CENTRAL RESEARCH LIBRARY
DOCUMENT COLLECTION

OAK RIDGE NATIONAL LABORATORY LIBRARY
3 4456 0023204 0

cy. 2

ORNL-4244
UC-4 – Chemistry

DIFFRACTION PATTERN AND STRUCTURE OF AQUEOUS AMMONIUM FLUORIDE SOLUTIONS

M. D. Danford

OAK RIDGE NATIONAL LABORATORY
CENTRAL RESEARCH LIBRARY
DOCUMENT COLLECTION
LIBRARY LOAN COPY
DO NOT TRANSFER TO ANOTHER PERSON
If you wish someone else to see this document, send in name with document and the library will arrange a loan.
UCN-7969
(3 3-67)

OAK RIDGE NATIONAL LABORATORY
operated by
UNION CARBIDE CORPORATION
for the
U.S. ATOMIC ENERGY COMMISSION

Printed in the United States of America. Available from Clearinghouse for Federal Scientific and Technical Information, National Bureau of Standards, U.S. Department of Commerce, Springfield, Virginia 22151
Price: Printed Copy $3.00; Microfiche $0.65

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

ORNL-4244

Contract No. W-7405-eng-26

CHEMISTRY DIVISION

DIFFRACTION PATTERN AND STRUCTURE OF AQUEOUS AMMONIUM FLUORIDE SOLUTIONS

M. D. Danford

JUNE 1968

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee
operated by
UNION CARBIDE CORPORATION
for the
U.S. ATOMIC ENERGY COMMISSION

OAK RIDGE NATIONAL LABORATORY LIBRARY

3 4456 0023204 0

ABSTRACT

The scattering of x-rays from the free surface of 1.18 M and 10.87 M solutions of NH_4F in water has been measured and analyzed at 25°C. In this report, both the raw data and the intensity and radial distribution functions derived from them are presented in tabulated form.

The data have been interpreted in terms of the proposed model for pure liquid water. Experimental intensity and radial distribution functions are compared to those for water, along with theoretical intensity functions calculated from the model parameters.

CONTENTS

ABSTRACT iii

1. INTRODUCTION 1

2. EXPERIMENTAL 1

   2.1 Diffractometer 1

   2.2 Materials and Sample Holders 2

   2.3 Data Collection 2

3. RESULTS 3

   3.1 Raw Data 3

   3.2 Reduced Intensity and Radial Distribution Functions 18

4. DISCUSSION 32

5. REFERENCES 38

1. INTRODUCTION

The diffraction pattern of liquid water[1] has been interpreted in terms of a simple model which gives a detailed description of the average arrangement of the oxygen atoms[2]. In this study, the radial distribution functions (RDF) of aqueous ammonium fluoride solutions are compared with the RDF of water. Both the raw data and the intensity and radial distribution functions derived from them are presented in tabulated form. The structural changes which occur when ammonium fluoride is added to water can be explained in terms of the proposed water model.

2. EXPERIMENTAL

The diffractometer, the procedure for data collection, the various corrections applied to the raw data, and their final evaluation have been discussed in detail elsewhere[3]. Only a short outline will be given in this section.

2.1 Diffractometer. The diffraction measurements were made with a diffractometer specially designed for the study of liquids. The diffraction pattern from the horizontal surface of the liquid sample was obtained with a divergent beam technique similar to the Bragg-Brentano system used for powder samples. The instrument provides for simultaneous angular motion of the x-ray tube and detector about a horizontal axis lying in the liquid surface. This method eliminates sample

holder absorption and scattering. Monochromatic MoKα radiation is obtained through the use of a bent and ground crystal monochromator mounted in the diffracted beam.

2.2 Materials and Sample Holders. The solutions were prepared from reagent grade ammonium fluoride*, and contained in a Lucite tray at 25°C. An air-tight cover with a window of 0.005" polystyrene foil prevented evaporation of the samples (Ref. 1, Fig. 1). Analysis of the two solutions studied yielded 1.18 M and 10.87 M NH_4F with densities of 1.01723 and 1.10223 g cm^{-3} respectively.

2.3 Data Collection. Scattered intensities were measured with various beam divergences, ranging from 0.5 degrees at the lowest scattering angles to 4 degrees at the highest angles. The times for a fixed number of counts, ranging from 100,000 to 700,000, were measured at 0.25 to 1 degree intervals in scattering angle. The accumulated counts were chosen to hold statistical errors in the reduced intensity function approximately uniform. The diffraction pattern showed interference throughout the observable range of the instrument[3] (to $s_{max} = (4\ \pi/\lambda)\ \sin\ \theta_{max} = 16$, θ being half the scattering angle).

---

*Allied Chemical Co., New York, N. Y.

3. RESULTS

In this section the experimental data and the results derived directly from them are tabulated in the format of the computer programs used. The procedure for data treatment falls into two stages. In the first, the raw data in various scattering angle ranges are placed on a consistent scale and appropriate corrections are applied[3]. In the second, data reduction and Fourier inversion are carried out. A brief description of each program is given in order to explain its function and clarify the nomenclature.

3.1 Raw Data. The output of this program is divided into two parts. The first presents the experimental data under the heading INPUT DATA. The second part, called TOTAL SCATTERED INTENSITIES, lists the various corrections applied to the raw data, and the corrected relative intensities, normalized to a certain size divergence slit. In the following table the definitions of various terms are given in the order of their appearance (some are omitted since they are self-explanatory).

INPUT DATA IN COUNTS PER MINUTE

SECTION	refers to the portion of scattering angles covered; each section is characterized by a certain size divergence slit and angular increment.
N	is a running index.

THETA is half the scattering angle in degrees.

COUNTS is the accumulated count, summed over all repeat runs, for each θ.

RUN is the sequence number of the repeat run over a particular section.

TOTAL SCATTERED INTENSITIES IN COUNTS PER MINUTE

S is the value $(4\ \pi/\lambda)\ \sin\ \theta$.

DIV. is the size of the divergence slit, in degrees.

I,RAW is the raw intensity, for each θ, averaged over all repeat runs.

BKG. is the measured background radiation.

POL. is the polarization correction[3].

PEN. is the penetration correction[3]; the atomic absorption coefficients for fluorine, oxygen, nitrogen and hydrogen were obtained from the literature [4].

I,CORR. is the corrected intensity, computed from
I,CORR = (I,RAW - BKG.)/(POL. x PEN.).

ERROR is the statistical error associated with I,CORR, computed from
ERROR = I,CORR x $(\text{COUNTS})^{1/2}$/COUNTS.

I,SCALED is the relative intensity, not as yet normalized to the independent atomic scattering, but corrected for background, polarization and absorption, and scaled to the size divergence slit listed in the caption of this column.

ERROR is the statistical error associated with I,SCALED.

NH4F*45.8H20 AT 25C.

SECTION 1, 0.500 DEGREE DIVERGENCE SLIT.

RAW INTENSITY IN COUNTS PER MINUTE

N	THETA	COUNTS	1 RUN	2 RUN
1	4.00	100000.00	2398.08	2452.18
2	4.25	100000.00	2641.31	2745.74
3	4.50	100000.00	3037.67	3162.56
4	4.75	100000.00	3584.23	3706.45
5	5.00	100000.00	4184.10	4374.45
6	5.25	100000.00	4965.24	5175.98
7	5.50	100000.00	5903.19	6053.27
8	5.75	100000.00	6784.26	7012.62
9	6.00	100000.00	7462.68	7763.98
10	6.25	100000.00	7886.43	8196.72
11	6.50	100000.00	7898.89	8250.83
12	6.75	100000.00	7552.87	7936.51
13	7.00	100000.00	6944.44	7256.89
14	7.25	100000.00	6369.43	6648.93
15	7.50	100000.00	5807.20	6329.11
16	7.75	100000.00	5376.34	5617.98
17	8.00	100000.00	4970.18	5263.16
18	8.25	100000.00	4708.10	4911.59
19	8.50	100000.00	4504.50	4681.65
20	8.75	100000.00	4374.45	4557.88
21	9.00	100000.00	4226.54	4409.17
22	9.25	100000.00	4074.98	4269.86
23	9.50	100000.00	3881.99	4045.31
24	9.75	100000.00	3568.88	3714.71
25	10.00	100000.00	3223.73	3342.25
26	10.25	100000.00	2818.49	2908.67
27	10.50	100000.00	2465.48	2553.63
28	10.75	100000.00	2130.38	2207.51
29	11.00	100000.00	1901.14	1955.42

NH4F*45.8H20 AT 25C.

SECTION 2, 2.000 DEGREE DIVERGENCE SLIT.

RAW INTENSITY IN COUNTS PER MINUTE

N	THETA	COUNTS	1 RUN	2 RUN
1	10.00	200000.00	22935.79	22779.05
2	10.50	200000.00	17762.00	17699.11
3	11.00	200000.00	14164.31	14204.55
4	11.50	200000.00	12254.90	12210.01
5	12.00	200000.00	11210.76	11273.96
6	12.50	200000.00	10834.24	10787.48
7	13.00	200000.00	10626.99	10570.82
8	13.50	200000.00	10416.66	10405.83
9	14.00	200000.00	10193.68	10224.95
10	14.50	200000.00	9832.84	9891.20
11	15.00	200000.00	9442.87	9487.66
12	15.50	200000.00	9017.13	8944.54
13	16.00	200000.00	8389.26	8403.36
14	16.50	200000.00	7806.40	7800.31
15	17.00	200000.00	7178.75	7173.60
16	17.50	200000.00	6574.62	6570.30
17	18.00	200000.00	6042.29	6045.95
18	18.50	200000.00	5595.97	5546.31
19	19.00	200000.00	5202.91	5149.33
20	19.50	200000.00	4873.29	4837.93
21	20.00	200000.00	4614.67	4597.70
22	20.50	200000.00	4416.96	4363.00
23	21.00	200000.00	4219.41	4205.21
24	21.50	200000.00	4051.86	4045.31
25	22.00	200000.00	3910.83	3872.97
26	22.50	200000.00	3721.62	3721.62
27	23.00	200000.00	3547.36	3542.33
28	23.50	200000.00	3368.14	3369.27
29	24.00	200000.00	3182.69	3156.57
30	24.50	200000.00	2980.63	2975.31
31	25.00	200000.00	2790.18	2777.78
32	25.50	200000.00	2596.05	2584.65
33	26.00	200000.00	2422.48	2405.00

NH4F*45.8H20 AT 25C.

SECTION 3, 4.000 DEGREE DIVERGENCE SLIT.

RAW INTENSITY IN COUNTS PER MINUTE

N	THETA	COUNTS	1 RUN	2 RUN	3 RUN	4 RUN	5 RUN	6 RUN	7 RUN
1	25.00	400000.00	7067.14	7017.54	6787.33	6703.91	6936.41	6920.41	6928.41
2	25.50	400000.00	6600.66	6607.93	6389.78	6302.52	6571.74	6507.59	6493.50
3	26.00	400000.00	6289.31	6217.61	6018.05	5982.05	6122.45	6122.45	6147.54
4	26.50	400000.00	5934.72	5808.32	5649.71	5617.98	5785.92	5719.73	5763.69
5	27.00	400000.00	5547.85	5459.51	5305.04	5267.78	5434.78	5386.00	5420.05
6	27.50	400000.00	5215.12	5172.41	5033.55	4938.27	5084.74	5123.82	5102.04
7	28.00	400000.00	4920.05	4901.96	4728.13	4724.41	4834.81	4889.97	4862.23
8	28.50	400000.00	4555.81	4636.79	4521.48	4494.38	4626.06	4583.65	4524.89
9	29.00	400000.00	4343.11	4415.01	4276.55	4225.35	4376.37	4395.60	4369.99
10	29.50	400000.00	4153.69	4172.46	4103.96	4043.13	4172.46	4149.38	4160.89
11	30.00	400000.00	3952.57	4016.06	3888.53	3851.09	3981.42	3978.78	3963.01
12	30.50	400000.00	3759.40	3828.97	3717.47	3694.58	3828.97	3828.97	3809.52
13	31.00	400000.00	3629.76	3642.99	3539.82	3523.19	3631.96	3634.16	3623.19
14	31.50	400000.00	3445.31	3494.47	3384.10	3363.23	3442.34	3458.21	3448.28
15	32.00	400000.00	3297.61	3300.33	3231.02	3220.61	3289.47	3302.15	3267.97
16	32.50	400000.00	3110.42	3154.57	3095.98	3031.83	3123.37	3123.37	3118.50
17	33.00	400000.00	2985.07	2971.77	2911.21	2873.56	2967.36	2973.24	2968.83
18	33.50	400000.00	2801.12	2836.88	2756.09	2749.77	2801.12	2814.26	2811.62
19	34.00	400000.00	2661.34	2712.48	2615.52	2579.54	2666.67	2671.42	2667.85
20	34.50	400000.00	2538.07	2553.19	2496.88	2470.15	2557.54	2561.91	2543.45
21	35.00	400000.00	2409.64	2427.18	2386.63	2323.78	2412.55	2434.08	2420.33
22	35.50	400000.00	2308.14	2318.39	2259.89	2245.51	2313.92	2321.98	2311.25
23	36.00	400000.00	2212.39	2221.40	2164.50	2126.91	2218.93	2209.94	2230.48
24	36.50	400000.00	2114.16	2140.56	2079.00	2057.61	2124.65	2128.41	2119.39
25	37.00	400000.00	2040.82	2049.88	1999.33	1970.44	2037.35	2035.28	2060.44
26	37.50	400000.00	1970.44	1993.36	1941.12	1897.39	1979.54	1982.82	1985.44
27	38.00	400000.00	1917.55	1915.71	1892.74	1849.00	1916.93	1928.64	1907.79
28	38.50	400000.00	1855.29	1892.15	1823.15	1795.33	1868.58	1867.41	1869.74
29	39.00	400000.00	1794.53	1808.86	1781.47	1739.63	1818.73	1810.50	1807.23
30	39.50	400000.00	1756.70	1770.96	1732.10	1694.44	1763.15	1766.26	1778.83
31	40.00	400000.00	1713.80	1719.20	1676.45	1653.35	1718.71	1727.12	1712.82
32	40.50	400000.00	1670.84	1685.39	1651.53	1614.64	1678.32	1680.20	1671.77
33	41.00	400000.00	1646.09	1649.26	1623.82	1599.82	1652.89	1658.37	1646.99
34	41.50	400000.00	1601.92	1612.47	1588.98	1533.35	1599.57	1614.64	1605.57
35	42.00	400000.00	1572.33	1579.36	1546.39	1512.48	1578.53	1591.93	1569.45
36	42.50	400000.00	1541.98	1544.80	1510.57	1459.50	1545.20	1560.47	1527.49
37	43.00	400000.00	1495.89	1514.39	1482.95	1440.92	1507.16	1522.84	1505.27
38	43.50	400000.00	1468.43	1479.29	1459.50	1403.18	1469.51	1482.21	1477.10
39	44.00	400000.00	1455.66	1444.39	1420.45	1429.59	1449.28	1459.50	1441.27
40	44.50	400000.00	1410.44	1422.81	1399.91	1379.63	1419.78	1427.89	1418.78
41	45.00	400000.00	1386.96	1392.11	1374.57	1344.39	1404.82	1419.78	1394.05
42	45.50	400000.00	1373.15	1376.46	1381.22	1309.76	1374.57	1383.44	1383.76
43	46.00	400000.00	1353.64	1356.55	1347.10	1298.14	1360.85	1369.86	1355.32
44	46.50	400000.00	1340.93	1341.38	1306.90	1289.77	1338.99	1349.22	1342.58
45	47.00	400000.00	1323.19	1333.63	1298.42	1275.51	1330.67	1341.38	1330.97
46	47.50	400000.00	1324.50	1318.39	1290.05	1261.56	1322.75	1332.15	1320.13
47	48.00	400000.00	1320.13	1319.84	1285.07	1257.07	1318.97	1328.90	1318.10
48	48.50	400000.00	1298.28	1307.76	1280.14	1252.87	1315.50	1333.63	1304.06

NH4F*45.8H20 AT 25C.

SECTION 4, 4.000 DEGREE DIVERGENCE SLIT.

RAW INTENSITY IN COUNTS PER MINUTE

N	THETA	COUNTS	1 RUN	2 RUN	3 RUN	4 RUN	5 RUN	6 RUN	7 RUN
1	46.50	640000.00	1350.26	1361.47	1344.09	1340.93	1314.06	1350.80	1355.56
2	47.50	640000.00	1321.18	1335.65	1323.28	1324.50	1278.94	1329.08	1322.23
3	48.50	640000.00	1315.44	1325.38	1311.48	1298.28	1279.75	1309.24	1317.87
4	49.50	640000.00	1310.16	1317.87	1305.31	1294.92	1265.82	1303.95	1308.56
5	50.50	640000.00	1294.83	1317.35	1299.21	1308.90	1268.87	1299.21	1304.97
6	51.50	640000.00	1300.22	1315.10	1298.53	1314.49	1264.54	1296.51	1312.34
7	52.50	640000.00	1307.53	1314.92	1298.03	1308.47	1272.43	1303.95	1311.13
8	53.50	640000.00	1304.80	1316.66	1310.79	1310.19	1273.24	1308.90	1330.85
9	54.50	640000.00	1317.87	1338.51	1317.52	1314.06	1295.00	1311.48	1321.53
10	55.50	640000.00	1328.02	1348.44	1322.93	1342.73	1296.85	1328.73	1344.99
11	56.50	640000.00	1342.46	1358.70	1333.69	1344.54	1308.56	1339.76	1343.18
12	57.50	640000.00	1365.19	1367.61	1357.77	1354.55	1322.93	1359.99	1367.24
13	58.50	640000.00	1384.66	1404.30	1383.51	1377.41	1336.54	1377.22	1389.28
14	59.50	640000.00	1414.63	1428.98	1404.69	1400.07	1365.75	1413.43	1415.43
15	60.50	640000.00	1423.89	1452.43	1423.08	1418.44	1384.27	1435.96	1439.06
16	61.50	640000.00	1460.49	1485.00	1463.70	1466.28	1422.27	1462.63	1475.80
17	62.50	640000.00	1502.40	1521.61	1495.66	1491.42	1449.70	1498.58	1501.05
18	63.50	640000.00	1546.79	1563.48	1537.75	1543.81	1490.98	1534.92	1535.63
19	64.50	640000.00	1578.28	1596.42	1569.86	1569.24	1532.80	1582.03	1578.78
20	65.50	640000.00	1612.38	1629.73	1606.43	1603.21	1563.97	1620.75	1623.99

TOTAL SCATTERED INTENSITIES IN COUNTS PER MINUTE

NH4F*45.8H2O AT 25C.

