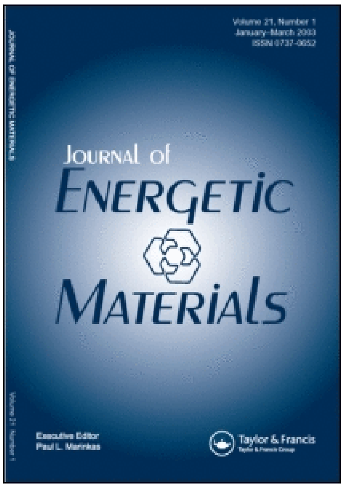

Journal of Energetic Materials
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713770432

On predicting properties of explosives - detonation velocity

J. R. Stine[a]
[a] Los Alamos National Laboratory Group, Los Alamos, NM

To cite this Article Stine, J. R.(1990) 'On predicting properties of explosives - detonation velocity', Journal of Energetic Materials, 8: 1, 41 — 73

To link to this Article: DOI: 10.1080/07370659008017245

URL: http://dx.doi.org/10.1080/07370659008017245

ON PREDICTING PROPERTIES OF EXPLOSIVES - DETONATION VELOCITY

J. R. Stine

Los Alamos National Laboratory

Group M-1 MS-C920

Los Alamos, NM 87545

ABSTRACT

A systematic method of representing an explosive, based on its composition, is presented. This method is used to display performance data for existing explosives, and suggests an alternate definition for oxygen balance and determines compositions that might produce high-performance explosives. A new method for predicting the detonation velocity of a proposed explosive is also presented. This is a simple method that also yields insight into which factors are important in predicting performance.

INTRODUCTION

An important aspect of explosives technology is the search for new explosives with particular performance, sensitivity, and physical properties. Initially, performance is usually of primary importance. The particular performance property one is

Journal of Energetic Materials vol. 8, 041-073 (1990)
Published in 1990 by Dowden, Brodman & Devine, Inc.

interested in will depend, of course, on the intended application of the explosive. However, one basic performance property is the detonation velocity. Indeed, other performance properties may be expressed in terms of the detonation velocity (along with other parameters). For example, the Chapman-Jouget pressure can be shown to vary as the square of the detonation velocity. Being of fundamental importance and also one of the few detonation parameters that can be measured precisely, the detonation velocity has been the subject of a number of predictive schemes. For the most part, these schemes have been limited to organic explosives containing only carbon, hydrogen, nitrogen, and oxygen. Such will also be the case in the present paper although our method can easily be extended to include explosives containing other elements.

These predictive methods can be grouped into three basic types. The first involves solving the hydrodynamic equations derived from the conservation of mass, momentum, and energy conditions.[1] The latter condition requires that the equation of state of the products be known. Toward this end, Kistiakowsky and Wilson suggested a functional form to describe the equation of state for each of the products. The advent of computers facilitated the solving of these equations and led to the development of the sophisticated BKW,[2,3] RUBY,[4] and TIGER[5] computer codes. However, little is known about the actual composition of the detonation products or their equations-of-state at these high temperatures and pressures. Hence, these methods must calibrate the equation-of-state parameters (e.g., covolumes) to detonation measurements.

The BKW and RUBY codes are similar in nature and were written in the early 1960s. The BKW code required that two sets of parameters be used to describe most explosives: a set derived from TNT detonation data for high-carbon-containing explosives, and a set derived from RDX detonation data for the more oxygen-balanced explosives. It was later realized that an additional set of parameters was needed for non-hydrogen containing explosives like hexanitrobenzene.

The RUBY code later evolved into the more flexible TIGER[6] code that allows for alternate forms for the equation of state, and one can use just one set of parameters for all explosives. It is interesting to note that because the TIGER code allows formic acid to be a detonation product and the BKW program does not, the types and relative amounts of detonation products predicted for HMX by the two codes are quite different. The effect of including formic acid as a detonation product for various explosives has been discussed by Kerley.[7] Over the years, numerous equations of state have been proposed,[8] and it is not unusual that significantly different product species and concentrations can be predicted by any two such equations of state.[9]

The second type of method involves simplified parametric fits to results calculated by the above mentioned methods.

These include a method originally proposed by Kamlet and Jacobs[10] and another proposed by Wu.[11] These are attractive methods because they are simple and do not require a computer or sophisticated programs. However, one cannot expect them to predict performance properties any better than the methods of the first type. Indeed, if one is interested in a predicted performance of a proposed compound to guide a synthetic organic effort, a method's simplicity should not be the main reason for using it.

The third type of performance-prediction method is simply parametric fits to experimental performance data. These fits may involve functional forms derived from a theory or observation, or may be more of a regression analysis involving factors thought to be important for predicting performance. The early method of Martin and Yallop,[12] for example, tried to correlate detonation velocities of explosives at a given density with oxygen balance. Aizenshtadt's[13] method is similar, but also included parameters related to heat of formation and number of gram atoms in the explosive. The resulting detonation velocity is then adjusted to the desired density using a linear extrapolation formula with an assumed slope. Rothstein and Petersen[14,15] suggested a functional form that uses the compound's composition and some of its constituent groups to predict the detonation velocity of the compound at it's theoretical maximum density. Jain[16,17] suggested using parameters related to the number of oxidizing and reducing valencies in the compound to predict it's detonation velocity also at its theoretical maximum density. It should be noted that none of these methods considers the detonation velocity explicitly as a function of the compound's composition, density, and heat of formation as is the case in the other classes of methods described above.

Although all these methods have been shown to yield reasonable results for the existing explosives their predictive capabilities for new explosives is suspect. One reason for this is that the amount of detonation velocity data for pure explosives is limited to only a few dozen compounds. Hence, the methods that are parametric fits to the existing data may produce erroneous results when applied to new compounds of a different nature than those in the basis set. Indeed, this seems to be the case with some recently synthesized explosives:[18] the calculated detonation velocity may be greatly overestimated (in which case, the synthesized explosive may not be any better than existing ones) or may be greatly underestimated (in which case no attempt is made to synthesize the proposed explosive). In other cases the various methods yield widely different predicted detonation velocities, making it difficult for one to decide which one is the most realistic.

