

The  $\alpha(v)$  curve *per se* provides a means of estimating the validity of the  $\alpha(v)$  approximation. In the limit of low pressures,  $\alpha$  should emerge smoothly into the van der Waals  $b$ . Hence, as a covolume,  $\alpha$  should be about four times greater than the actual volume  $v_m$  of the molecules. Hence one should have for the internal energy increase due to the applied pressure  $p$ ,

$$E_i = -\frac{1}{4} \int_0^p p d\alpha \cong -\frac{nRT}{4} \int_0^v d\alpha/(v - \alpha).$$

The integral has as an upper limit for CHNO explosives a value of about 2.5 giving an upper limit value for  $E_i$  of about 200 cal/g. But  $Q$  (the heat of explosion) plus the Hugoniot energy  $\frac{1}{2}p(v_1 - v_2)$  is in this upper limit case about 1800 cal g<sup>-1</sup> giving  $E_i/(Q + \frac{1}{2}p(v_1 - v_2)) = 0.1$  to 0.15.

One may also estimate  $E_i$  directly by the methods used here for thermal expansion and compressibility of solids. Thus

$$E_i = \Delta T = \int_0^p p dv = \int_0^p v_m p \left( \frac{1}{v_m} \frac{dv_m}{dp} \right) dp < v_m \beta p^2/2.$$

The theory for molecules of the type considered here also gives  $\beta_0 \leq 10^{-6}$  atm<sup>-1</sup>. Since  $\bar{v}_m$  should have an upper limit of 0.5 cm<sup>3</sup> g<sup>-1</sup>, one thus obtains  $E_i \sim 200$  cal g<sup>-1</sup> in agreement with the above estimate.

According to these estimates therefore, while the  $\alpha(v)$  equation of state gives an upper limit for  $T_2$ , the actual value should be no more than 10-15 % (or about 500° K) less. This is, however, in sharp contrast with the approximately 3000° K lower values for  $T_2$  computed for PETN at  $\rho_1 = 1.7$  g cm<sup>-3</sup> by Cottrell and Paterson.<sup>19</sup>

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