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X-RAY DIFFRACTION DATA ON LIQUID 2,2-DIMETHYLPROPANE (NEOPENTANE) AT 25°C

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CHEMISTRY DIVISION

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APRIL 1967

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ABSTRACT

The scattering of x-rays from the free surface of liquid neopentane in equilibrium with its vapor has been measured at 25°C. The diffractometer used was specially designed for the study of liquid structure. In this report, both the raw data and the intensity and radial distribution functions derived from them are presented in tabulated form. Intramolecular distances obtained in this study are in agreement with those derived from gas diffraction experiments.

1. INTRODUCTION

An x-ray diffraction study of liquid carbon tetrachloride[1] has yielded considerable insight both into the geometry of this tetrahedal molecule and into the packing of the molecules themselves. Replacement of the chlorine atoms in CCl_4 by the somewhat smaller and considerably less polarizable methyl groups of neopentane (CMe_4) should yield an even better approximation of a globular molecule. Since these molecules can be assumed to interact with short-range, two-body central forces, an x-ray diffraction study of liquid neopentane should provide useful information on the structure of a "simple" liquid, against which some results of the molecular theory of such systems can be checked.

Our results are presented in tabulated form in this report.

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[2]. 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 Material and Sample Holder. Neopentane of 99.91 mol % purity* was used in the experiments. The liquid was contained under its own vapor pressure in a cylindrical beryllium cup (1.625" I.D., 0.020" wall) with the liquid surface in the diffractometer axis.

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 200,000 to 500,000, 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[2] (to $s_{max} = (4\ \pi/\lambda) \sin \theta_{max} = 16$, θ being half the scattering angle).

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[2]. 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

*The Matheson Co., Inc., East Rutherford, N. J.

definitions of various terms are given in the order of their appearance (some are omitted since they are self-explanatory).

3.1.1 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.

3.1.2 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[2].

PEN. is the penetration correction[2]; the atomic absorption coefficients for carbon and hydrogen were obtained from the literature[3].

I,CORR. is the corrected intensity, computed from

I,CORR = (I,RAW - BKG.)/(POL.xPEN.).

ERROR is the statistical error associated with I,CORR, computed from

ERROR = I,CORRx$(\text{COUNTS})^{\frac{1}{2}}$/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.

NEOPENTANE 25C

SECTION 1, 0.500 DEGREE DIVERGENCE SLIT.

RAW INTENSITY IN COUNTS PER MINUTE

N	THETA	COUNTS	1 RUN	2 RUN
1	2.50	200000.00	2987.16	3275.47
2	2.75	200000.00	3552.40	3981.95
3	3.00	200000.00	4547.86	5131.71
4	3.25	200000.00	6340.48	7165.89
5	3.50	200000.00	9678.98	10791.36
6	3.75	200000.00	12162.99	13689.26
7	4.00	200000.00	9557.18	10643.96
8	4.25	200000.00	5550.93	6114.34
9	4.50	200000.00	3210.27	3534.19
10	4.75	200000.00	2113.57	2348.98
11	5.00	200000.00	1549.63	1701.69
12	5.25	200000.00	1225.24	1343.03
13	5.50	200000.00	1056.38	1171.21
14	5.75	200000.00	958.15	1061.67
15	6.00	200000.00	896.65	970.03
16	6.25	200000.00	849.97	922.58
17	6.50	200000.00	823.72	890.54
18	6.75	200000.00	765.54	871.84
19	7.00	200000.00	717.79	845.28
20	7.25	200000.00	706.06	809.59
21	7.50	200000.00	677.59	781.56
22	7.75	200000.00	657.06	794.41
23	8.00	200000.00	634.14	778.48
24	8.25	200000.00	604.36	761.13
25	8.50	200000.00	591.65	736.72
26	8.75	200000.00	569.15	716.44
27	9.00	200000.00	550.53	707.05
28	9.25	200000.00	530.93	677.47
29	9.50	200000.00	506.15	616.73

NEOPENTANE 25C

SECTION 2, 2.000 DEGREE DIVERGENCE SLIT.

RAW INTENSITY IN COUNTS PER MINUTE

N	THETA	COUNTS	1 RUN	2 RUN	3 RUN
1	9.00	300000.00	7125.04	7142.86	7139.46
2	9.50	300000.00	6628.37	6664.45	6675.57
3	10.00	300000.00	5993.41	5963.62	6072.87
4	10.50	300000.00	5269.63	5274.72	5346.16
5	11.00	300000.00	4624.28	4617.16	4627.48
6	11.50	300000.00	4042.31	4046.13	4075.81
7	12.00	300000.00	3603.60	3568.67	3631.52
8	12.50	300000.00	3251.86	3266.02	3246.23
9	13.00	300000.00	2970.89	2975.60	2982.26
10	13.50	300000.00	2808.99	2824.33	2812.41
11	14.00	300000.00	2671.65	2660.40	2651.82
12	14.50	300000.00	2592.02	2574.00	2578.21
13	15.00	300000.00	2521.11	2492.52	2554.82

N	THETA	COUNTS	1 RUN	2 RUN	3 RUN
14	15.50	300000.00	2450.88	2457.81	2550.91
15	16.00	300000.00	2374.08	2400.29	2464.07
16	16.50	300000.00	2329.64	2325.76	2382.94
17	17.00	300000.00	2234.64	2229.74	2264.15
18	17.50	300000.00	2127.06	2117.30	2119.24
19	18.00	300000.00	1993.82	1995.74	1931.19
20	18.50	300000.00	1853.68	1839.25	1785.77
21	19.00	300000.00	1698.90	1672.47	1633.28
22	19.50	300000.00	1549.39	1526.72	1485.88
23	20.00	300000.00	1386.90	1394.02	1344.72
24	20.50	300000.00	1231.68	1253.00	1212.98
25	21.00	300000.00	1106.81	1121.81	1101.75
26	21.50	300000.00	1008.15	1007.47	999.42
27	22.00	300000.00	924.91	921.59	908.93
28	22.50	300000.00	855.29	856.80	849.56
29	23.00	300000.00	802.92	810.67	802.00

NEOPENTANE 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
1	22.00	500000.00	4362.68	4324.32	4323.39	4405.61	4350.98
2	22.50	500000.00	4101.72	4058.44	4074.70	4132.80	4107.62
3	23.00	500000.00	3906.50	3842.21	3843.44	3929.79	3916.70
4	23.50	500000.00	3695.95	3673.54	3695.72	3722.55	3728.33
5	24.00	500000.00	3566.97	3509.80	3524.85	3562.31	3570.37
6	24.50	500000.00	3419.58	3393.86	3397.51	3452.84	3443.13
7	25.00	500000.00	3311.26	3262.11	3300.51	3313.64	3294.53
8	25.50	500000.00	3171.08	3140.21	3157.06	3202.56	3201.37
9	26.00	500000.00	3043.68	3016.59	3028.93	3079.29	3069.68
10	26.50	500000.00	2919.14	2894.36	2907.40	2923.55	2936.28
11	27.00	500000.00	2772.00	2751.03	2768.93	2806.23	2771.87
12	27.50	500000.00	2651.11	2625.02	2632.96	2674.75	2649.59
13	28.00	500000.00	2502.40	2473.51	2493.56	2514.88	2497.50
14	28.50	500000.00	2371.92	2335.27	2359.42	2380.29	2357.84
15	29.00	500000.00	2235.72	2188.90	2225.11	2256.15	2235.64
16	29.50	500000.00	2092.20	2066.04	2081.31	2129.62	2095.63
17	30.00	500000.00	1967.79	1953.76	1985.05	2008.10	1973.81
18	30.50	500000.00	1871.96	1844.79	1867.36	1886.02	1875.94
19	31.00	500000.00	1769.44	1744.29	1770.12	1797.97	1787.95
20	31.50	500000.00	1695.25	1682.84	1692.00	1714.87	1697.02
21	32.00	500000.00	1601.97	1600.21	1604.62	1650.66	1629.11
22	32.50	500000.00	1552.96	1538.42	1552.55	1575.63	1558.48
23	33.00	500000.00	1490.57	1481.23	1501.69	1510.12	1497.34
24	33.50	500000.00	1445.75	1425.38	1449.70	1469.51	1461.28
25	34.00	500000.00	1402.69	1395.84	1394.51	1419.78	1411.86
26	34.50	500000.00	1350.07	1346.44	1364.88	1376.40	1369.02
27	35.00	500000.00	1314.58	1310.44	1318.71	1340.33	1419.85
28	35.50	500000.00	1270.30	1270.11	1269.73	1296.99	1281.91
29	36.00	500000.00	1234.90	1231.76	1239.13	1244.01	1236.22
30	36.50	500000.00	1190.76	1186.83	1195.36	1207.15	1197.82
31	37.00	500000.00	1148.81	1148.57	1151.15	1175.99	1165.50
32	37.50	500000.00	1121.68	1113.88	1113.36	1132.80	1122.23
33	38.00	500000.00	1074.86	1071.45	1074.42	1097.59	1090.00
34	38.50	500000.00	1045.57	1039.88	1038.87	1062.04	1058.84
35	39.00	500000.00	1016.29	1016.97	1015.21	1030.59	1023.40
36	39.50	500000.00	989.09	996.05	992.60	1007.27	1000.33