In the next section we present an analysis of detonation velocity with respect to an explosive's composition, heat of formation, and density. We also present a method for estimating the detonation velocity of a new material. The real advantage of this method lies in its simplicity, which quantitatively relates composition to performance and, hence, indicates alternative compositions that might prove to be good performers. We also discuss the results of this method and how it relates to some of the other methods.

METHODS

Our Analysis of C, H, N, O Explosives

Here we will be concerned with organic explosives containing carbon, hydrogen, nitrogen, and oxygen with the formula $C_aH_bN_cO_d$. We will assume that the detonation velocity is dependent on the chemical composition (a, b, c, d); the bulk density, ρ, of the explosive; and the heat of formation, ΔH_f. In fact, it appears that only the relative composition is of importance for determining the detonation velocity. For example, HMX ($C_4H_8N_8O_8$) and RDX ($C_3H_6N_6O_6$) have nearly identical detonation velocities if pressed to the same density. This being the case, we can "normalize" the chemical formula such that,

$$A + B + C + D = 1 \qquad \text{Eq. 1}$$

where

$A=a/m$, $B=b/m$, $C=c/m$, $D=d/m$, and, $m=a+b+c+d$.

This makes for a convenient reference formula so that different compositions can be compared. Of course, RDX and HMX would have the same normalized formula; namely, $A=1/7$, and, $B=C=D=2/7$.

We can now take advantage of the geometric properties of a regular tetrahedron to systematically locate every such organic compound. A regular tetrahedron has the property that the sum of the four distances from any interior point to each of the four sides is a constant (which we can arbitrarily take to be unity). Hence, every normalized chemical formula is represented by a unique point in a tetrahedron whose corners represent carbon, hydrogen, nitrogen, and oxygen. This is the three-dimensional analog of using an equilateral triangle for plotting three component systems.

The tetrahedron is positioned such that the cartesian coordinates (x, y, z) of each of the four corners are:

Nitrogen: $(0, 0, 3/4)$
Oxygen: $(\sqrt{2}/2, 0, -1/4)$
Carbon: $(-\sqrt{2}/2, \sqrt{6}/4, -1/4)$
Hydrogen: $(-\sqrt{2}/4, -\sqrt{6}/4, -1/4)$.

This is a tetrahedron centered at the origin and where the four distances from any interior point to each of the four sides sum to unity. The following equations can be used to locate any organic compound in this tetrahedron:

$$x = \sqrt{2}(3D - 1 + C)/4$$

$$y = \sqrt{6}(A - B)/4$$

$$z = C - 1/4$$

where A, B, C, and D are given in Equation 1. Thus, for example, TATB ($C_6H_6N_6O_6$) is located at the center of the tetrahedron. Of course, these formulas are applicable to either pure compounds or mixtures. In the latter case, one need only find the equivalent chemical formula for the mixture.

For purposes of illustration, we have selected some common pure explosives and listed them in Table I. Their positions in this tetrahedron space are shown in the stereo picture given in Figure 1. It is seen that most of these 23 explosives are in a cluster that contains TNT (explosives 1, 4, 6, 7, 9, 10, 12, 14, 16, 18, 19, 20, 21, and 23). These are all relatively oxygen-deficient explosives. The remaining explosives are relatively close to the oxygen-balance plane. It is also evident that only a small portion of the tetrahedron is characterized by any performance data on existing explosives. It is not surprising that a set of BKW parameters appropriate for TNT and a set appropriate for RDX would fit most of the existing explosive data, because the other explosives are not qualitatively different from these two explosives. The problem would come if one were to try to use either of these sets of parameters for compounds in another region of the tetrahedron. These observations apply not only to the BKW calculations but to all methods that rely on empirical data for their calibration. There simply is not enough experimental performance data on compounds that are representative of the whole tetrahedron space.

Another parameter related to just the molecular formula of a compound is its oxygen balance. This is a parameter that has been used in some predictive schemes related to detonation velocity[12,13] and sensitivity[19-21] and represents the compound's lack or excess of oxygen needed to produce the most stable products.

Hence, its definition requires the specification of the products of the reaction. Usually these products are taken to be carbon dioxide, nitrogen, and water. These three compounds are represented by three points in the tetrahedron and, hence, define an "oxygen-balance" plane, and is also shown in Figure 1.

It seems reasonable to define the oxygen balance of the particular compound as the perpendicular distance from its position in the tetrahedron to the oxygen-balance plane. One can easily show that this leads to the expression,

$$OB = \frac{d - 2a - b/2}{5(a+b+c+d)} \qquad \text{Eq. 2}$$

This differs from the more common definition of oxygen balance[21] given by,

$$OB = \frac{d - 2a - b/2}{M} \qquad \text{Eq. 3}$$

where M is the molecular weight of the compound. Equation (2) has been previously suggested,[12] but only on the basis that Eq. (2) is "simpler" than Eq. (3). Although neither formula will enter into the discussion for estimating the detonation velocity given below, we feel that Eq. (2) is the preferred definition based on the above arguments. If the explosive does not contain much hydrogen, then these two formulas produce similar results (except for a multiplicative factor).

It is also interesting to display the positions of the known pure explosives reported in the literature,[23,24] which are primarily nitroaromatics, aliphatic nitramines, and heterocyclics. Their positions are displayed in Figure 2. It is seen that only a limited portion of the tetrahedron space is characterized by known explosives.

