 17 18 19 20 21      F(V)            C(K)     0<V<L
C     21 22 23 24 25 26 27 28 29 30 31      (2L-V)*F(V)     Z2(K)    L<V<2L
```

TABLE H.5 (cont.)

```
C       1  4  2  4  2  4  2  4  2  4  1      SIMPSON WEIGHTS
C
      DO 5000 LD=1,NMAX
      SR2=R2*SIN(T(2,LD))**2
C
C     THE *1.0001 THAT FOLLOWS IS NECESSARY TO THE BEAT THE FINITE
C     ARITHEMATIC OPERATIONS.
C
      DO 410 K=1,NL
      TWOT(K)=(ARSIN(SQRT((SR2+U(K))/(R2+U(K)))))*1.0001
      I=LD
      DO 405 M=1,9
      IF(TWOT(K).GE.T(2,I).AND.TWOT(K).LE.T(2,I+1)) GO TO 425
      I=I+1
405   CONTINUE
      WRITE (6,406) LD,I,K
406   FORMAT(//,10X,'*** SEARCH ERROR FOR TWOTHETA ***',3I10)
      WRITE (6,407) TWOT(K)
407   FORMAT(/,10X,'TWOTHETA = ',1PE11.4,', TEST PARAMETERS FOLLOW.',/)
      LD12=LD+12
      WRITE (6,408) (T(2,J),J=LD,LD12)
408   FORMAT(/,10X,1PE13.6)
      GO TO 9999
425   C(K)=T(1,I)+(T(1,I+1)-T(1,I))*(TWOT(K)-T(2,I))/DELTA
410   CONTINUE
      DO 510 K=1,NI
      Z1(K)=V(K)*C(K)
      Z2(K)=(L2-V(K+20))*C(K+20)
510   CONTINUE
      A1=0.
      A2=0.
      A3=0.
      DO 582 K=2,10,2
```


TABLE H.5 (cont.)

```
      A1=A1+C(K+10)
      A2=A2+Z1(K)
      A3=A3+Z2(K)
582   CONTINUE
      A1=2.*A1
      A2=2.*A2
      A3=2.*A3
      DO 583 K=3,9,2
      A1=A1+C(K+10)
      A2=A2+Z1(K)
      A3=A3+Z2(K)
583   CONTINUE
      A1=2.*A1+C(11)+C(21)
      A2=2.*A2+Z1(1)+Z1(11)
      A3=2.*A3+Z2(1)+Z2(11)
      RESULT(1,LD)=DELTAV*2*(L2*A1+A2+A3)/3/FOURL2
      PRT1=57.295*T(2,LD)
      PRT2=57.295*TWCT(NL)
      RATIO=RESULT(1,LD)/T(1,LD)
      WRITE (6,482) LD,PRT1,T(1,LD),RESULT(1,LD),PRT2,RATIO
482   FORMAT(5X,I3,5X,F7.2,2(5X,1PE11.4),5X,0PF7.2,5X,F7.4)
5000  CONTINUE
      K1=NMAX+1
      DO 879 K=K1,NP
      RESULT(1,K)=T(1,K)
      WRITE (6,878) K,RESULT(1,K)
878   FORMAT(5X,I3,17X,1PE11.4)
879   CONTINUE
      WRITE (6,990)
990   FORMAT(//,10X,'THE QUANTITY MAX-ANGLE IS THE MAXIMUM ANGLE A PHOTO
     1N CAN BE SCATTERED THROUGH AND STILL BE ACCEPTED BY THE DETECTOR')
      WRITE (6,991)
991   FORMAT(10X,'POSITIONED AT TWOTHETA.')
```

TABLE H.5 (cont.)

```
      WRITE (6,992)
992   FORMAT(/,10X,'THE QUANTITY DESIGNATED AS RATIO ABOVE IS THE DISTOR
     1TED INTENSITY DIVIDED BY THE TRUE INTENSITY.')
      WRITE (19) RESULT
C
C     PLOT CARDS FOLLOW.
C
      IF(PCODE.EQ.0) GO TO 9999
      READ (5,117) TITLE
117   FORMAT(4A4)
      READ (5,118) YMAX
118   FORMAT(F10.0)
      CALL LABEL(0.,0.,0.,10.,15.,10,'4*PIE*SIN()/LAMBDA',18,0)
      CALL SYSSYM(8.,9.,0.25,'SMEAR IT',8,0.)
      CALL SYSSYM(8.,8.,0.25,TITLE,16,0.)
      CALL SYSSYM(8.,7.5,0.1,'X IS INFINITY',13,0.)
      CALL XYPLT(NP,X1,Y1,0.,10.,0.,YMAX,DD,0,4)
      DO 119 K=1,NMAX
119   Y1(K)=RESULT(1,K)
      CALL XYPLT(NMAX,X1,Y1,0.,10.,0.,YMAX,DD,-1,2)
9999  WRITE (6,9090)
9090  FORMAT(//,10X,'END OF JOB.')
      RETURN
      END
```

TABLE H.5 (cont.)