N	THETA	COUNTS	1 RUN	2 RUN	3 RUN	4 RUN	5 RUN
37	40.00	500000.00	965.16	967.91	966.53	986.08	975.05
38	40.50	500000.00	953.90	948.63	958.15	965.16	965.94
39	41.00	500000.00	945.33	940.19	945.02	957.01	952.41
40	41.50	500000.00	933.16	927.86	929.83	947.81	933.02
41	42.00	500000.00	931.68	929.93	932.76	934.20	928.98
42	42.50	500000.00	926.43	923.69	929.89	937.53	935.60
43	43.00	500000.00	921.98	924.74	929.51	933.55	933.62
44	43.50	500000.00	929.37	926.97	931.23	935.91	934.81
45	44.00	500000.00	934.90	926.11	938.78	940.73	951.08
46	44.50	500000.00	939.33	939.35	940.28	950.53	953.73
47	45.00	500000.00	940.87	941.15	944.42	949.35	952.46
48	45.50	500000.00	945.64	948.39	950.59	959.52	957.73
49	46.00	500000.00	955.69	949.02	946.96	962.60	959.19
50	46.50	500000.00	953.59	953.88	950.53	962.09	963.36
51	47.00	500000.00	953.67	952.73	960.08	961.69	965.67
52	47.50	500000.00	951.73	949.98	960.14	958.71	960.71
53	48.00	500000.00	951.17	951.22	956.50	961.92	960.20
54	48.50	500000.00	949.23	944.21	948.95	951.32	947.93
55	49.00	500000.00	942.95	939.53	946.48	949.80	953.62
56	49.50	500000.00	932.55	935.16	934.83	945.33	945.25
57	50.00	500000.00	932.68	932.52	937.00	942.63	951.44
58	50.50	500000.00	932.82	929.89	939.19	939.95	936.49
59	51.00	500000.00	936.43	930.67	938.79	939.94	939.35
60	51.50	500000.00	940.07	931.45	938.41	939.94	945.69

NEOPENTANE 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
1	49.50	500000.00	660.07	614.24	626.37	642.46	664.49
2	50.50	500000.00	643.22	595.50	607.00	625.53	643.02
3	51.50	500000.00	626.50	583.67	594.52	606.88	629.40
4	52.50	500000.00	613.60	568.79	584.07	590.81	611.55
5	53.50	500000.00	606.97	567.05	576.70	590.17	607.34
6	54.50	500000.00	602.35	566.83	570.66	585.44	604.50
7	55.50	500000.00	606.83	568.90	576.50	590.26	605.36
8	56.50	500000.00	611.43	581.07	584.97	599.90	616.20
9	57.50	500000.00	623.90	588.85	594.06	605.98	624.54
10	58.50	500000.00	637.83	598.64	607.07	619.51	639.24
11	59.50	500000.00	655.68	612.70	625.41	635.26	651.10
12	60.50	500000.00	673.45	627.47	642.12	652.20	669.81
13	61.50	500000.00	690.28	645.36	661.39	665.56	682.59
14	62.50	500000.00	710.37	675.71	683.33	690.55	701.94
15	63.50	500000.00	727.67	693.99	697.50	722.15	720.82
16	64.50	500000.00	751.53	714.01	712.16	732.23	744.72

TOTAL SCATTERED INTENSITIES IN COUNTS PER MINUTE

NEOPENTANE 25C

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

N	THETA	S	DIV.	I,RAW	BKG.	POL.	PEN.	I,CORR.	ERROR
1	2.50	0.771	0.50	3124.67	3.10	1.00	0.38	8267.10	18.49
2	2.75	0.848	0.50	3754.93	3.10	1.00	0.35	10647.81	23.81
3	3.00	0.925	0.50	4822.18	3.10	0.99	0.33	14595.72	32.64
4	3.25	1.002	0.50	6727.96	3.10	0.99	0.31	21656.59	48.43
5	3.50	1.079	0.50	10204.95	3.10	0.99	0.30	34817.47	77.85
6	3.75	1.156	0.50	12881.07	3.10	0.99	0.28	46439.71	103.84
7	4.00	1.233	0.50	10071.34	3.10	0.99	0.27	38261.09	85.55
8	4.25	1.310	0.50	5819.03	3.10	0.99	0.25	23234.35	51.95
9	4.50	1.387	0.50	3364.45	3.10	0.99	0.24	14085.62	31.50
10	4.75	1.464	0.50	2225.07	3.10	0.99	0.23	9747.08	21.80
11	5.00	1.541	0.50	1622.10	3.10	0.99	0.22	7420.95	16.59
12	5.25	1.618	0.50	1281.44	3.10	0.98	0.21	6112.16	13.67
13	5.50	1.695	0.50	1110.83	3.10	0.98	0.20	5516.28	12.33
14	5.75	1.771	0.50	1007.25	3.10	0.98	0.20	5200.49	11.63
15	6.00	1.848	0.50	931.89	3.10	0.98	0.19	4995.95	11.17
16	6.25	1.925	0.50	884.79	3.10	0.98	0.18	4919.59	11.00
17	6.50	2.002	0.50	855.83	3.10	0.98	0.18	4929.91	11.02
18	6.75	2.078	0.50	815.24	3.10	0.97	0.17	4859.64	10.87
19	7.00	2.155	0.50	776.34	3.10	0.97	0.17	4784.04	10.70
20	7.25	2.231	0.50	754.29	3.10	0.97	0.16	4800.96	10.74
21	7.50	2.308	0.50	725.87	3.10	0.97	0.16	4767.56	10.66
22	7.75	2.384	0.50	719.23	3.10	0.97	0.15	4871.32	10.89
23	8.00	2.461	0.50	698.93	3.10	0.96	0.15	4877.22	10.91
24	8.25	2.537	0.50	673.75	3.10	0.96	0.14	4840.12	10.82
25	8.50	2.614	0.50	656.26	3.10	0.96	0.14	4850.38	10.85
26	8.75	2.690	0.50	634.36	3.10	0.96	0.14	4820.23	10.76
27	9.00	2.766	0.50	619.05	3.10	0.95	0.13	4833.27	10.81
28	9.25	2.842	0.50	595.31	3.10	0.95	0.13	4772.58	10.67
29	9.50	2.918	0.50	555.99	3.10	0.95	0.13	4573.55	10.23
30	9.00	2.766	2.00	7135.78	4.60	0.95	0.41	18145.27	33.13
31	9.50	2.918	2.00	6656.07	4.60	0.95	0.40	17634.44	32.20
32	10.00	3.070	2.00	6009.61	4.60	0.94	0.38	16570.50	30.25
33	10.50	3.222	2.00	5296.61	4.60	0.94	0.37	15183.96	27.72
34	11.00	3.374	2.00	4622.97	4.60	0.93	0.36	13765.38	25.13
35	11.50	3.525	2.00	4054.70	4.60	0.93	0.35	12529.07	22.87
36	12.00	3.676	2.00	3601.08	4.60	0.92	0.34	11537.90	21.07
37	12.50	3.827	2.00	3254.68	4.60	0.91	0.33	10804.44	19.73
38	13.00	3.978	2.00	2976.24	4.60	0.91	0.32	10229.34	18.68
39	13.50	4.128	2.00	2815.23	4.60	0.90	0.31	10011.52	18.28
40	14.00	4.278	2.00	2661.27	4.60	0.89	0.30	9785.84	17.87
41	14.50	4.427	2.00	2581.39	4.60	0.89	0.30	9809.32	17.91
42	15.00	4.576	2.00	2522.56	4.60	0.88	0.29	9900.51	18.08
43	15.50	4.725	2.00	2485.71	4.60	0.87	0.28	10070.80	18.39
44	16.00	4.874	2.00	2412.22	4.60	0.86	0.28	10083.00	18.41
45	16.50	5.022	2.00	2345.83	4.60	0.86	0.27	10111.43	18.46
46	17.00	5.170	2.00	2242.74	4.60	0.85	0.26	9963.62	18.19
47	17.50	5.317	2.00	2121.19	4.60	0.84	0.26	9708.04	17.72
48	18.00	5.464	2.00	1973.12	4.60	0.83	0.25	9298.43	16.98
49	18.50	5.610	2.00	1825.76	4.60	0.82	0.25	8855.46	16.17
50	19.00	5.757	2.00	1667.78	4.60	0.82	0.24	8321.82	15.19
51	19.50	5.902	2.00	1520.21	4.60	0.81	0.24	7800.31	14.24
52	20.00	6.047	2.00	1374.86	4.60	0.80	0.24	7251.21	13.24

