

explained if their molar volume were to coincide with the smallest extreme of their lattice parameter uncertainty ($4.462 \pm 0.002 \text{ \AA}$ vs. the x-ray value of $4.4638 \text{ \AA}$).⁷ The agreement with the theoretical calculation is good above 7 K for the $n = 12$ model, although the volume dependence of C_V as calculated on this model is not correct.³⁰ The difficulty most likely lies in the form of the two-body potential which was used for these calculations, and there are prospects for better potentials in the near future.⁵

The comparison in Fig. 7 of the present results and the values of Θ which are derived from C_P data is not very satisfactory since the earlier data have been processed in two ways. First, the smoothed values of C_P have been converted to C_V using

$$C_P = C_V(1 + \beta\gamma T) \quad (8)$$

where γ is given by Eq. (5), and second, the values of C_V for each temperature have been adjusted to make them correspond to the 0 K equilibrium volume. The present results suggest a simple model for solid neon in which C_V is a function only of the reduced temperature $T/\Theta_0(V)$. Hence, the known thermal expansion for solid neon⁷ can be used to determine the molar volume and Θ_0 at $P = 0$ for each temperature, after which C_V can be obtained from the reduced curve. In practice, the relationships of Figs. 5 and 6 are used together with a tabulation of the Debye function. The values of Θ_0 which result from the use of the equation-of-state expression for γ_0 ($\gamma_0 = 0.197 \pm 0.002 \text{ cm}^{-3} \cdot V$) range from 75.1 K at $V_0 = 13.391 \text{ cm}^3/\text{mole}$ to $66.8 \pm 0.5 \text{ K}$ at the triple point (24.6 K, $14.02 \text{ cm}^3/\text{mole}$), where $T/\Theta_0 = 0.37$. The use of a constant value $\gamma_0 = 2.51$ would not alter these results appreciably. C_P then is calculated from Eq. (8), using Eq. (5) to calculate γ and the x-ray values⁷ for the thermal expansion coefficient β .

The resulting relationship for $C_P(T, P = 0)$ is given as the solid line in Fig. 8, where it is compared with direct determinations of C_P .^{11,12,17} The

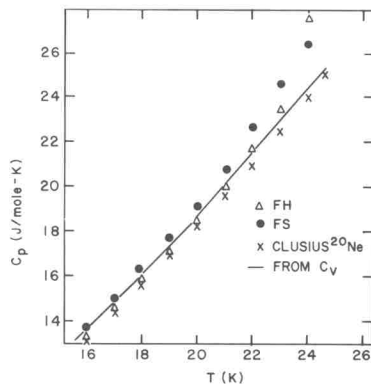


Fig. 8. A comparison of C_P as calculated from the present results and as obtained from the smoothed results of Refs. 11 (FH), 12 (FS), and 17 (Clusius).

agreement below 20 K is well within the experimental uncertainties, especially if the data of Clusius *et al.*¹⁷ (taken for the pure isotope ^{20}Ne , $T > 8$ K) are increased slightly to compensate for the 1% isotopic mass difference between their sample and natural neon. Above 20 K, the smoothed results of Fenichel and Serin¹² begin to deviate systematically from the other data, as do the data of Fagerstroem and Hollis-Hallet¹¹ above 23 K. The latter authors give only a plot for this temperature region, and the points in Fig. 8 were read from the smooth curve in this plot. If the values of γ which are used in Eq. (8) to calculate C_p from our model for C_v are calculated from experimental thermodynamic quantities⁷⁻⁹ in a self-consistent fashion instead of using our equation of state, the predicted curve for C_p would tend to bend over above 21 K to a value of roughly 24 J/mole·K at the triple point.

The agreement for C_p between the relation which is calculated from our C_v data and the results of Clusius *et al.*¹⁷ is excellent at all temperatures, as is the agreement with Fagerstroem and Hollis-Hallet¹¹ at 23 K and below. The reason for the rapid increase in C_p , which both Fenichel and Serin¹² and Fagerstroem and Hollis-Hallet¹¹ observe near the melting point, is not clear. None of our samples show a premelting anomaly of this magnitude (see Fig. 4, for instance, where the melting temperature is 46.8 K, and Fig. 6), in basic agreement with the results of Clusius *et al.*¹⁷ Schoknecht and Simmons³¹ have shown recently that vacancy effects should be quite small in C_p for solid neon near these temperatures. Our calculated values of C_p also are in excellent agreement with those given by Goldman *et al.*² for their $m = 12$ ISC calculation.

The present data can be used to test the Lindeman melting relation which associates the melting temperature T_m with the relative mean square amplitude $x^2 = \langle \delta r^2 \rangle / r_s^2$, $(4\pi r_s^3/3) = V_m$ of the atomic vibrations in the solid at the melting line. The usual relation³³

$$x^2 = (9\hbar^2/mk_B)(T_m/\Theta^2 r_s^2) = 41.11 (\text{cm}^2 \cdot \text{K})(T_m/\Theta^2 V_m^{2/3}) \quad (9)$$

(where $\hbar$ and k_B are the Planck and Boltzmann constants, respectively, and m is the mass of the atom) is applicable only for $T_m > \Theta$, whereas the melting temperatures of solid neon in Table I all are less than $0.6\Theta_0$. Hence, we have calculated a Debye model generalization of Eq. (9) following Ziman's approach,³² in which x^2 becomes [with $x_{\text{classical}}^2$ given by Eq. (9)]

$$x^2 = x_{\text{classical}}^2 [1 + (z^2/36) - (z^4/3600) + (z^6/2.12 \times 10^5) - \dots] \quad (10)$$

where $z = \Theta/T_m$. This expression is valid for the present range of z and is based on a series expansion³³ of the integrand of Ziman's equation (2.111).³²

Figure 9 gives a plot of x as calculated from the present data (Table I) for both Eqs. (9) and (10), with $\Theta = \Theta_0$. This plot is given in terms of T_m/Θ_0