Measurement of PVT Data for Molten Potassium Chloride to 1320 K and 6 kbar

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PVT data of molten KCl as a typical example for an ionic melt have been measured between 770 and 1050 °C at pressures up to 6 kbar. The experiments were performed in an internally heated pressure vessel containing argon as pressure transmitting medium. The salt was enclosed in a stainless steel cell the volume of which could be varied by means of a metal bellows and measured by monitoring the displacement of one end of the cell using an inductive transducer. The accuracy of the density data obtained is 0.15% for pressures below 2 kbar and 0.4% for higher pressures.

1. Introduction

Molten alkali halides are considered to be the simplest molten salts because they consist of only two different types of monovalent spherical ions. Therefore, the first computer simulation calculations on molten salts by the Monte Carlo [1] and the molecular dynamics [2] methods have been performed on the alkali halides, especially on potassium chloride. One purpose of these computer simulations is to calculate the macroscopic properties of ionic liquids and their temperature and density dependences from suitable pair potentials, since this cannot yet be done by rigorous statistical mechanical methods.

In order to test the validity of the results of such computer calculations a comparison with experimental data is necessary. Extensive experimental work has been done on the alkali halides at ordinary pressure, whereas an almost complete lack of information is existing for the high-pressure range. So far, only conductivity measurements up to 1 kbar have been published by Cleaver et alias [3]. Measurement of the PVT data over a wide range of temperature and pressure for molten potassium chloride as a first example of an ionic melt can provide valuable information, because they enable:

1. the derivation of an equation of state for a melt with long range forces between the constituent particles,
2. a comparison of the thermodynamic properties calculated from the equation of state with the properties of other types of liquids,
3. a discussion of the properties of molten KCl, e.g. the electrical conductivity, which have been measured as a function of pressure and temperature in terms of density or average particle distance,
4. a test of the results of computer calculations at high pressures or high densities.

The experimental effort necessary is outlined by the following facts:

1. in order to allow for a 15% isothermal density change a pressure range of about 6 kbar is necessary,
2. at that pressure the melting temperature of KCl is almost 900 °C; consequently the temperature range of the experiments should exceed 1000 °C,
3. under those conditions of temperature and pressure the alkali halides are highly corrosive,
4. in order to be useful for the purposes mentioned above the accuracy of the densities should be about 0.5% or even better.

One experimental method suitable to match all those requirements utilizes as a volumometer a closed all-metal container the volume of which is variable by means of a metal bellows mounted in an internally heated pressure vessel.

2. Experimental

2.1 Pressure System

The pressure apparatus consists essentially of an internally heated pressure vessel and the pressure generating and measuring equipment. The inner cylinder of the composite pressure vessel which is shown schematically in Fig. 1 has an inner diameter of 60 mm and is made of maraging steel (Suprafort 200, Krupp). For the outer cylinder a heat-treatable

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high strength steel is chosen. The outer surface of the pressure vessel is equipped with a water cooling system to keep the wall of the vessel at low temperatures. The bore of the pressure vessel is closed by Bridgman seals at either end.

The internal furnace (Fig. 2) consists of four independently controlled resistance heaters made of molybdenum wire insulated by thin-walled alumina tubes. Between the furnace and the wall of the pressure vessel zirconia, fired, and unfired pyrophyllite tubings are inserted for thermal insulation purposes. In order to avoid convection in the pressure transmitting compressed argon the insulating tubes fit smoothly and the gaps between them are sealed by 0-rings at the upper end. In addition all cavities are filled carefully with alumina powder. The complete furnace is connected to the lower Bridgman plug through which the electrical leads enter the high-pressure chamber. Small electrically insulated Bridgman plugs made from copper-beryllium bronze which are positioned in inclined bores in the lower Bridgman plug serve as feed-throughs for the power leads.

The temperature is measured by three sheathed chromel-alumel thermocouples distributed along the volumometer. They enter the pressure vessel at a position indicated in Fig. 1 through small Bridgman plugs into which they are soldered. The thermocouples are calibrated at the melting points of antimony and silver according to the International Practical Temperature Scale of 1968 (Sb: 630.74 °C; Ag: 961.93 °C) and at the melting point of KCl for which the value $T_F = 770.3$ °C of Roberts [4] is chosen which was confirmed by Johnson and Bredig [5] and was used in recent studies [6, 7].

The accuracy of temperature measurement including errors caused by temperature inhomogeneities is ± 2 K.

The vessel is pressurized by compressed argon. A two-stage diaphragm gas compressor (Nova) compresses argon from commercial cylinder supplies into the pressure vessel through the upper Bridgman

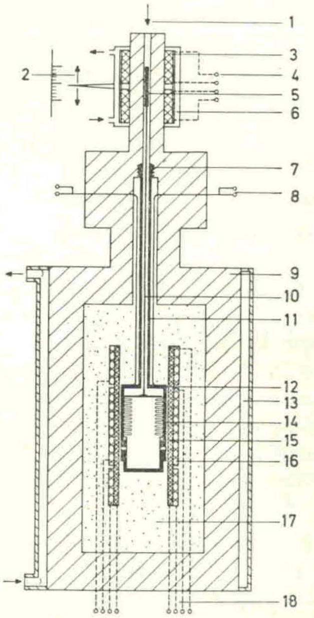

Fig. 1. Schematic diagram of high pressure apparatus: 1 gas inlet; 2 micrometer screw; 3 differential transformer; 4 leads to carrier frequency amplifier; 5 ferromagnetic tip; 6 thermostat; 7 fixed point of suspension system; 8 thermocouple inlets; 9 pressure vessel; 10 wire; 11 suspension tubing; 12 bracket; 13 cooling jacket; 14 volumometer with bellows; 15 main heater; 16 auxiliary heaters; 17 thermal insulation; 18 power leads.

