X-ray analysis of the structure of liquid Rb and Cs

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X-ray-transmission measurements have been performed and the diffraction patterns using Ag $K\alpha$ and Mo $K\alpha$ radiation have been determined for liquid rubidium at 40 and 90 °C and for liquid cesium at 65 and 100 °C, respectively. A new sample holder has been used. The structure factors a(q) do not agree very well with measurements of neutron diffraction, but there is good agreement with the x-ray pattern of Huijben *et al.* in the case of Cs.

I. INTRODUCTION

One of the most important quantities of the liquid state is the structure factor a(q) which is the Fourier transform of the correlation function [g(r)-1]. The structure factors can be obtained both from x-ray and neutron diffraction experiments. The structure factors a(q) of alkali metals (Li, Na, K, Rb, Cs) were determined by Gingrich et al. in 1961 from neutron diffraction measurements.¹ Greenfield et al. (1971) repeated the measurement on liquid Na and K with x rays.² The agreement with Gingrich's data is satisfactory,³ while the x-ray data on K of Thomas *et al.* (1938) disagree.⁴ Gamertsfelder is the first who published x-ray data of liquid Li.⁵ Huijben et al. recently (1976) published x-ray data on liquid Cs, which differ from Gingrich's data, because the maxima are shifted.⁶ However, in the case of liquid gallium, there is no significant difference between the x-ray and neutron data.7,8

It is one aim of this paper to find out which data are reliable. This is important for the structure analysis. A second aim is to obtain x-ray diffraction data of liquid Rb, which are till now unknown. Hence, an attempt was made to use x-ray diffraction to determine the structure factors of liquid Rb and Cs. We have employed a transmission geometry which is different from the system used by Greenfield $et al.^2$ and by Huijben $et al.^6$ Mo radiation was taken to determine the structure factors of liquid Cs and Ag radiation was taken to determine both the structure factors of liquid Rb and Cs. The use of two wavelengths serves to prove the internal consistency of data on Cs. The experimental data were obtained and analyzed at different temperatures.

II. EXPERIMENTAL

Our x-ray diffraction pattern was taken using MoK α and AgK α radiations in a transmission geometry and the measurements were made using

the Bragg-Brentano focusing, Philips horizontal goniometer (Fig. 1). The primary radiation emitted from the line focus (L) passed through the Soller slit (p) and $\frac{1}{2}^{\circ}$ divergences slit (D). The scattered beam from the sample S was limited by a 0.2-mm receiving slit (R) and the K_B radiation was removed by a filter of 0.05-mm Pd or Zr foil (F). The scattering intensity arising from the continuous spectrum and the Compton radiation was mostly removed by a bent graphite monochromator (M). The resolution $(\Delta\lambda/\lambda)$ is about 3×10^{-2} . The scattered intensity was measured by a scintillation counter (C).

The purity of the sample Rb and Cs is 99.98% which is given by Light Laboratories, Ltd., England. The elements for Rb and Cs are the most reactive metals. When these are contaminated with a trace of air or moisture, oxide and hydroxide are formed immediately. Therefore the sample was filled in a glass capillary ($\phi = 0.57$ mm with wall thickness of 0.007 mm) [Fig. 2(a)] under high vacuum (< 10⁻⁶ Torr). After filling, the glass capillary was end fused and mounted in the heating unit which is described in details in Fig. 2(b). The absorption of Mo radia-



FIG. 1. Focusing system of the Philips horizontal goniometer.

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III. ANALYSIS OF THE X-RAY DIFFRACTION MEASUREMENTS

The experimentally determined x-ray intensities were corrected for the effects of absorption, polarization, and dispersion. The corrected intensities were normalized and then converted into structure factors a(q).

A. Corrections for polarization, absorption, and empty glass capillary scattering

The measurements were carried out, one with the sample holder filled with the sample $[I_{sc}(\theta)]$ and one with the empty capillary $[I_c(\theta)]$. Both the intensities $I_{sc}(\theta)$ and $I_{c}(\theta)$ are reduced due to the absorption in the liquid sample and the glass capillary. The cylindrical absorption factor for scattering in the glass capillary and absorption in both sample and capillary A_c has been calculated.⁹ In the present case the absorption due to the glass capillary $[\exp(-\mu l) \cong 1$, where μ and l are the linear absorption coefficient and the path length in the glass capillary, respectively] was found to be negligible (wall thickness of the glass capillary =0.0007 cm). The cylindrical absorption factor for scattering and self-absorption in sample $A_{s}(\theta)$ is thus a function of μr , where μ is the linear absorption coefficient of the specimen and r is its radius. The absorption factors $A_{s}(\theta)$ and μ are taken from the international tables for x-ray crystallography.¹⁰ The generally valid formula for the absorption correction in cylindrical samples, derived by Paalman et al.,11 goes over into the simpler form

$$I_s = (I_{sc} - I_c A_c) / [A_s P(\theta)]$$

under the conditions of the present experiment. Here $P(\theta)$ is the polarization factor. The contribution of incoherent scattering to the intensity counted by the detector is less than 2% at all scattering angles of the present experiment. The correction of the Compton scattering has been therefore omitted.



FIG. 2. (a) Microscopic picture of the glass capillary. (b) Sample holder and associated heating unit. A: Stainless-steel cylinder for fixing the glass capillary. B: Soapstone cylinder wrapped by nickel wire for heating. C,D: Stainless tube and brass tube, respectively. W: Window sealed with Mylar foil.

tion is too high for the Rb sample and the fluorescence is correspondingly very high. Therefore, only Mo radiation was used to measure Cs. The Ag radiation measurements were carried out both for Rb and Cs. The use of two different wavelengths is applied to check the internal consistency of the data for Cs. The temperature is monitored by means of a copper-Constantan thermocouple. For both the full and empty glass capillary, at each temperature, data were taken at $\Delta \theta = 0.125^{\circ}$ interval from $\theta = 3^{\circ}$ to 30° . Data were taken at constant time of 2000 sec. The statistical deviation of the measured intensity was below 1%. Before the x-ray diffraction pattern of liquid

(a)

α) and Cs(Mo $K\alpha$).										
	a(q) (Rb)	- <u>) a stant</u> () () () () () ()		a(q) (Cs)	l					
	40 °C	90 °C	q	65 °C	100 °C					
)	1.206	1.197	2.272	0.855	0.852					
2	1.189	1.182	2.310	0.916	0.905					
3	1.164	1.159	2.348	0.975	0.957					
3	1.133	1.130	2.387	1.031	1.008					
5	1.098	1.096	2.425	1.082	1.054					
3	1.060	1.060	2.463	1.127	1.096					
2	1.023	1.025	2.501	1.163	1.130					
)	0.988	0.991	2.540	1.190	1.157					
2	0.957	0.961	2.578	1.208	1.176					

TABLE I. Experimental values of a(q) for $Rb(Ag K\alpha)$:

2e q 40°C 90°C q 65°C 100°C 0.000 1.5250 2.578 1.164 1.132 2.330 0.483 0.024 0.000 0.000 1.650 0.000 0.483 0.024 0.001 1.650 3.200 0.680 0.981 0.981 0.981 1.183 1.133 1.133 1.133 1.134 1.130 1.137 2.000 0.000 0.022 0.011 1.650 3.220 0.860 0.981 0.981 0.981 0.912 1.183 1.134 1.134 1.134 1.134 1.134 1.1343 1.134 1.145		a(q) (Rb)				a(q) (Cs)) ,	a(q) (Rb)			a(q) (Cs)			
	2Θ	q	40 °C	90 °C	q	65 °C	100 °C	20	q	40 °C	90 °C	q	65 °C	100 °C
0.000 0.000 <th< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td> </td><td></td><td></td><td></td><td></td><td></td><td></td></th<>														
0.250 0.494 0.000 0.000 0.000 0.000 15.000 2.222 1.189 1.182 2.130 0.936 0.985 0.750 0.447 0.000 0.000 0.161 0.000 0.000 1.55 0.285 1.081 1.130 2.337 1.631 1.130 2.337 1.631 1.130 2.337 0.631 1.031 1.030 2.345 0.061 0.060 0.060 1.650 3.275 1.085 1.085 1.085 1.131 1.130 2.337 1.061 1.600 2.425 1.051 1.131 1.130 2.337 1.131 1.130 2.337 1.131 1.130 1.337 1.131 1.1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	14.750	2.880	1.206	1.197	2.272	0.855	0.852
0.500 0.099 0.000 0.000 0.116 0.000 0.000 15.500 3.026 1.333 1.333 2.337 1.031 1.039 1.500 0.294 0.000 0.000 0.154 0.000 0.000 1.550 3.075 1.098 1.092 2.433 1.021 1.039 1.500 0.294 0.000 0.000 0.232 0.013 0.014 16.500 3.122 0.058 0.093 2.051 1.133 1.331 1.136 1.334 1.331 1.331 1.330 1.331 1.331 1.330 1.331 1.332 1.337 1.331 1.332 1.337 1.331 1.332 1.335 1.335 1.331 1.331 1.335 1.331 1.331 1.331 1.331 1.331 1.331 1.335 1.331 1.331 1.335 1	0.250	0.049	0.000	0.000	0.039	0.000	0.000	15.000	2.292	1.189	1.182	2.310	0.916	0.905
0.750 0.147 0.000 0.000 0.154 0.000 15.50 3.028 1.133 1.130 2.371 1.031 1.030 2.372 1.031 1.030 2.372 1.031 1.030 2.372 1.031 1.030 2.372 1.031 1.060 2.451 1.051 1.031 1.050 2.721 1.031 1.060 2.452 1.051 1.331 1.330 1.331 1.330 1.331 <td< td=""><td>0.500</td><td>0.098</td><td>0.000</td><td>0.000</td><td>0.077</td><td>0.000</td><td>0.000</td><td>15.250</td><td>2.978</td><td>1.164</td><td>1.159</td><td>2.348</td><td>0.975</td><td>0.957</td></td<>	0.500	0.098	0.000	0.000	0.077	0.000	0.000	15.250	2.978	1.164	1.159	2.348	0.975	0.957
1.000 0.156 0.000 0.154 0.000 0.000 1.750 3.075 1.098 1.096 2.452 1.021 1.054 1.560 0.244 0.000 0.000 0.332 0.001 0.270 0.232 0.001 0.270 0.222 0.011 1.650 3.123 1.060 0.660 2.450 1.163 1.330 2.000 0.392 0.002 0.032 0.023 0.021 16.500 3.172 1.023 0.661 0.661 1.163 1.330 2.500 0.440 0.004 0.348 0.038 0.031 17.500 3.161 0.583 0.613 0.031 17.500 3.161 0.683 0.862 1.061 1.173 3.500 0.638 0.638 0.638 0.638 1.300 1.750 3.462 0.893 0.891 1.017 1.154 3.500 0.658 0.611 0.638 0.638 1.500 3.550 0.893 0.893 2.921	0.750	0.147	0.000	0.000	0.116	0.000	0.000	15.500	3.026	1.133	1.130	2.387	1.031	1.008
1.250 0.244 0.000 0.000 0.133 0.002 0.004 16.250 3.123 1.060 1.065 2.661 1.127 1.096 1.750 0.244 0.000 0.022 0.017 16.250 3.123 1.025 2.601 1.357 1.025 2.601 1.460 1.025 2.610 1.137 2.500 0.441 0.044 0.044 0.044 0.038 0.031 17.250 3.617 0.932 0.936 2.611 1.216 1.137 2.500 0.400 0.044 0.444 0.438 0.038 17.500 3.414 0.900 0.901 2.621 1.266 1.357 3.500 0.638 0.038 0.038 18.200 3.510 0.883 0.897 2.731 1.139 1.134 3.750 0.637 0.038 0.038 18.200 3.510 0.899 0.911 2.971 1.074 1.080 4.500 0.532 0.338 0.438	1.000	0.196	0.000	0.000	0.154	0.000	0.000	15.750	3.075	1.098	1.096	2.425	1.082	1.054
1.500 0.294 0.000 0.000 0.232 0.013 0.014 16.500 3.172 1.025 2.501 1.163 1.301 2.000 0.392 0.002 0.009 0.382 0.001 0.270 0.538 0.991 2.540 1.163 1.301 2.500 0.440 0.004 0.048 0.038 0.031 17.50 3.260 0.587 0.991 2.541 1.216 1.187 2.500 0.490 0.006 0.007 0.386 0.038 0.031 17.50 3.462 0.883 0.896 2.761 1.156 1.157 1.153 3.500 0.685 0.017 0.733 0.038 0.038 15.500 3.690 0.910 2.465 1.161 1.156 4.260 0.733 0.646 0.048 0.038 1.550 3.650 0.910 2.465 1.101 1.016 4.260 0.832 0.634 0.638 0.638 1.550 1.675 <t< td=""><td>1.250</td><td>0.245</td><td>0.000</td><td>0.000</td><td>0.193</td><td>0.002</td><td>0.004</td><td>16.000</td><td>3.123</td><td>1.060</td><td>1.060</td><td>2.463</td><td>1.127</td><td>1.096</td></t<>	1.250	0.245	0.000	0.000	0.193	0.002	0.004	16.000	3.123	1.060	1.060	2.463	1.127	1.096
1756 0.343 0.000 0.001 0.77 0.622 0.017 2.250 0.444 0.004 0.044 0.044 0.044 0.044 0.044 0.044 0.044 0.044 0.044 0.044 0.044 0.044 0.044 0.044 0.046 0.07 0.386 0.028 17.700 3.317 0.932 0.936 2.641 1.268 1.175 2.500 0.460 0.004 0.444 0.463 0.038 0.038 17.500 3.414 0.900 0.939 2.768 1.167 1.156 3.500 0.658 0.021 0.038 0.038 18.200 3.510 0.893 0.991 2.676 1.167 1.156 3.500 0.652 0.038 0.034 0.038 18.250 3.607 0.996 0.910 2.676 1.047 1.068 4.500 0.532 0.638 0.038 0.387 1.555 0.590 0.997 2.951 1.041 1.051 4.500 0.532 0.538 0.640 0.638 0.038 1.575	1.500	0.294	0.000	0.000	0.232	0.013	0.014	16.250	3.172	1.023	1.025	2.501	1.163	1.130