PROPOSITION I.

The technique presented by White, et al,[1] for computing chemical equilibria in a complex gas mixture may be extended to include the presence of a nondistributing, nonmixing solid phase.

The free energy of a system of gases and nondistributing, nonmixing solids containing x_i moles of component i may be expressed as:

$$F(X) = \sum_{g=1}^{n} f_g + \sum_{s=1}^{m} x_s c_s \qquad (1)$$

where there are n gases and m solids in the system. For the gases:

$$f_g = x_g\left[c_g + \ln(x_g/\bar{x})\right] \qquad (2)$$

$$c_g = (F^o/RT)_g + \ln(P) \qquad (3)$$

$$\bar{x} = \sum_{g=1}^{n} x_g \qquad (4)$$

and P is the total pressure in atmospheres. For the solids:

$$c_s = (F^o/RT)_s + \delta \qquad (5)$$

The quantity δ is usually set equal to zero as will be here. F° is the molal standard free energy at the temperature T, and R is the gas constant.

The equilibrium composition is then the set of mole numbers that minimizes F(X), are all positive, and satisfy the mass balance constraint:

$$\sum_{i=1}^{n+m} a_{ij} x_i = b_j \quad \text{for } j = 1,2,.....,k \qquad (6)$$

where a_{ij} is the formula coefficient of component i, indicating the number of atoms of element j in that component, b_j is the total number of atomic weights of element j in the system, and there are k elements in the system. The total number of components is t = n+m.

The free energy of the system may be approximated by a Taylor's series through the second order terms about any set of mole numbers, $(Y)_{i=1}^{t}$, that satisfies Eq. (6). Letting $\Delta_i = x_i - y_i$, the approximation is:

$$Q(X) = F(Y) + \sum_{i}^{t} \partial F/\partial x_i \Big|_{x=y} \Delta_i + \tfrac{1}{2} \sum_{i}^{t} \sum_{q}^{t} \partial^2 F/\partial x_i \partial x_q \Big|_{x=y} \Delta_i \Delta_q \qquad (7)$$

where the summations all begin with the index set at one. From the previous equations the following partial derivatives for the gas components may be obtained:

$$\partial F/\partial x_g = c_g + \ln(x_g/\bar{x}) \qquad (8)$$

$$\partial^2 F/\partial x_g^2 = 1/x_g - 1/\bar{x} \qquad (9)$$

$$\partial^2 F/\partial x_g \partial x_{g'} = -1/\bar{x} \quad \text{for } g \neq g' \qquad (10)$$

For the solid components, noting that there is no free energy contribution due to mixing, the following is obtained:

$$\partial F/\partial x_s = c_s \qquad (11)$$

Eq. (7) now becomes:

$$Q(X) = F(Y) + \sum_g \left[c_g + \ln(y_g/\bar{y})\right] \Delta_g + \tfrac{1}{2}\sum_g y_g(\Delta_g/y_g - \bar{\Delta}/\bar{y})^2 + \sum_s c_s \Delta_s \qquad (12)$$

where $\Delta_g = x_g - y_g$, $\bar{y} = \sum_g y_g$, $\bar{\Delta} = \sum_g \Delta_g$, g sums over the gases and s sums over the solids.

Adding the mass balance constraint, Eq. (6) to Eq. (12), using Lagrange multipliers, π_j, yields:

$$G(X) = Q(X) + \sum_j \pi_j(-\sum_i a_{ij}x_i + b_j) \qquad (13)$$

where j sums over all elements and i sums over all components.

Now minimize G(X) by taking the partial derivative with respect to component i and setting it equal to zero. For the gas components this yields:

$$\partial G/\partial x_g = \left[c_g + \ln(y_g/\bar{y})\right] + (x_g/y_g - \bar{x}/\bar{y}) - \sum_j \pi_j a_{gj} = 0 \qquad (14)$$

Solving for x_g yields:

$$x_g = -f_g(Y) + (y_g/\bar{y})\bar{x} + (\sum_j \pi_j a_{gj})y_g \qquad (15)$$

The above equation for x_g may be summed over all g to yield:

$$\sum_g f_g(Y) = \sum_g (\sum_j \pi_j a_{gj})y_g = \sum_j \pi_j \sum_g a_{gj} y_g \qquad (16)$$

Consider now the partial of G(X) with respect to a solid component mole number:

$$\partial G/\partial x_s = c_s - \sum_j \pi_j a_{sj} = 0 \qquad (17)$$

The expression for x_g, Eq. (15), may be substituted into the mass balance constraint, Eq. (6), thus

eliminating the gas mole numbers. This yields:

$$\sum_g a_{gj}\left[-f_g(Y) + (y_g/\bar{y})\bar{x} + \left(\sum_{j'} \pi_{j'} a_{gj'}\right)y_g\right]$$

$$+ \sum_s a_{sj}x_s = b_j \qquad (18a)$$

This equation may be rearranged to the following:

$$\sum_g a_{gj}\left(\sum_{j'} \pi_{j'} a_{gj'}\right)y_g + (\bar{x}/\bar{y})\sum_g a_{gj}y_g + \sum_s a_{sj}x_s$$

$$= b_j + \sum_g a_{gj}f_g(Y) \qquad (18b)$$

In the previous two equations, j' sums over all elements.