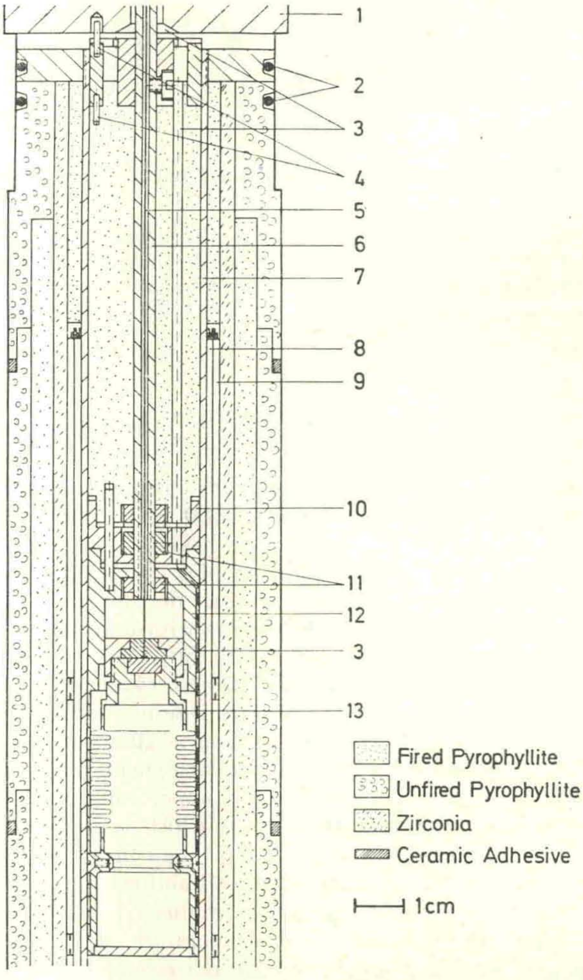

Fig. 2. Volumometer, heaters, and insulation: 1 upper Bridgman plug; 2 O-rings; 3thermocouples; 4 anti-torsion pins; 5 wire; 6 suspension tubing; 7 inner tube of furnace; 8 main heater; 9 auxiliary heaters; 10 centering device; 11 nuts; 12 bracket; 13 volumometer with bellows.

plug and into a pressure intensifier (Autoclave Engineers) to pressures of 3000 bar. Higher pressures are generated by the intensifier operated by an air-driven hydraulic pump.

The gas pressure is measured by a set of Bourdon gauges (Heise) with ranges of 1000, 3000, and 7000 bar and an accuracy of 0.1% of full scale reading. The gauges are calibrated against a deadweight tester.

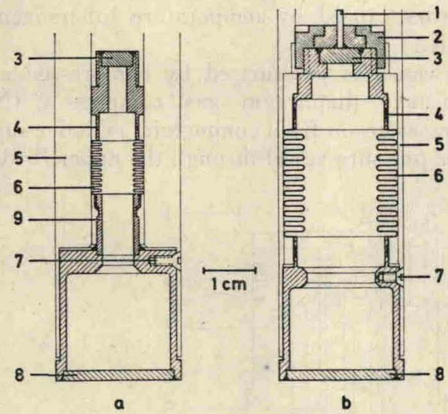

Fig. 3. Volumometers for different density ranges: a) type 1 for low densities, b) type 2 for high densities. 1 wire for displacement measurement; 2 gland; 3 lid (argon welded); 4 welded seam; 5 bracket; 6 metal bellows; 7 screw; 8 bottom part; 9 spacer.

2.2 Volumometer

The volumometer shown in Fig. 3 is a closed system of fixed salt content consisting of a rigid stainless steel cell (Remanit 1880 SST, Deutsche Edelstahl-Werke) and a metal bellows (material: Inconel 600, Henry Wiggin and Co.) which allows for pressure equilibration between the salt and the pressurizing argon. Metal bellows with different diameters are used depending on the density range leading to volumes between 7.2 and 14.3 cm^3. The lower end of the volumometer is rigidly attached to a bracket which is suspended from a stainless steel tubing connected to the upper Bridgman plug as indicated in Figure 1. To the upper end of the volumometer a wire is attached which is made of the same material as the tubing, thus compensating for most of the thermal expansion and compression effects along the temperature gradient from measuring temperature to room temperature and in the upper Bridgman seal. The wire is carrying a ferromagnetic tip. Hence changes in volume of the volumometer can be measured via displacements of its upper end by a thermostatted differential transformer outside the high-pressure system which can be moved up and down by a micrometer screw to find the relative zero position with respect to the ferromagnetic tip, which is monitored by a carrier frequency amplifier (Hottinger Meßtechnik). With this experimental set-up it is also possible to carry out quasi-isochoric measurements by adjusting the pressure in a way that the upper end of the volumometer is kept at the same (zero-) position when the salt is heated or cooled slowly.