				********** BEFORE NORMALIZATION **********						NORMALIZED TO 2.CC DEG.		
N	THETA	S	DIV.	I,RAW	BKG.	PCL.	PEN.	I,CORR.	ERROR	N	S	I,SCALED
1	4.00	1.233	0.50	2424.83	5.85	0.99	0.63	3885.67	12.29	1	1.233	13284.46
2	4.25	1.310	0.50	2692.52	5.85	0.99	0.61	4443.69	14.05	2	1.310	15192.21
3	4.50	1.387	0.50	3098.85	5.85	0.99	0.59	5265.07	16.65	3	1.387	18000.38
4	4.75	1.464	0.50	3644.31	5.85	0.99	0.58	6371.32	20.15	4	1.464	21782.45
5	5.00	1.541	0.50	4277.16	5.85	0.99	0.56	7690.44	24.32	5	1.541	26292.31
6	5.25	1.618	0.50	5068.42	5.85	0.98	0.55	9367.70	29.62	6	1.618	32026.57
7	5.50	1.695	0.50	5977.29	5.85	0.98	0.54	11350.28	35.89	7	1.695	38804.66
8	5.75	1.771	0.50	6896.55	5.85	0.98	0.52	13447.91	42.53	8	1.771	45976.10
9	6.00	1.848	0.50	7610.35	5.85	0.98	0.51	15230.95	48.16	9	1.848	52072.01
10	6.25	1.925	0.50	8038.59	5.85	0.98	0.50	16504.05	52.19	10	1.925	56424.55
11	6.50	2.002	0.50	8071.03	5.85	0.98	0.49	16991.16	53.73	11	2.002	58089.87
12	6.75	2.078	0.50	7739.94	5.85	0.97	0.48	16699.98	52.81	12	2.078	57094.40
13	7.00	2.155	0.50	7097.23	5.85	0.97	0.47	15687.62	49.61	13	2.155	53633.29
14	7.25	2.231	0.50	6506.18	5.85	0.97	0.46	14726.79	46.57	14	2.231	50348.39
15	7.50	2.308	0.50	6056.93	5.85	0.97	0.45	14034.11	44.38	15	2.308	47980.22
16	7.75	2.384	0.50	5494.50	5.85	0.97	0.44	13026.70	41.19	16	2.384	44536.05
17	8.00	2.461	0.50	5112.47	5.85	0.96	0.43	12398.30	39.21	17	2.461	42387.67
18	8.25	2.537	0.50	4807.69	5.85	0.96	0.42	11921.86	37.70	18	2.537	40758.82
19	8.50	2.614	0.50	4591.37	5.85	0.96	0.41	11638.23	36.80	19	2.614	39789.13
20	8.75	2.690	0.50	4464.29	5.85	0.96	0.40	11563.83	36.57	20	2.690	39534.76
21	9.00	2.766	0.50	4315.93	5.85	0.95	0.40	11420.58	36.12	21	2.766	39045.01
22	9.25	2.842	0.50	4170.14	5.85	0.95	0.39	11269.28	35.64	22	2.842	38527.74
23	9.50	2.918	0.50	3961.97	5.85	0.95	0.38	10930.72	34.57	23	2.918	37370.28
24	9.75	2.994	0.50	3640.34	5.85	0.95	0.37	10250.02	32.41	24	2.994	35043.06
25	10.00	3.070	0.50	3281.92	5.85	0.94	0.37	9427.95	29.81	25	3.070	32157.15
26	10.25	3.146	0.50	2862.87	5.85	0.94	0.36	8387.75	26.52	26	3.146	28676.27
27	10.50	3.222	0.50	2508.78	5.85	0.94	0.36	7494.41	23.70	27	3.222	25507.38
28	10.75	3.298	0.50	2168.26	5.85	0.94	0.35	6602.00	20.88	28	3.298	22571.11
29	11.00	3.374	0.50	1927.90	5.85	0.93	0.34	5982.02	18.92	29	3.374	20590.95
30	10.00	3.070	2.00	22857.15	7.37	0.94	0.75	32081.77	71.74			
31	10.50	3.222	2.00	17730.50	7.37	0.94	0.74	25392.63	56.78			
32	11.00	3.374	2.00	14184.40	7.37	0.93	0.73	20730.38	46.35			
33	11.50	3.525	2.00	12232.42	7.37	0.93	0.72	18246.64	40.80	30	3.525	18246.64
34	12.00	3.676	2.00	11242.27	7.37	0.92	0.71	17118.27	38.28	31	3.676	17118.27
35	12.50	3.827	2.00	10810.81	7.37	0.91	0.70	16805.56	37.58	32	3.827	16805.56
36	13.00	3.978	2.00	10598.84	7.37	0.91	0.69	16822.18	37.62	33	3.978	16822.18
37	13.50	4.128	2.00	10411.24	7.37	0.90	0.68	16872.77	37.73	34	4.128	16872.77
38	14.00	4.278	2.00	10209.29	7.37	0.89	0.68	16895.19	37.78	35	4.278	16895.19
39	14.50	4.427	2.00	9861.93	7.37	0.89	0.67	16665.85	37.27	36	4.427	16665.85
40	15.00	4.576	2.00	9465.21	7.37	0.88	0.66	16334.53	36.53	37	4.576	16334.53

N	THETA	S	DIV.	I,RAW	BKG.	POL.	PEN.	I,CORR.	ERROR
41	15.50	4.725	2.00	8950.69	7.37	0.87	0.65	15827.16	35.39
42	16.00	4.874	2.00	8396.30	7.37	0.86	0.64	15111.18	33.79
43	16.50	5.022	2.00	7803.36	7.37	0.86	0.63	14341.93	32.07
44	17.00	5.170	2.00	7176.18	7.37	0.85	0.63	13468.77	30.12
45	17.50	5.317	2.00	6572.46	7.37	0.84	0.62	12596.85	28.17
46	18.00	5.464	2.00	6044.12	7.37	0.83	0.61	11829.23	26.45
47	18.50	5.610	2.00	5571.03	7.37	0.82	0.61	11133.59	24.90
48	19.00	5.757	2.00	5175.98	7.37	0.82	0.60	10562.21	23.62
49	19.50	5.902	2.00	4855.55	7.37	0.81	0.59	10116.91	22.62
50	20.00	6.047	2.00	4606.17	7.37	0.80	0.59	9798.98	21.91
51	20.50	6.192	2.00	4389.81	7.37	0.79	0.58	9534.41	21.32
52	21.00	6.337	2.00	4212.30	7.37	0.78	0.57	9340.03	20.88
53	21.50	6.480	2.00	4048.58	7.37	0.77	0.57	9163.91	20.49
54	22.00	6.624	2.00	3891.81	7.37	0.77	0.56	8991.67	20.11
55	22.50	6.766	2.00	3721.62	7.37	0.76	0.56	8775.77	19.62
56	23.00	6.909	2.00	3544.84	7.37	0.75	0.55	8530.29	19.07
57	23.50	7.051	2.00	3368.70	7.37	0.74	0.55	8271.60	18.50
58	24.00	7.192	2.00	3169.57	7.37	0.73	0.54	7939.99	17.75
59	24.50	7.332	2.00	2977.96	7.37	0.72	0.54	7609.70	17.02
60	25.00	7.473	2.00	2783.97	7.37	0.72	0.53	7255.48	16.22
61	25.50	7.612	2.00	2590.34	7.37	0.71	0.53	6883.87	15.39
62	26.00	7.751	2.00	2413.71	7.37	0.70	0.53	6539.68	14.62
63	25.00	7.473	4.00	6898.93	5.98	0.72	0.73	13217.21	20.90
64	25.50	7.612	4.00	6489.29	5.98	0.71	0.72	12638.45	19.98
65	26.00	7.751	4.00	6119.02	5.98	0.70	0.72	12114.08	19.15
66	26.50	7.890	4.00	5743.82	5.98	0.69	0.72	11558.08	18.27
67	27.00	8.027	4.00	5394.47	5.98	0.68	0.71	11032.36	17.44
68	27.50	8.164	4.00	5088.41	5.98	0.68	0.71	10575.23	16.72
69	28.00	8.301	4.00	4832.09	5.98	0.67	0.71	10204.18	16.13
70	28.50	8.437	4.00	4563.09	5.98	0.66	0.71	9789.74	15.48
71	29.00	8.572	4.00	4342.16	5.98	0.65	0.70	9462.80	14.96
72	29.50	8.707	4.00	4135.22	5.98	0.64	0.70	9152.39	14.47
73	30.00	8.841	4.00	3946.33	5.98	0.64	0.70	8868.81	14.02
74	30.50	8.974	4.00	3781.43	5.98	0.63	0.69	8627.20	13.64
75	31.00	9.107	4.00	3631.66	5.98	0.62	0.69	8339.68	13.19
76	31.50	9.239	4.00	3432.59	5.98	0.62	0.69	8064.70	12.75
77	32.00	9.370	4.00	3271.18	5.98	0.61	0.69	7795.91	12.33
78	32.50	9.500	4.00	3107.77	5.98	0.60	0.69	7510.54	11.88
79	33.00	9.630	4.00	2947.90	5.98	0.60	0.68	7221.93	11.42
80	33.50	9.759	4.00	2795.25	5.98	0.59	0.68	6939.48	10.97
81	34.00	9.887	4.00	2652.52	5.98	0.58	0.68	6670.70	10.55
82	34.50	10.015	4.00	2530.85	5.98	0.58	0.68	6444.94	10.19
83	35.00	10.142	4.00	2401.11	5.98	0.57	0.68	6188.99	9.79
84	35.50	10.268	4.00	2296.08	5.98	0.57	0.67	5987.86	9.47
85	36.00	10.393	4.00	2196.48	5.98	0.56	0.67	5792.79	9.16

N	S	I,SCALED
38	4.725	15827.16
39	4.874	15111.18
40	5.022	14341.93
41	5.170	13468.77
42	5.317	12596.85
43	5.464	11829.23
44	5.610	11133.59
45	5.757	10562.21
46	5.902	10116.91
47	6.047	9798.98
48	6.192	9534.41
49	6.337	9340.03
50	6.480	9163.91
51	6.624	8991.67
52	6.766	8775.77
53	6.909	8530.29
54	7.051	8271.60
55	7.192	7939.99
56	7.332	7609.70
57	7.473	7225.87
58	7.612	6882.51
59	7.751	6567.66
60	7.890	6292.93
61	8.027	6006.70
62	8.164	5757.80
63	8.301	5555.78
64	8.437	5330.13
65	8.572	5152.13
66	8.707	4983.12
67	8.841	4828.72
68	8.974	4697.18
69	9.107	4540.63
70	9.239	4390.91
71	9.370	4244.57
72	9.500	4089.20
73	9.630	3932.06
74	9.759	3778.28
75	9.887	3631.94
76	10.015	3509.02
77	10.142	3369.67
78	10.268	3260.16
79	10.393	3153.95

N	THETA	S	DIV.	I,RAW	BKG.	POL.	PEN.	I,CORR.	ERROR
86	36.50	10.517	4.00	2108.48	5.98	0.56	0.67	5620.91	8.89
87	37.00	10.641	4.00	2026.55	5.98	0.55	0.67	5458.25	8.63
88	37.50	10.764	4.00	1961.54	5.98	0.55	0.67	5335.88	8.44
89	38.00	10.886	4.00	1903.04	5.98	0.54	0.67	5224.03	8.26
90	38.50	11.007	4.00	1852.45	5.98	0.54	0.67	5129.61	8.11
91	39.00	11.127	4.00	1794.04	5.98	0.54	0.66	5008.34	7.92
92	39.50	11.247	4.00	1751.02	5.98	0.53	0.66	4925.46	7.79
93	40.00	11.366	4.00	1702.13	5.98	0.53	0.66	4821.04	7.62
94	40.50	11.483	4.00	1664.03	5.98	0.53	0.66	4743.05	7.50
95	41.00	11.600	4.00	1637.47	5.98	0.53	0.66	4694.09	7.42
96	41.50	11.716	4.00	1592.93	5.98	0.52	0.66	4589.41	7.26
97	42.00	11.831	4.00	1563.54	5.98	0.52	0.66	4524.59	7.15
98	42.50	11.946	4.00	1524.74	5.98	0.52	0.66	4428.67	7.00
99	43.00	12.059	4.00	1495.16	5.98	0.52	0.66	4355.99	6.89
100	43.50	12.171	4.00	1461.99	5.98	0.52	0.66	4269.35	6.75
101	44.00	12.283	4.00	1442.12	5.98	0.52	0.66	4218.43	6.67
102	44.50	12.393	4.00	1411.13	5.98	0.52	0.66	4131.89	6.53
103	45.00	12.503	4.00	1387.72	5.98	0.52	0.66	4064.49	6.43
104	45.50	12.611	4.00	1368.22	5.98	0.52	0.66	4005.57	6.33
105	46.00	12.719	4.00	1348.16	5.98	0.52	0.66	3942.45	6.23
106	46.50	12.826	4.00	1329.08	5.98	0.52	0.66	3879.63	6.13
107	47.00	12.932	4.00	1318.52	5.98	0.52	0.66	3839.31	6.07
108	47.50	13.036	4.00	1308.77	5.98	0.52	0.66	3798.92	6.01
109	48.00	13.140	4.00	1305.74	5.98	0.52	0.66	3775.70	5.97
110	48.50	13.243	4.00	1298.45	5.98	0.52	0.66	3737.79	5.91
111	46.50	12.826	4.00	1345.56	5.98	0.52	0.66	3927.94	4.91
112	47.50	13.036	4.00	1318.53	5.98	0.52	0.66	3827.36	4.78
113	48.50	13.243	4.00	1308.93	5.98	0.52	0.66	3768.25	4.71
114	49.50	13.445	4.00	1301.29	5.98	0.53	0.66	3705.39	4.63
115	50.50	13.644	4.00	1297.96	5.98	0.53	0.66	3646.55	4.56
116	51.50	13.838	4.00	1298.70	5.98	0.54	0.67	3591.26	4.49
117	52.50	14.028	4.00	1301.63	5.98	0.55	0.67	3534.74	4.42
118	53.50	14.214	4.00	1307.48	5.98	0.56	0.67	3479.49	4.35
119	54.50	14.395	4.00	1316.68	5.98	0.57	0.67	3427.06	4.28
120	55.50	14.572	4.00	1329.01	5.98	0.58	0.68	3377.17	4.22
121	56.50	14.744	4.00	1337.99	5.98	0.59	0.68	3313.94	4.14
122	57.50	14.913	4.00	1356.48	5.98	0.60	0.69	3270.05	4.09
123	58.50	15.076	4.00	1378.84	5.98	0.62	0.69	3231.09	4.04
124	59.50	15.235	4.00	1406.44	5.98	0.63	0.69	3200.17	4.00
125	60.50	15.389	4.00	1425.64	5.98	0.64	0.70	3146.67	3.93
126	61.50	15.539	4.00	1461.69	5.98	0.66	0.71	3127.21	3.91
127	62.50	15.684	4.00	1494.32	5.98	0.68	0.71	3096.85	3.87
128	63.50	15.824	4.00	1535.18	5.98	0.69	0.72	3080.36	3.85
129	64.50	15.959	4.00	1572.56	5.98	0.71	0.72	3053.87	3.82
130	65.50	16.090	4.00	1610.39	5.98	0.72	0.73	3026.00	3.78

N	S	I,SCALED
80	10.517	3060.37
81	10.641	2971.81
82	10.764	2905.18
83	10.886	2844.28
84	11.007	2792.87
85	11.127	2726.85
86	11.247	2681.72
87	11.366	2624.87
88	11.483	2582.41
89	11.600	2555.75
90	11.716	2498.76
91	11.831	2463.46
92	11.946	2411.24
93	12.059	2371.67
94	12.171	2324.49
95	12.283	2296.77
96	12.393	2249.65
97	12.503	2212.96
98	12.611	2180.88
99	12.719	2146.51
100	12.826	2115.54
101	12.932	2090.36
102	13.036	2066.44
103	13.140	2055.73
104	13.243	2033.86
105	13.445	1998.73
106	13.644	1966.99
107	13.838	1937.17
108	14.028	1906.68
109	14.214	1876.88
110	14.395	1848.59
111	14.572	1821.68
112	14.744	1787.58
113	14.913	1763.90
114	15.076	1742.89
115	15.235	1726.21
116	15.389	1697.35
117	15.539	1686.85
118	15.684	1670.48
119	15.824	1661.58
120	15.959	1647.29
121	16.090	1632.26

NH4F*3.57H20 AT 25C.

SECTION 1, 0.500 DEGREE DIVERGENCE SLIT.

RAW INTENSITY IN COUNTS PER MINUTE

N	THETA	COUNTS	1 RUN	2 RUN	3 RUN
1	4.00	150000.0C	2525.25	2551.02	2554.93
2	4.25	150000.0C	2774.69	2857.14	2873.56
3	4.50	150000.0C	3178.64	328C.84	3217.50
4	4.75	150000.0C	3673.77	3728.56	3748.13
5	5.00	150000.0C	4317.79	4413.06	4405.29
6	5.25	150000.0C	5122.95	5133.47	5170.63
7	5.50	150000.0C	6016.85	6157.63	6142.50
8	5.75	150000.0C	7062.15	7183.91	7267.44
9	6.00	150000.0C	8250.83	8333.33	8319.47
10	6.25	150000.0C	8912.66	9242.14	9208.11
11	6.50	150000.0C	9451.80	9523.81	9615.38
12	6.75	150000.0C	9157.51	9451.80	9433.96
13	7.00	150000.0C	8591.07	8756.57	8818.34
14	7.25	150000.0C	7727.97	7936.51	8000.00
15	7.50	150000.0C	7002.80	72C4.61	7183.91
16	7.75	150000.0C	6353.24	651C.42	6518.90
17	8.00	150000.0C	5834.30	5959.48	5966.59
18	8.25	150000.0C	5399.57	5561.73	5561.73
19	8.50	150000.0C	5159.96	53C2.23	5296.61
20	8.75	150000.0C	4960.32	5C76.14	5096.84
21	9.00	150000.0C	4950.49	5C5C.50	5050.50
22	9.25	150000.0C	4835.59	4926.11	4975.12
23	9.50	150000.0C	4690.43	483C.91	4821.60
24	9.75	150000.0C	4476.27	4591.37	4638.22
25	10.00	150000.0C	4142.5C	4273.50	4284.49
26	10.25	150000.0C	3736.92	3863.99	3849.11
27	10.50	150000.0C	3317.85	3394.43	3417.64
28	10.75	150000.0C	2871.91	2958.58	2965.60
29	11.00	150000.0C	2483.86	2597.40	2601.46
30	11.25	150000.0C	2224.20	23C4.15	2309.47
31	11.50	150000.0C	2008.03	2C62.71	2077.27
32	11.75	150000.0C	1832.84	1923.82	1936.48
33	12.00	150000.0C	1747.64	1797.91	1814.22

NH4F*3.57H20 AT 25C.

SECTION 2, 2.000 DEGREE DIVERGENCE SLIT.

