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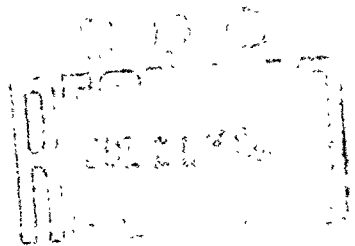
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COMPUTATION OF DETONATION PROPERTIES
OF FLUOROEXPLOSIVES (U)

10 JUNE 1966

NOL

UNITED STATES NAVAL ORDNANCE LABORATORY, WHITE OAK, MARYLAND



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COMPUTATION OF DETONATION PROPERTIES
OF FLUROEXPLOSIVES (U)

By
Harold Hurwitz

ABSTRACT: The RUBY code has been used to compute detonation properties for a number of fluorinated explosives. Results are given for fluorinated TNB, RDX, tetryl, TNT, DATB, and trinitrobenzotrifluoride, and for fluorodinitropropane and fluorodinitromethane. When necessary densities and heats of formation of the explosives were estimated for input to RUBY. In general, the calculated detonation properties of the fluorinated explosives, compared with the properties of the non-fluorinated parent compounds, showed increased detonation velocity, increased detonation pressure, and decreased detonation energy. It should be noted that if lower densities had been assumed, the computed detonation pressures and velocities would have been lower. For example, the computed detonation velocity for 2,2,4,6-tetrafluoro-RDX at the initial density $\rho_0 = 2.17$ gm/cc is 9.25 mm/ μ sec (compared with 8.80 for RDX at TMD), and the computed detonation pressure is 0.409 megabars (compared with 0.344 for RDX). At $\rho_0 = 2.05$ gm/cc, the values computed for the same compound are 8.65 mm/ μ sec and 0.352 megabars. Computed detonation velocities of the fluorinated TNB's at measured densities show an average deviation of 2.1% from literature values.

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10 June 1966

COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U)

The work described in this report was carried out under Eglin Air Force Base MIPR PG-3-19, dated September 1963. The purpose of the work was to calculate the detonation properties of a number of fluoroexplosives. This makes possible a preliminary evaluation of the compounds, thus serving as a guide for possible experimental effort.

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COMPUTATION OF DETONATION PROPERTIES OF FLUOROEXPLOSIVES (U)

INTRODUCTION

1. The research described in this report was conducted by the Naval Ordnance Laboratory for the Air Force under Eglin Air Force Base MIPR PG-3-19, dated September 1963. Under this contract NOL was to calculate the detonation properties of a number of fluorinated explosive compounds. Previously, the Denver Research Institute on an Air Force contract had shown by chemical synthesis and subsequent measurements that the replacement of hydrogen atoms by fluorine atoms in explosive materials could lead to improvements in desirable properties (Ref. 1).^{*} The need for actual synthesis and measurement, however, could be kept to a minimum by the use of available computational methods that predict the properties of hypothetical compounds.

2. Detonation characteristics of explosive compositions can be estimated using the RUBY code, a digital computer program developed at the Lawrence Radiation Laboratories (Ref. 2) and now in use at NOL (Refs. 3,4). An important feature of RUBY is the use of the Kistiakowsky-Wilson equation of state (which may be written as in Equation (1)) to represent the behavior of the explosion product gases.

$$\begin{aligned} PV/RT &= 1 + x \exp(\beta x) \\ x &= k/V(T + \theta)^\alpha \\ k &= \sum_i f_i x_i k_i \end{aligned} \quad (1)$$

In Equation (1), V is the molar gas volume, P is the pressure, T is the absolute temperature, and x_i is the mole fraction of component i . The quantities α , β , f , θ , and k_i are constants, the k_i being covolumes. The use of this equation of state for representing gaseous explosion products has been discussed by Mader (Ref. 5).