Since the suspension system described above does not compensate for all expansion and compression effects completely, the small resultant erroneous zero point shift of the arrangement is determined by replacing the volumometer by a solid piece of metal of the same material and size and then measuring the movement of the ferromagnetic tip as a function of pressure and temperature. The resultant shift which is found to be reproducible to ± 0.07 mm with an additional uncertainty of 0.07 mm for the zero point position is taken into account as a correction to the displacements measured. The uncertainty in the final density values caused by this effect is only small for volumometers of type 1, but it is appreciable (0.25%) for type 2 volumometers. In this case it can be diminished by finding the zero point position with the aid of density values obtained with type 1 volumometers (see also Sect. 2.4 and Table 1).

2.3 Experimental Procedure

The zero point volume at 20 °C of the volumometer is determined before an experiment by differential weighing with water and carbon tetrachloride. The salt (E. Merck and Co., >99.5%) is dried carefully under vacuum at about 450 °C for at least six hours [8], then fused in a quartz glass funnel and introduced into the volumometer. After filling and cooling down the volumometer the amount of salt is determined by differential weighing. Then the volumometer is closed by welding under dry argon gas and placed into the pressure vessel.

For densities smaller than the density of the fused salt at its melting point at 1 bar pressure cells of type 1 (Fig. 3) are used. They are heated at ordinary pressure until the salt fills the zero point volume of the volumometer completely. Upon further heating the pressure is adjusted in a way, that a quasi-isochoric measurement can be performed. For densities higher than the density of the liquid at its ordinary melting point volumometers of type 2 are chosen because the larger bellows allow for the volume increase of the salt upon fusion without irreversible deformations caused by large elongations. In order to check the consistency of the isochores in this range additional isothermal measurements are made. For this purpose the volume of the volumometers is calibrated as a function of the displacement of its upper end using density values obtained by isochoric measurements. It turns out that for volume changes smaller than about $\pm 15\%$ even under these extreme conditions the volume-displacement relation is reproducible although not linear, as was also observed by Babb et al. [9] at room temperature. If the volume change of the bellows caused by melting of the salt at 1 bar exceeds about 15% it may be partly irreversible. In this case a redetermination of the zero point volume of the bellows and of its crossection is necessary with the aid of density values determined with volumometers of type 1. This leads to an additional uncertainty in the final density values of about 0.15% (see also Sect. 2.4 and Table 1).

2.4 Determination of Density

The density of molten KCl corresponding to a measured pair of temperature and pressure is calculated from

$$\varrho(\mathrm{P,T}) = m/V_0(\mathrm{P,T}) = m/[V_0(1\,\mathrm{bar}, 20\,^\circ\mathrm{C}) + \Delta V_{\mathrm{T,C}} + \Delta V_{\mathrm{T,B}} + \Delta V_{\mathrm{P}}] \quad (1)$$

where m is the amount of salt in the volumometer, $V_0(\mathrm{P,T})$ the volume of the volumometer at P and T and zero displacement, V_0 (1 bar, 20 °C) the calibrated volume at 1 bar and 20 °C, $\Delta V_{\mathrm{T,C}}$ the volume correction of the total volumometer due to thermal expansion as if it were totally made from the material of the rigid part. $\Delta V_{\mathrm{T,B}}$ a correction to $\Delta V_{\mathrm{T,C}}$ taking into account, that the bellows and the rigid part are made from different materials, ΔV_{P} the correction due to compression of the volumometer. All the corrections are temperature and pressure dependent.

The corrections due to thermal expansion are calculated according to

$$\Delta V_{\mathrm{T,C}} = 3\,V_0(1\,\mathrm{bar}, 20\,^\circ\mathrm{C})\alpha_{\mathrm{C}}\,[t-20]\,, \quad (2)$$

$$\Delta V_{\mathrm{T,B}} = -2\,V_{0,\mathrm{B}}(1\,\mathrm{bar}, 20\,^\circ\mathrm{C})\,\Delta\alpha_{\mathrm{C-B}}\,[t-20]\,, \quad (3)$$

where α is the average linear thermal expansion coefficient between 20 °C and the measuring temperature, $\Delta\alpha_{\mathrm{C-B}} = \alpha_{\mathrm{C}} - \alpha_{\mathrm{B}}$ is the difference between the coefficients for cell and bellows materials, t is the measuring temperature in degrees centigrade, and $V_{0,\mathrm{B}}$ (1 bar, 20 °C) is the volume of the bellows at 1 bar, 20 °C, and zero displacement. Equation (3) is taking into account that the correction for the difference in thermal expansion between the cell and bellows materials in axial direction is already included in the displacement measurement.