RAW INTENSITY IN COUNTS PER MINUTE

N	THETA	COUNTS	1 RUN	2 RUN	3 RUN
1	11.00	300000.00	15974.45	15479.88	15552.11
2	11.50	300000.00	13227.52	12836.97	13020.84
3	12.00	300000.00	11876.48	11494.25	11668.61
4	12.50	300000.00	11235.95	10787.48	11001.10
5	13.00	300000.00	10989.01	10582.01	10729.61
6	13.50	300000.00	10741.14	10427.53	10604.46
7	14.00	300000.00	10638.30	10266.94	10449.32
8	14.50	300000.00	10362.69	10060.36	10256.41
9	15.00	300000.00	10080.64	9643.20	9881.42
10	15.50	300000.00	9606.15	9276.44	9442.87
11	16.00	300000.00	9066.18	8748.91	8992.80
12	16.50	300000.00	8503.40	8196.72	8424.60
13	17.00	300000.00	7880.22	7593.01	7770.01
14	17.50	300000.00	7278.02	7002.80	7163.32
15	18.00	300000.00	6680.02	6435.00	6618.13
16	18.50	300000.00	6184.29	5970.15	6101.28
17	19.00	300000.00	5707.76	5537.10	5611.67
18	19.50	300000.00	5330.49	5189.41	5257.62
19	20.00	300000.00	5020.08	4830.91	4955.40
20	20.50	300000.00	4730.37	4597.70	4686.04
21	21.00	300000.00	4504.50	4364.91	4480.29
22	21.50	300000.00	4330.88	4201.68	4269.85
23	22.00	300000.00	4156.27	4033.88	4115.22
24	22.50	300000.00	4000.00	3847.63	3941.66
25	23.00	300000.00	3808.07	3691.40	3790.75
26	23.50	300000.00	3645.64	3523.61	3599.71
27	24.00	300000.00	3465.00	3356.83	3432.89
28	24.50	300000.00	3262.64	3159.56	3241.49
29	25.00	300000.00	3070.31	3005.71	3034.90
30	25.50	300000.00	2871.09	2781.64	2847.38
31	26.00	300000.00	2683.12	2597.40	2653.93

NH4F*3.57H20 AT 25C.

SECTION 3, 4.000 DEGREE DIVERGENCE SLIT.

RAW INTENSITY IN COUNTS PER MINUTE

N	THETA	COUNTS	1 RUN	2 RUN	3 RUN	4 RUN	5 RUN	6 RUN	7 RUN	8 RUN	9 RUN
1	25.00	540000.00	7317.07	7407.41	7416.56	7343.94	7509.39	7398.27	7371.01	7042.25	6779.66
2	25.50	540000.00	6904.49	6993.01	6944.45	6912.44	7025.76	7009.35	7025.76	6571.74	6382.98
3	26.00	540000.00	6479.48	6578.95	6557.37	6514.66	6600.66	6543.07	6615.21	6243.50	6048.39
4	26.50	540000.00	6103.77	6185.57	6160.16	6109.98	6211.18	6166.50	6198.35	5882.35	5703.42
5	27.00	540000.00	5747.13	5802.71	5747.13	5819.59	5865.10	5741.62	5830.90	5499.54	5347.59
6	27.50	540000.00	5400.54	5459.51	5434.78	5420.05	5444.64	5459.51	5499.54	5172.41	5033.55
7	28.00	540000.00	5115.09	5181.35	5123.82	5110.73	5194.80	5128.20	5163.51	4838.71	4716.98
8	28.50	540000.00	4838.71	4914.00	4850.44	4846.53	4930.16	4862.23	4905.97	4640.37	4491.02
9	29.00	540000.00	4569.69	4636.79	4576.66	4597.70	4647.56	4618.94	4676.54	4363.63	4243.28
10	29.50	540000.00	4382.76	4411.76	4373.18	4363.63	4402.05	4373.18	4444.44	4181.18	4032.26
11	30.00	540000.00	4146.51	4187.02	4135.08	4137.93	4181.18	4178.27	4270.46	3960.40	3841.23
12	30.50	540000.00	3960.40	4010.70	3949.97	3978.78	4029.55	3994.67	4034.97	3804.69	3651.86
13	31.00	540000.00	3795.07	3807.11	3780.72	3816.79	3833.87	3833.87	3888.53	3649.64	3484.32
14	31.50	540000.00	3625.38	3685.50	3621.00	3605.77	3645.20	3625.38	3680.98	3466.20	3329.63
15	32.00	540000.00	3476.25	3486.35	3460.21	3440.37	3510.83	3470.21	3548.20	3300.33	3181.34
16	32.50	540000.00	3316.75	3333.33	3303.97	3275.11	3320.42	3320.42	3363.23	3157.89	3047.23
17	33.00	540000.00	3138.08	3181.34	3154.57	3134.80	3191.49	3167.90	3188.10	3019.63	2904.16
18	33.50	540000.00	3001.50	3056.55	3016.59	3001.50	3056.55	3019.63	3065.92	2898.55	2752.29
19	34.00	540000.00	2866.70	2904.16	2892.96	2850.36	2884.62	2870.81	2936.86	2722.32	2616.66
20	34.50	540000.00	2719.86	2739.73	2724.80	2703.92	2754.82	2732.24	2777.78	2603.04	2497.92
21	35.00	540000.00	2596.28	2623.52	2580.65	2587.32	2636.20	2597.40	2652.52	2494.80	2373.42
22	35.50	540000.00	2464.07	2493.77	2477.29	2472.19	2505.22	2489.63	2531.65	2388.53	2267.57
23	36.00	540000.00	2373.42	2398.08	2389.49	2350.18	2380.01	2367.80	2418.38	2277.90	2157.50
24	36.50	540000.00	2271.87	2309.47	2254.79	2252.25	2287.46	2282.24	2309.47	2187.39	2070.39
25	37.00	540000.00	2159.83	2203.45	2181.82	2169.98	2194.59	2181.82	2225.52	2103.05	1988.73
26	37.50	540000.00	2086.23	2120.14	2100.84	2086.23	2127.66	2118.64	2139.80	2029.77	1915.71
27	38.00	540000.00	2014.10	2051.98	2022.93	2033.21	2044.99	2042.21	2054.79	1962.07	1867.41
28	38.50	540000.00	1956.95	1984.13	1966.57	1964.64	1982.16	1983.47	2002.67	1900.54	1800.72
29	39.00	540000.00	1909.00	1934.24	1923.69	1901.74	1928.64	1927.40	1953.12	1841.62	1757.47
30	39.50	540000.00	1838.24	1887.39	1869.74	1849.00	1880.88	1873.83	1892.74	1802.88	1706.00
31	40.00	540000.00	1822.60	1853.57	1837.67	1802.88	1842.19	1837.11	1869.16	1770.43	1660.21
32	40.50	540000.00	1762.63	1802.88	1792.11	1773.57	1793.72	1803.43	1804.51	1716.25	1610.74
33	41.00	540000.00	1738.63	1753.87	1739.13	1731.60	1755.41	1757.47	1756.95	1693.00	1586.04
34	41.50	540000.00	1704.06	1729.60	1705.51	1696.35	1711.84	1707.46	1729.11	1664.82	1548.79
35	42.00	540000.00	1668.06	1692.52	1672.71	1651.07	1690.62	1678.32	1685.39	1611.60	1518.22
36	42.50	540000.00	1631.32	1658.37	1647.90	1624.26	1648.35	1648.35	1661.13	1589.40	1500.37
37	43.00	540000.00	1601.28	1621.18	1618.56	1593.63	1622.94	1607.29	1638.00	1563.72	1449.63
38	43.50	540000.00	1563.72	1597.87	1586.46	1551.59	1592.78	1598.72	1602.99	1544.00	1438.50
39	44.00	540000.00	1543.61	1555.21	1556.02	1531.00	1551.19	1566.17	1571.09	1511.72	1419.45
40	44.50	540000.00	1507.16	1532.57	1527.11	1502.25	1534.92	1536.49	1552.79	1486.25	1376.78
41	45.00	540000.00	1496.26	1517.83	1504.89	1490.31	1512.48	1519.76	1512.48	1466.63	1362.40
42	45.50	540000.00	1472.03	1484.41	1483.68	1460.92	1492.91	1486.99	1495.14	1437.81	1331.56
43	46.00	540000.00	1447.88	1468.07	1460.56	1438.50	1478.56	1479.29	1471.67	1425.52	1327.73
44	46.50	540000.00	1427.89	1458.08	1456.31	1425.18	1447.18	1455.96	1465.56	1396.32	1307.19
45	47.00	540000.00	1414.09	1426.53	1423.83	1406.80	1446.13	1431.64	1448.58	1385.36	1288.66
46	47.50	540000.00	1402.52	1426.87	1416.43	1387.93	1421.80	1427.21	1429.59	1374.89	1270.65
47	48.00	540000.00	1399.91	1414.09	1401.54	1386.32	1415.09	1420.12	1405.48	1368.93	1265.56
48	48.50	540000.00	1385.68	1415.76	1410.77	1381.53	1389.85	1414.76	1417.10	1363.02	1260.77

NH4F*3.57H20 AT 25C.

SECTION 4, 4.000 DEGREE DIVERGENCE SLIT.

RAW INTENSITY IN COUNTS PER MINUTE

N	THETA	COUNTS	1 RUN	2 RUN	3 RUN	4 RUN	5 RUN	6 RUN	7 RUN
1	46.50	700000.00	1345.53	1347.53	1359.44	1401.54	1362.21	1382.17	1329.61
2	47.50	700000.00	1316.48	1306.34	1321.00	1374.76	1333.87	1348.44	1299.38
3	48.50	700000.00	1307.02	1275.19	1311.13	1354.65	1308.22	1331.56	1286.51
4	49.50	700000.00	1283.37	1251.88	1297.86	1338.69	1296.51	1325.03	1272.91
5	50.50	700000.00	1286.67	1262.79	1290.82	1332.62	1291.66	1318.57	1272.59
6	51.50	700000.00	1280.90	1273.56	1296.01	1329.61	1302.25	1314.58	1262.95
7	52.50	700000.00	1288.33	1280.25	1303.95	1337.08	1297.02	1329.43	1261.03
8	53.50	700000.00	1294.00	1289.49	1299.21	1347.17	1311.99	1332.80	1280.25
9	54.50	700000.00	1308.56	1304.80	1318.04	1356.12	1326.26	1350.62	1280.90
10	55.50	700000.00	1325.38	1322.75	1334.94	1365.75	1339.94	1350.80	1307.36
11	56.50	700000.00	1328.37	1339.41	1338.33	1385.43	1358.14	1376.08	1312.16
12	57.50	700000.00	1351.53	1347.17	1359.80	1402.92	1377.98	1390.05	1328.90
13	58.50	700000.00	1356.85	1370.61	1376.46	1413.83	1402.52	1418.84	1345.53
14	59.50	700000.00	1387.35	1394.12	1403.11	1453.07	1413.43	1432.25	1374.19
15	60.50	700000.00	1415.63	1422.68	1418.44	1468.64	1440.30	1466.06	1400.36
16	61.50	700000.00	1440.51	1453.28	1461.78	1492.98	1467.57	1505.12	1417.23
17	62.50	700000.00	1471.89	1476.67	1482.80	1523.46	1495.44	1520.91	1451.38
18	63.50	700000.00	1502.18	1512.40	1512.86	1546.55	1533.51	1554.97	1472.97

TOTAL SCATTERED INTENSITIES IN COUNTS PER MINUTE

NH4F*3.57H20 AT 25C.

**********BEFORE NORMALIZATION**********

N	THETA	S	DIV.	I,RAW	BKG.	POL.	PEN.	I,CORR.	ERROR
1	4.00	1.233	0.50	2543.67	5.85	0.99	0.65	3964.77	10.24
2	4.25	1.310	0.50	2834.47	5.85	0.99	0.63	4544.55	11.73
3	4.50	1.387	0.50	3225.11	5.85	0.99	0.61	5316.95	13.73
4	4.75	1.464	0.50	3716.55	5.85	0.99	0.60	6297.61	16.26
5	5.00	1.541	0.50	4378.28	5.85	0.99	0.58	7622.14	19.68
6	5.25	1.618	0.50	5142.27	5.85	0.98	0.57	9193.22	23.74
7	5.50	1.695	0.50	6105.00	5.85	0.98	0.55	11203.38	28.93
8	5.75	1.771	0.50	7170.17	5.85	0.98	0.54	13500.41	34.86
9	6.00	1.848	0.50	8301.05	5.85	0.98	0.53	16029.26	41.39
10	6.25	1.925	0.50	9118.54	5.85	0.98	0.52	18049.84	46.60
11	6.50	2.002	0.50	9529.86	5.85	0.98	0.51	19329.27	49.91
12	6.75	2.078	0.50	9345.79	5.85	0.97	0.49	19415.20	50.13
13	7.00	2.155	0.50	8720.93	5.85	0.97	0.48	18548.46	47.89
14	7.25	2.231	0.50	7886.43	5.85	0.97	0.47	17166.23	44.32
15	7.50	2.308	0.50	7129.28	5.85	0.97	0.46	15875.66	40.99
16	7.75	2.384	0.50	6459.95	5.85	0.97	0.45	14711.44	37.98
17	8.00	2.461	0.50	5919.50	5.85	0.96	0.45	13781.80	35.58
18	8.25	2.537	0.50	5506.61	5.85	0.96	0.44	13102.78	33.83
19	8.50	2.614	0.50	5252.10	5.85	0.96	0.43	12768.64	32.97
20	8.75	2.690	0.50	5043.71	5.85	0.96	0.42	12524.61	32.34
21	9.00	2.766	0.50	5016.72	5.85	0.95	0.41	12721.13	32.85
22	9.25	2.842	0.50	4911.59	5.85	0.95	0.41	12714.18	32.83
23	9.50	2.918	0.50	4780.11	5.85	0.95	0.40	12628.21	32.61
24	9.75	2.994	0.50	4567.60	5.85	0.95	0.39	12311.26	31.79
25	10.00	3.070	0.50	4232.50	5.85	0.94	0.39	11635.68	30.04
26	10.25	3.146	0.50	3815.82	5.85	0.94	0.38	10696.29	27.62
27	10.50	3.222	0.50	3376.10	5.85	0.94	0.37	9646.80	24.91
28	10.75	3.298	0.50	2931.41	5.85	0.94	0.37	8535.70	22.04
29	11.00	3.374	0.50	2559.73	5.85	0.93	0.36	7593.50	19.61
30	11.25	3.450	0.50	2278.60	5.85	0.93	0.36	6885.07	17.78
31	11.50	3.525	0.50	2048.90	5.85	0.93	0.35	6304.64	16.28
32	11.75	3.601	0.50	1896.57	5.85	0.92	0.34	5942.16	15.34
33	12.00	3.676	0.50	1786.14	5.85	0.92	0.34	5697.11	14.71
34	11.00	3.374	2.00	15665.80	7.37	0.93	0.75	22445.87	40.98
35	11.50	3.525	2.00	13026.49	7.37	0.93	0.74	19034.04	34.75
36	12.00	3.676	2.00	11677.70	7.37	0.92	0.73	17404.15	31.78
37	12.50	3.827	2.00	11005.13	7.37	0.91	0.72	16731.98	30.55
38	13.00	3.978	2.00	10764.26	7.37	0.91	0.71	16697.43	30.49
39	13.50	4.128	2.00	10589.48	7.37	0.90	0.70	16760.82	30.60
40	14.00	4.278	2.00	10449.32	7.37	0.89	0.69	16877.19	30.81
41	14.50	4.427	2.00	10224.95	7.37	0.89	0.68	16853.57	30.77

NORMALIZED TO 2.00 DEG. SLITS

N	S	I,SCALED	ERROR
1	1.233	11933.79	30.81
2	1.310	13678.92	35.32
3	1.387	16003.82	41.32
4	1.464	18955.58	48.94
5	1.541	22942.36	59.24
6	1.618	27671.26	71.45
7	1.695	33721.75	87.07
8	1.771	40635.72	104.92
9	1.848	48247.48	124.57
10	1.925	54329.35	140.28
11	2.002	58180.40	150.22
12	2.078	58439.04	150.89
13	2.155	55830.17	144.15
14	2.231	51669.72	133.41
15	2.308	47785.14	123.38
16	2.384	44280.88	114.33
17	2.461	41482.71	107.11
18	2.537	39438.89	101.83
19	2.614	38433.13	99.23
20	2.690	37698.60	97.34
21	2.766	38290.12	98.86
22	2.842	38269.22	98.81
23	2.918	38010.43	98.14
24	2.994	37056.44	95.68
25	3.070	35022.98	90.43
26	3.146	32195.43	83.13
27	3.222	29036.52	74.97
28	3.298	25692.14	66.34
29	3.374	22651.01	59.01
30	3.450	20723.82	53.51
31	3.525	19005.39	49.00
32	3.601	17885.68	46.18
33	3.676	17276.12	44.28
34	3.827	16731.98	30.55
35	3.978	16697.43	30.49
36	4.128	16760.82	30.60
37	4.278	16877.19	30.81
38	4.427	16853.57	30.77

N	THETA	S	DIV.	I,RAW	BKG.	POL.	PEN.	I,CORR.	ERROR
42	15.00	4.576	2.00	9865.18	7.37	0.88	0.68	16594.92	30.30
43	15.50	4.725	2.00	9439.90	7.37	0.87	0.67	16206.71	29.59
44	16.00	4.874	2.00	8933.89	7.37	0.86	0.66	15654.42	28.58
45	16.50	5.022	2.00	8372.87	7.37	0.86	0.65	14974.32	27.34
46	17.00	5.170	2.00	7745.93	7.37	0.85	0.64	14139.19	25.81
47	17.50	5.317	2.00	7146.26	7.37	0.84	0.64	13313.99	24.31
48	18.00	5.464	2.00	6576.06	7.37	0.83	0.63	12504.62	22.83
49	18.50	5.610	2.00	6083.96	7.37	0.82	0.62	11807.63	21.56
50	19.00	5.757	2.00	5617.98	7.37	0.82	0.62	11128.00	20.32
51	19.50	5.902	2.00	5258.54	7.37	0.81	0.61	10630.59	19.41
52	20.00	6.047	2.00	4934.21	7.37	0.80	0.60	10180.02	18.59
53	20.50	6.192	2.00	4670.71	7.37	0.79	0.60	9834.20	17.95
54	21.00	6.337	2.00	4449.05	7.37	0.78	0.59	9559.34	17.45
55	21.50	6.480	2.00	4266.82	7.37	0.77	0.59	9355.05	17.08
56	22.00	6.624	2.00	4101.16	7.37	0.77	0.58	9174.89	16.75
57	22.50	6.766	2.00	3928.76	7.37	0.76	0.58	8967.32	16.37
58	23.00	6.909	2.00	3762.70	7.37	0.75	0.57	8761.51	16.00
59	23.50	7.051	2.00	3588.95	7.37	0.74	0.57	8524.50	15.56
60	24.00	7.192	2.00	3417.64	7.37	0.73	0.56	8279.39	15.12
61	24.50	7.332	2.00	3220.61	7.37	0.72	0.56	7956.37	14.53
62	25.00	7.473	2.00	3036.75	7.37	0.72	0.55	7649.39	13.97
63	25.50	7.612	2.00	2832.86	7.37	0.71	0.55	7274.55	13.28
64	26.00	7.751	2.00	2644.34	7.37	0.70	0.54	6921.25	12.64
65	25.00	7.473	4.00	7280.57	5.98	0.72	0.74	13668.67	18.60
66	25.50	7.612	4.00	6856.27	5.98	0.71	0.74	13081.86	17.80
67	26.00	7.751	4.00	6459.33	5.98	0.70	0.74	12524.66	17.04
68	26.50	7.890	4.00	6075.61	5.98	0.69	0.73	11971.10	16.29
69	27.00	8.027	4.00	5706.44	5.98	0.68	0.73	11424.50	15.55
70	27.50	8.164	4.00	5365.13	5.98	0.68	0.73	10912.75	14.85
71	28.00	8.301	4.00	5058.55	5.98	0.67	0.72	10452.29	14.22
72	28.50	8.437	4.00	4804.70	5.98	0.66	0.72	10083.85	13.72
73	29.00	8.572	4.00	4543.55	5.98	0.65	0.72	9684.09	13.18
74	29.50	8.707	4.00	4325.54	5.98	0.64	0.72	9361.28	12.74
75	30.00	8.841	4.00	4111.47	5.98	0.64	0.71	9033.13	12.29
76	30.50	8.974	4.00	3931.28	5.98	0.63	0.71	8766.59	11.93
77	31.00	9.107	4.00	3761.76	5.98	0.62	0.71	8512.24	11.58
78	31.50	9.239	4.00	3583.76	5.98	0.62	0.71	8226.83	11.20
79	32.00	9.370	4.00	3426.84	5.98	0.61	0.70	7978.32	10.86
80	32.50	9.500	4.00	3267.98	5.98	0.60	0.70	7714.19	10.50
81	33.00	9.630	4.00	3117.24	5.98	0.60	0.70	7458.26	10.15
82	33.50	9.759	4.00	2982.27	5.98	0.59	0.70	7229.76	9.84
83	34.00	9.887	4.00	2834.95	5.98	0.58	0.70	6960.95	9.47
84	34.50	10.015	4.00	2692.19	5.98	0.58	0.69	6692.82	9.11
85	35.00	10.142	4.00	2568.62	5.98	0.57	0.69	6462.63	8.79
86	35.50	10.268	4.00	2451.98	5.98	0.57	0.69	6240.93	8.49
87	36.00	10.393	4.00	2343.24	5.98	0.56	0.69	6030.84	8.21