We would also like to display the detonation velocities of the compounds listed in Table I. The experimental detonation velocities, ρ_{TMD}, ρ_{actual}, ΔH_f for the compounds listed in Table I are given in Table II along with an adjusted detonation velocity, D^*, which we will describe. The detonation velocity is a function of the density and heat of formation of the compound as well as its composition. Hence, it is necessary to consider each of the compounds at the same density and heat of formation before the detonation velocities can be plotted or compared. That is, the experimental detonation velocity data of these explosives must be adjusted to correspond to a new compound that has the same composition, but has a given density and heat of formation. We have arbitrarily chosen a density of 1.8 g/cm^3 and a heat of formation of 0 kcal/mole for purposes of illustration. The experimental detonation velocities were then adjusted to these values. This adjustment was made in the following way. The detonation velocity of the actual explosive at its measured heat of formation and density at which it was fired was calculated using the TIGER code. The difference between this value and the observed detonation velocity is the correction needed to bring the TIGER value into agreement with the observed value. The TIGER code was then used to calculate the detonation velocity of this explosive using a heat of formation of 0 kcal/mole and a density of 1.8 g/cm^3. It is assumed that the correction needed for this value is the same as that found for the calculation on the actual explosive. These adjusted values, denoted by D*, are also in Table II. It should be remembered that these values correspond to an imaginary compound even though they are labeled with the designation of the real explosive. For most of the explosives, this adjustment was a relatively minor one because most explosives have a density around 1.8 g/cm^3 and a heat of formation of 0 kcal/mole. However, for some explosives like PETN (which has a heat of formation of -128 kcal/mole) or HNAB (which has a heat of formation of 145 kcal/mole) or NQ (which has a density of 1.55 g/cm^3) this adjustment was rather large. Nevertheless, it is thought that reasonable values were obtained for the purpose of displaying any trends. These detonation velocities are displayed in Figure 3 along with the oxygen balance plane described above. This figure shows two things. The first is that there is a rough correlation of detonation velocity with oxygen balance, meaning the closer to the oxygen balance plane the higher the detonation velocity. However, the compounds with similar detonation velocities are actually skewed from this plane. This observation is consistent with the early work of Martin and Yallop,[19] who tried to correlate detonation velocity with oxygen balance (they actually tried both definitions of oxygen balance). The other result is that the hydrogen side of the oxygen-balance plane contains higher performers than does the carbon side. This demonstrates the need for having hydrogen in the compound. For example, HMX, which is one of the best performers, has a lot of hydrogen relative to carbon. Indeed, if a compound can be found that has the composition of NQ but higher density (even a nominal density of 1.8 g/cm^3), it is expected to have a detonation velocity higher than HMX's. These data also show that a large nitrogen content is also favorable to producing a high detonation velocity.

A New Method for Predicting Detonation Velocities

In this section we will develop a new method for calculating the detonation velocity of a proposed explosive. Actually, this method is based on a method originally developed by Urizar at Los Alamos in the late 1940s for predicting the detonation velocity of a mixture. His method is described in the LLNL handbook of explosives[23] and is applicable to mixtures containing explosives, binders, additives, and voids. This method has been used for some time at Los Alamos for estimating the detonation velocity of a new mixture of explosives and, indeed, Price[24] has found this method to yield results within one percent of the observed detonation velocity for low porosities (low voids). For the present discussion, we will not be concerned with binders or additives.

In his method, Urizar assumed that the detonation velocity of a mixture, D, (not to be confused with the D in Eq. 1) is the sum of the detonation velocities of the components weighted by their corresponding volume fractions. That is,

$$D = \sum \hat{v}_i D_i \qquad \text{Eq. 4}$$

where D_i and $\hat{v}_i$ are the detonation velocity and volume fraction of the i-th explosive in the mixture. He also allows for voids in the mixture and derived a value of 1.5 km/s as a "characteristic velocity" for a void. We will reserve D_0 to represent this velocity.

We now assume that if the detonation velocity is dependent on just the chemical composition then a mixture with the same composition as the proposed compound should have the same detonation velocity (assuming the heat of formation and densities are the same). If we consider only C, H, N, O compounds and wish to compose a mixture of explosives that matches the chemical composition and heat of formation of the proposed compound, it is clear that five explosives are needed as a "basis set". We will assume that the chemical formulas, densities, heats of formation, and detonation velocities are known for these five explosives. We now construct a matrix, F, as follows:

$$F = \begin{pmatrix} a_1 & a_2 & a_3 & a_4 & a_5 \\ b_1 & b_2 & b_3 & b_4 & b_5 \\ c_1 & c_2 & c_3 & c_4 & c_5 \\ d_1 & d_2 & d_3 & d_4 & d_5 \\ H_1 & H_2 & H_3 & H_4 & H_5 \end{pmatrix} \qquad \text{Eq. 5}$$

where the i-th explosive has the formula $C_{a_i}H_{b_i}N_{c_i}O_{d_i}$ and heat of formation H_i. The five explosives must be chosen such that the matrix, **F**, is not singular. We now define a column vector $x=(a,b,c,d,\Delta H_f)$ where a, b, c, and d represent the chemical formula of the proposed compound and ΔH_f is its heat of formation in kcal/mole. We can now write,

$$x = \mathbf{F}\, n \qquad \text{Eq. 6}$$

where n is a column vector, whose elements represent the number of moles of each of the five basis set compounds needed to simulate the composition and heat of formation of the proposed compound. That is,

$$n = \mathbf{F}^{-1} x. \qquad \text{Eq. 7}$$

The weight of each explosive, w_i, needed for this mixture is then,

$$w_i = n_i M_i \qquad \text{Eq. 8}$$

where M_i is the molecular weight of the i-th explosive. Its corresponding volume is

$$v_i = w_i / \rho_i \qquad \text{Eq. 9}$$

where ρ_i is its density.

