TABLE I. Heats of formation of the explosives.

Explosive	$(\Delta H_f)_e$ kcal/mole at 25°C
RDX (cyclotrimethylenetrinitramine)	+14.71[a]
TNT (trinitrotoluene)	−17.81[b]
$C_{3.3}H_{6.2}O_6N_{5.6}$[c]	+0.49[d]

[a] E. J. Prosen (NBS), (private communication).
[b] G. Stegeman, NDRC Division-8 Interim Report PT-7 (1943).
[c] Explosive presently classified.
[d] L. Sitney (LASL) (unpublished data).

the final calculations, however, the set (9) was used in order to simplify the solution of the equilibrium equations and thereby reduce the machine time required. Although this set is rather restricted, components of differing size (H_2, CO_2) and with positive heat of formation (NO) are included. It was found that with this set of components the determination of the equilibrium composition, given k, n_0, V_0, and T, could be reduced analytically to the solution of one equation in one unknown. (With solid carbon present this unknown was n_{CO}; with carbon absent, n_{H_2}.)

The required reference-state thermodynamic functions and enthalpies of formation were taken from the tables published by the National Bureau of Standards.[19] For calculational purposes, it was convenient to have the temperature-dependent data represented by analytic fits; the functions which we used have been given elsewhere.[20] The enthalpies of formation of the explosives are given in Table I.

The calculations were done on IBM 701 digital computers. It was found quite feasible to code a single problem to calculate adiabatic or Hugoniot curves, as well as detonation velocities. In order to produce points on these curves, Eqs. (1), (2), and (3b), (4b) (for an adiabat), or (6) (for a Hugoniot) were solved by iteration to obtain values of V and T for the desired S or $h(=0)$, with the composition given by Eqs. (5) and the mass balance relations. The detonation velocity was determined by finding the point on the Hugoniot

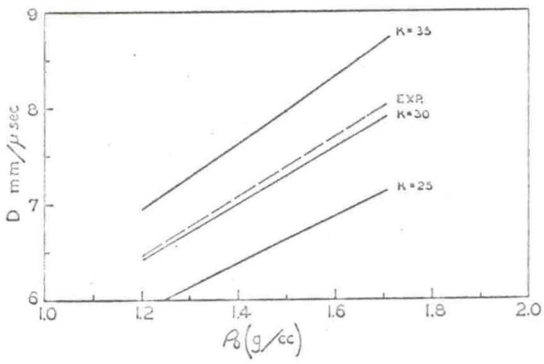

FIG. 1. The effect of κ on $D-\rho_0$; $\alpha=0.6$, $\beta=0.06$.

[19] U. S. National Bureau of Standards, *Selected Values of Chemical Thermodynamic Properties, Series III* (loose leaf).
[20] W. Fickett and R. D. Cowan, J. Chem. Phys. 23, 1349 (1955).

where

$$D=V_0[(p-p_0)/(V_0-V)]^{\frac{1}{2}} \tag{10}$$

had its minimum value; this is equivalent to satisfying the C−J condition (7) with $(\partial p/\partial V)_S$ evaluated with equilibrium composition. The time required for the calculation of one adiabat or Hugoniot point was about 20 sec; for a detonation velocity, an average of about 140 sec.

4. EFFECTS OF THE PARAMETERS

In order to determine the effects of the various equation-of-state parameters on the calculated $D-\rho_0$ curve and p_{CJ}, exploratory calculations were carried out for one explosive, 65/35 RDX/TNT. In order to save calculating time, these were carried out under the assumption of a fixed product composition resulting from the following decomposition equation:

$$C_qH_rO_sN_t=\frac{r}{2}H_2O+\left(s-\frac{r}{2}\right)CO+\left(q-s+\frac{r}{2}\right)C+\frac{t}{2}N_2. \tag{11}$$

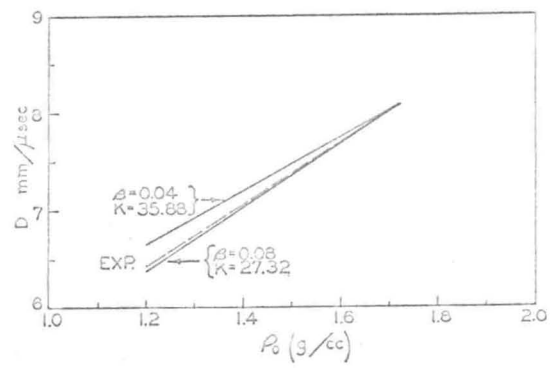

FIG. 2. The effect of β on $D-\rho_0$; κ chosen to match experimental D at one point; $\alpha=0.6$.

A set of geometrical covolume values was used, though with fixed composition the relative sizes of the individual k_i are unimportant. The other parameters were varied from the values

$$\alpha=0.6,\quad \beta=0.06,\quad \kappa=30, \tag{12}$$

which were found to give approximate agreement with the experimental $D-\rho_0$ and p_{CJ}. The results of the calculations are summarized in Figs. 1 through 5.[21]

Viewed from the standpoint of attempting to reproduce experimental data, the effects of the parameters

[21] These parameter studies differ from the final calculations in that they used a more incompressible equation of state for carbon than that which was finally adopted and used in the main calculations. This "harder" equation of state was based on an interpolation between the static measurements of P. W. Bridgman [Proc. Am. Acad. Arts Sci. 76, 55–87 (1948)] and Thomas-Fermi-Dirac calculations made by R. D. Cowan at this laboratory (unpublished results).