2.000 0.9192 0.002 0.038 0.021 16.750 3.265 0.947 0.936 2.751 1.208 1.176 2.500 0.449 0.004 0.348 0.028 0.038 0.031 17.500 3.365 0.936 2.614 1.216 1.139 2.750 0.538 0.009 0.010 0.425 0.038 0.038 17.500 3.462 0.936 2.694 1.216 1.139 3.750 0.738 0.011 0.018 0.038 0.038 1.800 3.550 0.898 2.769 1.139 1.134 4.000 0.783 0.626 0.636 0.048 1.550 3.650 0.931 2.461 1.061 4.250 0.520 0.632 0.636 0.042 0.038 115.500 3.650 0.931 2.461 1.061 4.250 0.520 0.632 0.636 0.042 0.038 115.50 3.650 0.931 3.656 0.661 1.061	1.750	0.343	0.000	0.001	0.270	0.022	0.017	16.500	3.220	0.988	0.991	2.540	1.190	1.157
2.250 0.441 0.004 0.044 0.048 0.038 0.028 17.000 3.217 0.322 0.363 2.616 1.216 1.130 2.750 0.458 0.009 0.010 0.425 0.638 0.031 17.500 3.365 0.901 2.682 1.261 1.131 3.250 0.636 0.011 0.445 0.638 0.038 1.850 3.462 0.838 0.897 2.731 1.150 1.134 3.750 0.734 0.028 0.579 0.038 0.038 185.00 3.655 0.899 0.901 2.845 1.108 1.164 4.250 0.532 0.034 0.668 0.044 0.038 185.00 3.655 0.599 0.301 2.845 1.041 1.051 4.500 0.532 0.590 0.500 0.570 0.577 2.590 1.022 1.041 1.051 4.500 0.591 0.591 0.591 0.591 0.591 0.591	2.000	0.392	0.002	0.002	0.309	0.038	0.021	16.750	3.268	0.957	0.961	2.578	1.208	1.176
2.500 0.440 0.006 0.007 0.386 0.038 0.031 17.250 3.365 0.432 0.264 1.261 1.363 3.260 0.363 0.013 0.014 0.463 0.038 0.038 17.500 3.414 0.000 0.637 2.731 1.190 1.175 3.260 0.365 0.071 0.023 0.541 0.038 0.038 1.167 1.365 0.283 0.893	2.250	0.441	0.004	0.004	0.348	0.038	0.028	17.000	3.317	0.932	0.936	2.616	1.216	1.187
2.756 0.538 0.009 0.610 0.425 0.038 0.033 17.500 3.414 0.900 0.603 0.487 1.190 1.173 3.250 0.636 0.017 0.118 0.502 0.038 0.038 1.8600 3.462 0.893 0.897 2.731 1.190 1.173 3.250 0.636 0.021 0.577 0.038 0.038 1.8500 3.650 0.893 0.292 1.181 1.190 1.134 3.750 0.686 0.041 0.635 0.042 0.638 1.674 1.680 3.460 0.877 0.937 2.991 1.041 1.051 4.750 0.830 0.079 0.772 0.635 0.042 0.088 19.500 3.752 0.937 2.991 1.041 1.052 5.000 0.79 0.121 0.077 0.733 0.660 0.038 19.500 3.752 0.937 2.991 1.041 1.042 5.000 1.077	2.500	0.490	0.006	0.007	0.386	0.038	0.031	17.250	3.365	0.912	0.916	2.654	1.216	1.190
3.000 0.557 0.013 0.014 0.463 0.038 17.750 3.442 0.893 2.871 1.190 1.173 3.250 0.635 0.021 0.028 0.541 0.038 0.038 1.8250 3.559 0.893 0.897 2.731 1.139 1.134 3.750 0.734 0.028 0.579 0.038 0.038 1.036 3.650 0.897 0.991 2.845 1.108 1.134 4.000 0.733 0.032 0.041 0.656 0.040 0.038 19.500 3.670 0.991 2.997 0.977 0.995 5.000 0.077 0.270 0.373 0.360 0.943 1.037 1.037 1.033 5.050 0.977 0.395 0.926 0.977 0.995 5.200 1.027 0.884 0.922 0.937 0.974 2.997 0.977 0.985 5.200 1.028 0.128 0.811 0.043 2.0007 2.250	2.750	0.538	0.009	0.010	0.425	0.038	0.033	17.500	3.414	0.900	0.903	2.692	1.206	1.185
3.250 0.636 0.017 0.018 0.502 0.038 0.038 0.890 0.899 0.890 2.890 1.147 1.156 3.750 0.636 0.021 0.023 0.541 0.038 0.038 0.899 0.910 2.845 1.108 1.134 3.750 0.632 0.034 0.618 0.038 0.038 18.500 3.607 0.990 0.910 2.845 1.108 1.080 4.500 0.832 0.044 0.618 0.038 19.500 3.762 0.957 0.974 2.997 0.977 0.999 0.910 1.022 1.001 1.002 1.002 1.002 1.002 1.002 1.002 1.002 1.002 1.002 1.002 1.002 1.003 1.003 1.003 0.035 0.950 0.970 0.971 0.941 1.002 0.949 0.955 0.970 0.971 0.974 1.018 1.019 1.011 1.022 0.893 1.030 1.031 0.933 0.933 0.930 0.935 0.949 0.955 0.970 0.944 0.9	3.000	0.587	0.013	0.014	0.463	0.038	0.038	17.750	3.462	0.893	0.897	2.731	1.190	1.173
3.500 0.685 0.021 0.028 0.541 0.038 0.038 0.038 0.859 0.990 2.807 1.139 1.134 4.000 0.733 0.032 0.034 0.618 0.038 0.038 0.038 0.038 0.038 0.038 1.061 1.062 4.200 0.831 0.043 0.662 0.696 0.042 0.038 19.500 3.774 0.939 2.921 1.041 1.051 4.500 0.881 0.047 0.773 0.650 0.043 19.500 3.760 0.977 0.977 0.995 5.000 0.077 0.290 0.121 0.062 0.696 0.043 20.000 3.897 1.007 1.063 0.414 1.035 0.435 0.956 0.943 0.957 0.974 2.997 0.977 0.995 0.926 0.949 0.911 0.911 0.914 0.914 0.914 0.914 0.373 0.926 0.949 0.911 0.914 0.411 0.433 0.311 0.960 0.914 0.914 0.433 0.3149 0.8	3.250	0.636	0.017	0.018	0.502	0.038	0.038	18.000	3.510	0.893	0.896	2.769	1.167	1.156
3.750 0.734 0.028 0.679 0.038 0.038 0.038 0.038 0.041 0.618 0.038 0.038 0.041 0.656 0.038 0.038 0.670 0.923 0.924 0.938 0.910 0.944 0.926 0.924 0.934 0.930 0.931 0.945 0.949 0.931 0.945 0.949 0.931 0.946 0.949 0.943 0.946 0.948 0.941 0.931 0.946 0.948 0.949 0.945 0.944 0.943 0.944 0.944 0.944 0.944 0.944 0.944 0.944 0.944 0.944 0.944 <td< td=""><td>3.500</td><td>0.685</td><td>0.021</td><td>0.023</td><td>0.541</td><td>0.038</td><td>0.038</td><td>18.250</td><td>3.559</td><td>0.899</td><td>0.901</td><td>2.807</td><td>1.139</td><td>1.134</td></td<>	3.500	0.685	0.021	0.023	0.541	0.038	0.038	18.250	3.559	0.899	0.901	2.807	1.139	1.134