The total mass is simply the molecular weight, M, ($M=\Sigma w_i$) of the proposed compound and the total volume, V, is given by,

$$V = v_0 + \sum v_i \qquad \text{Eq. 10}$$

where v_0 is the volume of the voids. We require that the volume of the voids be chosen such that,

$$\rho = M / V \qquad \text{Eq. 11}$$

where ρ is the density of the proposed compound. Substituting Equations 7 through 11 into Equation 4 we have,

$$D = \hat{v}_0 D_0 + \sum \hat{v}_i D_i = \frac{V_0 D_0}{V} + \frac{1}{V} \sum v_i D_i \qquad \text{Eq. 12}$$

where $\hat{v}_i = v_i/V$ is the volume fraction of component i. This can then be shown to be equivalent to,

$$D = D_0 + \sum n_i g_i \qquad \text{Eq. 13}$$

where g_i is an element of a column vector, G, given by,

$$g_i = m_i (D_i - D_0)/\rho_i . \qquad \text{Eq. 14}$$

Thus we have,

$$D = D_0 + \rho M^{-1}(G^T n) = D_0 + \rho M^{-1}(G^T F^{-1}) x. \qquad \text{Eq. 15}$$

For purposes of illustration, we have arbitrarily chosen five well-characterized explosives to serve as the basis set. These explosives are BTNEU, RDX, TNETB, ABH, and ExplD (see Tables I and II for their formulas and experimental properties). Note that the appropriate density for each of the basis compounds is that at which the detonation velocity was measured. No special consideration was given as to the five explosives selected. It had been observed, by selecting other sets of five explosives, that each of them should have the same detonation products. That is, oxygen-rich explosives should not be included with oxygen-deficient explosives. For this reason, NG, which is oxygen-rich, was not included in the basis set of five explosives.

We should also note, that some of the explosives have an abundance of data while others have very little. We have selected only pure explosives so that the results would not be biased toward mixtures containing only a few of the common explosives. We also selected just one point to represent the performance of a particular explosive. In most cases a decision had to be made as to what is the most representative value. Figures 4 and 5 show some of the experimental data for two of the explosives listed in Table I. It is clear that the experimental detonation velocities derived from different references can be quite different. For this reason, Tetryl and PETN were also not selected as basis-set compounds. The calculated detonation velocities for the other explosives listed in Table I using this method are given in Table III.

It is clear from Eq. 15 that once a set of basis-set explosives is selected, then the vector given by G^TF^{-1}, which has elements $(\alpha,\beta,\gamma,\delta,h)$, is determined. Thus, we can rewrite Eq. 15 as,

$$D = D_0 + \rho\ (\alpha\ a + \beta\ b + \gamma\ c + \delta\ d + h\ \Delta H_f)/M. \qquad \text{Eq. 16}$$

This equation can be considered as a general form that describes the detonation velocity in terms of the compound's composition, heat of formation, and density. We can now determine a set of values for α, β, γ, δ, h, and D_0 such that the best agreement (in the least-squares sense) is obtained between the experimental and observed detonation values given in Table II. Again, NG was omitted from consideration because it is oxygen rich. The results are:

$\alpha = -13.85$, $\beta = 3.95$, $\gamma = 37.74$,

$\delta = 68.11$, $D_0 = 3.69$, $h = 0.6917$.

Values for the detonation velocities are given in Table III using the above values in Equation 16 and are also shown in Figure 7, where the calculated values of the detonation velocities plotted versus the observed values. The straight line is for reference and represents perfect agreement between the calculated and observed values. It is seen that there is good agreement between the calculated and the observed results.

It is interesting to note a few properties of the above equations. It is clear from the Urizar assumption that the detonation velocities of the constituents be weighted by their volume fractions implies that detonation velocity is exactly linear with densities. Indeed, for many explosives this is seen to be the case, detonation velocity is linear or nearly linear over a wide range in densities. One can also immediately deduce from Equation 16 that

$$\frac{dD}{d\rho} = \frac{D - D_0}{\rho} \qquad \text{Eq. 17}$$

indicating that an approximation to the slope of this line can be obtained from one detonation-velocity measurement and the transmission velocity of a void.

Rothstein and Petersen[14] had found that the liquid explosive, NM (nitromethane), is anamolous where their calculated detonation velocity differed by 13 percent from the observed value. If we use Eq. 16 to estimate the detonation velocity of NM, where ΔH_f = -27 kcal/mole and ρ = 1.13 g/cm^3, we obtain a value of 6.79 km/s, which compares with the observed value of 6.35 km/s.[20] Note that this point was not used in the determination of the parameters used in Eq. 16.

CONCLUSIONS

We have suggested a graphical method for carbon-, hydrogen-, nitrogen-, and oxygen-containing compounds, based on the properties of a regular tetrahedron, for displaying performance related to an explosive's composition. This method allows one to see the regions of the composition space that produce good performing explosives and suggests other uninvestigated regions that may produce higher-performing explosives than we have now. This graphical technique also suggests a different definition for oxygen balance than usually used, which may be more useful for comparing explosives of different compositions and also for use in other theories that relate sensitivity or performance to oxygen balance.

We have also presented a new method for estimating the detonation velocity of a proposed compound that is based on the method of Urizar that was developed for mixtures. Estimates of the detonation velocity using this method rival those using any of the existing methods including the more sophisticated hydrodynamic-thermodynamic (BKW) methods. The only assumptions made in this method are:

1) The detonation velocity of a mixture of explosives is the sum of the detonation velocities of the components weighted by their corresponding volume fractions.
2) A characteristic velocity associated with a void exists and is independent of the explosive.
3) The performance of a pure compound with a particular carbon, hydrogen, nitrogen, and oxygen atomic composition, heat of formation, and density is the same as that of a mixture of explosives (and voids) of the same composition, heat of formation, and density.

The first two assumptions are those originally made by Urizar in his method.