3. Certain properties of the explosive material (HE) and the product species are required as input to RUBY. For the HE these are chemical composition, density, and heat of formation. The input quantities required for the gaseous product species are chemical composition, thermodynamic properties, and covolumes (k_i). The only condensed product considered in the present work is solid graphite, and the information on graphite required as input to RUBY includes thermodynamic properties, molar volume, and constants for an appropriate equation of state (note that Equation (1) applies only to gases). The equation of state used for this purpose is

$$\begin{aligned} P &= -2.4673 + 6.7692Y - 6.9555Y^2 + 3.0405Y^3 - 0.3869Y^4 \\ &\quad + (-1.9534 + 2.3368Y) \times 10^{-5}T \\ &\quad + (6.1742 - 5.794/Y + 2.277/Y^2) \times 10^{-10}T^2 \\ Y &= \frac{V_0}{V} \end{aligned}$$

^{*}References may be found
on page 8.

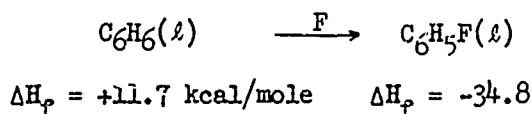
where P is in megabars, and T in degrees Kelvin, as given in Refs. 2 and 6.

4. In this report, lengthy chemical names have been abbreviated to short symbols for convenience. These short names are defined in Table 1, which also includes definitions of conventional HE names (RDX, DATB, etc.). The explosives investigated were mono-, di-, and trifluorinated TNB; mono-, di-, and tetrafluorinated RDX; mono- and difluorinated tetryl; mono- and difluorinated TWT; fluorinated DATB; trinitrobenzotrifluoride, and its mono- and difluoro derivatives; and fluorodinitropropane, fluorodinitromethane, and mixtures of the two. In general, the calculated detonation properties, compared with the properties of the non-fluorinated parent explosive compounds, show increased detonation velocity and detonation pressure, and decreased detonation energy.

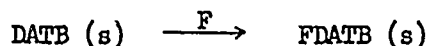
SOURCES OF INPUT DATA

5. The thermodynamic properties--enthalpy of formation, Gibbs free energy of formation, and constants giving the constant-pressure heat capacity as a function of temperature--required for the product species, were obtained from the JANAF Thermochemical Tables (Ref. 7). Covolumes used for the gaseous products were those given in Ref. 8, with the revisions for H₂O and CO₂ suggested in Ref. 5.

6. The heats of formation (ΔH_f) required for hypothetical explosive compositions had to be estimated. There are a number of useful methods (e.g. Refs. 9 and 10) for estimating heats of formation by summing the contributions of various structural features over the entire molecule. However, since the compounds treated in the present work are simple derivatives of known chemical species, the estimation of their heats of formation was approached by taking as a starting point molecules whose heats of formation were already known. The method may be illustrated by taking monofluorodiaminotrinitrobenzene (FDATB) as an example:



$$\Delta H = -34.8 - 11.7 = -46.5$$



$$\Delta H_f = -29.2 \quad \Delta H_f = ?$$

$$\Delta H_f(\text{FDATB}) = -29.2 + (-46.5) = -75.7 \text{ kcal/mole}$$

The difference in heat of formation between benzene and monofluorobenzene is -46.5 kcal/mole. When this is added to the heat of formation of DATB (-29.2 kcal/mole) the result is -75.7 kcal/mole, the estimated heat of formation of FDATB. In this procedure, the ΔH_f difference due to

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fluorination of a liquid to form a liquid is assumed to be approximately equal to the ΔH_f difference due to fluorination of a solid to form another solid. Appendix A shows the computation of the ΔH_f estimates for the various compounds treated in this report. The resulting estimated ΔH_f values are listed in Table 2.

7. In making the detonation calculations for the hypothetical compositions it is also necessary to estimate densities. Pavlath and Leffler (Ref. 11) suggest that densities be estimated by examining the molar volumes of similar compounds rather than from densities of similar compounds directly. Although these authors stress that their method is strictly applicable only to liquids, in the present work it was considered to give an adequate approximation for solids when no other information was available. It should be noted that the computed detonation properties are strongly influenced by these density estimates. Consideration of other factors which sometimes affect the densities of solids (such as charge distribution and symmetry) might have led to lower densities and lower detonation velocities and pressures.