N	S	I,SCALED	ERROR
39	4.576	16594.92	30.30
40	4.725	16206.71	29.59
41	4.874	15654.42	28.58
42	5.022	14974.32	27.34
43	5.170	14139.19	25.81
44	5.317	13313.99	24.31
45	5.464	12504.62	22.83
46	5.610	11807.63	21.56
47	5.757	11128.00	20.32
48	5.902	10630.59	19.41
49	6.047	10180.02	18.59
50	6.192	9834.20	17.95
51	6.337	9559.34	17.45
52	6.480	9355.05	17.08
53	6.624	9174.89	16.75
54	6.766	8967.32	16.37
55	6.909	8761.51	16.00
56	7.051	8524.50	15.56
57	7.192	8279.39	15.12
58	7.332	7956.37	14.53
59	7.473	7625.21	13.97
60	7.612	7274.63	13.28
61	7.751	6943.06	12.64
62	7.890	6657.03	9.06
63	8.027	6353.07	8.65
64	8.164	6068.49	8.26
65	8.301	5812.43	7.91
66	8.437	5607.55	7.63
67	8.572	5385.24	7.33
68	8.707	5205.73	7.08
69	8.841	5023.25	6.84
70	8.974	4875.03	6.63
71	9.107	4733.59	6.44
72	9.239	4574.87	6.23
73	9.370	4436.68	6.04
74	9.500	4289.80	5.84
75	9.630	4147.48	5.64
76	9.759	4020.41	5.47
77	9.887	3870.93	5.27
78	10.015	3721.82	5.06
79	10.142	3593.82	4.89
80	10.268	3470.53	4.72
81	10.393	3353.70	4.56

N	THETA	S	DIV.	I,RAW	BKG.	PEN.	POL.	I,CORR.	ERROR
88	36.50	10.517	4.00	2244.66	5.98	0.56	0.69	5839.51	7.95
89	37.00	10.641	4.00	2154.31	5.98	0.55	0.69	5661.25	7.70
90	37.50	10.764	4.00	2078.36	5.98	0.55	0.69	5514.75	7.50
91	38.00	10.886	4.00	2008.71	5.98	0.54	0.68	5378.90	7.32
92	38.50	11.007	4.00	1947.21	5.98	0.54	0.68	5259.31	7.16
93	39.00	11.127	4.00	1895.60	5.98	0.54	0.68	5161.34	7.02
94	39.50	11.247	4.00	1842.75	5.98	0.53	0.68	5055.05	6.88
95	40.00	11.366	4.00	1808.56	5.98	0.53	0.68	4995.61	6.80
96	40.50	11.483	4.00	1760.05	5.98	0.53	0.68	4892.11	6.66
97	41.00	11.600	4.00	1721.88	5.98	0.53	0.68	4813.14	6.55
98	41.50	11.716	4.00	1686.87	5.98	0.52	0.68	4738.93	6.45
99	42.00	11.831	4.00	1650.27	5.98	0.52	0.68	4656.30	6.34
100	42.50	11.946	4.00	1621.77	5.98	0.52	0.68	4592.86	6.25
101	43.00	12.059	4.00	1598.75	5.98	0.52	0.68	4512.94	6.14
102	43.50	12.171	4.00	1562.46	5.98	0.52	0.68	4448.69	6.05
103	44.00	12.283	4.00	1532.61	5.98	0.52	0.68	4370.93	5.95
104	44.50	12.393	4.00	1504.51	5.98	0.52	0.68	4294.95	5.84
105	45.00	12.503	4.00	1485.44	5.98	0.52	0.68	4241.73	5.77
106	45.50	12.611	4.00	1458.87	5.98	0.52	0.68	4164.12	5.67
107	46.00	12.719	4.00	1442.73	5.98	0.52	0.68	4113.60	5.60
108	46.50	12.826	4.00	1424.99	5.98	0.52	0.68	4055.79	5.52
109	47.00	12.932	4.00	1406.36	5.98	0.52	0.68	3992.90	5.43
110	47.50	13.036	4.00	1393.58	5.98	0.52	0.68	3944.25	5.37
111	48.00	13.140	4.00	1384.76	5.98	0.52	0.68	3904.44	5.31
112	48.50	13.243	4.00	1370.47	5.98	0.52	0.68	3875.11	5.27
113	46.50	12.826	4.00	1360.78	5.98	0.52	0.68	3872.27	4.63
114	47.50	13.036	4.00	1328.17	5.98	0.52	0.68	3758.32	4.49
115	48.50	13.243	4.00	1310.15	5.98	0.52	0.68	3676.85	4.39
116	49.50	13.445	4.00	1294.59	5.98	0.53	0.68	3593.96	4.30
117	50.50	13.644	4.00	1293.28	5.98	0.53	0.68	3542.82	4.23
118	51.50	13.838	4.00	1293.90	5.98	0.54	0.68	3489.32	4.17
119	52.50	14.028	4.00	1299.11	5.98	0.55	0.69	3441.11	4.11
120	53.50	14.214	4.00	1307.46	5.98	0.56	0.69	3394.56	4.06
121	54.50	14.395	4.00	1320.31	5.98	0.57	0.69	3353.49	4.01
122	55.50	14.572	4.00	1335.04	5.98	0.58	0.69	3311.41	3.96
123	56.50	14.744	4.00	1347.84	5.98	0.59	0.70	3259.54	3.90
124	57.50	14.913	4.00	1365.05	5.98	0.60	0.70	3214.34	3.84
125	58.50	15.076	4.00	1383.02	5.98	0.62	0.71	3166.40	3.78
126	59.50	15.235	4.00	1407.77	5.98	0.63	0.71	3130.71	3.74
127	60.50	15.389	4.00	1432.75	5.98	0.64	0.72	3092.09	3.70
128	61.50	15.539	4.00	1462.11	5.98	0.66	0.72	3059.86	3.66
129	62.50	15.684	4.00	1488.54	5.98	0.68	0.73	3018.92	3.61
130	63.50	15.824	4.00	1518.90	5.98	0.69	0.73	2983.93	3.57

N	S	I,SCALED	ERROR
82	10.517	3247.31	4.42
83	10.641	3148.18	4.28
84	10.764	3066.71	4.17
85	10.886	2991.16	4.07
86	11.007	2924.66	3.98
87	11.127	2870.18	3.91
88	11.247	2811.07	3.83
89	11.366	2778.02	3.78
90	11.483	2720.46	3.70
91	11.600	2676.55	3.64
92	11.716	2635.28	3.59
93	11.831	2589.33	3.52
94	11.946	2554.05	3.48
95	12.059	2509.61	3.42
96	12.171	2473.88	3.37
97	12.283	2430.64	3.31
98	12.393	2388.38	3.25
99	12.503	2358.79	3.21
100	12.611	2315.63	3.15
101	12.719	2287.54	3.11
102	12.826	2258.47	3.07
103	12.932	2220.42	3.02
104	13.036	2194.19	2.98
105	13.140	2171.23	2.95
106	13.243	2151.17	2.93
107	13.445	2099.02	2.51
108	13.644	2069.15	2.47
109	13.838	2037.90	2.44
110	14.028	2009.74	2.40
111	14.214	1982.56	2.37
112	14.395	1958.57	2.34
113	14.572	1933.99	2.31
114	14.744	1903.70	2.28
115	14.913	1877.12	2.24
116	15.076	1849.30	2.21
117	15.235	1828.46	2.19
118	15.389	1805.90	2.16
119	15.539	1787.08	2.14
120	15.684	1763.17	2.11
121	15.824	1742.73	2.08

3.2 Reduced Intensity and Radial Distribution Functions.

The output of this program is divided into two parts. The first part lists the reduced intensity functions, computed from

$$i\ (s) = C[(I(s) - I_c(s)] - \sum_i f_i^2\ (s) \qquad (3.2.1)$$

where I(s) is the relative intensity I,SCALED listed in section 3.1, I_c is the correction for incoherent or Compton scattering[3], C is the scaling factor[3], and $\sum_i f_i^2(s)$ is the part of the scattering ascribable to independent atoms, summed over the stoichiometric unit, $(NH_4)_yF_y(H_2O)_x$, with x = 0.9582, y = 0.0209 for the 1.18 M, and x = 0.6410, y = 0.1795 for the 10.87 M solution. The coherent and incoherent form factors for fluorine, oxygen, nitrogen and hydrogen were obtained from the literature[4]. The values of the relative intensities I(s) were extrapolated at low angle to θ equal to zero and I(O) equal to zero.

The second part of the program lists the radial distribution function (RDF) obtained by Fourier inversion of (3.2.1) according to

$$D(r) = 4\ \pi r^2 \rho_o + (2\ r/\pi) \int_o^{s_{max}} si(s)M(s)\sin(sr)ds \qquad (3.2.2)$$

where ρ_o is the average number density of stoichiometric units and M(s) is a modification function included to sharpen the features of the RDF[5]. The integral in (3.2.2) was evaluated numerically, using the trapezoidal method; summation was done with increments in s and r listed. The

modification function used in this study was

$$M(s) = [\sum_i f_i\ (s)]^{-2} \qquad (3.2.3)$$

where f refers to the coherent scattering amplitudes of fluorine, oxygen, nitrogen and hydrogen, and summation is again over the stoichiometric unit. This modification function removes the average breadth of the distribution of electron density in the atoms; it also changes the scale so that if i(s) is in electron units, i(s)M(s) and D(r) are in units characteristic of one stoichiometric unit of the sample.

The function D(r) represents a superposition of modified atomic pair distribution functions $D_{ij}(r)$ for the various kinds of atom pairs:

$$D(r) = \sum_i \sum_j D_{ij}(r)$$

The modification inherent in (3.2.2) of a given pair distribution function ρ_{ij} is expressed by[5]

$$D_{ij}(r) = 4\pi r \int_{-\infty}^{\infty} u\rho_{ij}(u)\ T_{ij}(u - r)\ du \qquad (3.2.4)$$

with

$$T_{ij}(r) = (1/\pi) \int_{o}^{s_{max}} f_i(s)f_j(s)M(s)\ \cos(sr)\ ds \qquad (3.2.5)$$

Thus D(r), the function accessible from experiment, is a kind of linear combination of true radial pair distributions which are convoluted with the known functions $T_{ij}(r)$ given by

(3.2.5). The function $(r/r_0)T(r)$ may be thought of as representing the modified appearance in D(r) of an idealized $\rho(r)$ having a single delta-function peak at $r = r_o$.

The reduced intensity curve, computed from (3.2.1), usually shows a more or less pronounced low frequency perturbation. This perturbation may be caused by incorrect data treatment, by the use of incorrect atomic scattering factors, or by an apparatus function. It will cause a peak at small distances r in the RDF. The perturbation can be removed by repeated Fourier transformations as discussed in Ref. 3. The basic assumption is here that there are no atom pair interactions in the RDF at distances r shorter than interatomic distances. In this study, all interactions in the RDF shorter than 2.3 Å were eliminated. This includes O—H and N—H interactions around 1 Å about which reliable information cannot be obtained by the x-ray diffraction method, because of the low scattering amplitude of the one electron in the hydrogen atom.

In the following table the definitions of the terms of the program are again given in the order of appearance.

REDUCED INTENSITY FUNCTIONS

S	is the value $(4\ \pi/\lambda)\ \sin\ \theta$.
SI*M 1	is the reduced intensity i(s) defined by (3.2.1), multiplied by s and by the modification function M(s) defined in (3.2.3).

SI*M 2 is the corrected[3] reduced intensity in the same terms as SI*M 1.

ERROR is the statistical error associated with SI*M 2.

DELTA SI*M is the difference between SI*M 1 and SI*M 2.

RADIAL DISTRIBUTION FUNCTIONS

R is the radial distance in angstrom.

D1 is the RDF D(r), obtained by Fourier inversion of SI*M 1.

G1 is the function $G(r) \equiv D(r)/4\ \pi r^2 \rho_o$, obtained from D1.

D2 is the RDF D(r), obtained by Fourier inversion of SI*M 2.

G2 is the function $G(r) \equiv D(r)/4\ \pi r^2 \rho_o$, obtained from D2.

ERROR is the statistical error associated with the quantity in the preceding column.

NH4F*45.8H20 AT 25C.

	S	SI*M 1	SI*M 2	ERRCR	DELTA SI*M
2	0.077	-0.050400	-0.103255	0.000066	0.052855
3	0.154	-0.099710	-0.204901	0.000265	0.105191
4	0.231	-0.147900	-0.304247	0.000600	0.156347
5	0.309	-0.195100	-0.400621	0.001074	0.205521
6	0.386	-0.241100	-0.492611	0.001691	0.251511
7	0.463	-0.286000	-0.579439	0.002459	0.293439
8	0.540	-0.329800	-0.660210	0.003386	0.330410
9	0.617	-0.372400	-0.734479	0.004482	0.362079
10	0.694	-0.413700	-0.802058	0.005759	0.388358
11	0.771	-0.453900	-0.863256	0.007261	0.409356
12	0.848	-0.492400	-0.917514	0.008951	0.425114
13	0.925	-0.529300	-0.964883	0.010870	0.435583
14	1.002	-0.564500	-1.004984	0.013030	0.440484
15	1.079	-0.597700	-1.037338	0.015450	0.439639
16	1.156	-0.628900	-1.061875	0.018170	0.432975
17	1.233	-0.657600	-1.078444	0.000715	0.420844
18	1.310	-0.665200	-1.069180	0.000898	0.403980
19	1.387	-0.649300	-1.032669	0.001161	0.383369
20	1.464	-0.603500	-0.963473	0.001529	0.359974
21	1.541	-0.527000	-0.861503	0.002004	0.334503
22	1.618	-0.402000	-0.709345	0.002650	0.307345
23	1.695	-0.224400	-0.503041	0.003479	0.278641
24	1.771	0.001408	-0.247567	0.004478	0.248975
25	1.848	0.228600	0.010559	0.005486	0.218041
26	1.925	0.433800	0.246745	0.006421	0.187055
27	2.002	0.572600	0.415455	0.007137	0.157145
28	2.078	0.624600	0.494817	0.007556	0.129783
29	2.155	0.578500	0.473504	0.007652	0.104996
30	2.231	0.527700	0.444086	0.007730	0.083614
31	2.308	0.515700	0.450950	0.007952	0.064750
32	2.384	0.433700	0.385390	0.007936	0.048310
33	2.461	0.408900	0.375445	0.008125	0.033454
34	2.537	0.406300	0.385645	0.008396	0.020655
35	2.614	0.443700	0.433484	0.008808	0.010216
36	2.690	0.530700	0.527383	0.009396	0.003317
37	2.766	0.611600	0.611067	0.009964	0.000533
38	2.842	0.693500	0.691599	0.010540	0.001901
39	2.918	0.725700	0.719142	0.010970	0.006558
40	2.994	0.647300	0.634391	0.011020	0.012909
41	3.070	0.495900	0.476824	0.010850	0.019076
42	3.146	0.252300	0.228648	0.010330	0.023652
43	3.222	0.003596	-0.022573	0.009863	0.026169
44	3.298	-0.257300	-0.284587	0.009272	0.027287
45	3.374	-0.432100	-0.460582	0.008977	0.028482
46	3.525	-0.624500	-0.661323	0.006605	0.036823
47	3.676	-0.674800	-0.729092	0.007047	0.054293
48	3.827	-0.592200	-0.661940	0.007834	0.069740
49	3.978	-0.420700	-0.492968	0.008890	0.072268
50	4.128	-0.206300	-0.271434	0.010080	0.065134
51	4.278	0.031980	-0.027043	0.011340	0.059023
52	4.427	0.235600	0.177928	0.012560	0.057672
53	4.576	0.426000	0.368711	0.013790	0.057289
54	4.725	0.568400	0.511028	0.014930	0.057371
55	4.874	0.600000	0.535920	0.015800	0.064080
56	5.022	0.595700	0.513749	0.016640	0.081951
57	5.170	0.502500	0.393295	0.017290	0.109205
58	5.317	0.335800	0.193161	0.017750	0.142639
59	5.464	0.190300	0.006880	0.018310	0.183420
60	5.610	0.037930	-0.194901	0.018890	0.232831
61	5.757	-0.079840	-0.368501	0.019530	0.288661
62	5.902	-0.117900	-0.462364	0.020380	0.344464
63	6.047	-0.067770	-0.466237	0.021470	0.398467
64	6.192	0.031320	-0.419253	0.022670	0.450573
65	6.337	0.200000	-0.298929	0.023950	0.498929
66	6.480	0.401800	-0.137318	0.025360	0.539118
67	6.624	0.625000	0.055117	0.026810	0.569883