Our method can be employed in two ways. One is to use a set of five well-characterized explosives to make a mixture having the same atomic composition, heat of formation, and density as the proposed compound. Voids are added to yield a mixture with the appropriate density. The detonation velocity is then calculated using Urizar's method. This method has no adjustable parameters (except for the "characteristic transmission velocity" of a void derived by Urizar). The only experimental data needed are the detonation velocity and density for each of the five basis-set explosives.

This method can be tested on explosives not used in the basis set to ascertain how well such a simple method performs. In practice, one would probably want to select five well-characterized explosives that are similar (i.e., in the same portion of the composition space) as the proposed compound.

The present method can also be employed in a second way. The mixture concept suggests a form as to how the detonation velocity behaves with respect to composition, heat of formation, and density. There are six parameters that can be adjusted to yield the best fit with known detonation-velocity data for a wide selection of explosives.

These two ways of applying the method complement one another. The first is conceptionally simple, yielding basic relationships, that give one an analysis of performance as related to composition, heat of formation, and density. It also makes clear exactly what assumptions and adjustable parameters are inherent in the method. The latter way of employing the method is appropriate for producing the best estimate for the detonation velocity of a proposed compound based on all available empirical data. One difference seen between the two ways of applying the method is in the values found for D_0. Urizar had originally estimated this value to be 1.5 km/s, whereas here we find a value of 3.69 km/s. Although this disparity is significant and should be investigated, at this point, neither value can be ruled out as being more physically reasonable than the other.

In the final analysis, the utility of this, or indeed any other prediction method, is going to be how well it does for compounds that were not used in its parameterization and for compounds that are quite different in structure from existing explosives. Unfortunately, the data base of performance data for pure compounds is not large enough to sufficiently test these methods, particularly if much of this same data were used in the method's parameterization.

ACKNOWLEDGEMENTS

I would like to thank Manual J. Urizar and John F. Kramer for some helpful discussions.

REFERENCES

1) W. Fickett and W. C. Davis, "Detonation," University of California Press, Berkeley, 1979.

2) C. L. Mader, "FORTRAN BKW: A Code for Computing the Detonation Properties of Explosives," Los Alamos Scientific Laboratory report LA-3704 (1967).

3) C. L. Mader, "Numerical Modeling of Detonations," University of California Press, Berkeley, 1979.

4) H. B. Levine and R. E. Sharples, "Operator's Manual for RUBY," Lawrence Livermore Laboratory report UCRL-6815 (1962).

5) M. Cowperthwaite and W. H. Zwisler, "TIGER Computer Program Documentation," Stanford Research Institution publication No. Z106 (1973).

6) M. Cowperthwaite and W. H. Zwisler, "Proceedings Sixth Symposium (International) on Detonation," San Diego, California, August 24-27, 1976, ONR report ACR 221 pp 162-172.

7) G. I. Kerely, "Proceedings Eight Symposium (International) on Detonation," Albuquerque, New Mexico, July 15-19, 1985, pp. 540-547.

8) See for example, R. Chirat and J. Baute, "Proceedings Eighth Symposium (International) on Detonation," Albuquerque, New Mexico, July 15-19, 1985, pp. 751-761; O. Heuze, P. Bauer, H. N. Presles, and C. Brochet, ibid. pp. 762-769; K. K. Feng, W. K. Chung and B. C.-Y. Lu, ibid. pp. 805-813; K. Tanaka, ibid. pp. 548-557.

9) Wu Xiong, J. Energetic Mat. 3, 263 (1985).

10) M. J. Kamlet and S. J. Jacobs, J. Chem. Phys. 48, 23 (1968).

11) Wu Xiong, J. Energetic Mat. 3, 263 (1985).

12) A. R. Martin and H. J. Yallop, Trans. Faraday Soc. 54, 257 (1958).

13) I. N. Aizenshtadt, Fiz. Goreniya i Vzryva 12, 754 (1976).

14) L. R. Rothstein and R. Petersen, Propellants and Explosives 4, 56 (1979) and 4, 86 (1979).

15) L. R. Rothstein, Propellants and Explosives 6, 91 (1981).

16) S. R. Jain, Propellants, Explosives, and Pyrotechnics 12, 188 (1987).

17) R. Sundararajan and S. R. Jain, Combustion and Flame 45, 47 (1982).

18) M. D. Coburn and C. Storm, Los Alamos National Laboratory, private communication.

19) M. J. Kamlet, "Proceedings Sixth Symposium (International) on Detonation," San Diego, California, August 24-27, 1976, ONR report ACR 221 pp 312-322.

20) M. J. Kamlet and H. G. Adolph, Propellants and Explosives 4, 30 (1979).

21) H. G. Adolph, J. R. Holden, and D. A. Cichra, "Relationships Between the Impact Sensitivity of High Energy Compounds and Some Molecular Properties Which Determine Their Performance; N, M, and ρ_0" Naval Surface Weapons Center report NSWC TR 80-495 (April, 1981).

22) R. Meyer, "Explosives," Verlag Chemie, New York, 1977.

23) B. M. Dobratz and P. C. Crawford, "LLNL Explosives Handbook - Properties of Chemical Explosives and Explosive Simulants," Lawrence Livermore National Laboratory report UCRL-52997 (January, 1985).

24) D. Price, J. Energetic Mat. 1, 55 (1983).

25) "Engineering Design Handbook - Explosives Series - Properties of Explosives of Military Interest," U. S. Army Materiel Command pamphlet AMCP 706-177 (January, 1971).

26) P. E. Rouse, Jr., J. Chem. Eng. Data 21, 16 (1976).

27) J. R. Holden and C. Dickinson, "Prediction of Crystal Density Throygh Molecular Packing Analysis," Naval Surface Weapons Center report NSWC MP 79-185 (September, 1979).

28) M. J. Kamlet and H. Hurwitz, J. Chem. Phys. 48, 3685 (1968).