The values used for the different thermal expansion coefficients in the range between 800 and 1050 °C are.

$$\alpha_{\mathrm{C}} = (16.4 + 0.003\,t \pm 0.3)\cdot 10^{-6}\ (\text{see [10]})\,,$$

$$\alpha_{\mathrm{B}} = (12.9 + 0.004\,t)\cdot 10^{-6}\ (\text{see [11]})\,,$$

$$\Delta\alpha_{\mathrm{C-B}} = (3.5 - 0.001\,t)\cdot 10^{-6}\,.$$

The relative uncertainty of α_{C} amounts to 1.6%, that of $\Delta\alpha_{\mathrm{C-B}}$ is estimated to be 8%. The corresponding errors in $V_0(\mathrm{P,T})$ are 0.09% and 0.02%, respectively. The pressure dependence of the thermal expansion coefficient is small and can therefore be neglected in the thermal expansion correction.

Since the overall correction for the compression of the volumometer is of the order 0.5% in $V_0(\mathrm{P,T})$, it is not necessary to distinguish between the compressibilities of the two different materials and to take into account the pressure dependence of the compressibility when calculating the correction which can then be written as

$$\Delta V_{\mathrm{P}} = -\beta(T)\,P[V_0(1\,\mathrm{bar}, 20\,^\circ\mathrm{C}) + \Delta V_{\mathrm{T,C}} + \Delta V_{\mathrm{T,B}}]\,. \quad (4)$$

The compressibility $\beta(T)$ may be calculated from

$$\beta(T) = \frac{3[1-2\,\nu(T)]}{E(T)} \quad (5)$$

with data for Young's modulus $E(T)$ [12] and Poisson's ratio $\nu(T)$ [13] extrapolated beyond 820 °C. It turns out that ν does not show a systematic variation with temperature. It thus has its usual value $\nu = 0.3$ over the whole temperature range. For $E(T)$ the following relation holds:

$$E(T) = 22860 - 11.6\,t\ (\text{in kp mm}^{-2})\,.$$

The value for β at room temperature obtained from Eq. (5) is $6.02\cdot 10^{-7}\,\mathrm{bar}^{-1}$. It is in good agreement with data for the constituent pure metals obtained by Bridgman [14] from high-pressure experiments. He also demonstrated that the pressure dependence of the compressibility may be expressed as a linear function of pressure and that the pressure dependent term is contributing less than 5% below 6 kbar. Hence it is justified to neglect it here.

The estimated error of the compressibility is about 10% below 2 kbar and about 20% for the highest pressures. This leads to errors in V_0 (P, T) of 0.025% and 0.13%, respectively.

2.4 Uncertainties in Density

The uncertainties in the final density values caused by various experimental errors may be obtained from

$$\Delta\varrho/\varrho = \Delta m/m + [\Delta V_0\,(1\text{ bar}, 20\,^\circ\text{C}) + \Delta V_0(\text{P},\text{T}) + q_0(\Delta l - \Delta l_0) + \Delta V_{\text{cal}}]/V_0(\text{P},\text{T}) + \alpha\,\Delta T + \beta\,\Delta P \qquad (6)$$

where the symbols appearing for the first time have the following significance: Δm: error in the amount of salt in the volumometer, ΔV_0 (1 bar, 20 °C): error in volume calibration; $\Delta V_0(\text{P},\text{T})$: error due to inaccuracies of the corrections $\Delta V_{\text{T,C}}$, $\Delta V_{\text{T,B}}$, and ΔV_{P}; Δl: uncertainty in displacement measurement; Δl_0: reduction of Δl by fixing the zero point of displacement for type 2 volumometers by calibration (see Sect. 2.2); ΔV_{cal}: uncertainty in calibration of $V_0(\text{P},\text{T})$ and q_0 of type 2 volumometers after an irreversible volume change (see Sect. 2.3); $\Delta T, \Delta P$: errors in temperature and pressure measurement, respectively (see Sect. 2.1); α, β: thermal expansion coefficient and isothermal compressibility of the salt, respectively.

The numerical values of the uncertainties for the two different types of volumometers are given in Table 1 for various pressures.

Table 1. Relative uncertainties of final density value due to various experimental errors.

Volumometers	Type 1		Type 2
Pressure	1 bar	2000 bar	6000 bar
$\Delta m/m$	0.017	0.017	0.008
ΔV_0(1 bar, 20 °C)$/V_0$(P,T)	0.035	0.035	0.042
ΔV_0(P,T)$/V_0$(P,T)	0.090	0.115	0.240
$q_0\Delta l/V_0$(P,T)	0.050	0.080	0.250
$q_0\Delta l_0/V_0$(P,T)	—	—	−0.150
$\Delta V_{\text{cal}}/V_0$(P,T)	—	—	0.150
$\alpha\,\Delta T$	0.085	0.062	0.041
$\beta\,\Delta P$	0.006	0.009	0.012
total $\Delta\varrho/\varrho$	0.28	0.32	0.59
$\Delta\varrho/\varrho$ when based on values at 1 bar	0.1	0.14	0.41

3. Results

Following the procedure described above twenty quasi-isochores with 431 experimental points and nine isotherms with 87 points are measured covering the temperature, pressure, and density ranges from 770 to 1050 °C, from 1 to 6000 bar, and from 1.36 to 1.67 g cm^{-3}, respectively. The uncorrected points of some of the quasi-isochores are shown in Fig. 4, where the points obtained upon heating and cooling in different cycles are marked by different symbols. As may be seen from the figure, the scatter of the experimental points is very small and statistical, thus indicating that there is neither hysteresis nor any time-dependent effect.