The resulting unknowns are the k Lagrange multipliers, the m mole numbers for the solids, and $\bar{x}$ for the gases. Hence, the total number of unknowns is k+m+1. However, there are k equations from Eq. (18b), one for each element, m equations from Eq. (17), one for each solid, and one equation from Eq. (16). Therefore, the total number of equations equals the number of unknowns.

Now define the following vectors:

$$\bar{\alpha} = \begin{bmatrix} \pi_1 \\ \pi_2 \\ \cdot \\ \cdot \\ \pi_k \\ \bar{x} \\ x_{s_1} \\ x_{s_2} \\ \cdot \\ \cdot \\ x_{s_m} \end{bmatrix} \tag{19}$$

and

$$\bar{\beta} = \begin{bmatrix} b_1 + \sum a_{g1} f_g(Y) \\ b_2 + \sum a_{g2} f_g(Y) \\ \cdot \\ b_k + \sum a_{gk} f_g(Y) \\ \sum f_g(Y) \\ c_{s_1} \\ c_{s_2} \\ \cdot \\ c_{s_m} \end{bmatrix} \tag{20}$$

where the sums above are over g.

The following matrix equation is obtained:

$$\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1k} & Z_1 & a_{s_1 1} & \cdots & a_{s_m 1} \\ r_{21} & r_{22} & \cdots & r_{2k} & Z_2 & a_{s_1 2} & \cdots & a_{s_m 2} \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ r_{k1} & r_{k2} & \cdots & r_{kk} & Z_k & a_{s_1 k} & \cdots & a_{s_m k} \\ \sum_g a_{g1} y_g & \cdots & & \sum_g a_{gk} y_g & 0 & 0 & \cdots & 0 \\ a_{s_1 1} & a_{s_1 2} & \cdots & a_{s_1 k} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ a_{s_m 1} & a_{s_m 2} & \cdots & a_{s_m k} & \cdots & & & \end{bmatrix} \bar{\alpha} = \bar{\beta} \qquad (21)$$

where:

$$r_{ij} = r_{ji} = \sum_g a_{gj} a_{gi} y_g \quad \text{for } j,i = 1,\ldots,k \qquad (22)$$

$$Z_j = \sum_g a_{gj} (y_g / \bar{y}) \qquad (23)$$

In the above equations the i subscript on s_i represents the i-th solid.

In using this computational technique one starts with any positive set of mole numbers, $(Y)_{i=1}^{t}$, that satisfies the mass balance constraint, Eq. (6), computes $f_i(Y)$ by Eq. (2) for all gases, and all the matrix elements of Eq. (21). Then Eq. (21) is solved for $\overline{a}$ and the improved set of mole numbers for the gases is obtained from Eq. (15). The improved mole numbers can then be used to repeat the calculation until the mole numbers do not appear to move any appreciable distance with each iteration.

It is possible to compute mole numbers that are less than zero, which, of course, is not allowed as an acceptable solution. Therefore, when an iteration yields negative mole numbers, the solution may be adjusted as follows. A number, λ, is computed such that $0 < \lambda < 1$ and $\lambda\Delta_i$ limits the computed changes in the mole numbers so that all are positive. Adjusting the new set of mole numbers in this manner does not violate the mass balance constraint. To show this, let $(X^o)_{i=1}^{t}$ be the computed mole numbers that are to be adjusted and let:

$$x_i = \lambda\left[(x_i^o - y_i)\right] + y_i \qquad (24)$$

Substituting this equation into Eq. (6) yields:

$$\sum_i a_{ij}\left[\lambda(x_i^o - y_i) + y_i\right] = b_j \qquad (25)$$

Simplifying Eq. (25) yields:

$$\lambda\sum_i a_{ij}x_i^o - \lambda\sum_i a_{ij}y_i + \sum_i a_{ij}y_i = b_j \qquad (26a)$$

or

$$\sum_i a_{ij}x_i^o = \sum_i a_{ij}y_i \qquad (26b)$$

Since both $(X^o)_{i=1}^t$ and $(Y)_{i=1}^t$ satisfy the initial constraint, Eq. (6), adjusting the mole numbers as described is acceptable.

Consider the following examples to illustrate the technique. The first example is calculable by hand and is presented to demonstrate the accuracy of the optimization technique. The second example is far more complex, and to obtain the result by hand computation would be rather tedious.