8. Table 3 gives the densities used for the RUBY calculations. In the case of the fluorinated trinitrobenzenes, only one density for each compound is given in the table although RUBY computations were also carried out for other densities for comparison with results reported by other investigators. Two separate densities are listed as estimated for each fluorinated RDX, and computations were carried out for each value. This was done because the volume increment derived by Pavlath and Leffler for aromatic compounds could not be applied with confidence to the aliphatic RDX's. For the TNBTF's the method of applying the theory to the side-chain fluorine atoms was uncertain, and the estimates are consequently given to only two significant figures.

9. The values of the equation-of-state parameters α , β , κ , and θ are those given by Mader in Ref. 5. The values of k_i were those given in Ref. 8 with the changes suggested in Ref. 5. The quantities α and β are dimensionless, the k_i have the dimensions of volume, θ has the dimensions of temperature, and κ has the dimensions of temperature raised to the α power. For β and κ , Mader recommended two sets of values. One set (called here RDX-type) is fitted to the properties of RDX, but then adjusted so that $(\partial P/\partial T)_V$ will always be positive. The other set (called here TNT-type) is fitted to the properties of TNT and recommended for dense explosives whose products contain relatively large amounts of solid graphite. The values of α , β , κ , and θ are as follows:

$$\alpha = 0.50$$

$$\theta = 400^\circ\text{K}$$

Parameter Type	β	κ ($^\circ\text{K}^\alpha$)
TNT	0.0958,	12.685
RDX	0.16	10.91

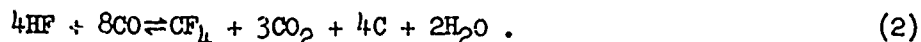
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The values of the k_1 are given in Table 4. It should be noted that consistency with the use of cubic centimeters as the units for other volume quantities in the computation requires that the units of the k_1 be considered as cubic centimeters. However, as is usual in RUBY-type computations, the numerical values of Mader's k_1 , which are computed in terms of cubic angstroms per molecule, have been used here without application of the appropriate factor (0.602) to convert to cubic centimeters per mole. This is equivalent to multiplying each k_1 by 1.66, which is the reciprocal of the conversion factor.

RESULTS OF COMPUTATIONS

10. Because of the uncertainty in some of the heat of formation estimates, it was of interest to observe the effect of changes in the heat of formation of the explosive composition on RUBY results. For this purpose, and also to compare the effects of the two sets of values of β and λ , computations were carried out for MFINT assuming the ΔH_f to be -50, -75, and -100 kcal/mole and using both sets of the equation of state parameters. The results are shown in Table 5, and in Figures 1, 2, and 3. In Tables 5-11, P, T, ρ , E, and S are pressure, temperature, density, energy, and entropy, respectively. The subscript J indicates the detonation products in the Chapman-Jouquet state, and the subscript o indicates the unreacted explosive at 298°K and 1 atm. pressure. ΔE_{chem} is the detonation energy, defined as the energy increase while going from the unreacted explosive at 298°K and 1 atm. pressure, to the Chapman-Jouquet gas mixture reduced to 298°K and 1 atm. pressure.

11. Decreasing the ΔH_f of the MFINT from -50 to -100 kcal/mole, using the TNT-type parameters, caused a 3.0% decrease in the computed detonation velocity, an 8.1% decrease in the Chapman-Jouquet (CJ) pressure, and a 451°K (or 16.0%) drop in the CJ temperature. The energy change for the chemical reaction (ΔE_{chem}) increased by 200 cal/gm or 49.0 kcal/mole, a value which suggests an immediate derivation from the decrease in ΔH_f of the explosive. The change in composition of the product mixture can be considered to result from a shift to the right of the equilibrium reaction



Such a shift would be expected to be associated with the decrease in temperature, although it would be opposed by the decrease in pressure.