NORMALIZED TO 2.00 DEG. SLITS

N	S	I,SCALED	ERROR
1	0.771	31456.27	70.34
2	0.848	40514.86	90.59
3	0.925	55536.66	124.18
4	1.002	82403.19	184.26
5	1.079	132480.31	296.23
6	1.156	176702.87	395.12
7	1.233	145583.25	325.53
8	1.310	88406.56	197.68
9	1.387	53595.71	119.84
10	1.464	37087.59	82.93
11	1.541	28236.66	63.14
12	1.618	23256.75	52.00
13	1.695	20989.41	46.93
14	1.771	19787.85	44.25
15	1.848	19009.58	42.51
16	1.925	18719.00	41.86
17	2.002	18758.27	41.94
18	2.078	18490.92	41.35
19	2.155	18203.26	40.70
20	2.231	18267.65	40.85
21	2.308	18140.55	40.56
22	2.384	18535.35	41.45
23	2.461	18557.79	41.50
24	2.537	18416.62	41.18
25	2.614	18455.68	41.27
26	2.690	18340.97	41.01
27	2.766	18267.91	41.12
28	2.842	18159.64	40.61
29	2.918	17518.38	38.91
30	3.070	16570.50	30.25
31	3.222	15183.96	27.72
32	3.374	13765.38	25.13
33	3.525	12529.07	22.87
34	3.676	11537.90	21.07
35	3.827	10804.44	19.73
36	3.978	10229.34	18.68
37	4.128	10011.52	18.28
38	4.278	9785.84	17.87
39	4.427	9809.32	17.91
40	4.576	9900.51	18.08
41	4.725	10070.80	18.39
42	4.874	10083.00	18.41
43	5.022	10111.43	18.46
44	5.170	9963.62	18.19
45	5.317	9708.04	17.72
46	5.464	9298.43	16.98
47	5.610	8855.46	16.17
48	5.757	8321.82	15.19
49	5.902	7800.31	14.24
50	6.047	7251.21	13.24

N	THETA	S	DIV.	I,RAW	BKG.	POL.	PEN.	I,CORR.	ERROR
53	20.50	6.192	2.00	1232.34	4.60	0.79	0.23	6677.76	12.19
54	21.00	6.337	2.00	1110.06	4.60	0.78	0.23	6177.72	11.28
55	21.50	6.480	2.00	1005.00	4.60	0.77	0.22	5742.02	10.48
56	22.00	6.624	2.00	918.42	4.60	0.77	0.22	5385.28	9.83
57	22.50	6.766	2.00	853.87	4.60	0.76	0.22	5136.81	9.38
58	23.00	6.909	2.00	805.18	4.60	0.75	0.21	4968.25	9.07
59	22.00	6.624	4.00	4353.19	4.00	0.77	0.38	14932.37	21.12
60	22.50	6.766	4.00	4094.89	4.00	0.76	0.38	14382.13	20.34
61	23.00	6.909	4.00	3887.37	4.00	0.75	0.37	13976.41	19.77
62	23.50	7.051	4.00	3703.11	4.00	0.74	0.37	13625.75	19.27
63	24.00	7.192	4.00	3546.69	4.00	0.73	0.36	13352.59	18.88
64	24.50	7.332	4.00	3421.22	4.00	0.72	0.36	13175.45	18.63
65	25.00	7.473	4.00	3296.31	4.00	0.72	0.35	12981.93	18.36
66	25.50	7.612	4.00	3174.27	4.00	0.71	0.35	12781.04	18.08
67	26.00	7.751	4.00	3047.45	4.00	0.70	0.35	12541.44	17.74
68	26.50	7.890	4.00	2916.08	4.00	0.69	0.34	12262.28	17.34
69	27.00	8.027	4.00	2773.90	4.00	0.68	0.34	11914.95	16.85
70	27.50	8.164	4.00	2646.58	4.00	0.68	0.34	11608.67	16.42
71	28.00	8.301	4.00	2496.30	4.00	0.67	0.33	11177.48	15.81
72	28.50	8.437	4.00	2360.85	4.00	0.66	0.33	10787.50	15.26
73	29.00	8.572	4.00	2228.08	4.00	0.65	0.33	10385.74	14.69
74	29.50	8.707	4.00	2092.75	4.00	0.64	0.33	9947.53	14.07
75	30.00	8.841	4.00	1977.54	4.00	0.64	0.32	9581.98	13.55
76	30.50	8.974	4.00	1869.11	4.00	0.63	0.32	9228.44	13.05
77	31.00	9.107	4.00	1773.76	4.00	0.62	0.32	8920.27	12.62
78	31.50	9.239	4.00	1696.33	4.00	0.62	0.32	8685.73	12.28
79	32.00	9.370	4.00	1617.08	4.00	0.61	0.31	8426.44	11.92
80	32.50	9.500	4.00	1555.52	4.00	0.60	0.31	8245.52	11.66
81	33.00	9.630	4.00	1496.13	4.00	0.60	0.31	8063.72	11.40
82	33.50	9.759	4.00	1450.17	4.00	0.59	0.31	7943.36	11.23
83	34.00	9.887	4.00	1404.87	4.00	0.58	0.31	7816.64	11.05
84	34.50	10.015	4.00	1361.27	4.00	0.58	0.31	7689.45	10.87
85	35.00	10.142	4.00	1339.58	4.00	0.57	0.30	7678.44	10.86
86	35.50	10.268	4.00	1277.72	4.00	0.57	0.30	7426.82	10.50
87	36.00	10.393	4.00	1237.19	4.00	0.56	0.30	7288.40	10.31
88	36.50	10.517	4.00	1195.54	4.00	0.56	0.30	7133.87	10.09
89	37.00	10.641	4.00	1157.90	4.00	0.55	0.30	6994.02	9.89
90	37.50	10.764	4.00	1120.75	4.00	0.55	0.30	6848.24	9.68
91	38.00	10.886	4.00	1081.57	4.00	0.54	0.30	6681.15	9.45
92	38.50	11.007	4.00	1048.95	4.00	0.54	0.30	6546.23	9.26
93	39.00	11.127	4.00	1020.46	4.00	0.54	0.29	6429.46	9.09
94	39.50	11.247	4.00	997.03	4.00	0.53	0.29	6337.65	8.96
95	40.00	11.366	4.00	972.09	4.00	0.53	0.29	6229.43	8.81
96	40.50	11.483	4.00	958.31	4.00	0.53	0.29	6186.88	8.75
97	41.00	11.600	4.00	947.95	4.00	0.53	0.29	6161.09	8.71
98	41.50	11.716	4.00	934.28	4.00	0.52	0.29	6108.21	8.64
99	42.00	11.831	4.00	931.51	4.00	0.52	0.29	6121.71	8.66
100	42.50	11.946	4.00	930.60	4.00	0.52	0.29	6142.76	8.69
101	43.00	12.059	4.00	928.66	4.00	0.52	0.29	6152.16	8.70
102	43.50	12.171	4.00	931.65	4.00	0.52	0.29	6189.50	8.75
103	44.00	12.283	4.00	938.25	4.00	0.52	0.29	6246.18	8.83
104	44.50	12.393	4.00	944.60	4.00	0.52	0.29	6296.30	8.90
105	45.00	12.503	4.00	945.63	4.00	0.52	0.29	6305.70	8.92
106	45.50	12.611	4.00	952.34	4.00	0.52	0.29	6348.12	8.98
107	46.00	12.719	4.00	954.65	4.00	0.52	0.29	6355.86	8.99
108	46.50	12.826	4.00	956.66	4.00	0.52	0.29	6356.43	8.99
109	47.00	12.932	4.00	958.74	4.00	0.52	0.29	6352.32	8.98
110	47.50	13.036	4.00	956.23	4.00	0.52	0.29	6312.72	8.93
111	48.00	13.140	4.00	956.18	4.00	0.52	0.29	6284.58	8.89
112	48.50	13.243	4.00	948.32	4.00	0.52	0.29	6200.41	8.77

N	S	I,SCALED	ERROR
51	6.192	6677.76	12.19
52	6.337	6177.72	11.28
53	6.480	5742.02	10.48
54	6.624	5363.66	9.83
55	6.766	5141.00	9.38
56	6.909	4984.14	9.07
57	7.051	4874.59	6.89
58	7.192	4776.87	6.76
59	7.332	4713.50	6.67
60	7.473	4644.27	6.57
61	7.612	4572.40	6.47
62	7.751	4486.68	6.35
63	7.890	4386.81	6.20
64	8.027	4262.56	6.03
65	8.164	4152.98	5.87
66	8.301	3998.73	5.66
67	8.437	3859.22	5.46
68	8.572	3715.48	5.25
69	8.707	3558.72	5.03
70	8.841	3427.94	4.85
71	8.974	3301.46	4.67
72	9.107	3191.22	4.51
73	9.239	3107.31	4.39
74	9.370	3014.55	4.26
75	9.500	2949.83	4.17
76	9.630	2884.79	4.08
77	9.759	2841.73	4.02
78	9.887	2796.39	3.95
79	10.015	2750.89	3.89
80	10.142	2746.95	3.88
81	10.268	2656.93	3.76
82	10.393	2607.42	3.69
83	10.517	2552.13	3.61
84	10.641	2502.10	3.54
85	10.764	2449.95	3.46
86	10.886	2390.17	3.38
87	11.007	2341.90	3.31
88	11.127	2300.13	3.25
89	11.247	2267.29	3.21
90	11.366	2228.57	3.15
91	11.483	2213.35	3.13
92	11.600	2204.12	3.12
93	11.716	2185.21	3.09
94	11.831	2190.03	3.10
95	11.946	2197.56	3.11
96	12.059	2200.93	3.11
97	12.171	2214.28	3.13
98	12.283	2234.56	3.16
99	12.393	2252.49	3.19
100	12.503	2255.86	3.19
101	12.611	2271.03	3.21
102	12.719	2273.80	3.22
103	12.826	2274.00	3.22
104	12.932	2272.54	3.21
105	13.036	2258.37	3.19
106	13.140	2248.30	3.18
107	13.243	2218.19	3.14