29) M. J. Urizar, E. Jones, Jr., and L. C. Smith, Phys. Fluids 4, 262 (1961).

TABLE I

SOME COMMON EXPLOSIVES AND THEIR FORMULAS

	Acronym	C	H	N	O	Chemical Name
1	ABH	24	6	14	24	Azo-bis(hexanitro) biphenyl
2	BTF	6	0	6	6	Benzotrifuroxan
3	BTNEU	5	6	8	13	bis(trinitroethyl) urea
4	DATB	6	5	5	6	Diamino-trinitrobenzene
5	DINA	4	8	4	8	Diethanolnitramine dinitrate
6	DIPAM	12	6	8	12	Dipicramide
7	ExplD	6	6	4	7	Ammonium picrate
8	HMX	4	8	8	8	Cyclotetramethylene tetranitramine
9	HNAB	12	4	8	12	Bis(trinitrophenyl) diazine
10	HNS	14	6	6	12	Hexanitrostilbene
11	NG	3	5	3	9	Nitroglycerine
12	NONA	18	5	9	18	Nonanitroterphenyl
13	NQ	1	4	4	2	Nitroguanidine
14	ONT	18	6	8	16	Octanitroterphenyl
15	PETN	5	8	4	12	Pentaerythritol tetranitrate
16	Picric	6	3	3	7	Trinitrophenol
17	RDX	3	6	6	6	Cyclotrimethylene trinitramine
18	TACOT	12	4	8	8	Tetranitrobenzotriazolobenzotriazole
19	TATB	6	6	6	6	Triamino-trinitrobenzene
20	Tetryl	7	5	5	8	N-methyl-N,2,4,6-tetranitroaniline
21	TNA	6	4	4	6	Trinitroaniline
22	TNETB	6	6	6	14	Trinitroethyltrinitrobutyrate
23	TNT	7	5	3	6	Trinitrotoluene

TABLE II

DETONATION VELOCITIES OF THE COMPOUNDS LISTED IN TABLE I

Acronym	ρ_{TMD} (g/cm^3)	ΔH_f (kcal/mole)	ρ (g/cm^3)	D (obs) (km/s)	D* (adjust.) (km/s)
ABH	1.780[a]	116.3[a]	1.78[b]	7.600[b]	7.47
BTF	1.901[a]	144.5[c]	1.86[c]	8.490[c]	7.55
BTNEU	1.861[d]	-72.9[d]	1.86[e]	9.01[e]	8.93
DATB	1.837[a]	-23.6[a]	1.79[c]	7.520[c]	7.78
DINA	1.670[f]	-75.4[g]	1.60[f]	7.720[f]	8.57
DIPAM	1.790[a]	-6.8[a]	1.76[c]	7.400[c]	7.51
ExplD	1.717[c]	-94.0[c]	1.55[c]	6.850[c]	8.09
HMX	1.905[c]	17.9[c]	1.89[c]	9.11[c]	8.76
HNAB	1.799[c]	67.9[a]	1.60[c]	7.311[c]	7.69
HNS	1.740[s]	18.7[c]	1.70[c]	7.000[c]	7.24
NG	1.596[c]	-88.6[c]	1.600[c]	7.700[c]	8.78
NONA	1.780[a]	27.4[a]	1.78[b]	7.560[b]	7.53
NQ	1.775[c]	-22.1[c]	1.550[c]	7.650[c]	8.99
ONT	1.800[a]	19.7[a]	1.800[b]	7.330[s]	7.29
PETN	1.780[c]	-128.7[c]	1.760[c]	8.260[c]	8.86
Picric	1.760[c]	-51.3[c]	1.710[c]	7.260[c]	7.76
RDX	1.806[c]	14.7[c]	1.770[c]	8.700[c]	8.76
TACOT	1.850[c]	110.5[c]	1.850[c]	7.250[c]	6.72
TATB	1.938[c]	-36.8[c]	1.880[c]	7.760[c]	7.71
Tetryl	1.730[c]	4.7[c]	1.710[c]	7.850[c]	8.01
TNA	1.760[h]	-29.9[h]	1.72[h]	7.300[h]	7.70
TNETB	1.783[i]	-118.5[h]	1.78[f]	8.460[h]	8.83
TNT	1.654[c]	-16.0[c]	1.609[j]	6.908[j]	7.67

[a] Ref. 26, [b] Ref. 3, [c] Ref. 23, [d] Ref. 27, [e] Ref. 28, [f] Ref. 24, [g] Ref. 22, [h] Ref. 25, [i] Ref. 21, [j] Ref. 29

TABLE III

COMPARISON OF OBSERVED AND CALCULATED DETONATION VELOCITIES

Acronym	D (km/s)	D(Eq. 15) (km/s)	D(Eq. 16) (km/s)
ABH	7.600	(7.60)	7.63
BTF	8.490	8.34	8.51
BTNEU	9.01	(9.01)	8.95
DATB	7.520	7.74	7.51
DINA	7.720	7.71	7.83
DIPAM	7.400	7.54	7.46
ExplD	6.850	(6.85)	6.86
HMX	9.11	9.18	9.03
HNAB	7.311	7.05	7.29
HNS	7.000	7.02	7.04
NG	7.700	....	....
NONA	7.560	7.50	7.49
NQ	7.650	7.86	7.78
ONT	7.330	7.38	7.29
PETN	8.260	8.38	8.38
Picric	7.260	7.33	7.30
RDX	8.700	(8.70)	8.70
TACOT	7.250	7.55	7.38
TATB	7.760	8.13	7.70
Tetryl	7.850	7.58	7.62
TNA	7.300	7.36	7.25
TNETB	8.460	(8.46)	8.48
TNT	6.908	6.73	6.77