	S	SI*M 1	SI*M 2	ERROR	DELTA SI*M
68	6.766	0.788900	0.197193	0.028030	0.591707
69	6.909	0.921900	0.315790	0.029190	0.606110
70	7.051	1.030000	0.417924	0.030250	0.612076
71	7.192	1.004000	0.394409	0.030910	0.609591
72	7.332	0.942200	0.340746	0.031400	0.601454
73	7.473	0.767400	0.176448	0.031710	0.590952
74	7.612	0.624700	0.045326	0.031820	0.579374
75	7.751	0.498700	-0.067476	0.031870	0.566176
76	7.890	0.434500	-0.118024	0.023410	0.552524
77	8.027	0.315600	-0.225886	0.023490	0.541486
78	8.164	0.257900	-0.276557	0.023640	0.534357
79	8.301	0.303000	-0.226719	0.023880	0.529719
80	8.437	0.258900	-0.266841	0.023970	0.525741
81	8.572	0.316300	-0.206258	0.024220	0.522558
82	8.707	0.382600	-0.138500	0.024460	0.521100
83	8.841	0.470600	-0.049697	0.024680	0.520297
84	8.974	0.608500	0.091193	0.025000	0.517307
85	9.107	0.657800	0.147548	0.025140	0.510252
86	9.239	0.702800	0.203082	0.025270	0.499718
87	9.370	0.741500	0.254905	0.025350	0.486595
88	9.500	0.707500	0.237445	0.025310	0.470055
89	9.630	0.638000	0.189847	0.025190	0.448153
90	9.759	0.531600	0.110747	0.025000	0.420853
91	9.887	0.428400	0.038100	0.024820	0.390300
92	10.010	0.368700	0.009065	0.024720	0.359635
93	10.140	0.238400	-0.087743	0.024500	0.326143
94	10.270	0.195500	-0.095272	0.024440	0.290772
95	10.390	0.110100	-0.146755	0.024320	0.256855
96	10.520	0.078890	-0.142053	0.024310	0.220943
97	10.640	0.017010	-0.173549	0.024260	0.190559
98	10.760	0.006857	-0.156340	0.024350	0.163197
99	10.890	0.049950	-0.086147	0.024540	0.136097
100	11.010	0.100300	-0.012932	0.024730	0.113232
101	11.130	0.058700	-0.034780	0.024760	0.093480
102	11.250	0.082180	0.004236	0.024940	0.077944
103	11.370	0.054920	-0.011459	0.025020	0.066379
104	11.480	0.073230	0.015192	0.025160	0.058038
105	11.600	0.204400	0.154137	0.025520	0.050263
106	11.720	0.156300	0.112432	0.025540	0.043868
107	11.830	0.214300	0.174488	0.025730	0.039812
108	11.950	0.169600	0.132217	0.025780	0.037383
109	12.060	0.165500	0.129427	0.025890	0.036073
110	12.170	0.091040	0.056503	0.025900	0.034537
111	12.280	0.115000	0.082587	0.026130	0.032413
112	12.390	0.019340	-0.010804	0.026120	0.030144
113	12.500	-0.021410	-0.049712	0.026210	0.028302
114	12.610	-0.037590	-0.064514	0.026340	0.026924
115	12.720	-0.075910	-0.101469	0.026440	0.025559
116	12.830	-0.101000	-0.124896	0.026510	0.023896
117	12.930	-0.118100	-0.140404	0.026690	0.022304
118	13.040	-0.112500	-0.133380	0.026930	0.020881
119	13.140	-0.027530	-0.047485	0.027240	0.019955
120	13.240	-0.037490	-0.056549	0.027450	0.019059
121	13.450	-0.002176	-0.018668	0.022810	0.016492
122	13.640	0.026940	0.010369	0.023190	0.016571
123	13.840	0.071930	0.051025	0.023570	0.020905
124	14.030	0.096370	0.073684	0.023960	0.022686
125	14.210	0.096820	0.074985	0.024340	0.021835
126	14.390	0.112400	0.088770	0.024810	0.023630
127	14.570	0.106900	0.082655	0.025190	0.024245
128	14.740	-0.001800	-0.019319	0.025400	0.017519
129	14.910	-0.044480	-0.052571	0.025680	0.008091
130	15.080	-0.051520	-0.053555	0.026080	0.002035
131	15.240	-0.036020	-0.031116	0.026530	-0.004904
132	15.390	-0.177300	-0.160555	0.026790	-0.016745
133	15.540	-0.097990	-0.069188	0.027300	-0.028802
134	15.680	-0.104600	-0.070631	0.027640	-0.033969
135	15.820	0.019240	0.053773	0.028070	-0.034533
136	15.960	0.029180	0.066063	0.028460	-0.036884
137	16.090	0.013990	0.056243	0.028810	-0.042253

OBSERVED RADIAL DISTRIBUTION FUNCTIONS, INTERACTIONS FROM 0.0 A TO 2.30 A CORRECTED.

	R	G1	D1	G2	ERROR	D2	ERROR
1	0.0	0.100E 01	0.0	0.100E 01	0.0	0.0	0.0
2	0.050	0.325E 02	0.347E-01	-0.290E 00	0.44E 01	-0.310E-03	0.46E-02
3	0.100	0.298E 02	0.127E 00	-0.204E 00	0.36E 01	-0.872E-03	0.16E-01
4	0.150	0.256E 02	0.246E 00	-0.946E-01	0.26E 01	-0.909E-03	0.25E-01
5	0.200	0.204E 02	0.349E 00	0.313E-02	0.16E 01	0.534E-04	0.27E-01
6	0.250	0.148E 02	0.394E 00	0.615E-01	0.12E 01	0.164E-02	0.31E-01
7	0.300	0.928E 01	0.357E 00	0.711E-01	0.11E 01	0.273E-02	0.40E-01
8	0.350	0.444E 01	0.232E 00	0.423E-01	0.93E 00	0.221E-02	0.48E-01
9	0.400	0.657E 00	0.449E-01	-0.143E-02	0.71E 00	-0.974E-04	0.49E-01
10	0.450	-0.189E 01	-0.163E 00	-0.353E-01	0.62E 00	-0.305E-02	0.53E-01
11	0.500	-0.319E 01	-0.340E 00	-0.440E-01	0.60E 00	-0.470E-02	0.64E-01
12	0.550	-0.344E 01	-0.444E 00	-0.275E-01	0.57E 00	-0.355E-02	0.74E-01
13	0.600	-0.292E 01	-0.448E 00	0.173E-02	0.50E 00	0.266E-03	0.76E-01
14	0.650	-0.197E 01	-0.354E 00	0.262E-01	0.46E 00	0.472E-02	0.83E-01
15	0.700	-0.876E 00	-0.183E 00	0.331E-01	0.45E 00	0.692E-02	0.95E-01
16	0.750	0.131E 00	0.315E-01	0.206E-01	0.42E 00	0.495E-02	0.10E 00
17	0.800	0.927E 00	0.253E 00	-0.244E-02	0.37E 00	-0.666E-03	0.10E 00
18	0.850	0.146E 01	0.451E 00	-0.222E-01	0.35E 00	-0.686E-02	0.11E 00
19	0.900	0.175E 01	0.604E 00	-0.278E-01	0.34E 00	-0.962E-02	0.12E 00
20	0.950	0.181E 01	0.698E 00	-0.169E-01	0.32E 00	-0.652E-02	0.13E 00
21	1.000	0.170E 01	0.727E 00	0.325E-02	0.29E 00	0.139E-02	0.13E 00
22	1.050	0.148E 01	0.695E 00	0.206E-01	0.29E 00	0.969E-02	0.13E 00
23	1.100	0.119E 01	0.614E 00	0.251E-01	0.28E 00	0.130E-01	0.15E 00
24	1.150	0.898E 00	0.507E 00	0.147E-01	0.27E 00	0.827E-02	0.15E 00
25	1.200	0.659E 00	0.405E 00	-0.426E-02	0.25E 00	-0.262E-02	0.15E 00
26	1.250	0.507E 00	0.338E 00	-0.203E-01	0.24E 00	-0.135E-01	0.16E 00
27	1.300	0.447E 00	0.322E 00	-0.239E-01	0.23E 00	-0.172E-01	0.17E 00
28	1.350	0.455E 00	0.354E 00	-0.131E-01	0.23E 00	-0.102E-01	0.18E 00
29	1.400	0.487E 00	0.407E 00	0.569E-02	0.21E 00	0.476E-02	0.18E 00
30	1.450	0.495E 00	0.445E 00	0.211E-01	0.21E 00	0.189E-01	0.19E 00
31	1.500	0.453E 00	0.435E 00	0.237E-01	0.21E 00	0.227E-01	0.20E 00
32	1.550	0.360E 00	0.369E 00	0.117E-01	0.20E 00	0.120E-01	0.21E 00
33	1.600	0.244E 00	0.267E 00	-0.782E-02	0.19E 00	-0.855E-02	0.21E 00
34	1.650	0.146E 00	0.170E 00	-0.231E-01	0.18E 00	-0.268E-01	0.21E 00
35	1.700	0.982E-01	0.121E 00	-0.244E-01	0.18E 00	-0.301E-01	0.22E 00
36	1.750	0.112E 00	0.146E 00	-0.102E-01	0.17E 00	-0.134E-01	0.23E 00
37	1.800	0.171E 00	0.237E 00	0.113E-01	0.17E 00	0.157E-01	0.23E 00
38	1.850	0.246E 00	0.359E 00	0.270E-01	0.17E 00	0.395E-01	0.24E 00
39	1.900	0.304E 00	0.469E 00	0.263E-01	0.16E 00	0.406E-01	0.25E 00
40	1.950	0.330E 00	0.536E 00	0.819E-02	0.16E 00	0.133E-01	0.25E 00
41	2.000	0.328E 00	0.560E 00	-0.173E-01	0.15E 00	-0.296E-01	0.26E 00
42	2.050	0.315E 00	0.565E 00	-0.343E-01	0.15E 00	-0.615E-01	0.27E 00
43	2.100	0.308E 00	0.580E 00	-0.300E-01	0.15E 00	-0.564E-01	0.28E 00
44	2.150	0.310E 00	0.612E 00	-0.363E-02	0.14E 00	-0.717E-02	0.28E 00
45	2.200	0.309E 00	0.638E 00	0.317E-01	0.14E 00	0.656E-01	0.28E 00
46	2.250	0.283E 00	0.613E 00	0.559E-01	0.14E 00	0.121E 00	0.29E 00
47	2.300	0.220E 00	0.498E 00	0.541E-01	0.13E 00	0.122E 00	0.30E 00
48	2.350	0.129E 00	0.305E 00	0.295E-01	0.13E 00	0.695E-01	0.31E 00
49	2.400	0.471E-01	0.116E 00	0.864E-02	0.13E 00	0.213E-01	0.31E 00
50	2.450	0.285E-01	0.729E-01	0.352E-01	0.12E 00	0.901E-01	0.32E 00
51	2.500	0.124E 00	0.332E 00	0.153E 00	0.12E 00	0.409E 00	0.33E 00
52	2.550	0.358E 00	0.995E 00	0.387E 00	0.12E 00	0.107E 01	0.33E 00
53	2.600	0.713E 00	0.206E 01	0.726E 00	0.12E 00	0.210E 01	0.33E 00
54	2.650	0.113E 01	0.338E 01	0.112E 01	0.11E 00	0.337E 01	0.34E 00
55	2.700	0.153E 01	0.475E 01	0.151E 01	0.11E 00	0.470E 01	0.35E 00
56	2.750	0.183E 01	0.590E 01	0.181E 01	0.11E 00	0.584E 01	0.35E 00
57	2.800	0.199E 01	0.665E 01	0.198E 01	0.11E 00	0.662E 01	0.36E 00
58	2.850	0.200E 01	0.692E 01	0.200E 01	0.11E 00	0.693E 01	0.37E 00
59	2.900	0.189E 01	0.678E 01	0.190E 01	0.10E 00	0.682E 01	0.37E 00
60	2.950	0.172E 01	0.640E 01	0.173E 01	0.10E 00	0.643E 01	0.37E 00
61	3.000	0.154E 01	0.594E 01	0.155E 01	0.10E 00	0.595E 01	0.38E 00
62	3.050	0.139E 01	0.554E 01	0.139E 01	0.99E-01	0.551E 01	0.39E 00
63	3.100	0.128E 01	0.525E 01	0.127E 01	0.97E-01	0.520E 01	0.40E 00
64	3.150	0.119E 01	0.506E 01	0.118E 01	0.95E-01	0.501E 01	0.40E 00
65	3.200	0.112E 01	0.490E 01	0.112E 01	0.94E-01	0.488E 01	0.41E 00
66	3.250	0.105E 01	0.474E 01	0.105E 01	0.93E-01	0.475E 01	0.42E 00

	R	G1	D1	G2	ERROR	D2	ERROR
67	3.300	0.986E 00	0.458E 01	0.993E 00	0.91E-01	0.462E 01	0.42E 00
68	3.350	0.933E 00	0.447E 01	0.940E 00	0.89E-01	0.450E 01	0.42E 00
69	3.400	0.904E 00	0.446E 01	0.906E 00	0.88E-01	0.447E 01	0.43E 00
70	3.450	0.902E 00	0.458E 01	0.898E 00	0.88E-01	0.456E 01	0.45E 00
71	3.500	0.922E 00	0.482E 01	0.915E 00	0.87E-01	0.478E 01	0.45E 00
72	3.550	0.951E 00	0.512E 01	0.945E 00	0.84E-01	0.509E 01	0.45E 00
73	3.600	0.976E 00	0.540E 01	0.975E 00	0.84E-01	0.539E 01	0.47E 00
74	3.650	0.989E 00	0.563E 01	0.993E 00	0.83E-01	0.565E 01	0.47E 00
75	3.700	0.990E 00	0.579E 01	0.997E 00	0.82E-01	0.583E 01	0.48E 00
76	3.750	0.986E 00	0.592E 01	0.993E 00	0.80E-01	0.596E 01	0.48E 00
77	3.800	0.985E 00	0.607E 01	0.988E 00	0.79E-01	0.609E 01	0.49E 00
78	3.850	0.992E 00	0.628E 01	0.990E 00	0.79E-01	0.627E 01	0.50E 00
79	3.900	0.101E 01	0.653E 01	0.100E 01	0.78E-01	0.650E 01	0.51E 00
80	3.950	0.102E 01	0.679E 01	0.102E 01	0.77E-01	0.677E 01	0.51E 00
81	4.000	0.103E 01	0.703E 01	0.103E 01	0.76E-01	0.704E 01	0.52E 00
82	4.050	0.103E 01	0.723E 01	0.104E 01	0.75E-01	0.726E 01	0.53E 00
83	4.100	0.103E 01	0.739E 01	0.104E 01	0.74E-01	0.744E 01	0.53E 00
84	4.150	0.103E 01	0.757E 01	0.103E 01	0.72E-01	0.760E 01	0.53E 00
85	4.200	0.103E 01	0.779E 01	0.104E 01	0.72E-01	0.780E 01	0.54E 00
86	4.250	0.105E 01	0.806E 01	0.104E 01	0.72E-01	0.805E 01	0.55E 00
87	4.300	0.106E 01	0.836E 01	0.106E 01	0.71E-01	0.834E 01	0.56E 00
88	4.350	0.107E 01	0.864E 01	0.107E 01	0.70E-01	0.863E 01	0.57E 00
89	4.400	0.107E 01	0.886E 01	0.107E 01	0.70E-01	0.886E 01	0.58E 00
90	4.450	0.106E 01	0.900E 01	0.107E 01	0.69E-01	0.902E 01	0.58E 00
91	4.500	0.105E 01	0.910E 01	0.106E 01	0.68E-01	0.912E 01	0.59E 00
92	4.550	0.104E 01	0.922E 01	0.105E 01	0.66E-01	0.924E 01	0.58E 00
93	4.600	0.104E 01	0.943E 01	0.104E 01	0.66E-01	0.943E 01	0.60E 00
94	4.650	0.106E 01	0.975E 01	0.105E 01	0.66E-01	0.972E 01	0.61E 00
95	4.700	0.107E 01	0.101E 02	0.107E 01	0.64E-01	0.101E 02	0.61E 00
96	4.750	0.109E 01	0.105E 02	0.109E 01	0.64E-01	0.105E 02	0.61E 00
97	4.800	0.109E 01	0.107E 02	0.109E 01	0.63E-01	0.107E 02	0.62E 00
98	4.850	0.108E 01	0.108E 02	0.108E 01	0.63E-01	0.109E 02	0.63E 00
99	4.900	0.105E 01	0.108E 02	0.106E 01	0.61E-01	0.108E 02	0.63E 00
100	4.950	0.102E 01	0.107E 02	0.102E 01	0.61E-01	0.107E 02	0.64E 00
101	5.000	0.992E 00	0.106E 02	0.990E 00	0.60E-01	0.106E 02	0.65E 00
102	5.050	0.971E 00	0.106E 02	0.967E 00	0.60E-01	0.105E 02	0.66E 00
103	5.100	0.960E 00	0.107E 02	0.956E 00	0.59E-01	0.106E 02	0.66E 00
104	5.150	0.956E 00	0.108E 02	0.954E 00	0.58E-01	0.108E 02	0.66E 00
105	5.200	0.955E 00	0.110E 02	0.956E 00	0.59E-01	0.110E 02	0.68E 00
106	5.250	0.953E 00	0.112E 02	0.955E 00	0.58E-01	0.112E 02	0.68E 00
107	5.300	0.946E 00	0.113E 02	0.948E 00	0.56E-01	0.114E 02	0.68E 00
108	5.350	0.937E 00	0.115E 02	0.938E 00	0.56E-01	0.115E 02	0.69E 00
109	5.400	0.928E 00	0.116E 02	0.928E 00	0.57E-01	0.115E 02	0.71E 00
110	5.450	0.922E 00	0.117E 02	0.920E 00	0.55E-01	0.117E 02	0.70E 00
111	5.500	0.919E 00	0.119E 02	0.917E 00	0.55E-01	0.118E 02	0.71E 00
112	5.550	0.917E 00	0.121E 02	0.918E 00	0.55E-01	0.121E 02	0.72E 00
113	5.600	0.916E 00	0.123E 02	0.918E 00	0.54E-01	0.123E 02	0.72E 00
114	5.650	0.914E 00	0.125E 02	0.917E 00	0.54E-01	0.125E 02	0.74E 00
115	5.700	0.911E 00	0.126E 02	0.914E 00	0.52E-01	0.127E 02	0.73E 00
116	5.750	0.909E 00	0.128E 02	0.911E 00	0.52E-01	0.129E 02	0.73E 00
117	5.800	0.910E 00	0.131E 02	0.910E 00	0.52E-01	0.131E 02	0.75E 00
118	5.850	0.914E 00	0.134E 02	0.914E 00	0.52E-01	0.134E 02	0.76E 00
119	5.900	0.922E 00	0.137E 02	0.921E 00	0.51E-01	0.137E 02	0.75E 00
120	5.950	0.930E 00	0.140E 02	0.930E 00	0.51E-01	0.141E 02	0.77E 00
121	6.000	0.937E 00	0.144E 02	0.939E 00	0.51E-01	0.144E 02	0.78E 00
122	6.050	0.945E 00	0.148E 02	0.947E 00	0.50E-01	0.148E 02	0.77E 00
123	6.100	0.953E 00	0.151E 02	0.955E 00	0.50E-01	0.152E 02	0.79E 00
124	6.150	0.964E 00	0.156E 02	0.965E 00	0.49E-01	0.156E 02	0.80E 00
125	6.200	0.978E 00	0.161E 02	0.978E 00	0.49E-01	0.160E 02	0.80E 00
126	6.250	0.995E 00	0.166E 02	0.994E 00	0.48E-01	0.166E 02	0.80E 00
127	6.300	0.101E 01	0.171E 02	0.101E 01	0.48E-01	0.171E 02	0.81E 00
128	6.350	0.102E 01	0.176E 02	0.102E 01	0.48E-01	0.176E 02	0.82E 00
129	6.400	0.103E 01	0.180E 02	0.103E 01	0.47E-01	0.180E 02	0.83E 00
130	6.450	0.103E 01	0.184E 02	0.103E 01	0.47E-01	0.184E 02	0.83E 00
131	6.500	0.103E 01	0.186E 02	0.103E 01	0.46E-01	0.186E 02	0.83E 00
132	6.550	0.103E 01	0.189E 02	0.103E 01	0.46E-01	0.189E 02	0.84E 00
133	6.600	0.103E 01	0.192E 02	0.103E 01	0.46E-01	0.192E 02	0.86E 00
134	6.650	0.104E 01	0.196E 02	0.104E 01	0.45E-01	0.196E 02	0.85E 00