4.000 0.733 0.032 0.034 0.038 0.038 18.750 3.655 0.923 0.924 2.881 1.074 1.060 4.250 0.832 0.045 0.041 0.655 0.042 0.038 19.000 3.762 0.937 0.937 2.921 1.014 1.061 4.750 0.831 0.045 0.067 0.772 0.633 0.038 19.500 3.800 0.974 2.995 1.008 1.022 5.250 1.077 0.290 0.128 0.811 0.069 0.731 0.208 0.977 0.995 0.506 0.977 0.995 0.506 0.977 0.995 0.506 0.977 0.995 0.506 0.977 0.995 0.506 0.977 0.995 0.506 0.977 0.995 0.506 0.977 0.995 0.506 0.977 0.995 0.506 0.377 0.916 0.331 0.506 0.506 0.507 0.411 0.33 0.506 0.506 0.506 <td>3.750</td> <td>0.734</td> <td>0.026</td> <td>0.028</td> <td>0.579</td> <td>0.038</td> <td>0.038</td> <td>18.500</td> <td>3.607</td> <td>0,909</td> <td>0.910</td> <td>2.845</td> <td>1.108</td> <td>1.108</td>	3.750	0.734	0.026	0.028	0.579	0.038	0.038	18.500	3.607	0,909	0.910	2.845	1.108	1.108
4.250 0.832 0.038 0.044 0.656 0.040 0.038 19.000 3.704 0.039 2.921 1.041 1.051 4.500 0.831 0.045 0.662 0.695 0.042 0.038 19.250 3.752 0.957 0.977 0.957 0.977 0.995 5.000 0.979 0.121 0.097 0.772 0.033 0.038 19.750 3.848 0.991 3.035 0.976 0.977 0.995 5.500 1.077 0.290 0.166 0.849 0.072 0.044 20.250 3.945 1.019 3.111 0.908 0.931 6.500 1.272 0.683 0.635 0.990 0.688 20.750 4.041 1.042 3.225 0.886 0.902 6.500 1.272 0.683 0.635 0.956 0.156 0.124 21.200 4.188 1.041 1.042 3.226 0.886 0.902 7.500 1.468 2.476 0.483 1.041 1.042 3.226 0.848 0.933 0.903 0.912	4.000	0.783	0.032	0.034	0.618	0.038	0.038	18.750	3.655	0.923	0.924	2.883	1.074	1.080
4.500 0.881 0.465 0.0645 0.0642 0.038 19.500 3.752 0.567 2.957 0.974 2.997 0.975 0.975 0.975 0.974 2.997 0.975 0.995 5.000 0.779 0.121 0.097 0.772 0.063 0.043 19.500 3.800 0.975 0.974 2.997 0.975 0.995 5.250 1.077 0.280 0.166 0.849 0.072 0.683 0.043 20.000 3.897 1.001 1.006 3.036 0.995 <t< td=""><td>4.250</td><td>0.832</td><td>0.038</td><td>0.041</td><td>0.656</td><td>0.040</td><td>0.038</td><td>19.000</td><td>3.704</td><td>0.939</td><td>0.939</td><td>2.921</td><td>1.041</td><td>1.051</td></t<>	4.250	0.832	0.038	0.041	0.656	0.040	0.038	19.000	3.704	0.939	0.939	2.921	1.041	1.051
4.750 0.930 0.070 0.070 0.077 0.733 0.650 0.038 19.500 3.095 0.991 0.991 3.035 0.990 0.970 0.520 1.028 0.180 0.128 0.811 0.063 0.043 19.750 3.848 0.991 0.991 3.035 0.990 0.990 0.949 5.500 1.028 0.180 0.128 0.811 0.063 0.043 20.250 3.945 1.0107 1.066 3.073 0.926 0.949 5.500 1.467 0.388 0.622 0.077 0.503 3.993 1.030 3.147 0.884 0.903 6.250 1.222 0.683 0.635 0.566 0.156 1.221 1.014 0.240 3.801 1.818 1.043 1.044 3.263 0.884 0.903 6.750 1.321 1.221 1.021 1.042 0.280 1.183 1.186 1.042 3.331 0.892 0.903 0.912 7.500 1.564 2.418 2.195 1.424 1.013 1.014 3.341	4.500	0.881	0.045	0.062	0.695	0.042	0.038	19.250	3.752	0.957	0.957	2.959	1.008	1.022
$ 5.000 0.979 0.121 0.097 0.712 0.653 0.038 0.043 \\ 5.250 1.028 0.190 0.128 0.811 0.063 0.043 \\ 5.001 0.077 0.290 0.166 0.649 0.072 0.048 0.025 3.945 1.019 1.019 3.111 0.98 0.931 \\ 5.750 1.126 0.380 0.249 0.888 0.062 0.077 0.200 3.993 1.030 1.030 3.149 0.894 0.931 \\ 5.750 1.126 0.380 0.249 0.888 0.062 0.077 0.200 0.3897 1.007 1.006 3.073 0.187 0.886 0.998 \\ 6.250 1.223 0.683 0.635 0.965 0.156 0.124 0.058 0.925 0.411 1.037 1.037 0.130 3.149 0.884 0.903 0.515 0.127 0.888 0.638 0.965 0.156 0.124 21.000 4.089 1.041 1.042 3.225 0.884 0.903 0.515 0.575 1.321 1.221 1.021 1.042 0.280 0.133 0.215 0.4.186 1.042 1.043 3.301 0.882 0.905 0.905 0.137 0.166 0.144 0.181 0.446 0.220 0.133 0.133 0.481 0.348 0.902 0.575 4.234 1.039 1.044 3.330 0.903 0.912 0.905 0.975 0.1468 2.478 2.287 1.158 0.689 0.490 22.550 4.330 1.031 0.313 3.415 0.932 0.905 0.975 0.156 0.166 1.469 1.041 0.423 0.320 0.922 0.006 4.274 1.031 0.101 3.415 0.932 0.904 0.922 0.006 4.373 0.166 0.303 0.221.50 4.186 0.104 0.333 0.903 0.912 0.935 0.985 0.976 0.976 0.976 0.978 0.437 0.166 0.922 0.955 0.161 2.211 0.15 0.148 0.474 0.753 0.22.50 4.330 1.031 0.313 0.415 0.932 0.934 0.996 0.962 0.962 0.975 0.156 0.148 0.168 0.164 0.200 0.474 0.1013 0.101 3.415 0.932 0.934 0.996 0.962 0.977 0.501 0.166 0.189 0.146 0.234 0.753 0.255 0.461 0.095 0.993 0.955 0.977 0.986 0.977 0.986 0.977 0.986 0.997 0.933 0.937 0.160 0.223 0.455 0.2450 0.476 0.750 0.044 0.007 3.566 0.1002 0.991 0.924 0.971 0.065 0.984 0.937 0.944 0.427 0.251 0.462 0.662 0.989 0.996 0.3664 0.1017 0.055 0.748 0.763 0.551 0.448 0.250 0.466 0.998 0.996 0.3664 0.1017 0.054 0.999 0.933 0.755 0.991 0.933 0.937 0.564 0.1251 0.262 0.431 0.991 0.992 0.992 0.992 0.994 0.1041 0.027 0.565 0.444 0.662 0.733 0.644 0.763 0.551 0.448 0.991 0.992 0.992 0.992 0.994 0.105 0.054 0.051 0.052 0.064 0.73 0.561 0.991 0.993 0.992 0.994 0.995 0.992 0.994 0.995 0.992 0.994 0.995 0.994 0.995 0.994 0.995 0.994 0.995 0.994 0.995 0.994 0.995 0.994 0.995 0.994 0.995 0.994 0.995 $	4.750	0.930	0.070	0.077	0.733	0.050	0.038	19.500	3.800	0.975	0.974	2.997	0.977	0.995