All unsmoothed experimental points corrected for the effects described in Sects. 2.2 and 2.4 are collected in Table 2.

Since PVT data for molten KCl at high pressures have not been published previously, a comparison with data from other sources is not feasible. Density values at normal pressure obtained by fitting a second order polynomial to the quasi-isochores shown in Fig. 4, subsequent numerical extrapolation of $T(\text{P})$ to normal pressure and calculating the corresponding density values from Eq. (1) are shown

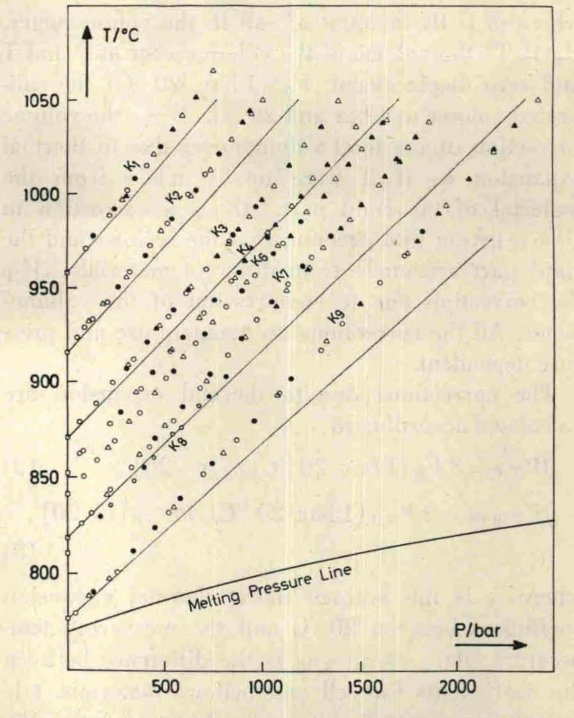

Fig. 4. Uncorrected experimental points on quasi-isochores and isochores (full lines) corresponding to quasi-isochores K_1, K_2, K_3, K_7, and K_9. ● heating first run, ○ cooling first run, △ heating second run, ▲ cooling second run, □ extrapolated points at 1 bar (see text).

Table 2. Unsmoothed corrected experimental points for density determinations of molten potassium chloride.