	R	G1	D1	G2	ERROR	D2	ERROR
135	6.700	0.104E 01	0.200E 02	0.104E 01	0.45E-01	0.200E 02	0.86E 00
136	6.750	0.105E 01	0.204E 02	0.105E 01	0.45E-01	0.204E 02	0.88E 00
137	6.800	0.105E 01	0.208E 02	0.105E 01	0.45E-01	0.207E 02	0.88E 00
138	6.850	0.105E 01	0.210E 02	0.105E 01	0.44E-01	0.210E 02	0.88E 00
139	6.900	0.105E 01	0.213E 02	0.105E 01	0.43E-01	0.213E 02	0.88E 00
140	6.950	0.105E 01	0.216E 02	0.105E 01	0.44E-01	0.216E 02	0.90E 00
141	7.000	0.105E 01	0.219E 02	0.105E 01	0.44E-01	0.219E 02	0.91E 00
142	7.050	0.105E 01	0.223E 02	0.105E 01	0.43E-01	0.222E 02	0.92E 00
143	7.100	0.105E 01	0.226E 02	0.105E 01	0.42E-01	0.226E 02	0.91E 00
144	7.150	0.105E 01	0.229E 02	0.105E 01	0.42E-01	0.229E 02	0.92E 00
145	7.200	0.104E 01	0.230E 02	0.104E 01	0.43E-01	0.230E 02	0.95E 00
146	7.250	0.103E 01	0.231E 02	0.103E 01	0.42E-01	0.231E 02	0.94E 00
147	7.300	0.102E 01	0.232E 02	0.102E 01	0.41E-01	0.232E 02	0.94E 00
148	7.350	0.101E 01	0.233E 02	0.101E 01	0.41E-01	0.233E 02	0.95E 00
149	7.400	0.101E 01	0.235E 02	0.101E 01	0.41E-01	0.235E 02	0.96E 00
150	7.450	0.101E 01	0.239E 02	0.101E 01	0.40E-01	0.239E 02	0.96E 00
151	7.500	0.101E 01	0.242E 02	0.101E 01	0.41E-01	0.243E 02	0.98E 00
152	7.550	0.101E 01	0.246E 02	0.101E 01	0.40E-01	0.246E 02	0.98E 00
153	7.600	0.101E 01	0.248E 02	0.101E 01	0.39E-01	0.249E 02	0.97E 00
154	7.650	0.998E 00	0.249E 02	0.100E 01	0.40E-01	0.250E 02	0.10E 01
155	7.700	0.988E 00	0.250E 02	0.989E 00	0.39E-01	0.250E 02	0.98E 00
156	7.750	0.979E 00	0.251E 02	0.979E 00	0.39E-01	0.251E 02	0.10E 01
157	7.800	0.974E 00	0.253E 02	0.974E 00	0.39E-01	0.253E 02	0.10E 01
158	7.850	0.976E 00	0.257E 02	0.975E 00	0.38E-01	0.257E 02	0.10E 01
159	7.900	0.980E 00	0.261E 02	0.981E 00	0.39E-01	0.261E 02	0.10E 01
160	7.950	0.986E 00	0.266E 02	0.987E 00	0.38E-01	0.266E 02	0.10E 01
161	8.000	0.990E 00	0.270E 02	0.991E 00	0.38E-01	0.271E 02	0.11E 01
162	8.050	0.990E 00	0.274E 02	0.991E 00	0.37E-01	0.274E 02	0.10E 01
163	8.100	0.987E 00	0.276E 02	0.987E 00	0.37E-01	0.277E 02	0.10E 01
164	8.150	0.984E 00	0.279E 02	0.983E 00	0.37E-01	0.279E 02	0.10E 01
165	8.200	0.982E 00	0.282E 02	0.981E 00	0.37E-01	0.282E 02	0.11E 01
166	8.250	0.983E 00	0.285E 02	0.981E 00	0.37E-01	0.285E 02	0.11E 01
167	8.300	0.984E 00	0.289E 02	0.983E 00	0.36E-01	0.289E 02	0.11E 01
168	8.350	0.986E 00	0.294E 02	0.985E 00	0.37E-01	0.293E 02	0.11E 01
169	8.400	0.987E 00	0.297E 02	0.986E 00	0.35E-01	0.297E 02	0.11E 01
170	8.450	0.986E 00	0.300E 02	0.985E 00	0.36E-01	0.300E 02	0.11E 01
171	8.500	0.985E 00	0.304E 02	0.984E 00	0.35E-01	0.303E 02	0.11E 01
172	8.550	0.986E 00	0.308E 02	0.985E 00	0.35E-01	0.307E 02	0.11E 01
173	8.600	0.991E 00	0.313E 02	0.989E 00	0.35E-01	0.312E 02	0.11E 01
174	8.650	0.997E 00	0.319E 02	0.996E 00	0.34E-01	0.318E 02	0.11E 01
175	8.700	0.100E 01	0.325E 02	0.100E 01	0.36E-01	0.324E 02	0.12E 01
176	8.750	0.101E 01	0.330E 02	0.101E 01	0.34E-01	0.330E 02	0.11E 01
177	8.800	0.101E 01	0.334E 02	0.101E 01	0.35E-01	0.333E 02	0.11E 01
178	8.850	0.101E 01	0.336E 02	0.100E 01	0.33E-01	0.336E 02	0.11E 01
179	8.900	0.999E 00	0.338E 02	0.999E 00	0.35E-01	0.338E 02	0.12E 01
180	8.950	0.995E 00	0.340E 02	0.995E 00	0.33E-01	0.340E 02	0.11E 01
181	9.000	0.995E 00	0.344E 02	0.994E 00	0.34E-01	0.344E 02	0.12E 01
182	9.050	0.999E 00	0.349E 02	0.999E 00	0.33E-01	0.349E 02	0.12E 01
183	9.100	0.101E 01	0.356E 02	0.101E 01	0.33E-01	0.356E 02	0.12E 01
184	9.150	0.101E 01	0.362E 02	0.101E 01	0.33E-01	0.362E 02	0.12E 01
185	9.200	0.101E 01	0.367E 02	0.102E 01	0.33E-01	0.367E 02	0.12E 01
186	9.250	0.101E 01	0.370E 02	0.101E 01	0.33E-01	0.370E 02	0.12E 01
187	9.300	0.101E 01	0.371E 02	0.101E 01	0.32E-01	0.372E 02	0.12E 01
188	9.350	0.999E 00	0.373E 02	0.100E 01	0.33E-01	0.373E 02	0.12E 01
189	9.400	0.994E 00	0.375E 02	0.995E 00	0.32E-01	0.375E 02	0.12E 01
190	9.450	0.993E 00	0.379E 02	0.995E 00	0.32E-01	0.379E 02	0.12E 01
191	9.500	0.996E 00	0.384E 02	0.997E 00	0.32E-01	0.384E 02	0.12E 01
192	9.550	0.100E 01	0.389E 02	0.100E 01	0.32E-01	0.390E 02	0.12E 01
193	9.600	0.100E 01	0.395E 02	0.100E 01	0.31E-01	0.395E 02	0.12E 01
194	9.650	0.100E 01	0.399E 02	0.100E 01	0.32E-01	0.399E 02	0.13E 01
195	9.700	0.100E 01	0.402E 02	0.100E 01	0.31E-01	0.403E 02	0.13E 01
196	9.750	0.999E 00	0.405E 02	0.999E 00	0.31E-01	0.405E 02	0.13E 01
197	9.800	0.996E 00	0.408E 02	0.997E 00	0.30E-01	0.409E 02	0.12E 01
198	9.850	0.996E 00	0.413E 02	0.996E 00	0.31E-01	0.413E 02	0.13E 01
199	9.900	0.998E 00	0.418E 02	0.998E 00	0.30E-01	0.418E 02	0.13E 01
200	9.950	0.100E 01	0.423E 02	0.100E 01	0.31E-01	0.423E 02	0.13E 01
201	10.000	0.100E 01	0.428E 02	0.100E 01	0.30E-01	0.428E 02	0.13E 01

NH4F*3.57H20 AT 25C.

	S	SI*M 1	SI*M 2	ERRCR	DELTA SI*M
2	0.077	-0.050750	-0.108067	0.000057	0.057317
3	0.154	-0.100600	-0.213426	0.000227	0.112826
4	0.231	-0.149600	-0.314814	0.000513	0.165214
5	0.309	-0.197700	-0.411683	0.000919	0.213983
6	0.386	-0.244900	-0.503876	0.001447	0.258976
7	0.463	-0.291300	-0.591761	0.002105	0.300461
8	0.540	-0.336800	-0.674983	0.002898	0.338183
9	0.617	-0.381300	-0.752778	0.003836	0.371478
10	0.694	-0.424900	-0.824059	0.004929	0.399159
11	0.771	-0.467700	-0.887661	0.006215	0.419961
12	0.848	-0.509200	-0.942256	0.007662	0.433056
13	0.925	-0.549400	-0.987855	0.009301	0.438455
14	1.002	-0.588200	-1.025124	0.011150	0.436924
15	1.079	-0.625600	-1.055202	0.013230	0.429603
16	1.156	-0.661400	-1.078932	0.015560	0.417533
17	1.233	-0.695200	-1.096415	0.000505	0.401215
18	1.310	-0.710900	-1.091341	0.000635	0.380541
19	1.387	-0.710500	-1.065573	0.000811	0.355074
20	1.464	-0.690100	-1.014705	0.001045	0.324605
21	1.541	-0.637400	-0.926993	0.001375	0.289593
22	1.618	-0.552000	-0.803320	0.001800	0.251320
23	1.695	-0.413600	-0.625190	0.002378	0.211590
24	1.771	-0.221200	-0.393880	0.003113	0.172680
25	1.848	0.023550	-0.111196	0.004001	0.134746
26	1.925	0.260200	0.161651	0.004869	0.098549
27	2.002	0.457100	0.393424	0.005627	0.063676
28	2.078	0.548300	0.518396	0.006090	0.029904
29	2.155	0.536700	0.540495	0.006272	-0.003795
30	2.231	0.451500	0.487365	0.006243	-0.035865
31	2.308	0.368500	0.434189	0.006232	-0.065689
32	2.384	0.280100	0.370929	0.006205	-0.090829
33	2.461	0.213900	0.324692	0.006253	-0.110792
34	2.537	0.177300	0.302284	0.006382	-0.124984
35	2.614	0.197300	0.332251	0.006684	-0.134951
36	2.690	0.235000	0.377259	0.007036	-0.142260
37	2.766	0.371000	0.519738	0.007668	-0.148738
38	2.842	0.474800	0.629914	0.008219	-0.155114
39	2.918	0.569300	0.730125	0.008750	-0.160825
40	2.994	0.611100	0.775338	0.009139	-0.164238
41	3.070	0.550000	0.713510	0.009246	-0.163510
42	3.146	0.394900	0.552537	0.009091	-0.157637
43	3.222	0.174900	0.322072	0.008762	-0.147172
44	3.298	-0.103700	0.030714	0.008267	-0.134414
45	3.374	-0.386100	-0.263450	0.007841	-0.122650
46	3.450	-0.563900	-0.448784	0.007591	-0.115116
47	3.525	-0.737800	-0.624110	0.007407	-0.113690
48	3.601	-0.846900	-0.728629	0.007441	-0.118271
49	3.676	-0.890200	-0.763386	0.007603	-0.126814
50	3.827	-0.875500	-0.731252	0.006087	-0.144248
51	3.978	-0.750000	-0.600263	0.006880	-0.149737
52	4.128	-0.576900	-0.426500	0.007798	-0.150400
53	4.278	-0.361800	-0.198131	0.008814	-0.163669
54	4.427	-0.144100	0.047646	0.009879	-0.191746
55	4.576	0.033710	0.254623	0.010890	-0.220913
56	4.725	0.186100	0.427022	0.011870	-0.240922
57	4.874	0.261600	0.516123	0.012700	-0.254523
58	5.022	0.284000	0.550594	0.013470	-0.266594
59	5.170	0.206800	0.480622	0.014060	-0.273822
60	5.317	0.065230	0.335056	0.014530	-0.269827
61	5.464	-0.098580	0.156323	0.014980	-0.254903
62	5.610	-0.238100	-0.003578	0.015490	-0.234422
63	5.757	-0.428600	-0.217866	0.015880	-0.210734
64	5.902	-0.516200	-0.333894	0.016510	-0.183106
65	6.047	-0.586200	-0.434249	0.017180	-0.151951
66	6.192	-0.581100	-0.459343	0.017980	-0.121757
67	6.337	-0.516500	-0.420131	0.018860	-0.096369

	S	SI*M 1	SI*M 2	ERROR	DELTA SI*M
68	6.480	-0.377100	-0.300826	0.019910	-0.076274
69	6.624	-0.197000	-0.136707	0.021030	-0.060293
70	6.766	-0.049690	0.000454	0.022020	-0.050144
71	6.909	0.115000	0.162299	0.023060	-0.047299
72	7.051	0.237100	0.288059	0.023950	-0.050959
73	7.192	0.340100	0.398159	0.024800	-0.058059
74	7.332	0.297700	0.364246	0.025230	-0.066546
75	7.473	0.238200	0.314377	0.025720	-0.076177
76	7.612	0.115900	0.201811	0.025870	-0.085911
77	7.751	0.003319	0.096920	0.025990	-0.093601
78	7.890	-0.046460	0.050398	0.020090	-0.096858
79	8.027	-0.163600	-0.068455	0.020160	-0.095145
80	8.164	-0.266200	-0.177107	0.020220	-0.089093
81	8.301	-0.327200	-0.248237	0.020280	-0.078963
82	8.437	-0.287400	-0.222794	0.020490	-0.064606
83	8.572	-0.313800	-0.267188	0.020570	-0.046612
84	8.707	-0.243200	-0.216697	0.020770	-0.026503
85	8.841	-0.194500	-0.188132	0.020890	-0.006368
86	8.974	-0.075290	-0.087747	0.021130	0.012457
87	9.107	0.050240	0.021014	0.021370	0.029226
88	9.239	0.100200	0.057339	0.021480	0.042861
89	9.370	0.194100	0.141762	0.021640	0.052338
90	9.500	0.228700	0.171665	0.021710	0.057035
91	9.630	0.250100	0.193370	0.021760	0.056730
92	9.759	0.286600	0.235054	0.021830	0.051546
93	9.887	0.222400	0.180338	0.021720	0.042062
94	10.010	0.110300	0.080501	0.021540	0.029799
95	10.140	0.072900	0.058288	0.021480	0.014612
96	10.270	0.024880	0.026727	0.021370	-0.001847
97	10.390	-0.061490	-0.043823	0.021240	-0.017667
98	10.520	-0.104800	-0.069893	0.021200	-0.034907
99	10.640	-0.174800	-0.124900	0.021130	-0.049900
100	10.760	-0.208800	-0.146076	0.021180	-0.062724
101	10.890	-0.203200	-0.129942	0.021280	-0.073258
102	11.010	-0.199600	-0.119739	0.021370	-0.079861
103	11.130	-0.163700	-0.079799	0.021520	-0.083901
104	11.250	-0.199600	-0.114057	0.021570	-0.085543
105	11.370	-0.087200	-0.002543	0.021850	-0.084657
106	11.480	-0.130100	-0.048343	0.021880	-0.081757
107	11.600	-0.078610	-0.001518	0.022070	-0.077092
108	11.720	-0.026980	0.044945	0.022280	-0.071925
109	11.830	-0.016910	0.050312	0.022420	-0.067222
110	11.950	0.057120	0.119058	0.022660	-0.061938
111	12.060	0.046680	0.103490	0.022750	-0.056810
112	12.170	0.071780	0.123775	0.022910	-0.051995
113	12.280	0.040630	0.089271	0.022950	-0.048641
114	12.390	0.000060	0.047569	0.023010	-0.047509
115	12.500	0.035120	0.083218	0.023200	-0.048098
116	12.610	-0.029900	0.018937	0.023240	-0.048837
117	12.720	-0.010530	0.037868	0.023440	-0.048398
118	12.830	-0.022230	0.024734	0.023610	-0.046964
119	12.930	-0.107700	-0.061552	0.023670	-0.046148
120	13.040	-0.104100	-0.056860	0.023860	-0.047240
121	13.140	-0.104200	-0.054236	0.024040	-0.049964
122	13.240	-0.090630	-0.037940	0.024280	-0.052690
123	13.450	-0.166900	-0.117364	0.021940	-0.049536
124	13.640	-0.111700	-0.076637	0.022340	-0.035063
125	13.840	-0.073440	-0.055051	0.022720	-0.018389
126	14.030	-0.011180	-0.009629	0.023140	-0.001551
127	14.210	0.048290	0.028146	0.023570	0.020144
128	14.390	0.161100	0.118143	0.024080	0.042957
129	14.570	0.205400	0.144925	0.024540	0.060475
130	14.740	0.157600	0.084646	0.024850	0.072954
131	14.910	0.080300	-0.002375	0.025200	0.082675
132	15.080	0.032470	-0.054507	0.025550	0.086977
133	15.240	0.043180	-0.041371	0.025950	0.084551
134	15.390	0.042510	-0.034873	0.026300	0.077383
135	15.540	0.052550	-0.013179	0.026710	0.065729
136	15.680	-0.013400	-0.064311	0.026990	0.050911
137	15.820	-0.034270	-0.068745	0.027330	0.034475

OBSERVED RADIAL DISTRIBUTION FUNCTIONS, INTERACTIONS FROM 0.0 A TO 2.30 A CORRECTED.

