

responds to the nearest-neighbor distance. The calculated Hugoniot which agree with the experimental Hugoniot have the following potential forms:

$$\text{LJD } \Phi(r) = [kT^*/(n-6)] [6(r/r^*)^{-n} - n(r/r^*)^{-6}], \quad (18)$$

$$\text{exp-6 } \Phi(r) = [kT^*/(\alpha-6)] \times \{6 \exp[\alpha(1-r/r^*)] - \alpha(r/r^*)^{-6}\}, \quad (19)$$

where r^* is the position of the potential minimum, T^* is the temperature equivalent of the energy of the potential minimum at $r=r^*$, r is the intermolecular distance, k is Boltzmann's constant, n is the repulsion term for the LJD form, and α is the steepness parameter for the exp-6 form. Table V is a list of the values for these "constants" from which the Hugoniot were calculated. Also included for comparison are the values used by others. Figure 12 shows the calculated and experimental Hugoniot. The most recent calculations²² are by Salzman, Collings, and Pings. These agree with the experimental Hugoniot and the parameters used except for the value of n in the repulsion term. A comparison of the parameters for the exp-6 potential used in this study with Fickett's values indicated close agreement. No significance was placed on the separation of the experimental and calculated Hugoniot curves about 170 kbar. The calculated Hugoniot indicates a stiffer material than observed.

IV. SUMMARY

Table VI summarizes the equation of state parameters obtained for each liquid and indicates the appropriate range, standard deviations, and initial conditions. The benzene and carbon disulfide U_s-U_p data are represented by a linear relationship while the carbon tetrachloride and liquid nitrogen data are represented equally well by a linear relationship or by a quadratic in U_p . A transition occurs in benzene and carbon disulfide with the possibility of a mixed phase region existing between the low and high pressure phases. The evidence for the occurrence of a transition in carbon tetrachloride and liquid nitrogen is not as strong as for the other two liquids. Considering Table VI, the values for the slope of the lower and upper line segments for each liquid are very similar.

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