N	THETA	S	DIV.	I,RAW	BKG.	POL.	PEN.	I,CORR.	ERROR
113	49.00	13.345	4.00	946.45	4.00	0.53	0.29	6151.28	8.70
114	49.50	13.445	4.00	938.59	4.00	0.53	0.29	6059.07	8.57
115	50.00	13.545	4.00	939.20	4.00	0.53	0.29	6017.83	8.51
116	50.50	13.644	4.00	935.65	4.00	0.53	0.29	5945.94	8.41
117	51.00	13.741	4.00	937.02	4.00	0.54	0.29	5901.70	8.35
118	51.50	13.838	4.00	939.09	4.00	0.54	0.30	5857.98	8.28
119	49.50	13.445	4.00	640.95	3.60	0.53	0.29	4132.01	5.84
120	50.50	13.644	4.00	622.26	3.60	0.53	0.29	3948.40	5.58
121	51.50	13.838	4.00	607.68	3.60	0.54	0.30	3784.32	5.35
122	52.50	14.028	4.00	593.28	3.60	0.55	0.30	3616.09	5.11
123	53.50	14.214	4.00	589.21	3.60	0.56	0.30	3506.09	4.96
124	54.50	14.395	4.00	585.54	3.60	0.57	0.30	3393.19	4.80
125	55.50	14.572	4.00	589.18	3.60	0.58	0.31	3317.54	4.69
126	56.50	14.744	4.00	598.39	3.60	0.59	0.31	3267.01	4.62
127	57.50	14.913	4.00	607.11	3.60	0.60	0.31	3207.33	4.54
128	58.50	15.076	4.00	620.03	3.60	0.62	0.32	3163.78	4.47
129	59.50	15.235	4.00	635.63	3.60	0.63	0.32	3127.23	4.42
130	60.50	15.389	4.00	652.56	3.60	0.64	0.33	3090.63	4.37
131	61.50	15.539	4.00	668.66	3.60	0.66	0.33	3044.04	4.30
132	62.50	15.684	4.00	692.16	3.60	0.68	0.34	3024.79	4.28
133	63.50	15.824	4.00	712.16	3.60	0.69	0.34	2983.63	4.22
134	64.50	15.959	4.00	730.59	3.60	0.71	0.35	2930.88	4.14

N	S	I,SCALED	ERROR
108	13.345	2200.61	3.11
109	13.445	2196.92	3.07
110	13.545	2152.87	3.04
111	13.644	2127.22	3.01
112	13.741	2111.32	2.99
113	13.838	2067.29	2.96
114	14.028	1948.26	2.76
115	14.214	1888.99	2.67
116	14.395	1828.17	2.59
117	14.572	1787.41	2.53
118	14.744	1760.18	2.49
119	14.913	1728.03	2.44
120	15.076	1704.57	2.41
121	15.235	1684.87	2.38
122	15.389	1665.15	2.35
123	15.539	1640.05	2.32
124	15.684	1629.68	2.30
125	15.824	1607.51	2.27
126	15.959	1579.09	2.23

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[2], C is the scaling factor[2], and $\sum_i f_i^2(s)$ is the part of the scattering ascribable to independent atoms, summed over the stochiometric unit (one neopentane molecule). The coherent and incoherent form factors for carbon and hydrogen were obtained from the literature[3]. The values of the relative intensities I(s) were extrapolated at low angle from θ equal to 2.5 degrees to θ equal to zero and I(0) 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

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

where ρ_o is the uniform number density obtained from the literature[4], 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 the 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 carbon and hydrogen,

and summation is again over the stochiometric 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 molecule.

The physical meaning of the function D(r) has been discussed in detail elsewhere[2,5].

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. 2. 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 1.0 Å were eliminated. This includes C-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.

3.2.1 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[2] 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.

3.2.2 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.

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	S	SI*M 1	SI*M 2	ERROR	DELTA SI*M
2	0.077	-0.007985	-0.007899	0.000046	-0.000086
3	0.154	-0.015140	-0.014993	0.000186	-0.000147
4	0.231	-0.021420	-0.021247	0.000421	-0.000173
5	0.309	-0.026830	-0.026657	0.000755	-0.000173
6	0.386	-0.031290	-0.031117	0.001193	-0.000173
7	0.463	-0.034740	-0.034538	0.001743	-0.000202
8	0.540	-0.037120	-0.036835	0.002410	-0.000285
9	0.617	-0.038300	-0.037871	0.003209	-0.000429
10	0.694	-0.038180	-0.037558	0.004150	-0.000622
11	0.771	-0.036140	-0.035296	0.000184	-0.000844
12	0.848	-0.021760	-0.020681	0.000269	-0.001079
13	0.925	0.009656	0.010976	0.000417	-0.001320
14	1.002	0.076720	0.078293	0.000694	-0.001573
15	1.079	0.219500	0.221368	0.001245	-0.001868
16	1.156	0.375300	0.377535	0.001845	-0.002235
17	1.233	0.319500	0.322207	0.001678	-0.002707
18	1.310	0.157100	0.160409	0.001126	-0.003309
19	1.387	0.041560	0.045614	0.000744	-0.004054
20	1.464	-0.019950	-0.015017	0.000559	-0.004933
21	1.541	-0.057670	-0.051742	0.000461	-0.005928
22	1.618	-0.082400	-0.075385	0.000411	-0.007015
23	1.695	-0.095910	-0.087731	0.000402	-0.008179
24	1.771	-0.104300	-0.094883	0.000414	-0.009417
25	1.848	-0.110900	-0.100088	0.000433	-0.010812
26	1.925	-0.114300	-0.101866	0.000464	-0.012434
27	2.002	-0.114800	-0.100428	0.000507	-0.014372
28	2.078	-0.117400	-0.100745	0.000544	-0.016655
29	2.155	-0.119900	-0.100559	0.000583	-0.019341
30	2.231	-0.118300	-0.096016	0.000637	-0.022284
31	2.308	-0.117400	-0.091962	0.000691	-0.025438
32	2.384	-0.109900	-0.081301	0.000770	-0.028599
33	2.461	-0.105900	-0.074086	0.000840	-0.031814
34	2.537	-0.103800	-0.068717	0.000904	-0.035083
35	2.614	-0.097800	-0.059089	0.000985	-0.038711
36	2.690	-0.094030	-0.051141	0.001059	-0.042889
37	2.766	-0.089950	-0.042040	0.001140	-0.047910
38	2.842	-0.084840	-0.030947	0.001219	-0.053893
39	2.918	-0.090870	-0.030110	0.001258	-0.060760
40	3.070	-0.097830	-0.021786	0.001202	-0.076044
41	3.222	-0.121800	-0.030273	0.001257	-0.091527
42	3.374	-0.156100	-0.048831	0.001284	-0.107269
43	3.525	-0.193800	-0.068171	0.001315	-0.125629
44	3.676	-0.231100	-0.082942	0.001357	-0.148158
45	3.827	-0.265400	-0.091879	0.001413	-0.173521
46	3.978	-0.297500	-0.097432	0.001493	-0.200068
47	4.128	-0.312400	-0.084184	0.001639	-0.228216
48	4.278	-0.330600	-0.070870	0.001775	-0.259730
49	4.427	-0.329000	-0.034690	0.001990	-0.294310
50	4.576	-0.318400	0.012412	0.002244	-0.330812
51	4.725	-0.296100	0.072788	0.002542	-0.368887
52	4.874	-0.289400	0.120042	0.002780	-0.409442
53	5.022	-0.275700	0.176701	0.003059	-0.452401
54	5.170	-0.283700	0.213358	0.003275	-0.497058