	R	G1	D1	G2	ERROR	D2	ERROR
1	0.0	0.100E 01	0.0	0.100E 01	0.0	0.0	0.0
2	0.050	-0.595E 01	-0.682E-02	-0.151E 00	0.35E 01	-0.173E-03	0.40E-02
3	0.100	-0.572E 01	-0.262E-01	-0.102E 00	0.29E 01	-0.467E-03	0.13E-01
4	0.150	-0.530E 01	-0.546E-01	-0.415E-01	0.21E 01	-0.428E-03	0.22E-01
5	0.200	-0.466E 01	-0.855E-01	0.873E-02	0.13E 01	0.160E-03	0.23E-01
6	0.250	-0.383E 01	-0.110E 00	0.340E-01	0.89E 00	0.976E-03	0.26E-01
7	0.300	-0.287E 01	-0.119E 00	0.319E-01	0.82E 00	0.132E-02	0.34E-01
8	0.350	-0.191E 01	-0.107E 00	0.116E-01	0.74E 00	0.654E-03	0.41E-01
9	0.400	-0.107E 01	-0.784E-01	-0.112E-01	0.57E 00	-0.823E-03	0.42E-01
10	0.450	-0.435E 00	-0.404E-01	-0.234E-01	0.48E 00	-0.218E-02	0.45E-01
11	0.500	-0.367E-01	-0.421E-02	-0.200E-01	0.48E 00	-0.229E-02	0.54E-01
12	0.550	0.171E 00	0.237E-01	-0.530E-02	0.46E 00	-0.735E-03	0.64E-01
13	0.600	0.283E 00	0.468E-01	0.105E-01	0.40E 00	0.173E-02	0.66E-01
14	0.650	0.403E 00	0.780E-01	0.179E-01	0.36E 00	0.347E-02	0.69E-01
15	0.700	0.595E 00	0.134E 00	0.135E-01	0.35E 00	0.304E-02	0.79E-01
16	0.750	0.864E 00	0.223E 00	0.124E-02	0.34E 00	0.320E-03	0.87E-01
17	0.800	0.115E 01	0.339E 00	-0.108E-01	0.30E 00	-0.317E-02	0.87E-01
18	0.850	0.138E 01	0.456E 00	-0.151E-01	0.27E 00	-0.501E-02	0.89E-01
19	0.900	0.146E 01	0.541E 00	-0.954E-02	0.27E 00	-0.354E-02	0.99E-01
20	0.950	0.137E 01	0.565E 00	0.201E-02	0.26E 00	0.830E-03	0.11E 00
21	1.000	0.114E 01	0.521E 00	0.121E-01	0.24E 00	0.554E-02	0.11E 00
22	1.050	0.849E 00	0.429E 00	0.144E-01	0.22E 00	0.730E-02	0.11E 00
23	1.100	0.597E 00	0.331E 00	0.781E-02	0.22E 00	0.434E-02	0.12E 00
24	1.150	0.450E 00	0.273E 00	-0.343E-02	0.22E 00	-0.208E-02	0.13E 00
25	1.200	0.427E 00	0.282E 00	-0.122E-01	0.20E 00	-0.803E-02	0.13E 00
26	1.250	0.496E 00	0.356E 00	-0.129E-01	0.18E 00	-0.922E-02	0.13E 00
27	1.300	0.593E 00	0.460E 00	-0.514E-02	0.18E 00	-0.398E-02	0.14E 00
28	1.350	0.653E 00	0.546E 00	0.613E-02	0.18E 00	0.512E-02	0.15E 00
29	1.400	0.638E 00	0.573E 00	0.137E-01	0.17E 00	0.123E-01	0.15E 00
30	1.450	0.551E 00	0.532E 00	0.126E-01	0.16E 00	0.122E-01	0.16E 00
31	1.500	0.429E 00	0.442E 00	0.331E-02	0.16E 00	0.342E-02	0.17E 00
32	1.550	0.317E 00	0.349E 00	-0.856E-02	0.16E 00	-0.943E-02	0.18E 00
33	1.600	0.252E 00	0.295E 00	-0.154E-01	0.15E 00	-0.181E-01	0.18E 00
34	1.650	0.240E 00	0.300E 00	-0.125E-01	0.14E 00	-0.156E-01	0.18E 00
35	1.700	0.265E 00	0.351E 00	-0.131E-02	0.14E 00	-0.173E-02	0.19E 00
36	1.750	0.294E 00	0.413E 00	0.114E-01	0.14E 00	0.159E-01	0.20E 00
37	1.800	0.303E 00	0.451E 00	0.172E-01	0.13E 00	0.255E-01	0.20E 00
38	1.850	0.288E 00	0.452E 00	0.116E-01	0.13E 00	0.183E-01	0.20E 00
39	1.900	0.263E 00	0.435E 00	-0.251E-02	0.13E 00	-0.416E-02	0.21E 00
40	1.950	0.252E 00	0.440E 00	-0.165E-01	0.13E 00	-0.287E-01	0.22E 00
41	2.000	0.273E 00	0.501E 00	-0.206E-01	0.12E 00	-0.379E-01	0.22E 00
42	2.050	0.322E 00	0.621E 00	-0.108E-01	0.12E 00	-0.208E-01	0.22E 00
43	2.100	0.374E 00	0.756E 00	0.789E-02	0.11E 00	0.159E-01	0.23E 00
44	2.150	0.394E 00	0.836E 00	0.232E-01	0.11E 00	0.492E-01	0.24E 00
45	2.200	0.357E 00	0.792E 00	0.232E-01	0.11E 00	0.516E-01	0.24E 00
46	2.250	0.263E 00	0.611E 00	0.647E-02	0.11E 00	0.150E-01	0.25E 00
47	2.300	0.147E 00	0.356E 00	-0.118E-01	0.11E 00	-0.286E-01	0.26E 00
48	2.350	0.648E-01	0.164E 00	-0.129E-03	0.10E 00	-0.326E-03	0.26E 00
49	2.400	0.773E-01	0.204E 00	0.789E-01	0.99E-01	0.209E 00	0.26E 00
50	2.450	0.223E 00	0.613E 00	0.254E 00	0.96E-01	0.698E 00	0.27E 00
51	2.500	0.501E 00	0.144E 01	0.529E 00	0.96E-01	0.151E 01	0.28E 00
52	2.550	0.870E 00	0.259E 01	0.877E 00	0.95E-01	0.262E 01	0.28E 00
53	2.600	0.126E 01	0.391E 01	0.125E 01	0.91E-01	0.386E 01	0.28E 00
54	2.650	0.160E 01	0.514E 01	0.157E 01	0.89E-01	0.506E 01	0.29E 00
55	2.700	0.182E 01	0.608E 01	0.180E 01	0.89E-01	0.602E 01	0.30E 00
56	2.750	0.191E 01	0.661E 01	0.190E 01	0.88E-01	0.660E 01	0.30E 00
57	2.800	0.187E 01	0.673E 01	0.188E 01	0.84E-01	0.677E 01	0.30E 00
58	2.850	0.176E 01	0.655E 01	0.177E 01	0.82E-01	0.660E 01	0.31E 00
59	2.900	0.161E 01	0.620E 01	0.162E 01	0.82E-01	0.623E 01	0.32E 00
60	2.950	0.146E 01	0.583E 01	0.146E 01	0.80E-01	0.583E 01	0.32E 00
61	3.000	0.134E 01	0.553E 01	0.133E 01	0.78E-01	0.549E 01	0.32E 00
62	3.050	0.124E 01	0.530E 01	0.123E 01	0.77E-01	0.526E 01	0.33E 00
63	3.100	0.116E 01	0.513E 01	0.116E 01	0.77E-01	0.510E 01	0.34E 00
64	3.150	0.109E 01	0.496E 01	0.109E 01	0.76E-01	0.497E 01	0.35E 00
65	3.200	0.102E 01	0.479E 01	0.103E 01	0.74E-01	0.483E 01	0.35E 00
66	3.250	0.958E 00	0.464E 01	0.968E 00	0.72E-01	0.469E 01	0.35E 00
67	3.300	0.913E 00	0.456E 01	0.919E 00	0.72E-01	0.459E 01	0.36E 00

	R	G1	D1	G2	ERROR	D2	ERROR
68	3.350	0.893E 00	0.460E 01	0.893E 00	0.71E-01	0.459E 01	0.37E 00
69	3.400	0.899E 00	0.477E 01	0.894E 00	0.69E-01	0.474E 01	0.37E 00
70	3.450	0.924E 00	0.504E 01	0.918E 00	0.68E-01	0.501E 01	0.37E 00
71	3.500	0.953E 00	0.536E 01	0.952E 00	0.68E-01	0.535E 01	0.38E 00
72	3.550	0.976E 00	0.564E 01	0.980E 00	0.67E-01	0.566E 01	0.39E 00
73	3.600	0.985E 00	0.585E 01	0.992E 00	0.66E-01	0.589E 01	0.39E 00
74	3.650	0.980E 00	0.599E 01	0.987E 00	0.65E-01	0.603E 01	0.40E 00
75	3.700	0.971E 00	0.609E 01	0.974E 00	0.65E-01	0.611E 01	0.41E 00
76	3.750	0.965E 00	0.622E 01	0.964E 00	0.64E-01	0.621E 01	0.41E 00
77	3.800	0.971E 00	0.643E 01	0.967E 00	0.62E-01	0.640E 01	0.41E 00
78	3.850	0.990E 00	0.673E 01	0.986E 00	0.62E-01	0.670E 01	0.42E 00
79	3.900	0.102E 01	0.709E 01	0.101E 01	0.62E-01	0.708E 01	0.43E 00
80	3.950	0.104E 01	0.746E 01	0.104E 01	0.61E-01	0.747E 01	0.44E 00
81	4.000	0.106E 01	0.778E 01	0.106E 01	0.60E-01	0.780E 01	0.44E 00
82	4.050	0.107E 01	0.802E 01	0.107E 01	0.59E-01	0.804E 01	0.44E 00
83	4.100	0.106E 01	0.819E 01	0.106E 01	0.58E-01	0.819E 01	0.45E 00
84	4.150	0.106E 01	0.834E 01	0.105E 01	0.58E-01	0.831E 01	0.46E 00
85	4.200	0.105E 01	0.851E 01	0.105E 01	0.56E-01	0.847E 01	0.46E 00
86	4.250	0.106E 01	0.875E 01	0.105E 01	0.56E-01	0.871E 01	0.46E 00
87	4.300	0.107E 01	0.906E 01	0.107E 01	0.56E-01	0.904E 01	0.47E 00
88	4.350	0.108E 01	0.941E 01	0.109E 01	0.56E-01	0.942E 01	0.48E 00
89	4.400	0.110E 01	0.975E 01	0.110E 01	0.54E-01	0.977E 01	0.48E 00
90	4.450	0.110E 01	0.100E 02	0.111E 01	0.54E-01	0.100E 02	0.49E 00
91	4.500	0.110E 01	0.102E 02	0.110E 01	0.54E-01	0.102E 02	0.50E 00
92	4.550	0.109E 01	0.104E 02	0.109E 01	0.53E-01	0.103E 02	0.50E 00
93	4.600	0.108E 01	0.105E 02	0.108E 01	0.52E-01	0.104E 02	0.50E 00
94	4.650	0.107E 01	0.106E 02	0.107E 01	0.51E-01	0.106E 02	0.51E 00
95	4.700	0.106E 01	0.108E 02	0.106E 01	0.51E-01	0.108E 02	0.52E 00
96	4.750	0.106E 01	0.109E 02	0.106E 01	0.51E-01	0.110E 02	0.52E 00
97	4.800	0.105E 01	0.111E 02	0.105E 01	0.50E-01	0.111E 02	0.52E 00
98	4.850	0.104E 01	0.112E 02	0.104E 01	0.49E-01	0.112E 02	0.53E 00
99	4.900	0.102E 01	0.112E 02	0.102E 01	0.49E-01	0.112E 02	0.53E 00
100	4.950	0.995E 00	0.112E 02	0.994E 00	0.48E-01	0.112E 02	0.54E 00
101	5.000	0.967E 00	0.111E 02	0.966E 00	0.47E-01	0.111E 02	0.54E 00
102	5.050	0.943E 00	0.110E 02	0.942E 00	0.47E-01	0.110E 02	0.55E 00
103	5.100	0.926E 00	0.110E 02	0.927E 00	0.47E-01	0.111E 02	0.56E 00
104	5.150	0.918E 00	0.112E 02	0.921E 00	0.46E-01	0.112E 02	0.56E 00
105	5.200	0.917E 00	0.114E 02	0.921E 00	0.46E-01	0.114E 02	0.57E 00
106	5.250	0.919E 00	0.116E 02	0.923E 00	0.45E-01	0.117E 02	0.57E 00
107	5.300	0.920E 00	0.118E 02	0.921E 00	0.45E-01	0.119E 02	0.58E 00
108	5.350	0.915E 00	0.120E 02	0.915E 00	0.45E-01	0.120E 02	0.59E 00
109	5.400	0.907E 00	0.121E 02	0.905E 00	0.44E-01	0.121E 02	0.59E 00
110	5.450	0.896E 00	0.122E 02	0.895E 00	0.43E-01	0.122E 02	0.59E 00
111	5.500	0.889E 00	0.123E 02	0.889E 00	0.44E-01	0.123E 02	0.61E 00
112	5.550	0.887E 00	0.125E 02	0.888E 00	0.43E-01	0.125E 02	0.61E 00
113	5.600	0.892E 00	0.128E 02	0.894E 00	0.42E-01	0.128E 02	0.60E 00
114	5.650	0.902E 00	0.132E 02	0.903E 00	0.43E-01	0.132E 02	0.62E 00
115	5.700	0.914E 00	0.136E 02	0.913E 00	0.42E-01	0.136E 02	0.62E 00
116	5.750	0.923E 00	0.140E 02	0.921E 00	0.41E-01	0.140E 02	0.62E 00
117	5.800	0.929E 00	0.143E 02	0.926E 00	0.41E-01	0.143E 02	0.63E 00
118	5.850	0.932E 00	0.146E 02	0.930E 00	0.41E-01	0.146E 02	0.64E 00
119	5.900	0.935E 00	0.149E 02	0.934E 00	0.40E-01	0.149E 02	0.64E 00
120	5.950	0.942E 00	0.153E 02	0.941E 00	0.40E-01	0.153E 02	0.65E 00
121	6.000	0.954E 00	0.157E 02	0.954E 00	0.40E-01	0.157E 02	0.66E 00
122	6.050	0.970E 00	0.163E 02	0.970E 00	0.39E-01	0.163E 02	0.65E 00
123	6.100	0.989E 00	0.169E 02	0.988E 00	0.39E-01	0.168E 02	0.67E 00
124	6.150	0.101E 01	0.175E 02	0.100E 01	0.39E-01	0.174E 02	0.68E 00
125	6.200	0.102E 01	0.180E 02	0.102E 01	0.38E-01	0.179E 02	0.67E 00
126	6.250	0.103E 01	0.184E 02	0.103E 01	0.38E-01	0.184E 02	0.68E 00
127	6.300	0.103E 01	0.188E 02	0.103E 01	0.38E-01	0.188E 02	0.69E 00
128	6.350	0.104E 01	0.192E 02	0.104E 01	0.38E-01	0.192E 02	0.70E 00
129	6.400	0.105E 01	0.196E 02	0.105E 01	0.37E-01	0.197E 02	0.70E 00
130	6.450	0.105E 01	0.201E 02	0.105E 01	0.37E-01	0.201E 02	0.70E 00
131	6.500	0.106E 01	0.206E 02	0.106E 01	0.37E-01	0.206E 02	0.71E 00
132	6.550	0.107E 01	0.210E 02	0.107E 01	0.36E-01	0.210E 02	0.71E 00
133	6.600	0.107E 01	0.214E 02	0.107E 01	0.36E-01	0.214E 02	0.72E 00
134	6.650	0.107E 01	0.216E 02	0.107E 01	0.36E-01	0.217E 02	0.73E 00

	R	G1	D1	G2	ERROR	D2	ERROR
135	6.700	0.106E 01	0.219E 02	0.106E 01	0.36E-01	0.219E 02	0.74E 00
136	6.750	0.106E 01	0.221E 02	0.106E 01	0.36E-01	0.221E 02	0.74E 00
137	6.800	0.105E 01	0.223E 02	0.105E 01	0.35E-01	0.224E 02	0.74E 00
138	6.850	0.105E 01	0.226E 02	0.105E 01	0.35E-01	0.226E 02	0.75E 00
139	6.900	0.105E 01	0.230E 02	0.105E 01	0.34E-01	0.230E 02	0.75E 00
140	6.950	0.105E 01	0.233E 02	0.105E 01	0.34E-01	0.233E 02	0.76E 00
141	7.000	0.105E 01	0.236E 02	0.105E 01	0.34E-01	0.236E 02	0.77E 00
142	7.050	0.104E 01	0.237E 02	0.104E 01	0.34E-01	0.238E 02	0.78E 00
143	7.100	0.103E 01	0.238E 02	0.103E 01	0.34E-01	0.239E 02	0.78E 00
144	7.150	0.102E 01	0.239E 02	0.102E 01	0.33E-01	0.240E 02	0.78E 00
145	7.200	0.101E 01	0.240E 02	0.101E 01	0.34E-01	0.241E 02	0.80E 00
146	7.250	0.101E 01	0.242E 02	0.101E 01	0.33E-01	0.243E 02	0.80E 00
147	7.300	0.100E 01	0.245E 02	0.100E 01	0.33E-01	0.245E 02	0.80E 00
148	7.350	0.100E 01	0.249E 02	0.100E 01	0.32E-01	0.248E 02	0.81E 00
149	7.400	0.100E 01	0.252E 02	0.100E 01	0.32E-01	0.251E 02	0.81E 00
150	7.450	0.998E 00	0.254E 02	0.996E 00	0.32E-01	0.254E 02	0.82E 00
151	7.500	0.990E 00	0.255E 02	0.988E 00	0.32E-01	0.255E 02	0.83E 00
152	7.550	0.980E 00	0.256E 02	0.979E 00	0.32E-01	0.256E 02	0.83E 00
153	7.600	0.971E 00	0.257E 02	0.971E 00	0.31E-01	0.257E 02	0.82E 00
154	7.650	0.967E 00	0.260E 02	0.966E 00	0.32E-01	0.259E 02	0.85E 00
155	7.700	0.968E 00	0.263E 02	0.967E 00	0.31E-01	0.263E 02	0.83E 00
156	7.750	0.973E 00	0.268E 02	0.971E 00	0.31E-01	0.267E 02	0.85E 00
157	7.800	0.980E 00	0.273E 02	0.977E 00	0.31E-01	0.273E 02	0.86E 00
158	7.850	0.984E 00	0.278E 02	0.982E 00	0.30E-01	0.278E 02	0.85E 00
159	7.900	0.986E 00	0.282E 02	0.985E 00	0.31E-01	0.282E 02	0.87E 00
160	7.950	0.984E 00	0.285E 02	0.984E 00	0.29E-01	0.285E 02	0.85E 00
161	8.000	0.982E 00	0.288E 02	0.982E 00	0.30E-01	0.288E 02	0.89E 00
162	8.050	0.980E 00	0.291E 02	0.980E 00	0.29E-01	0.291E 02	0.87E 00
163	8.100	0.981E 00	0.295E 02	0.981E 00	0.30E-01	0.295E 02	0.89E 00
164	8.150	0.984E 00	0.300E 02	0.984E 00	0.29E-01	0.300E 02	0.89E 00
165	8.200	0.988E 00	0.305E 02	0.988E 00	0.29E-01	0.305E 02	0.89E 00
166	8.250	0.991E 00	0.309E 02	0.992E 00	0.29E-01	0.309E 02	0.91E 00
167	8.300	0.993E 00	0.314E 02	0.994E 00	0.28E-01	0.314E 02	0.89E 00
168	8.350	0.992E 00	0.317E 02	0.994E 00	0.29E-01	0.318E 02	0.92E 00
169	8.400	0.992E 00	0.321E 02	0.994E 00	0.28E-01	0.321E 02	0.90E 00
170	8.450	0.992E 00	0.325E 02	0.994E 00	0.29E-01	0.325E 02	0.94E 00
171	8.500	0.994E 00	0.329E 02	0.996E 00	0.28E-01	0.330E 02	0.93E 00
172	8.550	0.998E 00	0.335E 02	0.100E 01	0.28E-01	0.335E 02	0.93E 00
173	8.600	0.100E 01	0.340E 02	0.100E 01	0.28E-01	0.341E 02	0.94E 00
174	8.650	0.101E 01	0.345E 02	0.101E 01	0.27E-01	0.346E 02	0.93E 00
175	8.700	0.101E 01	0.350E 02	0.101E 01	0.28E-01	0.350E 02	0.98E 00
176	8.750	0.101E 01	0.353E 02	0.101E 01	0.27E-01	0.354E 02	0.94E 00
177	8.800	0.100E 01	0.356E 02	0.100E 01	0.27E-01	0.357E 02	0.97E 00
178	8.850	0.100E 01	0.359E 02	0.100E 01	0.26E-01	0.360E 02	0.94E 00
179	8.900	0.100E 01	0.363E 02	0.100E 01	0.27E-01	0.363E 02	0.99E 00
180	8.950	0.100E 01	0.368E 02	0.100E 01	0.26E-01	0.368E 02	0.97E 00
181	9.000	0.101E 01	0.373E 02	0.100E 01	0.27E-01	0.373E 02	0.10E 01
182	9.050	0.101E 01	0.379E 02	0.101E 01	0.26E-01	0.378E 02	0.98E 00
183	9.100	0.101E 01	0.383E 02	0.101E 01	0.26E-01	0.383E 02	0.99E 00
184	9.150	0.101E 01	0.386E 02	0.101E 01	0.26E-01	0.386E 02	0.10E 01
185	9.200	0.100E 01	0.389E 02	0.100E 01	0.26E-01	0.389E 02	0.10E 01
186	9.250	0.997E 00	0.391E 02	0.995E 00	0.26E-01	0.390E 02	0.10E 01
187	9.300	0.992E 00	0.394E 02	0.990E 00	0.25E-01	0.393E 02	0.10E 01
188	9.350	0.991E 00	0.397E 02	0.988E 00	0.26E-01	0.396E 02	0.10E 01
189	9.400	0.991E 00	0.402E 02	0.989E 00	0.25E-01	0.401E 02	0.10E 01
190	9.450	0.993E 00	0.407E 02	0.992E 00	0.26E-01	0.406E 02	0.10E 01
191	9.500	0.996E 00	0.412E 02	0.995E 00	0.25E-01	0.412E 02	0.10E 01
192	9.550	0.999E 00	0.418E 02	0.998E 00	0.25E-01	0.417E 02	0.10E 01
193	9.600	0.100E 01	0.423E 02	0.100E 01	0.25E-01	0.422E 02	0.10E 01
194	9.650	0.100E 01	0.427E 02	0.100E 01	0.25E-01	0.427E 02	0.11E 01
195	9.700	0.100E 01	0.432E 02	0.100E 01	0.24E-01	0.431E 02	0.11E 01
196	9.750	0.100E 01	0.436E 02	0.100E 01	0.25E-01	0.436E 02	0.11E 01
197	9.800	0.100E 01	0.441E 02	0.100E 01	0.24E-01	0.441E 02	0.10E 01
198	9.850	0.100E 01	0.446E 02	0.100E 01	0.25E-01	0.446E 02	0.11E 01
199	9.900	0.100E 01	0.451E 02	0.100E 01	0.24E-01	0.451E 02	0.11E 01
200	9.950	0.100E 01	0.456E 02	0.100E 01	0.24E-01	0.456E 02	0.11E 01
201	10.000	0.100E 01	0.460E 02	0.100E 01	0.24E-01	0.460E 02	0.11E 01

