

Table 3 shows a comparison of the best set of computed values for some derived properties<sup>7</sup> with experimental data. Obviously, the temperature and pressure dependences of the quantities compiled in the table from the computer experiments are qualitatively correct. The numerical values, however, normally fall outside the experimental limits of error. The best agreement is achieved for the molar heat capacity, but this quantity, unfortunately, can only be derived from the experiments with poor accuracy. Thus it appears that computer simulation methods cannot produce *PVT* data and related quantities at high pressure with an accuracy comparable to that of precise experimental studies.

### 5. Estimate of High-pressure *PVT* Data for Molten Salts

Since precise measurements of high-pressure *PVT* data for molten salts are difficult and time consuming and since computer simulations in spite of long computing times cannot produce sufficiently accurate results at present, a method for satisfactory estimates of *PVT* data for other molten salts is highly desirable for the interpretation of experimental results obtained at high pressures, e. g. specific electrical conductivities of the alkali metal chlorides<sup>45</sup>. The Tait equation has proven to be an excellent equation of state for various types of liquids, if the parameters *A* and *B* are allowed to vary with temperature. It was also noticed that *A* varies only slightly with temperature and has similar values for quite different liquids. Kuss and Taslimi<sup>17</sup> found that the *PVT* data of many organic liquids could be well described by the Tait equation, when

*A* was held constant and the temperature dependence of *B* was expressed as

$$B(T) = 0.089/\kappa_T(1 \text{ bar}, T) + 40/\text{bar} \quad (10)$$

where  $\kappa_T(1 \text{ bar}, T)$  is the isothermal compressibility of the liquid at 1 bar. Equation (10) and Eq. (1) yield the equation of state

$$\begin{aligned} \rho(P, T) = \rho(1 \text{ bar}, T) / [1 - 0.1 \\ \cdot \ln \{ (0.089/\kappa_T(1 \text{ bar}, T) + 40 + P) \\ : (0.089/\kappa_T(1 \text{ bar}, T) + 40) \}] \end{aligned} \quad (11)$$

For *A* the value 0.1 has been introduced which seems to be the best choice for molten salts. Equation (11) enables the calculation of the density of a liquid at high pressure when its density and isothermal compressibility are known as functions of temperature at ordinary pressure. In Table 4 densities which were estimated with the aid of Eq. (11) are compared with experimental values for KCl, KNO<sub>3</sub>, and NaNO<sub>3</sub>. Up to 5 kbar the discrepancies are well below 1%. The *PVT* measurements for the nitrates above 1 kbar are performed in a piston-cylinder apparatus with an error limit which is comparable to the differences between the estimated and measured values listed in Table 4.

It appears that Eq. (11) enables an estimate of high-pressure densities for molten salts which is superior to the best results of computer simulations presently available.

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