	S	DI*M 1	SI*M 2	ERROR	DELTA SI*M
55	5.317	-0.311700	0.230795	0.003422	-0.542495
56	5.464	-0.366100	0.223362	0.003495	-0.589462
57	5.610	-0.433000	0.204726	0.003524	-0.637725
58	5.757	-0.527200	0.159944	0.003458	-0.687144
59	5.902	-0.626000	0.109923	0.003377	-0.735923
60	6.047	-0.738600	0.046394	0.003245	-0.784994
61	6.192	-0.865100	-0.030547	0.003059	-0.834553
62	6.337	-0.978900	-0.095304	0.002890	-0.883596
63	6.480	-1.087000	-0.156553	0.002741	-0.930446
64	6.624	-1.184999	-0.208641	0.002628	-0.976358
65	6.766	-1.240000	-0.218966	0.002611	-1.021033
66	6.909	-1.275999	-0.211296	0.002656	-1.064703
67	7.051	-1.296000	-0.190927	0.002115	-1.105073
68	7.192	-1.308000	-0.166233	0.002204	-1.141767
69	7.332	-1.302999	-0.126977	0.002324	-1.176023
70	7.473	-1.296000	-0.087146	0.002448	-1.208854
71	7.612	-1.285000	-0.046891	0.002573	-1.238109
72	7.751	-1.273000	-0.010402	0.002691	-1.262598
73	7.890	-1.264000	0.018664	0.002793	-1.282664
74	8.027	-1.263000	0.036673	0.002865	-1.299672
75	8.164	-1.252999	0.061065	0.002955	-1.314064
76	8.301	-1.254999	0.069168	0.002990	-1.324167
77	8.437	-1.256000	0.072783	0.003034	-1.328782
78	8.572	-1.257999	0.071031	0.003066	-1.329030
79	8.707	-1.266999	0.059402	0.003075	-1.326402
80	8.841	-1.263000	0.057640	0.003114	-1.320640
81	8.974	-1.259999	0.050213	0.003150	-1.310212
82	9.107	-1.249000	0.045750	0.003205	-1.294749
83	9.239	-1.224000	0.052009	0.003296	-1.276009
84	9.370	-1.204000	0.051332	0.003371	-1.255332
85	9.500	-1.171000	0.060903	0.003483	-1.231902
86	9.630	-1.141000	0.062817	0.003591	-1.203816
87	9.759	-1.099000	0.072473	0.003732	-1.171473
88	9.887	-1.058999	0.078315	0.003867	-1.137314
89	10.010	-1.023000	0.081321	0.003991	-1.104321
90	10.140	-0.953600	0.114747	0.004211	-1.068347
91	10.270	-0.947600	0.080930	0.004252	-1.028530
92	10.390	-0.921000	0.066598	0.004353	-0.987598
93	10.520	-0.896500	0.044644	0.004453	-0.941144
94	10.640	-0.877000	0.022281	0.004542	-0.899281
95	10.760	-0.865100	-0.006210	0.004613	-0.858890
96	10.890	-0.855600	-0.041298	0.004681	-0.814302
97	11.010	-0.844200	-0.074198	0.004756	-0.770002
98	11.130	-0.830100	-0.106950	0.004841	-0.723150
99	11.250	-0.815500	-0.138954	0.004939	-0.676546
100	11.370	-0.802100	-0.169539	0.005027	-0.632561
101	11.480	-0.771400	-0.177039	0.005161	-0.594361
102	11.600	-0.729100	-0.176148	0.005332	-0.552952
103	11.720	-0.696800	-0.186553	0.005475	-0.510247
104	11.830	-0.641600	-0.171162	0.005677	-0.470438
105	11.950	-0.578500	-0.150281	0.005908	-0.428219
106	12.060	-0.524300	-0.132449	0.006113	-0.391851
107	12.170	-0.458900	-0.101458	0.006350	-0.357442
108	12.280	-0.381600	-0.057637	0.006622	-0.323963
109	12.390	-0.307900	-0.017124	0.006888	-0.290776
110	12.500	-0.249600	0.008931	0.007110	-0.258531
111	12.610	-0.175300	0.053070	0.007380	-0.228370
112	12.720	-0.117700	0.083072	0.007607	-0.200772
113	12.830	-0.064220	0.110802	0.007825	-0.175021

	S	DI*M 1	SI*M 2	ERROR	DELTA SI*M
114	12.930	-0.013510	0.138686	0.008026	-0.152196
115	13.040	0.021430	0.148713	0.008195	-0.127283
116	13.140	0.058180	0.163686	0.008364	-0.105506
117	13.240	0.065850	0.151677	0.008450	-0.085827
118	13.340	0.090610	0.159750	0.008586	-0.069140
119	13.450	0.141200	0.195222	0.008739	-0.054022
120	13.540	0.117900	0.160989	0.008804	-0.043089
121	13.640	0.127700	0.158737	0.008902	-0.031037
122	13.740	0.151100	0.169366	0.009045	-0.018266
123	13.840	0.126100	0.131157	0.009122	-0.005057
124	14.030	0.007754	-0.009115	0.008866	0.016869
125	14.210	-0.018670	-0.047918	0.008939	0.029248
126	14.390	-0.054440	-0.090281	0.008991	0.035841
127	14.570	-0.056960	-0.098454	0.009144	0.041494
128	14.740	-0.040710	-0.086682	0.009347	0.045972
129	14.910	-0.039430	-0.086873	0.009518	0.047443
130	15.080	-0.017620	-0.063464	0.009746	0.045844
131	15.240	0.001765	-0.041265	0.009969	0.043030
132	15.390	0.015950	-0.024110	0.010170	0.040060
133	15.540	0.016650	-0.020219	0.010340	0.036869
134	15.680	0.045760	0.012108	0.010580	0.033652
135	15.820	0.042900	0.012890	0.010740	0.030010
136	15.960	0.016490	-0.009002	0.010840	0.025492

OBSERVED RADIAL DISTRIBUTION FUNCTIONS, INTERACTIONS FROM 0.0 A TO 1.00 A ELIMINATED.

	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	-0.630E 03	-0.970E-01	-0.162E 01	0.71E 01	-0.250E-03	0.11E-02
3	0.100	-0.567E 03	-0.349E 00	-0.105E 01	0.57E 01	-0.649E-03	0.35E-02
4	0.150	-0.471E 03	-0.653E 00	-0.366E 00	0.38E 01	-0.507E-03	0.52E-02
5	0.200	-0.356E 03	-0.878E 00	0.180E 00	0.19E 01	0.443E-03	0.46E-02
6	0.250	-0.236E 03	-0.910E 00	0.410E 00	0.14E 01	0.158E-02	0.54E-02
7	0.300	-0.125E 03	-0.695E 00	0.315E 00	0.16E 01	0.174E-02	0.88E-02
8	0.350	-0.344E 02	-0.260E 00	0.318E-01	0.15E 01	0.240E-03	0.11E-01
9	0.400	0.300E 02	0.296E 00	-0.232E 00	0.10E 01	-0.228E-02	0.10E-01
10	0.450	0.663E 02	0.827E 00	-0.315E 00	0.84E 00	-0.393E-02	0.10E-01
11	0.500	0.775E 02	0.119E 01	-0.181E 00	0.87E 00	-0.279E-02	0.13E-01
12	0.550	0.698E 02	0.130E 01	0.692E-01	0.85E 00	0.129E-02	0.16E-01
13	0.600	0.510E 02	0.113E 01	0.269E 00	0.68E 00	0.597E-02	0.15E-01
14	0.650	0.288E 02	0.749E 00	0.286E 00	0.61E 00	0.745E-02	0.16E-01
15	0.700	0.908E 01	0.274E 00	0.103E 00	0.63E 00	0.310E-02	0.19E-01
16	0.750	-0.458E 01	-0.159E 00	-0.167E 00	0.62E 00	-0.578E-02	0.21E-01
17	0.800	-0.112E 02	-0.443E 00	-0.342E 00	0.53E 00	-0.135E-01	0.21E-01
18	0.850	-0.120E 02	-0.532E 00	-0.284E 00	0.50E 00	-0.126E-01	0.22E-01
19	0.900	-0.899E 01	-0.449E 00	0.641E-02	0.50E 00	0.320E-03	0.25E-01
20	0.950	-0.482E 01	-0.268E 00	0.371E 00	0.48E 00	0.206E-01	0.27E-01
21	1.000	-0.138E 01	-0.852E-01	0.562E 00	0.42E 00	0.346E-01	0.26E-01
22	1.050	0.346E 00	0.235E-01	0.379E 00	0.40E 00	0.257E-01	0.27E-01
23	1.100	0.377E 00	0.281E-01	-0.199E 00	0.40E 00	-0.148E-01	0.30E-01
24	1.150	-0.572E 00	-0.466E-01	-0.948E 00	0.39E 00	-0.773E-01	0.32E-01
25	1.200	-0.151E 01	-0.134E 00	-0.147E 01	0.35E 00	-0.130E 00	0.31E-01
26	1.250	-0.163E 01	-0.156E 00	-0.133E 01	0.34E 00	-0.128E 00	0.32E-01
27	1.300	-0.555E 00	-0.578E-01	-0.284E 00	0.35E 00	-0.296E-01	0.36E-01
28	1.350	0.151E 01	0.170E 00	0.158E 01	0.34E 00	0.178E 00	0.38E-01
29	1.400	0.398E 01	0.480E 00	0.385E 01	0.30E 00	0.464E 00	0.37E-01
30	1.450	0.606E 01	0.785E 00	0.586E 01	0.30E 00	0.759E 00	0.38E-01
31	1.500	0.713E 01	0.988E 00	0.700E 01	0.30E 00	0.971E 00	0.42E-01
32	1.550	0.689E 01	0.102E 01	0.690E 01	0.29E 00	0.102E 01	0.43E-01
33	1.600	0.548E 01	0.864E 00	0.560E 01	0.27E 00	0.883E 00	0.42E-01
34	1.650	0.339E 01	0.569E 00	0.353E 01	0.26E 00	0.592E 00	0.44E-01
35	1.700	0.129E 01	0.230E 00	0.136E 01	0.26E 00	0.241E 00	0.47E-01
36	1.750	-0.233E 00	-0.439E-01	-0.270E 00	0.26E 00	-0.510E-01	0.48E-01
37	1.800	-0.866E 00	-0.173E 00	-0.966E 00	0.24E 00	-0.193E 00	0.47E-01
38	1.850	-0.641E 00	-0.135E 00	-0.732E 00	0.23E 00	-0.154E 00	0.49E-01
39	1.900	0.110E 00	0.245E-01	0.823E-01	0.23E 00	0.183E-01	0.52E-01
40	1.950	0.909E 00	0.213E 00	0.955E 00	0.23E 00	0.224E 00	0.54E-01
41	2.000	0.134E 01	0.329E 00	0.142E 01	0.21E 00	0.350E 00	0.53E-01
42	2.050	0.120E 01	0.310E 00	0.127E 01	0.21E 00	0.328E 00	0.55E-01
43	2.100	0.580E 00	0.158E 00	0.594E 00	0.21E 00	0.161E 00	0.58E-01
44	2.150	-0.199E 00	-0.567E-01	-0.242E 00	0.21E 00	-0.688E-01	0.59E-01
45	2.200	-0.743E 00	-0.221E 00	-0.811E 00	0.19E 00	-0.242E 00	0.58E-01
46	2.250	-0.747E 00	-0.233E 00	-0.798E 00	0.19E 00	-0.249E 00	0.60E-01
47	2.300	-0.130E 00	-0.424E-01	-0.135E 00	0.19E 00	-0.440E-01	0.63E-01
48	2.350	0.944E 00	0.321E 00	0.983E 00	0.19E 00	0.334E 00	0.64E-01
49	2.400	0.214E 01	0.758E 00	0.219E 01	0.18E 00	0.778E 00	0.63E-01
50	2.450	0.307E 01	0.114E 01	0.311E 01	0.18E 00	0.115E 01	0.65E-01
51	2.500	0.349E 01	0.134E 01	0.349E 01	0.18E 00	0.134E 01	0.68E-01
52	2.550	0.334E 01	0.134E 01	0.330E 01	0.17E 00	0.132E 01	0.69E-01
53	2.600	0.275E 01	0.114E 01	0.270E 01	0.16E 00	0.112E 01	0.69E-01
54	2.650	0.198E 01	0.855E 00	0.195E 01	0.16E 00	0.842E 00	0.71E-01
55	2.700	0.130E 01	0.583E 00	0.130E 01	0.17E 00	0.583E 00	0.74E-01