4. DISCUSSION

Radial distribution functions for the ammonium fluoride solutions, obtained from the experimental data, are compared with that of pure water in Fig. 1. The first prominent maximum in the RDF's shifts from 2.88 Å in water to 2.87 Å and 2.80 Å in the 1.18 M and 10.87 M solutions respectively. A corresponding shift toward shorter distances can be observed in the broad peak at about 5 Å, while the maximum centered at about 6.5 Å remains essentially unchanged. The structural changes which cause the differences in the RDF's of Fig. 1 can be explained in terms of the proposed model for liquid water. This model, described in detail elsewhere[2], assumes a modified ice framework surrounded by a continuous distribution of distances as an adequate description for the short range order (Fig. 2). Variable parameters in the model are the distances P_1, P_2, and P_3 indicated in Fig. 2, with all other distances (to about 8 Å) generated by the symmetry operations of the crystal space group (P_6/mmc). Occupancy of the large cavities typical of this structure is permitted, but constrained to conform to the experimental density.

Reduced intensity functions computed from the refined model parameters are shown in Fig. 3 along with those derived from experiment. A list of the values obtained for P_1, P_2 and P_3 of the model, along with their associated root-mean-square displacements (amplitudes), are presented in Table I. The x-ray scattering factors for nitrogen, fluorine and

oxygen are very nearly alike, so that the x-ray method does not distinguish between the different kinds of atoms.

There is very little difference between the model parameters for water and those for the 1.18 M solution. In each case, a framework molecule has one neighbor at about 2.77 Å (P_2 of Fig. 2) and three other framework neighbors at 2.94 Å (P_1 of Fig. 2). Each "interstitial" molecule has three network neighbors at about 2.95 Å (P_3 of Fig. 2). The 10.87 M solution shows a significant decrease in these distances, 2.88 Å for P_1, 2.69 Å for P_2 and 2.87 Å for P_3. Both in pure water and in the two solutions about half of the available cavities are occupied by "interstitial" molecules. The decrease in the model distances for the solutions indicates that ions and water molecules are distributed over both framework and interstitial positions.

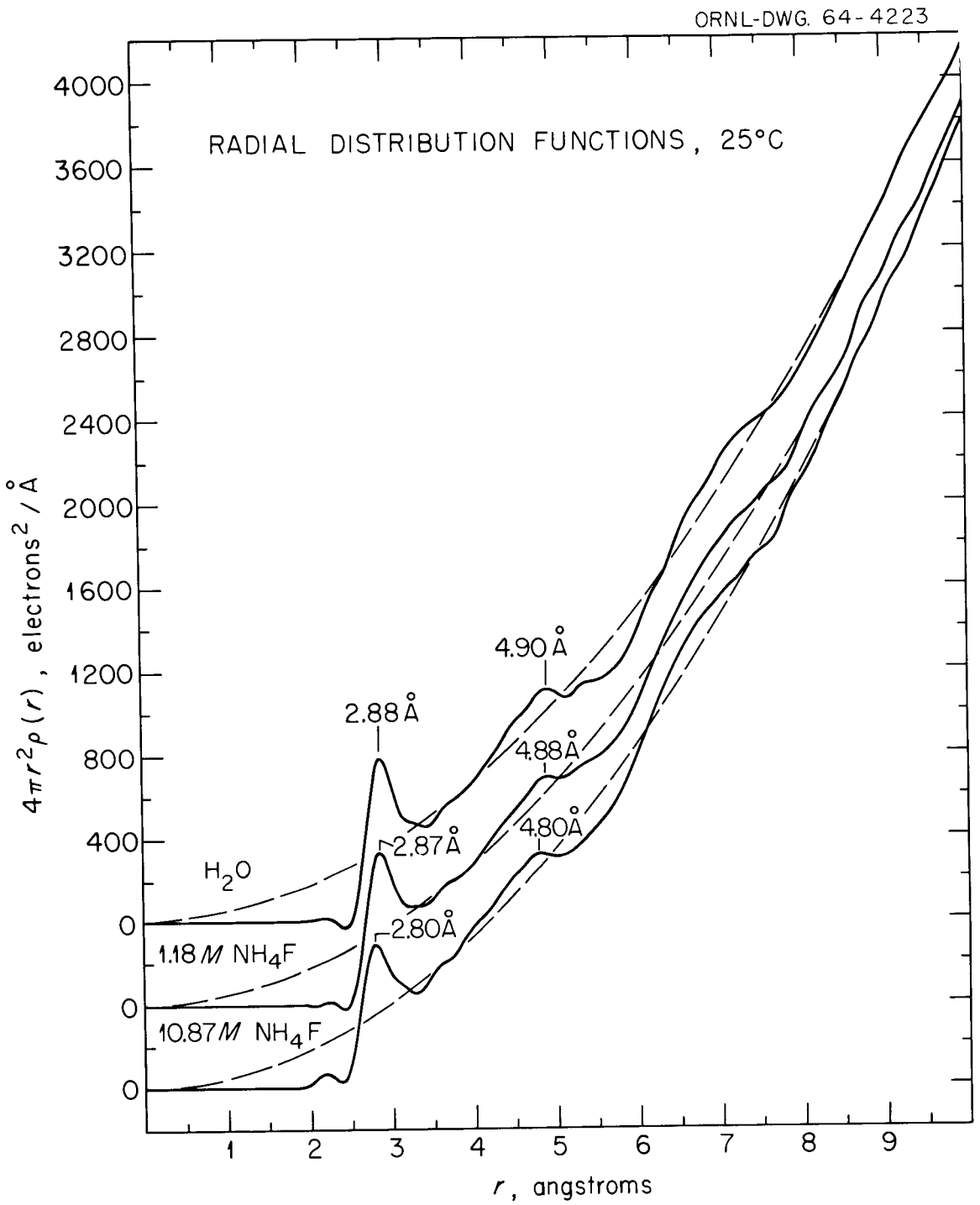

Fig. 1. Data of Section 3.2 Converted to Electron Units.

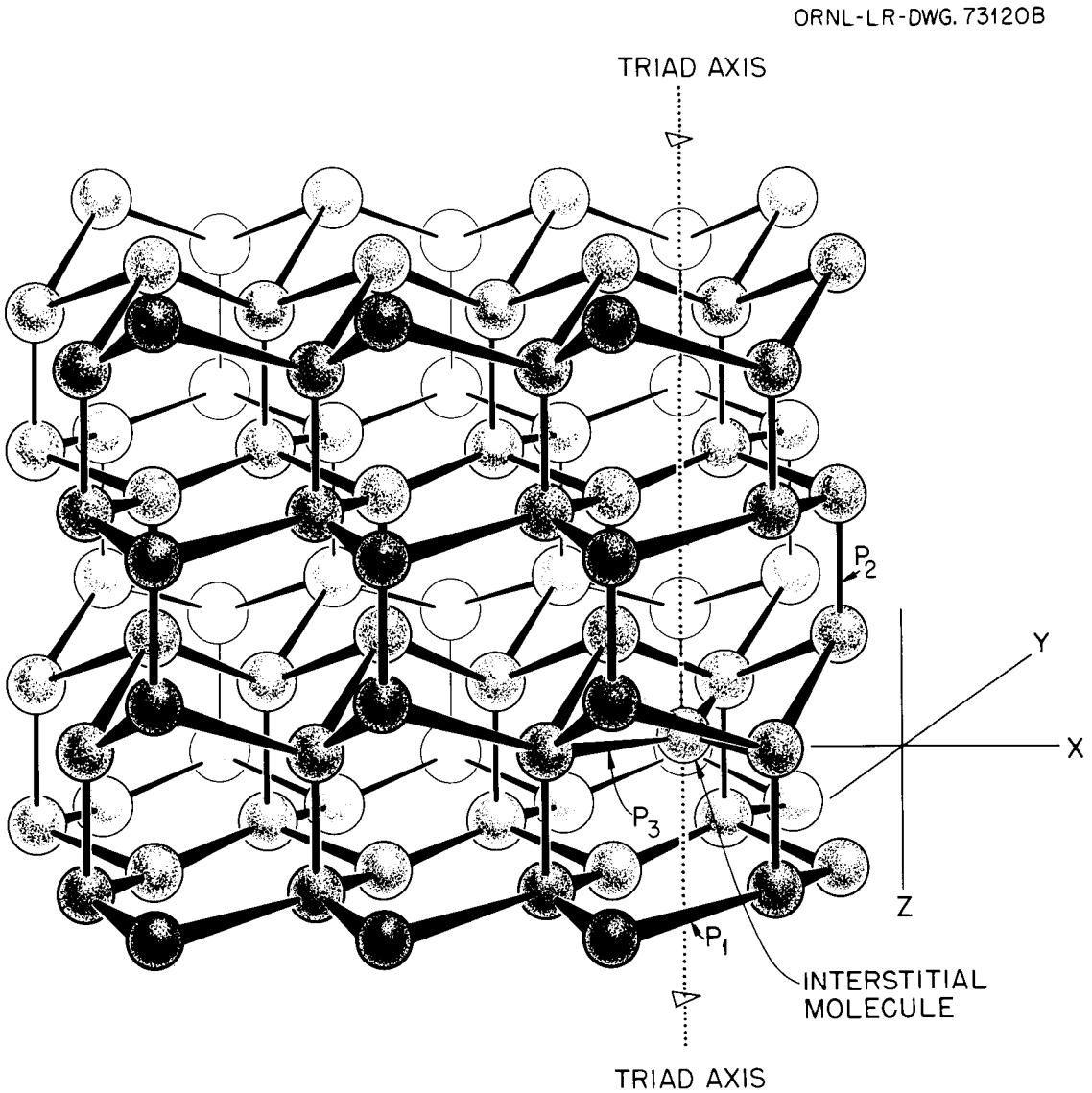

Fig. 2. Structural Model for the Short-Range Order in the H_2O-NH_4F System. The balls represent oxygen, nitrogen or fluorine atoms, the sticks hydrogen bonds.

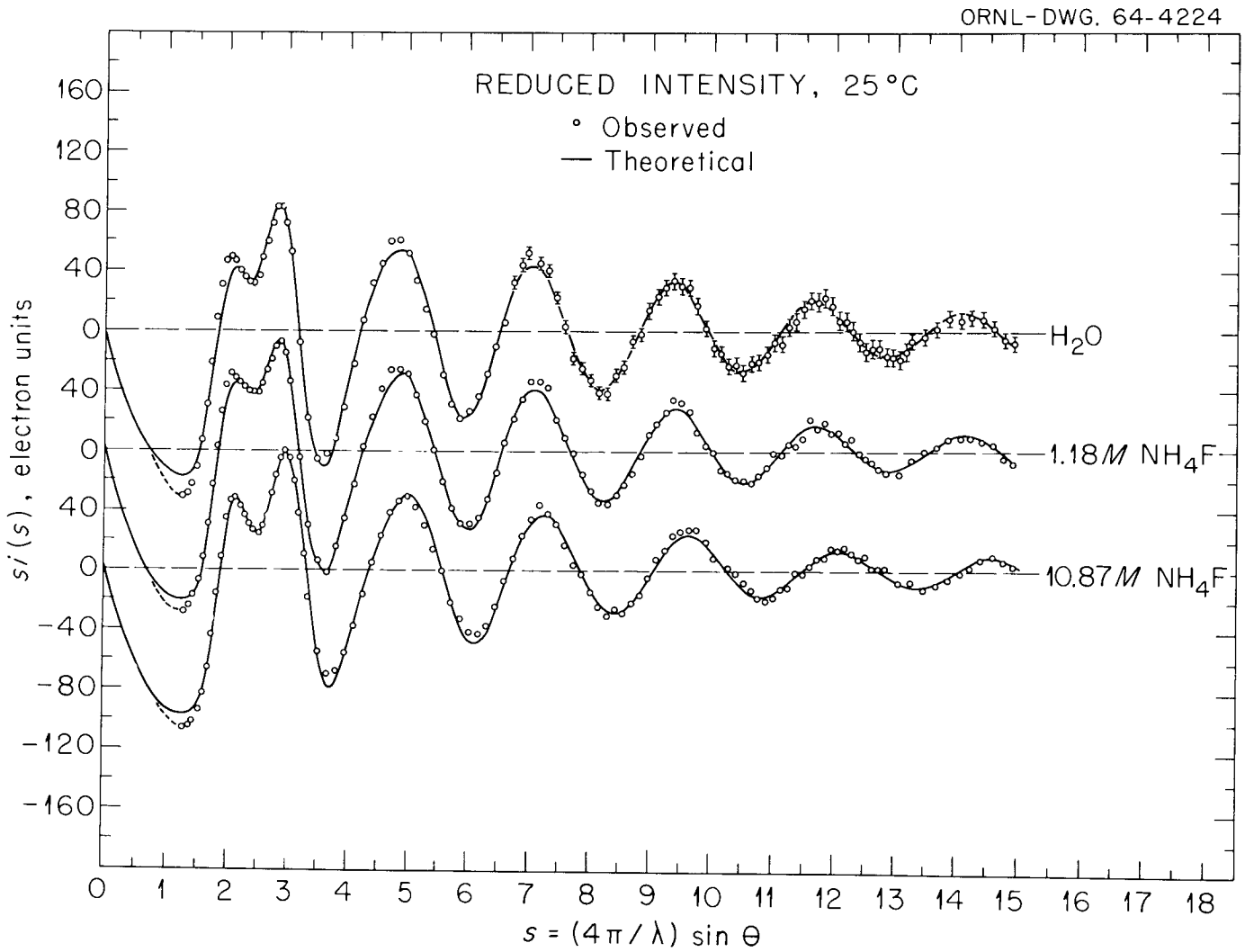

Fig. 3. Reduced Intensity Functions of Section 3.2, Converted to Electon Units. Solid lines computed from the model parameters of Table 1.

Table 1. Some Relevant Parameters of the Model for the H_2O-NH_4F System. The Atom Pair Interactions P_1, P_2 and P_3 (Fig. 2) Are Characterized by a Distance r (Å) and a RMS- Displacement $\langle \Delta r^2 \rangle^{1/2}$ (Å). The Fractional Occupancy of Cavity Sites Is Designated by f_2; w is the Fraction of Molecules or Ions in Network Positions (Network Occupancy $f_1 = 1$).

	H_2O		1.18 *M* NH_4F		10.87 *M* NH_4F	
	r	$\langle \Delta r^2 \rangle^{\frac{1}{2}}$	r	$\langle \Delta r^2 \rangle^{\frac{1}{2}}$	r	$\langle \Delta r^2 \rangle^{\frac{1}{2}}$
P_1	2.94	0.18	2.94	0.37	2.88	0.38
P_2	2.78	0.08	2.77	0.09	2.69	0.10
P_3	2.96	0.53	2.94	0.17	2.87	0.17
f_2	0.50		0.53		0.55	
w	0.80		0.79		0.78	

5. REFERENCES

1. A. H. Narten, M. D. Danford and H. A. Levy, X-Ray Diffraction Data on Liquid Water in the Temperature Range 4 to 200°C, ORNL-3997 (1966).

2. A. H. Narten, M. D. Danford and H. A. Levy, Disc. Farad. Soc., 43, 97 (1967).

3. H. A. Levy, M. D. Danford and A. H. Narten, Data Collection and Evaluation with an X-Ray Diffractometer Designed for the Study of Liquid Structure, ORNL-3960 (1966).

4. International Tables for X-Ray Crystallography, The Kynoch Press, Birmingham (England), 1959.

5. J. Waser and V. Schomaker, Rev. Mod. Phys., 25, 671 (1953).

ORNL-4244
UC-4 — Chemistry

INTERNAL DISTRIBUTION

1. Biology Library
2-4. Central Research Library
5-6. ORNL — Y-12 Technical Library Document Reference Section
7-41. Laboratory Records Department
42. Laboratory Records, ORNL R.C.
43. G. E. Boyd
44-53. M. D. Danford
54. L. O. Gilpatrick
55. H. B. Hupf
56. C. E. Larson
57. H. G. MacPherson
58-67. A. H. Narten
68. M. J. Skinner
69. G. P. Smith
70. D. A. Sundberg
71. E. H. Taylor
72. A. M. Weinberg
73. P. D. Bartlett (consultant)
74. G. Friedlander (consultant)
75. J. J. Katz (consultant)
76. F. A. Long (consultant)
77. J. E. Mayer (consultant)
78. G. Scatchard (consultant)
79. H. M. Sisler (consultant)

EXTERNAL DISTRIBUTION

80. J. A. Swartout, Union Carbide Corporation, New York
81. Laboratory and University Division, AEC, ORO
82-334. Given distribution as shown in TID-4500 under Chemistry category (25 copies — CFSTI)