Example 1. Consider a stream of 80 mole per cent N_2 and 20 mole per cent CO passing over solid FeO. The reaction occurring is:

$$CO + FeO \rightleftarrows CO_2 + Fe \qquad (27)$$

The conditions of the system are 1000°C and one atmosphere total pressure. $\Delta F_f/RT$ values may be obtained from the literature.[2] In order to start the computation, a set of mole numbers that satisfies the initial mass balance must be obtained. It is assumed that FeO is in excess. Table 1. presents the information used to start the calculation and the result for each iteration. A hand calculation reveals that the final amount of CO_2 should be 0.05496 moles.

Example 2. Consider now a system of steam and carbon briquettes in an iron reactor. Assume that the following components are present at equilibrium: H_2O, CH_4, H_2, O_2, CO, CO_2, C, Fe, and FeO. The temperature of the system is 600°C and the pressure is one atmosphere. As a basis for the calculation use one lb. mole of steam with carbon and iron in excess. $\Delta F_f/RT$ values at 600°C may be obtained from the literature.[2,3] Table 2. presents the information used to start the calculation and the result after 12 iterations. A hand calculation for this system would be very time consuming.

REFERENCES FOR PROPOSITION I.

1. W. B. White, S. M. Johnson and G. B. Dantzig, J. Chem. Phys. 28, 751(1958).

2. C. E. Wickes and F. E. Block, Bulletin 605, Bureau of Mines, (1963).

3. F. D. Rossini, et al, "Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds," API 44 Project, Carnegie Press, Pittsburgh, (1953).

TABLE 1.

Results for Example 1.

Input Data:

Component	CO	FeO	CO_2	Fe	N_2
$\Delta F_f/RT$	-21.207	-17.082	-37.319	0.	0.
Initial moles	0.02	1.82	0.18	0.18	0.8

Iteration #	0	1	2	3	Final
Comp.					
N_2	0.8	0.8	0.8	0.8	0.8
CO	0.02	0.077	0.145	0.145	0.14502
CO_2	0.18	0.122	0.055	0.054	0.05497
FeO	1.82	1.87	1.945	1.945	1.94502
Fe	0.18	0.122	0.055	0.054	0.05497

TABLE 2.

Results for Example 2.

Input Data:

Component	$\Delta F_f/RT$	Initial Moles
H_2O	-27.499	0.65
CH_4	0.758	0.10
H_2	0.	0.15
O_2	0.	0.05
CO	-26.066	0.10
CO_2	-54.412	0.05
C	0.	4.75
Fe	0.	4.95
FeO	-28.549	0.05

Result after 12 iterations:

Component	Moles	Mole Fract. in Gas
H_2O	0.189	0.1857
CH_4	0.134	0.1319
H_2	0.541	0.5306
O_2	~0	-
CO	0.085	0.0834
CO_2	0.069	0.0681
C	4.710	
Fe	4.440	
FeO	0.586	

PROPOSITION II.

The evaluation of semi-infinite Fourier integrals by Simpson's rule may be accomplished by using the Fast Fourier Transform.

The presentation of the Fast Fourier Transform (FFT) algorithm by Cooley and Tukey[1,2] greatly reduced the time required relative to other algorithms for the evaluation of Fourier transforms. The FFT is essentially a trapezoidal[3] integration and evaluates the sum:

$$X(j) = \sum_{k=0}^{N-1} A(k)\exp(i2\pi jk/N) \qquad (1)$$

$$\text{for } j = 0,1,\ldots\ldots,N-1$$

The number of operations required to evaluate Eq. (1) in a straight forward manner is N^2, but using the FFT the number of operations goes like $N*\log_e(N)$.

To be considered here is the evaluation of the semi-infinite Fourier integral by Simpson's rule[3] for integration using an available FFT routine.

In terms of the real and imaginary parts, the integrals of interest are:

$$I_c(k) = \int_0^\infty f(x)\cos(kx)dx \qquad (2)$$

and

$$I_s(k) = \int_0^\infty f(x)\sin(kx)dx \qquad (3)$$

Therefore, it is necessary to show that Simpson's rule for a semi-infinite integral on a grid spacing of Δx may be written in terms of two trapezoidal integrations on grid spacings of Δx and $2\Delta x$. The integration is to be carried out far enough in x space so that $f(x) \longrightarrow 0$.

Simpson's rule on the semi-infinite interval, $0 \leq x < \infty$, may be written as:

$$F_s(\Delta x) = (2\Delta x/3)\left[\sum_{\text{odd } i}^{\infty} y_i + 2 \sum_{\text{even } i}^{\infty} y_i - \tfrac{1}{2}y_1 \right] \qquad (4)$$

where $y_i = y(x_i)$ for $i = 1,2,\ldots$, and $x_1 = 0$.