P/bar	T/°C	ρ/gcm^{-3}	P/bar	T/°C	ρ/gcm^{-3}	P/bar	T/°C	ρ/gcm^{-3}	P/bar	T°C	ρ/gcm^{-3}
1	958.2	1.4180	485	980.0	1.4379	877	981.0	1.4605	526	911.5	1.4772
136	978.0	1.4166	631	1000.0	1.4363	768	967.0	1.4616	684	930.0	1.4758
244	992.5	1.4155	733	1013.5	1.4353	625	949.5	1.4630	950	963.5	1.4731
348	1008.5	1.4143	846	1029.0	1.4340	460	929.0	1.4646	1119	983.5	1.4714
476	1025.5	1.4130	943	1042.5	1.4329	1	852.3	1.4797	1334	1010.5	1.4692
407	1015.5	1.4138	938	1044.5	1.4327	274	884.0	1.4775	1206	995.0	1.4705
308	1002.0	1.4148	1006	1050.0	1.4323	441	905.5	1.4759	1058	977.5	1.4719
218	988.5	1.4158	899	1038.5	1.4332	596	924.0	1.4744	915	960.0	1.4733
96	971.0	1.4171	1	870.9	1.4689	752	943.5	1.4729	773	941.5	1.4749
278	997.0	1.4152	157	889.0	1.4676	882	958.5	1.4717	620	922.0	1.4764
447	1021.0	1.4134	304	907.0	1.4663	1028	977.0	1.4702	508	909.5	1.4774
589	1041.5	1.4118	413	921.5	1.4652	840	953.5	1.4721	394	895.5	1.4785
750	1065.5	1.4099	546	938.5	1.4639	701	936.5	1.4734	287	882.5	1.4794
659	1051.5	1.4110	852	978.0	1.4608	530	916.5	1.4750	186	870.5	1.4803
541	1034.0	1.4124	970	994.0	1.4594	378	896.5	1.4766	112	862.0	1.4809
305	999.0	1.4151	830	975.0	1.4610	217	877.5	1.4780	73	857.5	1.4812
1	916.0	1.4426	710	960.0	1.4622	79	863.5	1.4789	41	854.5	1.4814
261	950.5	1.4401	611	947.5	1.4632	61	862.5	1.4790	1	841.5	1.4860
402	967.5	1.4389	518	934.5	1.4642	354	894.5	1.4767	550	906.0	1.4813
536	986.5	1.4374	342	912.0	1.4660	534	917.0	1.4750	710	926.0	1.4797
658	1002.5	1.4362	236	899.5	1.4669	679	934.0	1.4736	895	949.0	1.4778
779	1022.0	1.4346	147	888.5	1.4677	860	955.0	1.4720	1058	968.0	1.4763
708	1010.5	1.4355	63	879.0	1.4683	1027	979.5	1.4699	1201	986.0	1.4748
622	1000.5	1.4363	313	909.0	1.4662	1156	994.0	1.4687	1106	974.0	1.4758
509	984.0	1.4376	473	930.0	1.4646	1265	1009.0	1.4675	964	957.0	1.4772
425	972.5	1.4385	638	950.0	1.4630	1486	1036.0	1.4652	815	940.0	1.4786
323	958.5	1.4395	824	973.5	1.4611	1338	1016.0	1.4669	660	921.0	1.4801
205	942.5	1.4407	935	988.0	1.4599	1203	999.5	1.4683	510	902.5	1.4816
131	933.5	1.4413	1066	1005.5	1.4585	1067	983.5	1.4696	373	884.0	1.4830
90	929.0	1.4417	1220	1026.0	1.4568	912	964.0	1.4712	247	869.0	1.4841
49	923.5	1.4420	1393	1049.5	1.4548	1	848.7	1.4818	154	859.0	1.4848
109	932.5	1.4414	1305	1036.0	1.4560	106	862.0	1.4809	83	850.5	1.4854
183	941.5	1.4408	1142	1015.5	1.4577	245	878.0	1.4798	209	865.0	1.4844
302	956.0	1.4397	1000	997.0	1.4592	410	897.5	1.4783	317	879.0	1.4834
448	894.0	1.4822	1313	971.5	1.4874	702	851.5	1.5184	1125	906.5	1.5110
600	913.5	1.4807	1450	987.0	1.4861	522	831.5	1.5200	1288	925.0	1.5095
748	931.5	1.4793	1600	1005.5	1.4845	257	801.0	1.5223	1161	910.0	1.5107
919	952.5	1.4775	1749	1025.0	1.4829	42	779.5	1.5238	1042	895.0	1.5122
1080	972.5	1.4759	1858	1038.5	1.4818	108	787.0	1.5232	905	879.5	1.5134
1230	991.0	1.4744	1790	1031.0	1.4824	212	797.5	1.5225	1294	879.0	1.5328
1380	1008.5	1.4729	1696	1019.0	1.4834	547	834.5	1.5197	1156	863.5	1.5341
1513	1024.0	1.4716	1705	1018.0	1.4835	803	862.5	1.5175	1005	847.0	1.5357
1639	1039.5	1.4703	1632	1010.0	1.4841	1078	893.0	1.5150	864	830.0	1.5371
1620	1038.0	1.4705	1510	995.0	1.4854	1329	921.5	1.5126	719	813.5	1.5381
1561	1030.5	1.4711	1404	982.0	1.4865	1510	943.0	1.5107	555	795.5	1.5386
1447	1016.0	1.4723	1235	960.0	1.4883	1736	968.5	1.5086	659	809.0	1.5381
1439	1015.5	1.4723	1072	940.5	1.4900	1950	994.5	1.5064	807	826.0	1.5373
1317	999.5	1.4737	1	811.0	1.5038	2195	1023.5	1.5041	951	841.5	1.5361
1146	977.5	1.4755	171	829.5	1.5025	2426	1050.5	1.5021	1099	857.5	1.5346
1	818.7	1.4993	393	854.5	1.5007	2300	1037.0	1.5031	1243	873.5	1.5333
449	870.0	1.4956	585	875.5	1.4991	2196	1025.0	1.5040	1411	893.5	1.5311
593	887.0	1.4943	730	892.5	1.4977	2067	1009.0	1.5053	1564	910.5	1.5291
736	904.5	1.4929	816	903.0	1.4969	1910	990.5	1.5068	1663	920.5	1.5281
894	923.5	1.4913	682	887.5	1.4981	1799	975.5	1.5080	1824	940.5	1.5259
