Fig. 4. Typical deviations of high-temperature data from a smooth curve. The rms deviation is 0.33 %.

uncorrected for bomb expansion) results. The rms deviation for the intermediate region (Fig. 3) is 0.07 %, while that for the high-temperature region is 0.33 %, with the major scatter occurring above 30 K.

4. DISCUSSION, NATURAL NEON

The plot of $\ln \Theta_0$ vs. $\ln V$ in Fig. 5 can be used to evaluate the limiting average value of the Grüneisen parameter, $\gamma_0 = -d \ln \Theta_0/d \ln V = 2.51$ (± 0.03). The error bars on this figure correspond to approximately $\pm 0.1 \%$ uncertainties in both Θ_0 and V. The value of Θ_0, which we obtain for the 0 K equilibrium state $\Theta_0(13.39 \text{ cm}^3/\text{mole}) = 75.1 (\pm 0.1)$ K, is in good agreement with that given by Fagerstroem and Hollis-Hallet [75.0 (± 0.5) K][11]
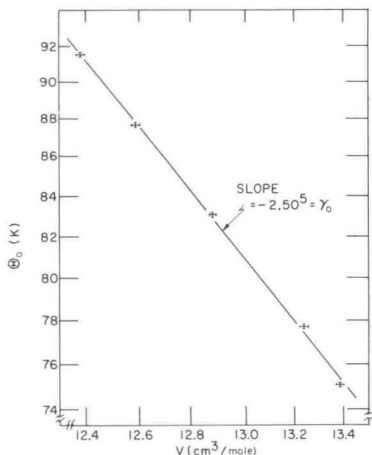

Fig. 5. A logarithmic plot of Θ_0 vs. V for the present data.

and by Fenichel and Serin [74.6 ($\pm$ 1) K].[12] γ_0 also can be calculated from the extrapolation of low-temperature thermal expansion data to $T = 0$, but the only available data[7] are not sufficiently precise to carry out this extrapolation. Our value of γ_0 does appear to be consistent with those values calculated from the higher temperature data, although, as we argue in Ref. 10, a more reasonable procedure involves the assumption of a volume dependence for γ, with one possibility being $\gamma_0 = 0.194 \pm 0.002 \, \text{cm}^{-3}$ V. This representation is not unique, and gives a $\Theta_0(V)$ relation which differs from the straight line of Fig. 5 by the width of the line. On this basis, we would predict γ_0 (13.39 cm^3/mole) = 2.60 $\pm$ 0.03.

The volume dependence of the lattice vibrational properties for a solid can be expected to a first approximation to scale with Θ_0; that is, in this approximation all lattice frequencies scale identically with volume, and the shape of the density of states curve is not a function of volume. This assumption is equivalent to that of a temperature-independent thermodynamic Grüneisen parameter

$$\gamma = \beta B_T V/C_V = V(\partial S/\partial V)_T/C_V = \sum_i \gamma_i c_i/C_V \tag{5}$$

at constant volume. The right-hand side of Eq. (5) gives the result for γ in the quasiharmonic approximation, with $\gamma_i = -d \ln \omega_i/d \ln V$ and c_i being, respectively, the Grüneisen parameters and specific heats for the individual modes. The present data indeed can be represented by a common curve to better than $\pm 1 \%$ at all temperatures when C_V is plotted as a function of $T/\Theta_0(V)$. Small deviations exist, however, and these are illustrated in Fig. 6, where the smoothed results from Tables II through VI are plotted in reduced form as $\Theta(T, V)/\Theta_0(V)$ vs. $T/\Theta_0(V)$. The internal consistency of the results is quite evident in this figure, with a maximum difference between the four experimental curves (the curve for 13.39 cm^3/mole is extrapolated) of 1.5 % near $T/\Theta_0 = 0.12$. This difference appears to be systematic and smooth to within our estimated experimental accuracy of $\pm 0.3 \%$ and to disappear for temperatures below roughly $0.08\Theta_0$ (6.5 K) and above $0.3\Theta_0$ (25 K). These results suggest that the higher frequency modes have γ_i's which are slightly larger than those for lower frequencies, and hence that γ [Eq. (5)] should show a slight increase with increasing temperature at constant volume.

The magnitude of this increase can be estimated in the following manner. If C_V can be represented approximately as a universal function $C_V(T/\Theta_0)$, then the entropy also can be represented in the same fashion and to the same approximation as $S(T/\Theta_0)$. In particular, the entropy curve for Ne 6 is chosen for the reduced expression, since these results are for an "average" volume, and the entropies for the other volumes are considered to deviate