The trapezoid rule on the same interval may be written as:

$$F_t(\Delta x) = \Delta x\left[\sum_{\text{all } i}^{\infty} y_i - \tfrac{1}{2}y_1 \right] \qquad (5)$$

Now consider the trapezoid rule written on the odd points:

$$F_t(2\Delta x) = 2\Delta x\left[\sum_{\text{odd } i}^{\infty} y_i - \tfrac{1}{2}y_1 \right] \qquad (6)$$

Hence, Simpson's rule may be written in terms of Eqs. (5) and (6) as:

$$F_s(\Delta x) = \left[4F_t(\Delta x) - F_t(2\Delta x)\right]/3 \qquad (7)$$

Define the error of the integration rules as:

$$E_t(\Delta x) = F_t(\Delta x) - \int_0^\infty h(x)dx \qquad (8)$$

$$E_s(\Delta x) = F_s(\Delta x) - \int_0^\infty h(x)dx \qquad (9)$$

Then the relation between the errors is:

$$E_s(\Delta x) = \left[4E_t(\Delta x) - E_t(2\Delta x)\right]/3 \qquad (10)$$

The above equation does not imply that Simpson's rule is better than the trapezoid rule for the same interval size, Δx, or the converse. This result may be somewhat unexpected for Simpson's rule is usually "believed" to be better than the trapezoid rule. However, de Balbine and Franklin[4] have shown that on the infinite interval the trapezoid rule is always at least as good as Simpson's rule.

A trial calculation using Eq. (7) and an available FFT routine[5] was made on the following integrals:[6]

$$I_c(k) = \int_0^\infty x*\exp(-x)\cos(kx)dx \qquad (11)$$

$$I_s(k) = \int_0^\infty x*\exp(-x)\sin(kx)dx \qquad (12)$$

A total of 512 points were used on the interval $0 \le x \le 51.1$. Error norms were defined as:

$$E_c = \sum \left| I_c(k) - (1-k^2)/(1+k^2)^2 \right| \qquad (13)$$

$$E_s = \sum \left| I_s(k) - 2k/(1+k^2)^2 \right| \qquad (14)$$

where the sums are over the first 50 points in the k domain.

Simpson's rule was better for the real (cos) integral, its error norm was 0.00098 while for the trapezoid rule it was 0.041. But the trapezoid rule was better for the imaginary (sin) integral, its error norm was 0.00013 while for Simpson's rule it was 0.00054.

In conclusion, the semi-infinite Fourier integrals defined by Eqs.(2) and (3) may be evaluated by a Simpson's rule by carrying out two evaluations of the integrals on grid spacings of Δx and $2\Delta x$ using an available FFT routine. At the present time there are no criteria to determine which integration rule yields more accurate

results. This is an important research topic because the errors for the trial case were in the fourth decimal place. Some numerical studies require iterative Fourier inversions, such as in liquid state physics,[7] and knowing which integration rule to use would be helpful in reducing overall errors. The only "advice" for the present time is to run test cases on known functions that mimic the functions to be studied.

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PROPOSITION III.

The criterion of optimality for the design of any number of continuous stirred tank reactors in series to achieve a specified conversion for certain rate expressions is: The tangent to the inverse rate curve as a function of conversion at each reactor exit conversion must be parallel to the corresponding line through the two points, (x,y), designated by the inlet conversion of that reactor and the value of the inverse rate at the exit conversion, and the outlet conversion of that reactor and the value of the inverse rate at the outlet conversion of the next downstream reactor, as illustrated in Figure 2.

The optimal design of a reactor system is defined as minimum total volume for a specified conversion. It is the purpose of this work to describe a graphical procedure to minimize the total volume of a series of continuous stirred tank reactors (CSTR's) for certain inverse reaction rate expressions, f(x), as a function of conversion, x.

Consider f(x) to have the following properties:

$$f(x) > 0, \quad f'(x) > 0, \quad f''(x) \geq 0 \qquad (1)$$

where the prime (') denotes a derivative. This type of inverse rate expression is concave upward. Also, it is assumed that there is no volume change occurring.

The volume of a single CSTR for a given reaction of this type is:[1]

$$T = C_*(x_f - x_i)f(x_f) \qquad (2)$$

where T is the volume of the reactor divided by the volumetric feed rate, C_* is the concentration on which the conversions are based, x_f is the final conversion and x_i is the inlet conversion. Graphically, T/C_* is seen to be the area of a rectangle with dimensions $x_f - x_i$ and $f(x_f)$ as shown in Figure 1.