	R	G1	D1	G2	ERROR	D2	ERROR
56	2.750	0.870E 00	0.405E 00	0.898E 00	0.16E 00	0.418E 00	0.74E-01
57	2.800	0.718E 00	0.347E 00	0.754E 00	0.15E 00	0.364E 00	0.74E-01
58	2.850	0.744E 00	0.372E 00	0.766E 00	0.15E 00	0.383E 00	0.77E-01
59	2.900	0.805E 00	0.417E 00	0.801E 00	0.15E 00	0.415E 00	0.80E-01
60	2.950	0.787E 00	0.422E 00	0.762E 00	0.15E 00	0.408E 00	0.79E-01
61	3.000	0.659E 00	0.365E 00	0.629E 00	0.14E 00	0.349E 00	0.80E-01
62	3.050	0.472E 00	0.270E 00	0.455E 00	0.14E 00	0.261E 00	0.82E-01
63	3.100	0.316E 00	0.187E 00	0.319E 00	0.14E 00	0.189E 00	0.85E-01
64	3.150	0.266E 00	0.163E 00	0.286E 00	0.14E 00	0.175E 00	0.85E-01
65	3.200	0.343E 00	0.216E 00	0.364E 00	0.13E 00	0.230E 00	0.84E-01
66	3.250	0.500E 00	0.325E 00	0.510E 00	0.13E 00	0.332E 00	0.88E-01
67	3.300	0.658E 00	0.441E 00	0.651E 00	0.13E 00	0.437E 00	0.90E-01
68	3.350	0.745E 00	0.515E 00	0.727E 00	0.13E 00	0.503E 00	0.90E-01
69	3.400	0.732E 00	0.521E 00	0.715E 00	0.13E 00	0.509E 00	0.90E-01
70	3.450	0.646E 00	0.474E 00	0.640E 00	0.13E 00	0.469E 00	0.93E-01
71	3.500	0.547E 00	0.413E 00	0.556E 00	0.13E 00	0.419E 00	0.96E-01
72	3.550	0.498E 00	0.387E 00	0.514E 00	0.12E 00	0.399E 00	0.95E-01
73	3.600	0.529E 00	0.422E 00	0.542E 00	0.12E 00	0.433E 00	0.97E-01
74	3.650	0.625E 00	0.513E 00	0.627E 00	0.12E 00	0.514E 00	0.99E-01
75	3.700	0.737E 00	0.621E 00	0.727E 00	0.12E 00	0.613E 00	0.10E 00
76	3.750	0.810E 00	0.701E 00	0.795E 00	0.12E 00	0.689E 00	0.10E 00
77	3.800	0.811E 00	0.721E 00	0.801E 00	0.11E 00	0.713E 00	0.10E 00
78	3.850	0.744E 00	0.679E 00	0.746E 00	0.11E 00	0.681E 00	0.10E 00
79	3.900	0.645E 00	0.604E 00	0.658E 00	0.11E 00	0.616E 00	0.11E 00
80	3.950	0.563E 00	0.541E 00	0.579E 00	0.11E 00	0.556E 00	0.11E 00
81	4.000	0.535E 00	0.528E 00	0.545E 00	0.11E 00	0.537E 00	0.11E 00
82	4.050	0.570E 00	0.576E 00	0.568E 00	0.11E 00	0.574E 00	0.11E 00
83	4.100	0.649E 00	0.672E 00	0.636E 00	0.11E 00	0.659E 00	0.11E 00
84	4.150	0.734E 00	0.779E 00	0.720E 00	0.10E 00	0.764E 00	0.11E 00
85	4.200	0.795E 00	0.863E 00	0.788E 00	0.10E 00	0.856E 00	0.11E 00
86	4.250	0.813E 00	0.905E 00	0.818E 00	0.10E 00	0.910E 00	0.11E 00
87	4.300	0.796E 00	0.906E 00	0.810E 00	0.10E 00	0.922E 00	0.12E 00
88	4.350	0.763E 00	0.890E 00	0.779E 00	0.10E 00	0.908E 00	0.12E 00
89	4.400	0.741E 00	0.884E 00	0.749E 00	0.98E-01	0.893E 00	0.12E 00
90	4.450	0.744E 00	0.908E 00	0.740E 00	0.99E-01	0.903E 00	0.12E 00
91	4.500	0.774E 00	0.966E 00	0.761E 00	0.98E-01	0.949E 00	0.12E 00
92	4.550	0.820E 00	0.105E 01	0.805E 00	0.95E-01	0.103E 01	0.12E 00
93	4.600	0.864E 00	0.113E 01	0.856E 00	0.94E-01	0.112E 01	0.12E 00
94	4.650	0.893E 00	0.119E 01	0.897E 00	0.93E-01	0.119E 01	0.12E 00
95	4.700	0.900E 00	0.122E 01	0.913E 00	0.92E-01	0.124E 01	0.13E 00
96	4.750	0.888E 00	0.123E 01	0.903E 00	0.91E-01	0.125E 01	0.13E 00
97	4.800	0.868E 00	0.123E 01	0.875E 00	0.89E-01	0.124E 01	0.13E 00
98	4.850	0.850E 00	0.123E 01	0.847E 00	0.89E-01	0.123E 01	0.13E 00
99	4.900	0.846E 00	0.125E 01	0.834E 00	0.88E-01	0.123E 01	0.13E 00
100	4.950	0.860E 00	0.130E 01	0.846E 00	0.87E-01	0.128E 01	0.13E 00
101	5.000	0.892E 00	0.137E 01	0.884E 00	0.86E-01	0.136E 01	0.13E 00
102	5.050	0.935E 00	0.147E 01	0.937E 00	0.86E-01	0.147E 01	0.14E 00
103	5.100	0.979E 00	0.157E 01	0.988E 00	0.85E-01	0.158E 01	0.14E 00
104	5.150	0.101E 01	0.165E 01	0.102E 01	0.83E-01	0.167E 01	0.14E 00
105	5.200	0.103E 01	0.171E 01	0.103E 01	0.83E-01	0.172E 01	0.14E 00
106	5.250	0.102E 01	0.174E 01	0.102E 01	0.83E-01	0.174E 01	0.14E 00
107	5.300	0.101E 01	0.175E 01	0.100E 01	0.81E-01	0.173E 01	0.14E 00
108	5.350	0.993E 00	0.175E 01	0.982E 00	0.80E-01	0.173E 01	0.14E 00
109	5.400	0.989E 00	0.178E 01	0.982E 00	0.81E-01	0.176E 01	0.15E 00
110	5.450	0.100E 01	0.184E 01	0.100E 01	0.80E-01	0.184E 01	0.15E 00
111	5.500	0.104E 01	0.193E 01	0.104E 01	0.79E-01	0.195E 01	0.15E 00
112	5.550	0.108E 01	0.205E 01	0.109E 01	0.78E-01	0.206E 01	0.15E 00
113	5.600	0.111E 01	0.215E 01	0.112E 01	0.77E-01	0.216E 01	0.15E 00
114	5.650	0.112E 01	0.220E 01	0.112E 01	0.78E-01	0.220E 01	0.15E 00