$ 5.250 1.028 0.190 0.128 0.811 0.063 0.043 \\ 5.500 1.077 0.290 0.166 0.849 0.072 0.048 \\ 5.750 1.126 0.380 0.249 0.888 0.082 0.077 0.063 0.993 1.030 1.019 3.111 0.908 0.931 \\ 0.500 1.174 0.487 0.388 0.926 0.099 0.088 \\ 0.052 0.223 0.638 0.635 0.956 0.156 0.124 20.500 3.993 1.030 1.030 3.149 0.884 0.903 \\ 0.500 1.272 0.888 0.708 1.003 0.211 0.145 21.000 4.089 1.041 1.042 3.225 0.848 0.902 \\ 0.700 1.370 1.666 1.469 1.041 0.346 1.044 3.263 0.886 0.902 \\ 0.710 1.370 1.666 1.469 1.041 0.346 0.346 0.220 21.750 4.234 1.033 1.044 3.330 0.892 0.903 \\ 0.750 1.468 2.478 2.287 1.188 0.589 0.490 22.000 4.282 1.035 1.036 3.347 0.916 0.922 \\ 0.750 1.566 2.418 2.341 1.196 0.844 0.753 22.500 4.378 1.024 1.025 3.453 0.930 0.948 \\ 0.900 1.565 2.418 2.341 1.196 0.824 0.753 22.506 4.378 1.024 1.025 3.453 0.956 0.948 \\ 0.900 1.565 2.418 2.145 1.389 2.545 2.266 23.500 4.570 1.004 1.002 3.664 1.001 0.998 \\ 0.961 1.005 0.977 0.506 1.663 1.693 1.469 1.345 2.450 2.2750 4.618 1.001 0.999 3.642 1.031 1.017 \\ 0.500 1.663 1.693 1.446 1.329 2.546 2.2450 4.761 0.995 0.994 3.781 1.044 \\ 1.025 2.005 0.744 0.73 1.561 1.446 1.242 1.043 1.047 1.045 \\ 0.991 0.991 0.992 3.861 1.041 1.027 \\ 0.500 0.574 0.631 0.681 1.77 1.668 1.691 0.091 0.992 3.681 1.041 1.07 \\ 0.55 0.006 0.743 0.746 0.775 2.650 4.951 0.991 0.992 3.861 1.041 1.027 \\ 0.55 0.000 0.746 0.73 0.581 0.997 0.860 0.991 0.992 3.861 1.041 1.027 \\ 0.55 0.000 0.746 0.73 0.581 0.977 0.566 0.693 0.992 3.991 0.051 0.041 \\ 0.002 0.54 0.633 0.643 0.73 0.766 0.775 2.650 0.993 0.992 3.991 0.041 0.063 \\ 0.991 0.992 3.991 0.041 0.068 0.991 $	5.000	0.979	0.121	0.097	0.772	0.053	0.038	19.750	3.848	0.991	0.991	3.035	0.950	0.970
$ 5.500 1.077 0.290 0.166 0.449 0.72 0.048 \\ 5.750 1.126 0.380 0.249 0.848 0.082 0.077 \\ 5.750 1.127 0.487 0.388 0.926 0.099 0.088 0.077 \\ 5.000 1.174 0.487 0.388 0.926 0.099 0.088 \\ 6.250 1.223 0.683 0.635 0.965 0.156 0.124 \\ 5.750 1.321 1.221 1.021 1.042 0.300 0.183 \\ 7.000 1.370 1.666 1.469 1.081 0.346 0.220 \\ 7.250 1.419 2.111 1.936 1.119 0.463 0.330 \\ 7.100 1.468 2.478 2.287 1.158 0.589 0.400 \\ 7.250 1.419 2.111 1.936 1.119 0.463 0.330 \\ 7.500 1.468 2.478 2.287 1.158 0.589 0.400 \\ 7.500 1.663 1.693 1.480 1.312 0.684 0.753 \\ 7.50 1.616 2.618 2.341 1.196 0.824 0.753 \\ 7.50 1.616 2.618 2.341 1.196 0.824 0.753 \\ 7.50 1.616 2.618 2.341 1.138 0.589 0.400 \\ 7.550 1.616 2.618 2.341 1.139 0.463 0.330 \\ 7.550 1.616 2.618 2.341 1.139 0.589 0.400 \\ 7.550 1.616 2.618 2.341 1.138 0.589 0.400 \\ 7.550 1.616 2.618 2.341 1.138 0.589 0.400 \\ 7.550 1.616 2.618 2.341 1.138 0.589 0.400 \\ 7.550 1.616 2.618 2.341 1.138 0.589 0.400 \\ 7.550 1.616 2.618 2.341 1.138 0.589 0.400 \\ 7.550 1.616 2.618 2.341 1.139 0.624 0.753 \\ 7.550 1.616 2.618 2.341 1.139 0.565 0.148 \\ 7.550 1.663 1.693 1.480 1.312 2.053 1.487 \\ 7.550 1.61 1.202 1.145 1.389 2.544 2.502 \\ 7.550 1.611 1.002 1.145 1.389 2.544 2.502 \\ 7.550 1.712 1.406 1.223 1.350 2.545 2.266 \\ 7.550 1.618 1.046 1.044 1.466 2.534 2.260 \\ 7.550 1.561 1.002 1.145 1.389 2.544 2.502 \\ 7.550 1.561 1.041 1.004 1.002 3.604 1.017 1.005 \\ 7.560 1.565 0.484 0.703 1.620 1.251 1.206 \\ 7.550 1.560 0.488 0.703 1.620 1.251 1.206 \\ 7.550 0.994 0.994 3.755 1.055 1.041 \\ 7.550 2.05 0.748 0.763 1.581 1.495 1.389 \\ 7.550 0.994 0.992 3.806 1.004 1.049 1.049 1.042 \\ 7.50 2.48 0.644 0.662 1.733 0.977 0.880 \\ 7.50 0.504 0.993 0.992 3.906 1.041 1.027 \\ 7.50 0.514 0.692 0.633 0.684 0.703 1.620 0.251 1.206 \\ 7.550 0.994 0.992 3.806 1.004 1.049 1.044 \\ 7.55 0.205 0.748 0.644 0.662 1.753 0.189 0.877 \\ 7.50 5.381 0.994 0.992 3.806 1.004 1.049 1.048 \\ 7.550 1.652 0.643 0.733 0.746 0.773 0.880 \\ 7.50 0.548 0.994 0.992 3.806 1.044 1.043 1.035 \\ 7.50 0.548 0.994 0.992 3.806 1.004 1.004 1.008 1.025 \\ 7.50 0.548 0.994 0$	5.250	1.028	0.190	0.128	0.811	0.063	0.043	20.000	3.897	1.007	1.006	3.073	0.926	0.949