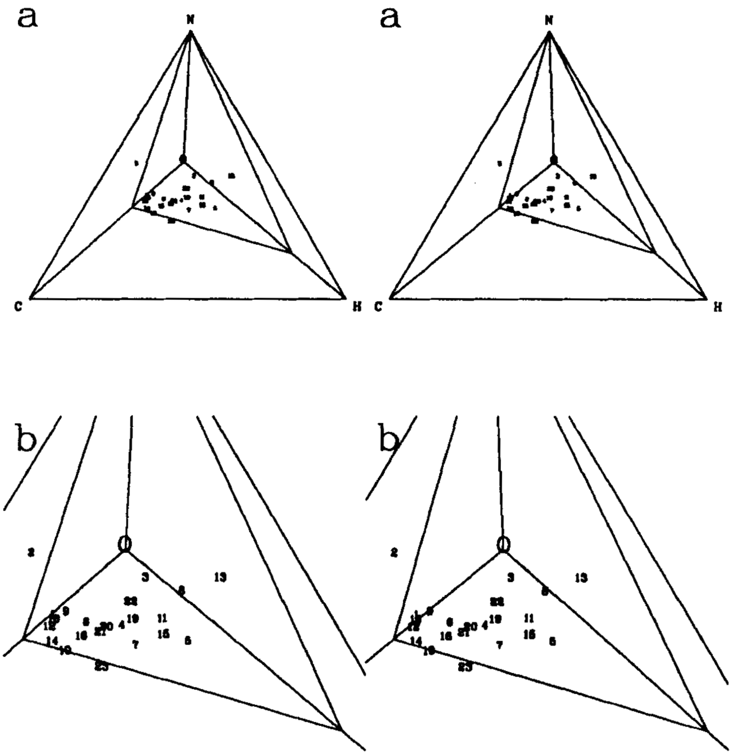

Figure 1. Stereo plot in the tetrahedron space of the explosives listed in Table I. Figure 1b is an expanded view of Figure 1a.

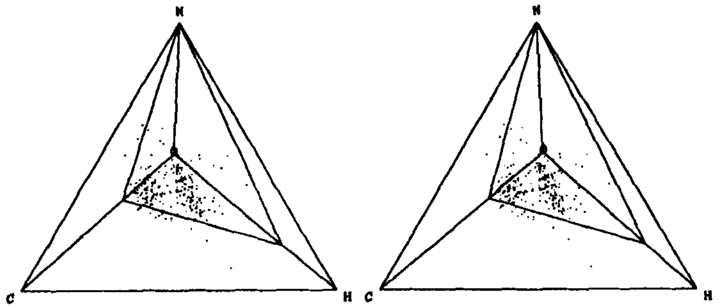

Figure 2. Stereo plot in the tetrahedron space for 351 known C, H, N, O explosives.

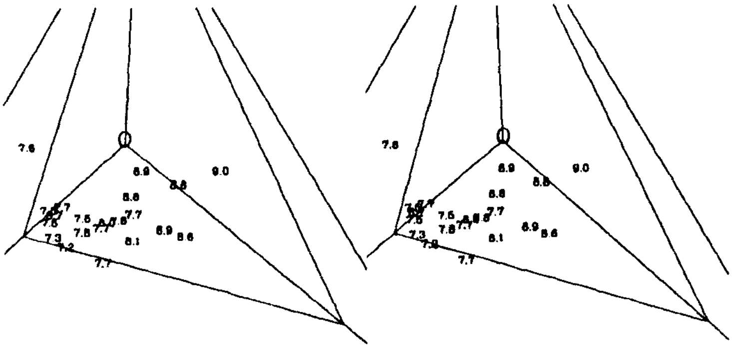

Figure 3. Detonation velocities in km/s of the explosives listed in Table II. These values have been adjusted as if the explosive had a density of 1.8 g/cm^3 and a heat of formation of 0 kcal/mole.

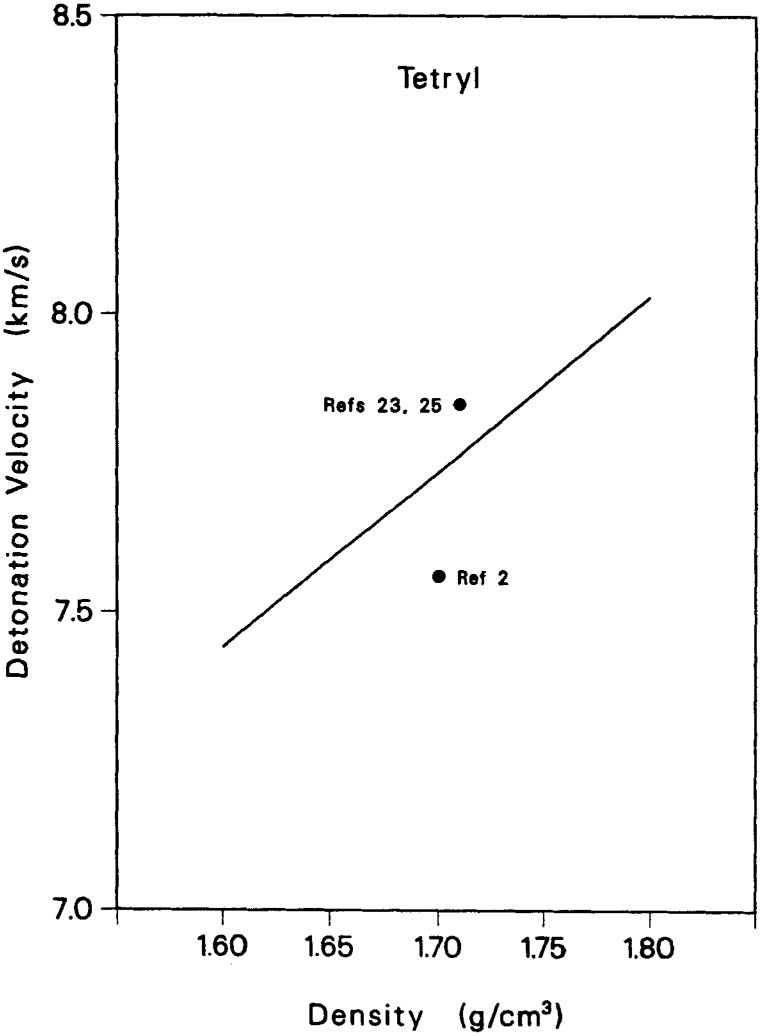

Figure 4. Experimental detonation velocities for Tetryl taken from the literature.