1049	942.5	1.4898	542	872.5	1.4993	1504	942.0	1.5108	1989	960.5	1.5237
1205	961.5	1.4882	443	860.0	1.5003	180	811.5	1.5137	2177	983.0	1.5215
1354	978.0	1.4868	343	848.0	1.5012	292	820.5	1.5148	2080	968.5	1.5229
1254	965.5	1.4878	223	835.5	1.5021	458	833.5	1.5153	1941	950.5	1.5249
1128	951.5	1.4890	1	776.5	1.5239	604	848.5	1.5150	1792	933.5	1.5267
973	933.0	1.4905	133	790.5	1.5230	773	867.0	1.5141	1477	879.0	1.5401
829	914.5	1.4921	338	812.0	1.5214	941	887.0	1.5128	1673	900.0	1.5381
686	897.0	1.4935	451	824.0	1.5205	855	875.5	1.5137	1847	916.5	1.5364
544	879.5	1.4949	577	839.0	1.5193	716	858.5	1.5148	1569	889.0	1.5391
421	866.0	1.4959	754	857.0	1.5179	568	842.0	1.5155	1383	870.0	1.5408
331	855.0	1.4968	961	879.5	1.5161	415	828.5	1.5156	1178	848.0	1.5428
222	843.0	1.4976	1152	902.0	1.5142	320	820.5	1.5156	967	825.0	1.5446
124	831.5	1.4985	1510	943.0	1.5107	205	810.5	1.5147	729	800.0	1.5464
72	826.0	1.4988	1826	980.0	1.5076	96	801.0	1.5139	1058	834.5	1.5439
201	840.5	1.4978	1732	968.0	1.5086	256	815.5	1.5146	1426	874.5	1.5405
370	861.5	1.4962	1607	953.0	1.5099	373	825.0	1.5153	1763	909.5	1.5372
502	876.5	1.4951	1415	931.5	1.5117	521	838.5	1.5155	1970	931.5	1.5351
716	900.5	1.4932	1298	917.5	1.5129	679	854.5	1.5148	2160	952.5	1.5329
914	923.5	1.4914	1088	894.0	1.5149	818	871.5	1.5140	2386	980.0	1.5304
1125	948.5	1.4893	872	869.5	1.5169	976	890.0	1.5125	2555	1000.5	1.5285
2776	1025.5	1.5263	2652	965.0	1.5493	2838	921.5	1.5741	4646	964.0	1.6153
2641	1009.5	1.5278	2873	992.5	1.5468	3071	947.5	1.5717	4567	955.5	1.6160
953	796.0	1.5580	3138	1025.5	1.5439	3287	971.0	1.5696	4389	935.5	1.6179
1104	813.0	1.5563	3286	1044.0	1.5422	3475	993.5	1.5675	4155	911.0	1.6202
1265	830.0	1.5549	3169	1027.0	1.5437	3671	1016.5	1.5654	4804	921.0	1.6352
1409	846.0	1.5530	3080	1017.0	1.5446	3953	1049.5	1.5625	4469	885.0	1.6386
1576	863.5	1.5510	2968	1002.0	1.5460	3817	1031.5	1.5641	4319	875.0	1.6396
1766	885.0	1.5487	2780	979.0	1.5480	3708	1018.0	1.5653	4583	899.0	1.6373
1585	863.5	1.5510	2585	954.5	1.5503	3573	1002.5	1.5667	4788	918.5	1.6354
1445	849.0	1.5528	2410	935.5	1.5520	3027	899.0	1.5889	4929	934.5	1.6339
1300	833.5	1.5543	2438	900.0	1.5681	3429	944.0	1.5847	5146	957.0	1.6318
1185	820.0	1.5557	2208	876.0	1.5704	3615	964.5	1.5828	5356	981.5	1.6295
1002	799.0	1.5577	1975	849.5	1.5728	3860	993.5	1.5802	5562	1003.5	1.6275
1000	799.0	1.5577	1723	822.5	1.5753	4064	1017.5	1.5780	5748	1023.5	1.6256
1143	815.0	1.5561	1847	837.5	1.5739	4208	1035.5	1.5764	6028	1055.5	1.6227
1335	836.0	1.5541	2025	856.5	1.5722	4081	1021.0	1.5777			
1506	856.5	1.5519	2164	871.5	1.5708	3948	1004.0	1.5792			
1685	877.5	1.5496	2359	893.5	1.5687	3744	980.5	1.5814			
1835	894.5	1.5476	2580	918.0	1.5665	3531	955.5	1.5837			
2007	913.5	1.5456	2769	938.5	1.5646	3320	931.5	1.5859			
1892	899.5	1.5470	2976	961.5	1.5625	3110	907.0	1.5882			
1720	881.5	1.5493	3174	985.0	1.5604	2900	884.0	1.5903			
1600	867.5	1.5507	3378	1007.5	1.5584	2668	858.5	1.5927			
1434	848.5	1.5528	3630	1038.0	1.5556	3637	920.0	1.6007			
1286	833.0	1.5544	3521	1024.0	1.5569	3443	899.5	1.6026			
1169	820.0	1.5557	3388	1008.0	1.5583	3252	879.0	1.6045			
2550	952.5	1.5504	3261	992.5	1.5597	3049	857.5	1.6065			
2353	927.5	1.5527	3051	969.0	1.5618	3049	860.0	1.6063			
2165	905.5	1.5547	2844	945.0	1.5640	2871	843.5	1.6078			
1961	883.5	1.5567	2955	935.5	1.5728	2973	852.5	1.6070			
1761	861.0	1.5588	3393	984.5	1.5683	3170	872.5	1.6051			
1567	838.0	1.5609	3155	955.5	1.5710	3360	892.0	1.6033			
1288	807.5	1.5637	2865	923.5	1.5739	3559	913.0	1.6014			
1397	822.0	1.5624	2600	892.5	1.5768	3771	935.5	1.5993			
1512	835.0	1.5612	2378	868.5	1.5790	3924	952.5	1.5977			
1671	853.5	1.5595	2192	847.5	1.5809	4104	907.5	1.6205			
1857	872.0	1.5578	1977	824.0	1.5831	4438	941.5	1.6173			
2064	897.0	1.5555	2140	844.5	1.5812	4712	972.5	1.6145			
2260	918.5	1.5535	2483	882.0	1.5777	4951	1001.5	1.6118			
2470	945.5	1.5511	2672	902.5	1.5758	4806	982.0	1.6136			