$ 5.750 1.126 0.380 0.249 0.888 0.962 0.077 \\ 0.000 1.174 0.487 0.388 0.962 0.099 0.088 \\ 0.000 1.074 0.487 0.388 0.965 0.156 0.124 \\ 0.223 0.683 0.635 0.965 0.156 0.124 \\ 0.122 0.888 0.708 1.003 0.211 0.145 \\ 0.750 1.321 1.221 1.021 1.042 0.280 0.183 \\ 21.500 4.186 1.043 1.044 3.233 0.886 0.903 \\ 0.700 1.370 1.666 1.469 1.081 0.346 0.220 \\ 7.500 1.468 2.478 2.287 1.158 0.589 0.490 \\ 22.150 4.186 1.042 1.043 3.10 0.482 0.905 \\ 7.000 1.370 1.666 1.469 1.081 0.346 0.220 \\ 7.500 1.468 2.478 2.287 1.158 0.589 0.490 \\ 22.250 4.138 1.035 1.036 3.377 0.916 0.922 \\ 7.500 1.648 2.478 2.287 1.158 0.589 0.490 \\ 22.250 4.330 1.035 1.036 3.347 0.916 0.922 \\ 7.50 1.614 2.060 1.808 1.273 1.550 1.408 \\ 2.250 1.614 2.060 1.808 1.273 1.550 1.408 \\ 2.250 1.614 2.060 1.808 1.273 1.550 1.408 \\ 2.250 1.614 2.061 1.808 1.273 1.550 1.408 \\ 2.250 1.614 2.061 1.808 1.273 1.550 1.408 \\ 2.250 1.663 1.693 1.480 1.312 2.053 1.867 \\ 2.250 4.570 1.004 1.002 3.664 1.001 \\ 0.000 1.761 1.202 1.145 1.389 2.854 2.502 \\ 2.3.50 4.570 1.004 1.002 3.664 1.001 0.999 \\ 3.642 1.041 1.027 \\ 9.500 1.858 1.046 1.044 1.442 2.851 2.482 \\ 24.500 4.616 0.998 0.996 3.680 1.041 1.027 \\ 9.500 1.956 0.834 0.763 1.581 1.495 1.389 \\ 25.500 4.857 0.994 0.992 3.781 1.041 1.027 \\ 9.500 1.956 0.834 0.763 1.581 1.495 1.389 \\ 25.500 4.857 0.994 0.992 3.881 1.057 1.044 \\ 1.055 2.005 0.748 0.763 1.581 1.495 1.389 \\ 25.500 4.857 0.994 0.992 3.811 1.057 1.044 \\ 1.055 1.041 1.027 \\ 9.500 0.538 0.644 0.662 1.773 0.819 0.817 \\ 25.500 4.857 0.994 0.992 3.81 1.057 1.041 \\ 1.027 1.045 \\ 1.050 2.448 0.643 1.676 1.021 0.993 \\ 3.755 1.041 0.995 0.994 3$	5.500	1.077	0.290	0.166	0.849	0.072	0.048	20.250	3.945	1.019	1.019	3.111	0.908	0.931
	5.750	1.126	0.380	0.249	0.888	0.082	0.077	20.500	3.993	1.030	1.030	3.149	0.894	0.917
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	6.000	1.174	0.487	0.388	0.926	0.099	0.088	20.750	4.041	1.037	1.037	3.187	0.886	0.908
	6.250	1.223	0.683	0.635	0.965	0.156	0.124	21.000	4.089	1.041	1.042	3.225	0.884	0.903
$ \begin{array}{c} 6.750 & 1.321 & 1.221 & 1.021 & 1.042 & 0.280 & 0.183 \\ 7.000 & 1.370 & 1.666 & 1.469 & 1.081 & 0.346 & 0.320 \\ 7.250 & 1.419 & 2.111 & 1.936 & 1.119 & 0.463 & 0.330 \\ 7.250 & 1.468 & 2.478 & 2.287 & 1.158 & 0.589 & 0.490 \\ 7.750 & 1.516 & 2.618 & 2.341 & 1.196 & 0.824 & 0.753 \\ 7.550 & 1.665 & 2.418 & 2.195 & 1.235 & 1.149 & 1.053 & 22.500 & 4.378 & 1.024 & 1.025 & 3.453 & 0.960 \\ 8.250 & 1.614 & 2.050 & 1.808 & 1.273 & 1.550 & 1.408 \\ 8.250 & 1.614 & 2.050 & 1.808 & 1.273 & 1.550 & 1.408 \\ 8.550 & 1.614 & 2.050 & 1.808 & 1.273 & 1.550 & 1.408 \\ 8.550 & 1.614 & 2.051 & 1.808 & 1.273 & 1.550 & 1.408 \\ 8.750 & 1.614 & 1.021 & 1.202 & 1.145 & 1.389 & 2.854 & 2.266 \\ 9.000 & 1.761 & 1.202 & 1.145 & 1.389 & 2.854 & 2.502 \\ 9.000 & 1.761 & 1.202 & 1.145 & 1.389 & 2.854 & 2.502 \\ 9.500 & 1.888 & 1.046 & 1.044 & 1.462 & 2.534 & 2.2400 \\ 9.500 & 1.888 & 1.046 & 1.044 & 1.427 & 2.851 & 2.482 \\ 24.100 & 4.666 & 0.998 & 0.996 & 3.6642 & 1.031 & 1.017 \\ 9.500 & 1.888 & 1.046 & 1.044 & 1.427 & 2.851 & 2.482 \\ 24.500 & 4.713 & 0.997 & 0.994 & 3.718 & 1.049 & 1.035 \\ 9.750 & 1.907 & 0.933 & 0.937 & 1.564 & 2.118 & 1.925 \\ 9.500 & 1.581 & 1.046 & 0.642 & 1.543 & 1.787 & 1.668 \\ 1.0250 & 2.005 & 0.748 & 0.763 & 1.620 & 1.251 & 1.206 \\ 1.050 & 2.053 & 0.684 & 0.703 & 1.620 & 1.251 & 1.206 \\ 1.050 & 2.480 & 0.662 & 1.658 & 1.091 & 0.892 & 2.550 & 4.995 & 0.992 & 3.881 & 1.057 & 1.044 \\ 10.750 & 2.102 & 0.642 & 0.662 & 1.658 & 1.091 & 0.82 \\ 11.500 & 2.248 & 0.644 & 0.662 & 1.773 & 0.819 & 0.817 & 26.505 & 5.040 & 0.992 & 3.984 & 1.042 & 1.038 \\ 11.250 & 2.200 & 0.633 & 0.803 & 1.888 & 0.717 & 0.760 & 27.50 & 5.314 & 0.980 & 0.991 & 4.094 & 1.008 & 1.012 \\ 12.500 & 2.443 & 0.642 & 0.662 & 1.773 & 0.819 & 0.817 & 26.505 & 5.046 & 0.981 & 0.989 & 4.244 & 0.981 & 0.982 \\ 13.000 & 2.540 & 0.990 & 2.992 & 1.655 & 0.663 & 28.500 & 5.143 & 0.990 & 0.992 & 3.944 & 1.042 & 1.038 \\ 1.750 & 2.443 & 0.642 & 0.662 & 1.773 & 0.819 & 0.667 & 27.103 & 27.505 & 5.334 & 0.886 & 0.889 & 4.247 & 0.986 & 0.989 \\ 1.500 & 2.443 & 0.642 & 0.662 $	6.500	1.272	0.888	0.708	1.003	0.211	0.145	21.250	4.138	1.043	1.044	3.263	0.886	0.902
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	6.750	1.321	1.221	1.021	1.042	0.280	0.183	21.500	4.186	1.042	1.043	3.301	0.892	0.905
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	7.000	1.370	1.666	1.469	1.081	0.346	0.220	21.750	4.234	1.039	1.040	3.339	0.903	0.912
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	7.250	1.419	2.111	1.936	1.119	0.463	0.330	22.000	4.282	1.035	1.036	3.377	0.916	0.922
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	7.500	1.468	2.478	2.287	1.158	0.589	0.490	22.250	4.330	1.030	1.031	3.415	0.932	0.934
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	7.750	1.516	2.618	2.341	1.196	0.824	0.753	22.500	4.378	1.024	1.025	3.453	0.950	0.948