	R	G1	D1	G2	ERROR	D2	ERROR
115	5.700	0.111E 01	0.221E 01	0.110E 01	0.76E-01	0.220E 01	0.15E 00
116	5.750	0.107E 01	0.219E 01	0.107E 01	0.74E-01	0.217E 01	0.15E 00
117	5.800	0.104E 01	0.216E 01	0.104E 01	0.75E-01	0.215E 01	0.16E 00
118	5.850	0.103E 01	0.216E 01	0.103E 01	0.76E-01	0.217E 01	0.16E 00
119	5.900	0.104E 01	0.223E 01	0.104E 01	0.73E-01	0.224E 01	0.16E 00
120	5.950	0.108E 01	0.234E 01	0.108E 01	0.72E-01	0.236E 01	0.16E 00
121	6.000	0.112E 01	0.248E 01	0.112E 01	0.73E-01	0.249E 01	0.16E 00
122	6.050	0.116E 01	0.261E 01	0.116E 01	0.72E-01	0.261E 01	0.16E 00
123	6.100	0.117E 01	0.268E 01	0.117E 01	0.72E-01	0.268E 01	0.17E 00
124	6.150	0.116E 01	0.270E 01	0.116E 01	0.71E-01	0.269E 01	0.17E 00
125	6.200	0.113E 01	0.268E 01	0.113E 01	0.70E-01	0.268E 01	0.17E 00
126	6.250	0.111E 01	0.267E 01	0.111E 01	0.70E-01	0.267E 01	0.17E 00
127	6.300	0.110E 01	0.270E 01	0.111E 01	0.70E-01	0.270E 01	0.17E 00
128	6.350	0.112E 01	0.278E 01	0.112E 01	0.68E-01	0.278E 01	0.17E 00
129	6.400	0.115E 01	0.290E 01	0.115E 01	0.67E-01	0.290E 01	0.17E 00
130	6.450	0.118E 01	0.303E 01	0.118E 01	0.68E-01	0.302E 01	0.17E 00
131	6.500	0.120E 01	0.311E 01	0.119E 01	0.67E-01	0.311E 01	0.17E 00
132	6.550	0.119E 01	0.314E 01	0.119E 01	0.66E-01	0.314E 01	0.17E 00
133	6.600	0.116E 01	0.311E 01	0.116E 01	0.66E-01	0.311E 01	0.18E 00
134	6.650	0.112E 01	0.305E 01	0.113E 01	0.66E-01	0.307E 01	0.18E 00
135	6.700	0.109E 01	0.303E 01	0.110E 01	0.65E-01	0.304E 01	0.18E 00
136	6.750	0.109E 01	0.305E 01	0.109E 01	0.64E-01	0.305E 01	0.18E 00
137	6.800	0.110E 01	0.313E 01	0.110E 01	0.64E-01	0.312E 01	0.18E 00
138	6.850	0.112E 01	0.325E 01	0.112E 01	0.63E-01	0.323E 01	0.18E 00
139	6.900	0.115E 01	0.336E 01	0.114E 01	0.63E-01	0.334E 01	0.18E 00
140	6.950	0.115E 01	0.343E 01	0.115E 01	0.62E-01	0.343E 01	0.18E 00
141	7.000	0.114E 01	0.345E 01	0.115E 01	0.63E-01	0.346E 01	0.19E 00
142	7.050	0.112E 01	0.342E 01	0.112E 01	0.62E-01	0.344E 01	0.19E 00
143	7.100	0.109E 01	0.338E 01	0.109E 01	0.61E-01	0.339E 01	0.19E 00
144	7.150	0.107E 01	0.336E 01	0.107E 01	0.60E-01	0.336E 01	0.19E 00
145	7.200	0.106E 01	0.338E 01	0.105E 01	0.62E-01	0.336E 01	0.20E 00
146	7.250	0.106E 01	0.343E 01	0.105E 01	0.61E-01	0.341E 01	0.20E 00
147	7.300	0.107E 01	0.352E 01	0.106E 01	0.59E-01	0.349E 01	0.19E 00
148	7.350	0.108E 01	0.360E 01	0.108E 01	0.59E-01	0.359E 01	0.20E 00
149	7.400	0.108E 01	0.366E 01	0.109E 01	0.60E-01	0.367E 01	0.20E 00
150	7.450	0.108E 01	0.369E 01	0.109E 01	0.59E-01	0.371E 01	0.20E 00
151	7.500	0.107E 01	0.370E 01	0.107E 01	0.58E-01	0.372E 01	0.20E 00
152	7.550	0.105E 01	0.369E 01	0.105E 01	0.57E-01	0.370E 01	0.20E 00
153	7.600	0.104E 01	0.369E 01	0.103E 01	0.57E-01	0.368E 01	0.20E 00
154	7.650	0.103E 01	0.370E 01	0.102E 01	0.58E-01	0.367E 01	0.21E 00
155	7.700	0.102E 01	0.372E 01	0.101E 01	0.56E-01	0.369E 01	0.21E 00
156	7.750	0.101E 01	0.375E 01	0.101E 01	0.56E-01	0.373E 01	0.21E 00
157	7.800	0.101E 01	0.379E 01	0.101E 01	0.56E-01	0.379E 01	0.21E 00
158	7.850	0.101E 01	0.382E 01	0.101E 01	0.56E-01	0.384E 01	0.21E 00
159	7.900	0.100E 01	0.385E 01	0.101E 01	0.56E-01	0.388E 01	0.21E 00
160	7.950	0.994E 00	0.387E 01	0.999E 00	0.54E-01	0.389E 01	0.21E 00
161	8.000	0.987E 00	0.389E 01	0.987E 00	0.55E-01	0.389E 01	0.22E 00
162	8.050	0.980E 00	0.391E 01	0.975E 00	0.54E-01	0.389E 01	0.22E 00
163	8.100	0.975E 00	0.394E 01	0.968E 00	0.54E-01	0.391E 01	0.22E 00
164	8.150	0.973E 00	0.398E 01	0.968E 00	0.54E-01	0.396E 01	0.22E 00
165	8.200	0.974E 00	0.404E 01	0.974E 00	0.53E-01	0.403E 01	0.22E 00
166	8.250	0.978E 00	0.410E 01	0.982E 00	0.53E-01	0.412E 01	0.22E 00
167	8.300	0.982E 00	0.417E 01	0.988E 00	0.52E-01	0.419E 01	0.22E 00
168	8.350	0.981E 00	0.422E 01	0.987E 00	0.53E-01	0.424E 01	0.23E 00
169	8.400	0.974E 00	0.424E 01	0.977E 00	0.51E-01	0.425E 01	0.22E 00
170	8.450	0.961E 00	0.423E 01	0.960E 00	0.52E-01	0.422E 01	0.23E 00
171	8.500	0.944E 00	0.420E 01	0.941E 00	0.51E-01	0.419E 01	0.23E 00
172	8.550	0.930E 00	0.419E 01	0.926E 00	0.51E-01	0.417E 01	0.23E 00
173	8.600	0.923E 00	0.420E 01	0.922E 00	0.51E-01	0.420E 01	0.23E 00

	R	G1	D1	G2	ERROR	D2	ERROR
174	8.650	0.926E 00	0.427E 01	0.927E 00	0.50E-01	0.427E 01	0.23E 00
175	8.700	0.937E 00	0.437E 01	0.940E 00	0.51E-01	0.438E 01	0.24E 00
176	8.750	0.950E 00	0.448E 01	0.954E 00	0.48E-01	0.450E 01	0.23E 00
177	8.800	0.958E 00	0.457E 01	0.960E 00	0.51E-01	0.458E 01	0.24E 00
178	8.850	0.956E 00	0.461E 01	0.956E 00	0.47E-01	0.461E 01	0.23E 00
179	8.900	0.943E 00	0.460E 01	0.942E 00	0.50E-01	0.459E 01	0.24E 00
180	8.950	0.925E 00	0.456E 01	0.923E 00	0.47E-01	0.456E 01	0.23E 00
181	9.000	0.910E 00	0.454E 01	0.909E 00	0.50E-01	0.453E 01	0.25E 00
182	9.050	0.904E 00	0.456E 01	0.904E 00	0.47E-01	0.456E 01	0.24E 00
183	9.100	0.911E 00	0.465E 01	0.910E 00	0.48E-01	0.464E 01	0.24E 00
184	9.150	0.926E 00	0.477E 01	0.926E 00	0.47E-01	0.477E 01	0.24E 00
185	9.200	0.943E 00	0.491E 01	0.942E 00	0.47E-01	0.491E 01	0.25E 00
186	9.250	0.953E 00	0.502E 01	0.953E 00	0.48E-01	0.502E 01	0.25E 00
187	9.300	0.953E 00	0.508E 01	0.954E 00	0.46E-01	0.508E 01	0.24E 00
188	9.350	0.944E 00	0.508E 01	0.945E 00	0.47E-01	0.509E 01	0.25E 00
189	9.400	0.931E 00	0.507E 01	0.932E 00	0.45E-01	0.507E 01	0.25E 00
190	9.450	0.921E 00	0.507E 01	0.921E 00	0.47E-01	0.507E 01	0.26E 00
191	9.500	0.919E 00	0.511E 01	0.918E 00	0.45E-01	0.510E 01	0.25E 00
192	9.550	0.926E 00	0.521E 01	0.923E 00	0.46E-01	0.519E 01	0.26E 00
193	9.600	0.939E 00	0.533E 01	0.935E 00	0.44E-01	0.531E 01	0.25E 00
194	9.650	0.950E 00	0.545E 01	0.947E 00	0.46E-01	0.543E 01	0.26E 00
195	9.700	0.956E 00	0.554E 01	0.955E 00	0.44E-01	0.554E 01	0.26E 00
196	9.750	0.954E 00	0.559E 01	0.957E 00	0.45E-01	0.560E 01	0.26E 00
197	9.800	0.948E 00	0.561E 01	0.953E 00	0.43E-01	0.564E 01	0.25E 00
198	9.850	0.943E 00	0.563E 01	0.947E 00	0.44E-01	0.566E 01	0.27E 00
199	9.900	0.943E 00	0.569E 01	0.946E 00	0.43E-01	0.571E 01	0.26E 00
200	9.950	0.949E 00	0.579E 01	0.950E 00	0.44E-01	0.579E 01	0.27E 00
201	10.000	0.961E 00	0.592E 01	0.960E 00	0.43E-01	0.591E 01	0.26E 00

4. DISCUSSION

The reduced intensity function for liquid neopentane is shown in Fig. 1; Fig. 2 shows the corresponding radial distribution function. Distinct maxima in the RDF at 1.54 and 2.52 Å correspond to intramolecular carbon-carbon interactions; the ratio of these two distances is, within experimental error, equal to $(8/3)^{\frac{1}{2}}$, indicating tetrahedal geometry. Distinct peaks which start at 3.8 Å, and are centered around a broad maximum at 6.5 Å, must be ascribed to interactions between atom pairs from different molecules. The intramolecular distances derived from this study are in agreement with values of 1.54 ± 0.02 and 2.52 Å, obtained from gas diffraction experiments[6].