Consider now n CSTR's in series and designate the inlet conversion to the series as x_o and the outlet conversion as x_n. For unit C_* and volumetric feed rate, the volume of the system is:

$$V = \sum_{i=1}^{n} (x_i - x_{i-1})f(x_i) \qquad (3)$$

To minimize V, or find a stationary point of V with respect to the intermediate conversions, $(x)_{k=1}^{n-1}$, differentiate with respect to x_k:

$$\partial \bar{V}/\partial x_k = (x_k - x_{k-1})f'(x_k) + f(x_k) - f(x_{k+1}) \quad (4)$$

Equating to zero yields:

$$f'(x_k) = \left[f(x_{k+1}) - f(x_k)\right] / \left[x_k - x_{k-1}\right] \quad (5)$$

The above equation says that for the volume to be a stationary point, the tangent to $f(x)$ at x_k is parallel to the line through the two points $\left[x_{k-1}, f(x_k)\right]$ and $\left[x_k, f(x_{k+1})\right]$. This is illustrated in Figure 2. for a two reactor system. For a two reactor system this stationary point is a local minimum because $\partial^2 V/\partial x_1^2 > 0$.

Examining the nature of the stationary point by infinitesimal variations, $\lambda_i = (x - x_i)$, about itself did not yield conclusive results for the n reactor case, $n > 2$. The problem is that arbitrary variations λ_i are not allowed. Recognize that the intermediate conversions are not allowed to merge or cross. Specifically, the desire is to maintain n distinct reactors for $f(x)$ as described in Eq. (1) and mimic a plug flow reactor for the specified x_o and x_n.

However, consider the following physical argument. Suppose that the system can be made smaller by appropriate λ_i variations. There is a physical constraint to the minimum size of the system and that is the case

of the plug flow reactor. That implies that there must be a minimum somewhere with respect to the intermediate conversions, and the minimum is a stationary point characterized by Eq. (5). The system may always be made larger by making all intermediate conversions very close to x_o but still distinct.

To show that the local minimum is unique, suppose that the inlet and outlet conversions, x_o and x_1, to the first reactor are specified. This then determines the outlet conversion to the second reactor, because for the optimum to occur, the following relation must be satisfied:

$$\left[f(x_2) - f(x_1)\right] / \left[x_1 - x_o\right] = f'(x_1) \qquad (6)$$

There can only be one value of x_2 because:

$$F(x_2) = f(x_2) - f(x_1) = \int_{x_1}^{x_2} f'(z)dz \qquad (7)$$

where $f'(z) > 0$, hence, $F(x_2)$ is always increasing. Thus, in general, each outlet conversion is uniquely determined by specifying x_1. The problem then is the proper choice of x_1 to "fit" the desired number of reactors between x_o and x_n, and a trial and error procedure results.

Also, the overall conversions of each reactor, $\Delta x_i = x_i - x_{i-1}$, form a decreasing sequence. Using, in general, Eqs. (6) and (7):

$$\int_{x_i}^{x_{i+1}} f'(z)dz = (x_i - x_{i-1})f'(x_i) \qquad (8)$$

Because $f'(z) \geq f'(x_1)$ in the range of integration, the following is obtained:

$$(x_{i+1} - x_i)f'(x_i) \leq (x_i - x_{i-1})f'(x_i) \qquad (9)$$

Or, for the equality, the overall conversions are equal.

As an example of the volume minimization, consider the following rate expression:

$$r = kC^{1.2} = kC_*^{1.2}(1 - x)^{1.2} \qquad (10)$$

Specify $x_o = 0.$, $x_n = 0.90$, $kC_*^{1.2} = 1.$, and unit volumetric flow rate. The results for a two and four reactor system are presented in Figures 2. and 3., and Table 1. Note the parallel lines and the decreasing overall conversions for the reactors in these Figures.

This reactor design procedure may be applied to experimental rate data that have the proper behavior since line estimating techniques that yield good first derivative estimates have recently been developed.[3,4]

The optimal policy of a sequence of continuous stirred tank reactors has also been investigated by Aris.[5] The approach by Aris is different than the one presented in this proposition and involves dynamic programming. The procedure presented here appears to be more adaptable for general computer programming, but the final result for a reactor system will be independent of the method of solution.