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	8.000	1.565	2.418	2.195	1.235	1.149	1.053	22.750	4.426	1.018	1.018	3.491	0.968	0.962
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	8.250	1.614	2.050	1.808	1.273	1.550	1.408	23.000	4.474	1.013	1.012	3.529	0.985	0.977
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	8.500	1.663	1.693	1.480	1.312	2.053	1.867	23.250	4.522	1.008	1.007	3.566	1.002	0.991
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	8.750	1.712	1.406	1.223	1.350	2.545	2.266	23.500	4.570	1.004	1.002	3.604	1.017	1.005
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	9.000	1.761	1.202	1.145	1.389	2.854	2.502	23.750	4.618	1.001	0.999	3.642	1.031	1.017
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	9.250	1.809	1.116	1.084	1.427	2.851	2.482	24.000	4.666	0.998	0.996	3.680	1.041	1.027
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	9.500	1.858	1.046	1.044	1.466	2.534	2.260	24.250	4.713	0.997	0.994	3.718	1.049	1.035
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	9.750	1.907	0.933	0.937	1.504	2.118	1.925	24.500	4.761	0.995	0.993	3.755	1.055	1.041
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	10.000	1.956	0.832	0.842	1.543	1.787	1.668	24.750	4.809	0.995	0.992	3.793	1.057	1.044
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	10.250	2.005	0.748	0.763	1.581	1.495	1.389	25.000	4.857	0.994	0.992	3.831	1.057	1.045
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	10.500	2.053	0.684	0.703	1.620	1.251	1.206	25.250	4.905	0.994	0.992	3.868	1.054	1.044
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	10.750	2.102	0.642	0.662	1.658	1.099	1.082	25.500	4.952	0.993	0.992	3.906	1.049	1.042
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	11.000	2.151	0.622	0.643	1.696	1.021	0.993	25.750	5.000	0.993	0.992	3.944	1.042	1.038
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	11.250	2.200	0.623	0.643	1.735	0.907	0.880	26.000	5.048	0.992	0.992	3.981	1.035	1.032
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	11.500	2.248	0.644	0.662	1.773	0.819	0.817	26.250	5.096	0.991	0.992	4.019	1.026	1.026
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	11.750	2.297	0.682	0.697	1.812	0.780	0.792	26.500	5.143	0.990	0.992	4.057	1.017	1.019
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	12.000	2.346	0.733	0.746	1.850	0.746	0.775	26.750	5.191	0.989	0.991	4.094	1.008	1.012
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	12.250	2.394	0.795	0.803	1.888	0.717	0.760	27.000	5.239	0.987	0.991	4.132	1.000	1.005
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	12.500	2.443	0.862	0.867	1.927	0.667	0.713	27.250	5.286	0.986	0.990	4.169	0.992	0.999
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	12.750	2.492	0.932	0.932	1.965	0.634	0.679	27.500	5.334	0.986	0.989	4.207	0.986	0.994
13.250 2.589 1.060 1.055 2.042 0.616 0.655 28.000 5.429 0.986 0.989 4.282 0.977 0.986 13.500 2.638 1.114 1.106 2.080 0.629 0.663 28.250 5.476 0.987 0.990 4.319 0.975 0.983 13.750 2.686 1.156 1.147 2.119 0.656 0.684 28.500 5.524 0.990 4.319 0.975 0.982 14.000 2.735 1.187 1.177 2.157 0.695 0.715 28.750 5.571 0.991 0.993 4.394 0.975 0.982 14.250 2.783 1.206 1.195 2.195 0.742 0.755 29.000 5.619 0.994 0.995 4.432 0.977 0.982 14.500 2.832 1.211 1.202 2.234 0.797 0.801 29.250 5.666 0.998 0.997 4.469 0.979 0.984	13.000	2.540	0.999	0.996	2.004	0.617	0.660	27.750	5.381	0.986	0.989	4.244	0.981	0.989
13.500 2.638 1.114 1.106 2.080 0.629 0.663 13.750 2.686 1.156 1.147 2.119 0.656 0.684 14.000 2.735 1.187 1.177 2.157 0.695 0.715 14.250 2.783 1.206 1.195 2.195 0.742 0.755 14.500 2.832 1.211 1.202 2.234 0.797 0.801	13.250	2.589	1.060	1.055	2.042	0.616	0.655	28.000	5.429	0.986	0.989	4.282	0.977	0.986
13.750 2.686 1.156 1.147 2.119 0.656 0.684 14.000 2.735 1.187 1.177 2.157 0.695 0.715 14.250 2.783 1.206 1.195 2.195 0.742 0.755 14.500 2.832 1.211 1.202 2.234 0.797 0.801	13.500	2.638	1.114	1.106	2.080	0.629	0.663	28.250	5.476	0.987	0.990	4.319	0.975	0.983
14.000 2.735 1.187 1.177 2.157 0.695 0.715 14.250 2.783 1.206 1.195 2.195 0.742 0.755 14.500 2.832 1.211 1.202 2.234 0.797 0.801	13.750	2.686	1.156	1.147	2.119	0.656	0.684	28.500	5.524	0.989	0.991	4.357	0.974	0.982
14.250 2.783 1.206 1.195 2.195 0.742 0.755 14.500 2.832 1.211 1.202 2.234 0.797 0.801	14.000	2.735	1.187	1.177	2.157	0.695	0.715	28.750	5.571	0.991	0.993	4.394	0.975	0.982
14.500 2.832 1.211 1.202 2.234 0.797 0.801 29.250 5.666 0.998 0.997 4.469 0.979 0.984	14.250	2.783	1.206	1.195	2.195	0.742	0.755	29.000	5.619	0.994	0.995	4.432	0.977	0.982
	14.500	2.832	1.211	1.202	2.234	0.797	0.801	29.250	5.666	0.998	0.997	4.469	0.979	0.984
		·						1						

