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

G. Goldmann and K. Tödheide

Institut für Physikalische Chemie und Elektrochemie der Universität Karlsruhe
Karlsruhe, Germany

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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.

Requests for reprints should be addressed to Dr. K. Tödheide, Institut für Physikalische Chemie und Elektrochemie, Universität Karlsruhe, Kaiserstr. 12, *D-7500 Karlsruhe 1.*

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