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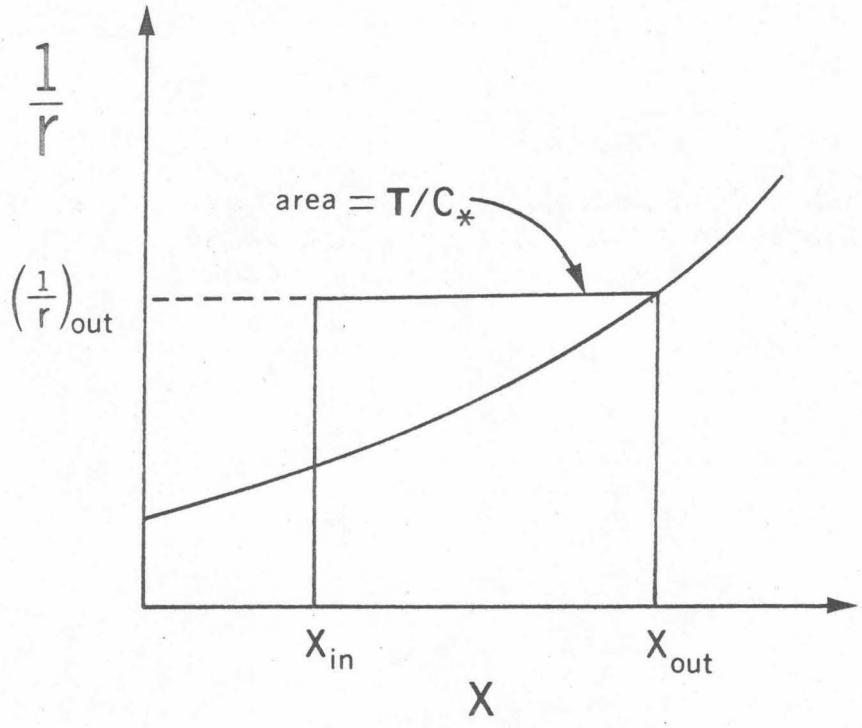

Figure 1. Graphical representation of the design equation for a continuous stirred tank reactor. (ref. 1)

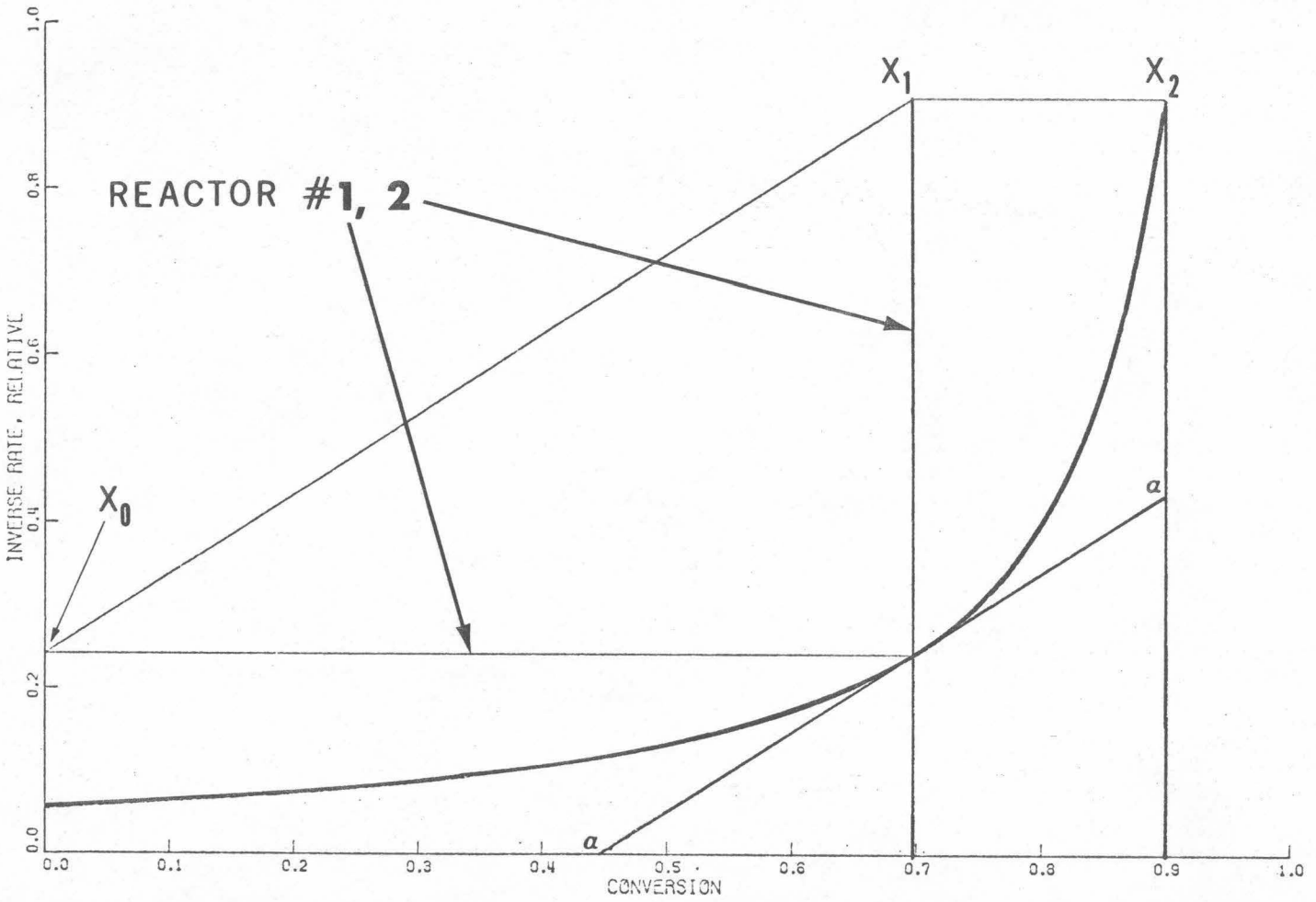

Figure 2. Graphical representation of the design of two CSTR's for minimum total volume. Note line *a,a* is parallel to line X_o, X_1

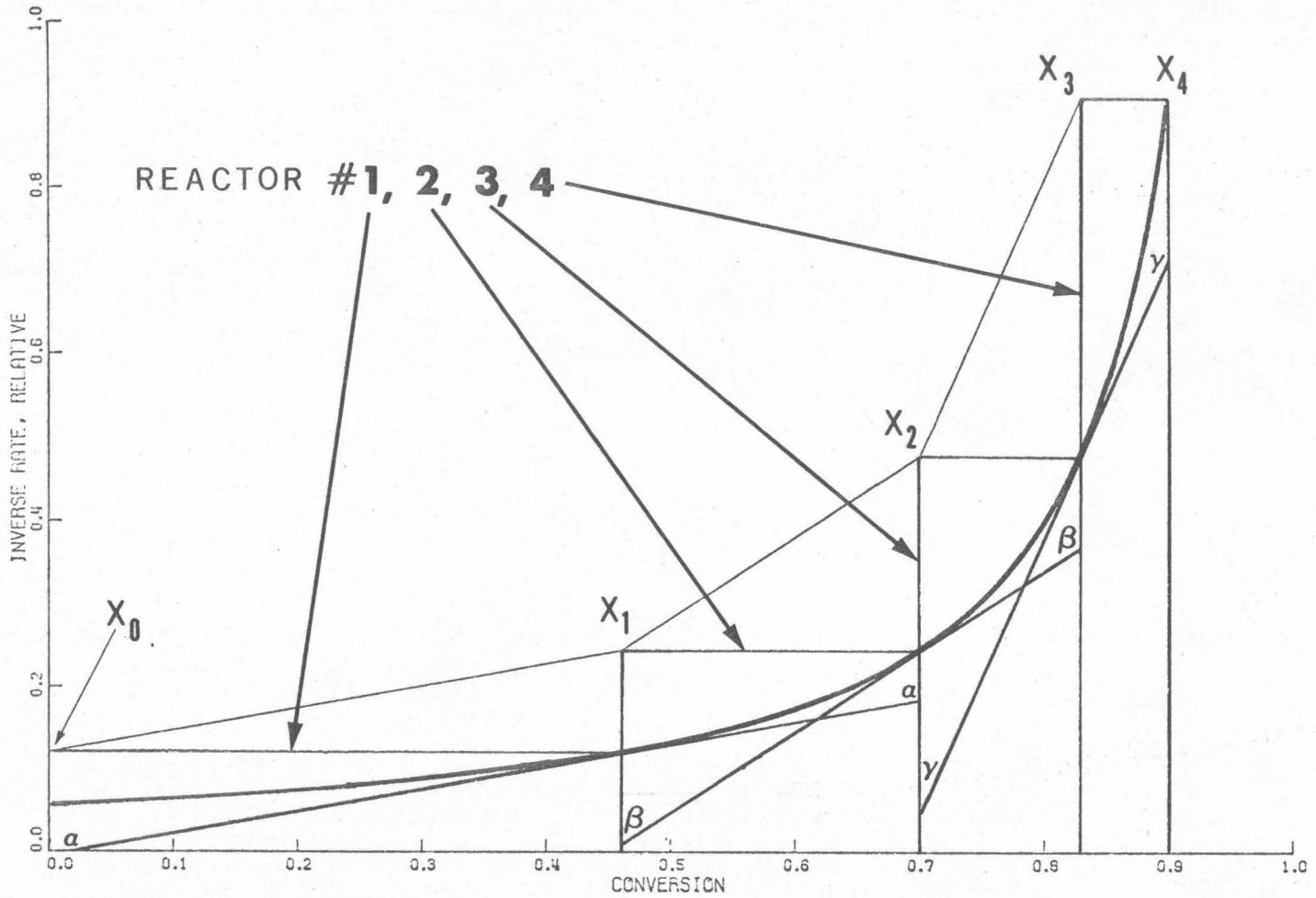

Figure 3. Graphical representation of the design of four CSTR's for minimum total volume. Note three sets of parallel lines.

TABLE 1.

Results of design calculation of two and four CSTR's for minimum total volume.

Inlet conversion = 0., Outlet conversion = 0.9

Unit kC_* and volumetric flow rate.

Inverse rate: f(x) = 1/(1-x)**1.2

Two reactors:

Intermediate conversion = 0.6977

Size reactor #1 = 2.933

Size #2/#1 = 1.0928

Total volume = 6.138

Four reactors:

Intermediate conversions: 0.4606, 0.7004, 0.8290

Size reactor #1 = 0.9633

Size normalized by #1: #2 = 1.054

#3 = 1.108

#4 = 1.163

Total volume = 4.179