in Fig. 5 in comparison with data from the literature [15–26] which show considerable discrepancies.

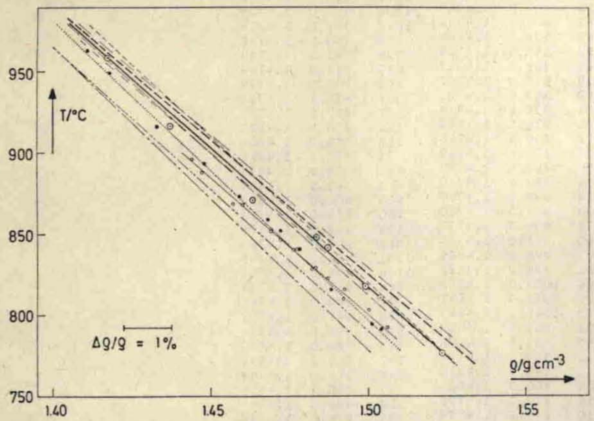

Fig. 5. Density of molten potassium chloride as a function of temperature at 1 bar. – – – – Grjotheim et al. (1971) [15], ——— Kirshenbaum et al. (1962) [16], ●······ Neithamer and Peake (1961) [17], ——— Van Artsdalen and Yaffe (1955) [18], ○——— Peake and Bothwell (1954) [20], –·–·– Bloom et al. (1953) [21], –··–··– Mashovetz and Lundina (1935) [22], – – – – – – Klemm (1926) [23], –··–··– Jäger (1917) [25], ——— Brunner (1904) [26], ⊙ This work.

Our extrapolated values, with the exception of two, agree to better than 0.1% with the data of Van Artsdalen and Yaffe [18, 19]. A linear fit of our extrapolated densities as a function of temperature is almost identical with that of Yaffe and Van Artsdalen [19] and may be expressed as

$$\varrho_0(T) = \varrho_{0\mathrm{YA}}(T) = 1.9767 - 0.5831 \cdot 10^{-3}\, t\,.$$

The good agreement with the accurate values of Van Artsdalen and Yaffe points out that our smoothed values at 1 bar pressure are accurate to about 0.1% rather than 0.28% as noted in the second last line of Table 1 and that the error limits of the high-pressure density values can be changed to the numbers given in the last line of Table 1, if the densities are based on the smoothed values at 1 bar rather than being regarded as absolute values.

The corrected experimental density values are fitted by an equation of state (modified Tait-equation) with temperature and pressure as independent variables with a standard deviation of 0.04% in density. The smoothed data are reported in Table 3.

Table 3. Smoothed density values in g/cm³ for molten potassium chloride.

T/°C P/bar	800	825	850	875	900	925	950	975	1000	1025	1050
1	1.510	1.496	1.481	1.467	1.452	1.437	1.423	1.408	1.394	1.379	1.364
250	1.523	1.509	1.495	1.481	1.468	1.454	1.440	1.426	1.412	1.398	1.384
500	1.536	1.522	1.509	1.495	1.482	1.469	1.455	1.442	1.428	1.415	1.402
750	1.547	1.534	1.521	1.508	1.495	1.482	1.469	1.457	1.444	1.431	1.418
1000	1.558	1.546	1.533	1.520	1.508	1.495	1.483	1.470	1.458	1.445	1.432
1250		1.556	1.544	1.532	1.519	1.507	1.495	1.483	1.471	1.459	1.446
1500		1.566	1.554	1.542	1.530	1.519	1.507	1.495	1.483	1.471	1.459
1750		1.576	1.564	1.552	1.541	1.529	1.518	1.506	1.495	1.483	1.472
2000		1.585	1.573	1.562	1.551	1.540	1.529	1.517	1.506	1.495	1.483
2250		1.594	1.583	1.572	1.561	1.550	1.540	1.528	1.518	1.506	1.495
2500			1.592	1.581	1.571	1.560	1.550	1.539	1.528	1.517	1.506
2750			1.600	1.590	1.580	1.569	1.559	1.548	1.538	1.527	1.517
3000			1.608	1.598	1.588	1.578	1.568	1.558	1.547	1.537	1.527
3250			1.616	1.606	1.596	1.587	1.577	1.567	1.557	1.547	1.536
3500			1.624	1.614	1.604	1.595	1.585	1.575	1.566	1.556	1.546
3750			1.631	1.622	1.612	1.603	1.593	1.584	1.574	1.564	1.555
4000			1.638	1.629	1.620	1.610	1.601	1.592	1.582	1.573	1.563
4250				1.636	1.627	1.618	1.609	1.600	1.590	1.581	1.572
4500				1.643	1.634	1.625	1.616	1.607	1.598	1.589	1.580
4750				1.649	1.641	1.632	1.623	1.615	1.606	1.597	1.588
5000				1.656	1.647	1.639	1.630	1.622	1.613	1.605	1.596
5250				1.662	1.654	1.646	1.637	1.629	1.621	1.612	1.603
5500				1.668	1.660	1.652	1.644	1.636	1.628	1.619	1.611
5750					1.666	1.659	1.651	1.643	1.634	1.626	1.618
6000					1.673	1.665	1.657	1.649	1.641	1.633	1.625

Smoothed isochores belonging to the uncorrected experimental points in Fig. 4 are shown as full lines in the same figure.

A discussion of the PVT data reported here, of the derivation of the equation of state used for fitting the results, and of some thermodynamic properties of molten potassium chloride calculated with the aid of this equation will be published in a subsequent paper [27].

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