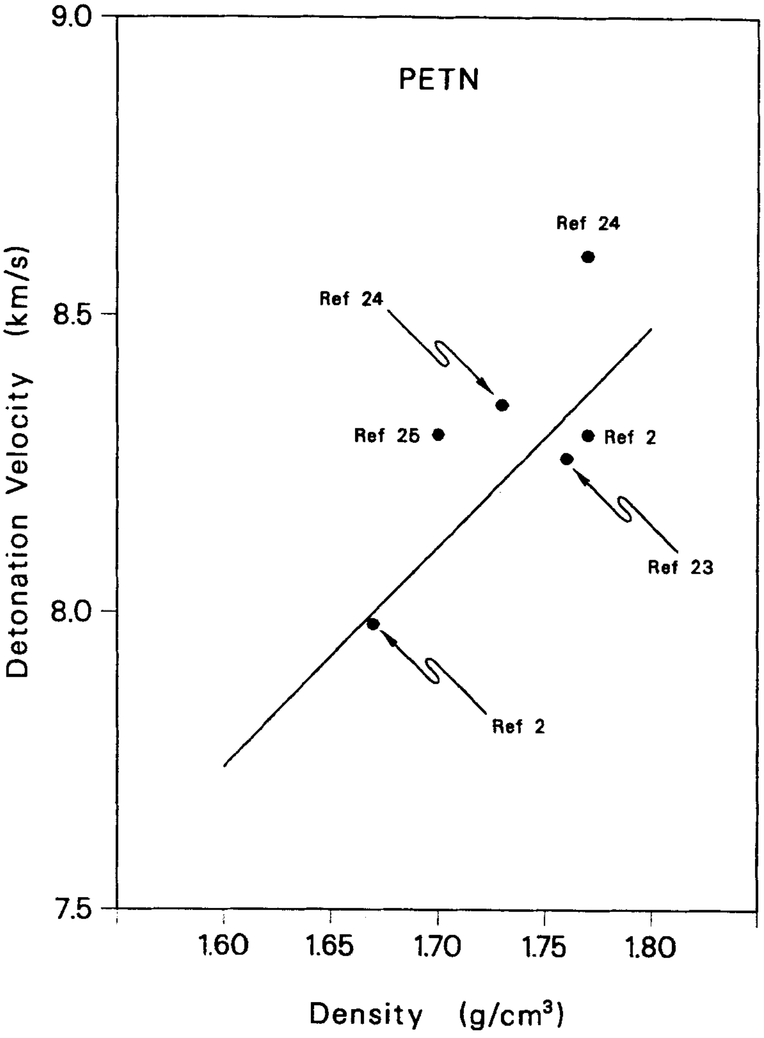

Figure 5. Experimental detonation velocities of PETN taken from the literature.

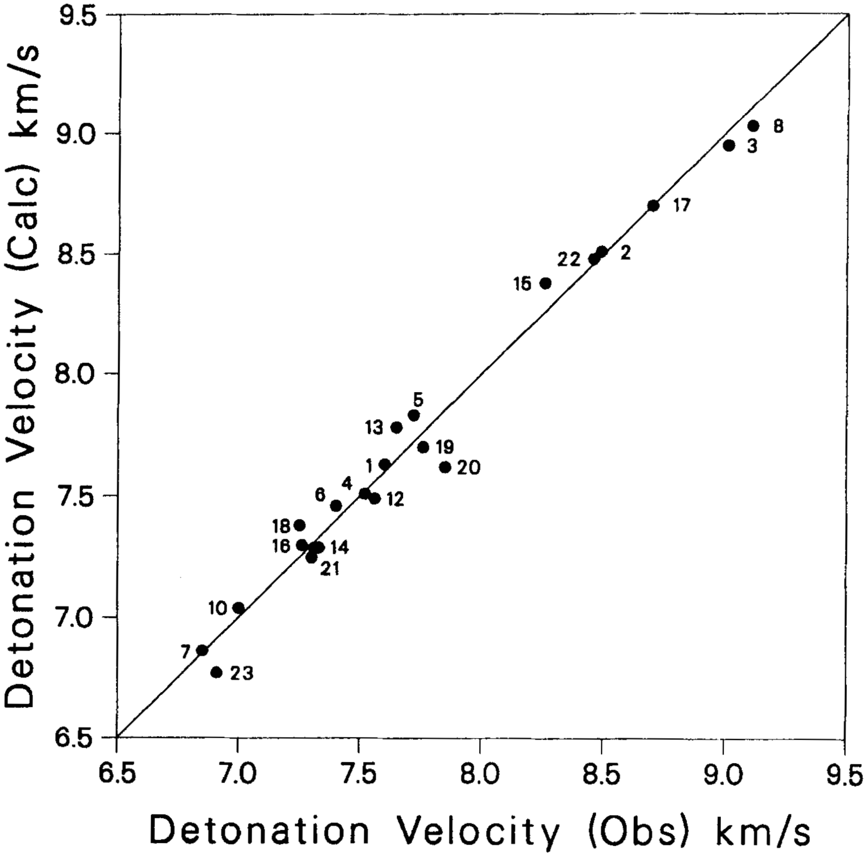

Figure 6. Comparison of the experimental and calculated detonation velocities for the explosives listed in Table I. The calculated values were obtained using Eq. 12.