A model structure for liquid neopentane, which gives a detailed description of the atomic and molecular configuration in the liquid state, will be described in a later report.

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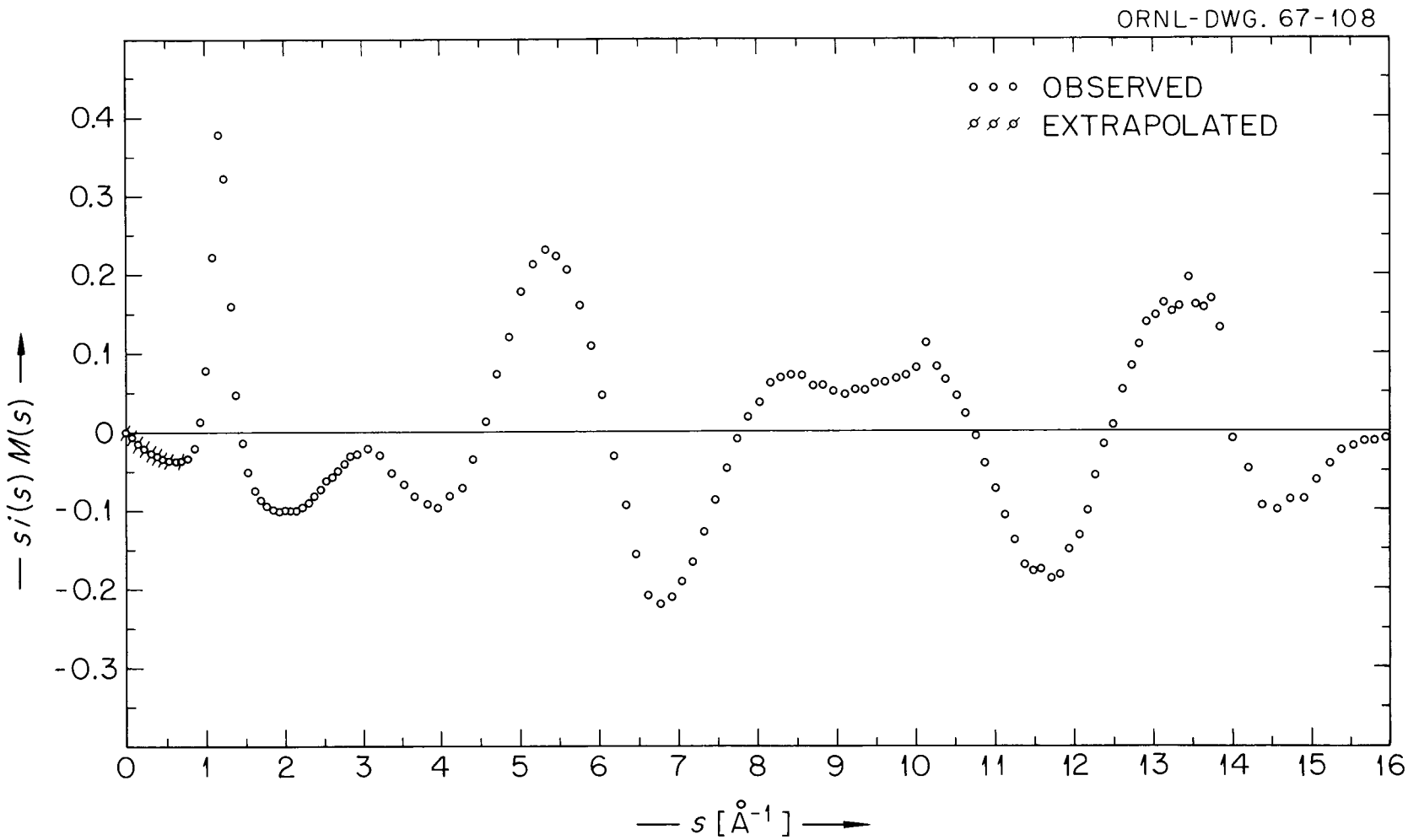

Fig. 1. Reduced Intensity Function of Liquid Neopentane at 25°C.

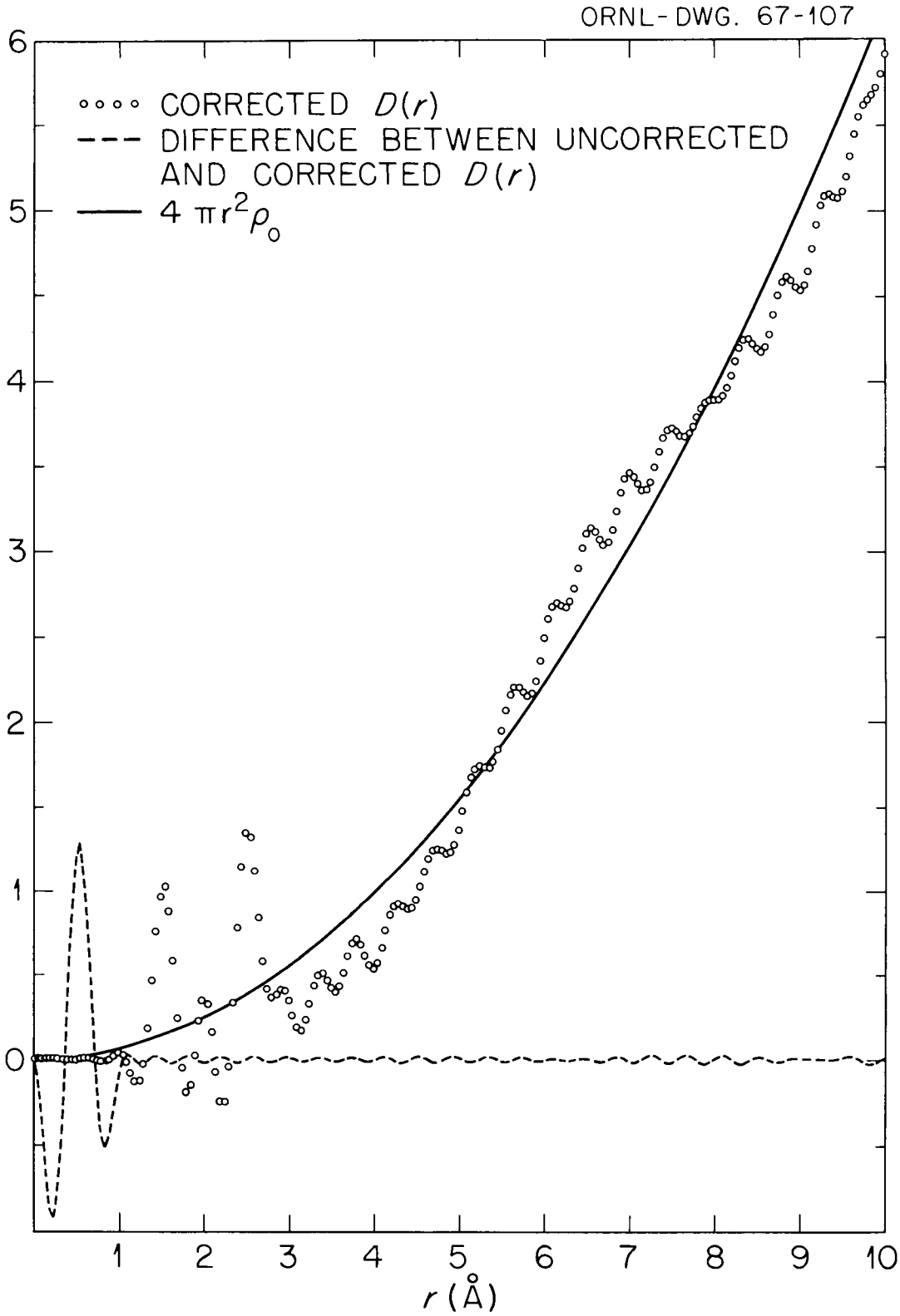

Fig. 2. Radial Distribution Function of Liquid Neopentane at 25°C.

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