i(q)

1.5

1.0

0.5 0

- 0.5

-1.0

5.808

5.855

1.009

1.013

4512

30.000

30.250

1.007

1.010

4.581

4.618

0.992

0.996

0.992

0.996

B. Normalization

The corrected intensity $I_s(\theta)$ has to be normalized. The normalization factor N was calculated according to the procedure published by Hosemann *et al.*¹² After multiplication of the corrected intensity $I_s(\theta)$ with the factor N,

$$I_n = NI_s(\theta),$$

the structure factor a(q) of the specimen is then given by

 $a(q) = [I_n(q)]/f^2(q)$.

The atomic scattering factors were calculated from a formula proposed by Cromer and Mann¹³ based on relativistic Hartree-Fock atomic wave functions. We have adopted the correction factor for anomalous dispersion calculated by Cromer and Liberman.¹⁴

C. Correlation function g(r) of Rb and Cs

The experimental structure factors of a liquid are related to the correlation function g(r) by the equation

$$4\pi r^2 g(r)\rho_0 = 4\pi r^2 \rho_0 + \frac{2r}{\pi} \int q i(q) \sin(qr) dq ,$$

where g(r) is the correlation function, ρ_0 is the average macroscopic density of the liquid, and i(q) = a(q) - 1. The related quantity $g(r)\rho_0$ gives the probability of finding an atom at a distance r

FIG. 3. Smoothed structure factors [a(q)-1] of Rb and Cs.

from a reference atom in the liquid. The ripples of the correlation functions which were produced by the termination error are removed using a procedure published by Zei *et al.*⁸

IV. RESULT AND DISCUSSION

Figure 3 shows the observed experimental structure factors [a(q) - 1] of liquid Rb and liquid Cs as functions of q at temperatures 40, 90 °C, and 65, 100 °C, respectively. With rising temperature, the heights of the peaks decrease while

TABLE II. The positions and amplitudes of the first maximum of i(q) for the present results on liquid Rb and Cs in comparison with the data of other authors.

Authors		Position of 1st maximum (Å ⁻¹)		Value of 1st maximum		Temperature (°C)	
		Rb	Cs	Rb	Cs	Rb	Cs
Zei	$\operatorname{Ag} K \alpha$	1.50	1.40	1.62	1.45	40	40
	$Mo K\alpha$		1.40		1.85		65
Huijben et al. (Ref. 6)	Mo $K\alpha$		1.40		1.70		65
Gingrich et al. (Ref. 1)	n^{*a}	1.53	1.47	2.0	1.34	40	30
Copley et al. (Ref. 21)	n	1.54		2.3		40	
Page et al. (Ref. 22)	n	1.54		1.8		40	
Suzuki et al. (Ref. 23)	n	1.52		1.45		55	
Wingfield et al. (Ref. 24)	n	1.57		1.71		45	

^a n^* neutron diffraction.



Rb 40° C

Rb 90°C



FIG. 4. Smoothed structure factors [a(q) - 1] of Rb and Cs compared with results from Huijben *et al.* and Gingrich *et al.*

their widths are slightly increasing. In Table I, we present our results for a(q) for Rb at T = 40, 90 °C and for Cs at 65, 100 °C. We compare our data with the x-ray data obtained by Huijben et al.6 and the neutron data from Gingrich $et al.^1$ in Fig. 4. In the case of Cs [Fig. 4(a)], our data (Mo radiation) are in good agreement with the data from Huijben et al., and show the same phase shift with respect to the neutron data. Only the value of the first maximum of Cs with MoKa radiation is a slightly larger (1.85 instead of 1.70, Table II). Such a nice agreement does not exist with the neutron measurements. In Fig. 4(b) we compare our data (Rb) with the neutron data from Gingrich et al. It can be seen that both values of the maxima and their positions are different. Although there exist more recent experimental investigations for



FIG. 5. Comparison of the structure factor of Cs obtained from Mo $K\alpha$ and Ag $K\alpha$ radiations.



FIG. 6. Experimental correlation function $[4\pi r^2 \rho_0 (g(r) - 1)]$ in comparison with results from Gingrich *et al.*

Rb, we have selected the data of Gingrich *et al.* because these are mostly used to compare with theoretical calculated structure factors.¹⁵⁻²⁰ A comparison with other recent experiments is given in Table II. The values listed there are taken from the curves in the respective publications, which is good enough for qualitative but not for quantitative comparison. It is remarkable that the first maximum is markedly shifted to higher qvalues in all neutron data, compared with our result. An explanation of this discrepancy is un-



FIG. 7. Experimental correlation functions $[4\pi r^2 \rho_0 (g(r)-1)]$ at different temperatures.

known to us. The third column of Table II shows that also the peak heights of the first maximum are quite different. Our Cs first maximum (Fig. 5) obtained from AgK α radiation is also somewhat smaller than for MoK α radiation. This can be explained by the large counting rate of the Ag radiation, which leads to a counting loss. Therefore we suspect that the sizable differences between the results of the other authors could also be due to the electronic counting systems.

Figure 6 shows the comparison of our correlation function g(r) with that of Gingrich *et al*. The position of the maxima of g(r) from Gingrich's data shifts to smaller r values, as is to be expected, since the function g(r) is the Fourier transform of the structure factor. A comparison of the correlation functions at different temperatures is shown in Fig. 7. The damping of g(r) increases with increasing temperature. This is plausible, since

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the magnitude of the distance fluctuations increases. This effect is stronger in the case of Cs than in the case of Rb. This may be due to a larger atomic diameter and a soft repulsive core in the pair potential of Cs.²⁵ In both cases (Rb and Cs) the positions of the maxima and minima remain unchanged. An attempt to analyze the structure of these liquids will be published elsewhere.

ACKNOWLEDGMENTS

We wish to thank Dr. D. Weick for helpful discussions and his critical revision of the manuscript. In addition we also acknowledge the efforts of A. Tavernier and S. Plass for their preparation of the glass capillaries. Financial support from the Deutsche Forschungsgemeinschaft is gratefully acknowledged.

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FIG. 2. (a) Microscopic picture of the glass capillary. (b) Sample holder and associated heating unit. A: Stainless-steel cylinder for fixing the glass capillary. B: Soapstone cylinder wrapped by nickel wire for heating. C,D: Stainless tube and brass tube, respectively. W: Window sealed with Mylar foil.