12. When the computations using the two sets of equation-of-state parameters are compared (both for $\Delta H_f = -50$ kcal/mole), it is seen that with the RDX-type parameters the detonation velocity is 5.2% higher, the CJ pressure is 5.2% higher, and the CJ temperature is 6.2% lower. The difference in ΔE_{chem} is negligible (0.16%). The difference in chemical composition of the product mixture can again be described as a righthand shift in Equation 2 (for a change from TNT-type parameters to RDX-type parameters), with the increase in pressure and decrease in temperature now acting in the same direction.

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13. RUBY computations were carried out for a series of fluorinated RDX's. The results are given in Table 6 for 0,1,2, and 4 fluorine atoms per molecule. The program would not converge for the trifluoro-RDX's. The detonation velocities, CJ pressures, and chemical energies are plotted in Figures 4, 5, and 6, respectively, the points for the difluoro and tetrafluoro compounds being plotted for the more probable higher densities (see paragraph 8).

14. It can be seen from the graphs that as the number of fluorine atoms per molecule increases, the detonation velocity increases, the CJ pressure increases, and the detonation energy ($-\Delta E_{\text{chem}}$) decreases. Although the ΔE_{chem} (Figure 6) seems to be strictly monotonic, the D and P_J curves (Figures 4 and 5) have humps at the two-fluorine-atom position. However, the estimated density of the difluoro-RDX is likely a few tenths of a percent too high, and a correction of this magnitude would smooth out the D and P_J curves. For the disubstituted and tetrasubstituted compounds, the differences between isomers are presented to RUBY simply as differences in heat of formation. Accordingly, the consequent differences in computed results are analogous to those discussed in paragraph 11.

15. Computed detonation parameters for fluorinated TNB, tetryl, TNT, TNBTF, and DATB are given in Tables 7-10, along with values computed for the unfluorinated materials for comparison. (See Figures 7-9 for plots of TNB results.) Since it was not clear which set of equation-of-state parameters was applicable in each case, computations were carried out using both sets, and both are listed in the tables.

16. Table 11 gives the results of computations suggested by Dr. J. M. Rosen of this Laboratory, for FDNP, FTNM, and mixtures of the two. As predicted by Rosen (Ref. 12) the maximum detonation energy is computed for a mixture containing approximately 50.3% FDNP, which is balanced for complete reaction to H_2O , CO_2 , CF_2 , and N_2 . The P_J maximum is at about the same composition, while the mixture with maximum detonation velocity seems to contain a little more FDNP.

COMPARISON WITH OTHER VALUES

17. Experimentally determined detonation velocities for several of the compounds treated here have been reported by other workers (Refs. 1, 13, 14). These values are given in Table 12, along with values computed by Amcel using RUBY (Ref. 14), and NOL RUBY results. The same information is presented graphically for DFTNB, MFTNB, and TNBTF in Figures 10, 11, and 12.

18. For MFTNB, DFTNB, and TFTNB, computations were carried out at the same loading densities (ρ_0) at which experimental detonation velocities had been reported by Schmidt-Collerus et al of the Denver Research Institute (Ref. 1). The RDX parameters were used for this comparison because, as seen in the Table, they seemed to give results that were closer to the experimental values.

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19. For MFTNB at $\rho_0 = 1.512, 1.615, \text{ and } 1.802 \text{ gm/cc}$, the deviations of the NOL computed values^o from the DRI experimental values are +0.14%, -1.6%, and +0.17%. Deviation from the Picatinny value (Ref. 13) at $\rho_0 = 1.80$ is +4.8%. If the value computed at NOL for $\rho_0 = 1.8383$ (RDX parameters) is compared with the experimental value reported by Amcel for $\rho_0 = 1.83$, the deviation is +0.026%.

20. For DFTNB the deviations from the DRI experimental values are not quite as good. For $\rho_0 = 1.695, 1.768, \text{ and } 1.841$, the deviations are -3.7%, -3.5%, and -3.0%, respectively. The deviation from the Picatinny value at $\rho_0 = 1.84$ is -0.94%. The deviation of the NOL computed value at $\rho_0 = 1.8564$ (RDX parameters) from the Amcel experimental value at $\rho_0 = 1.855$ is -2.1%. It should be noted that the NOL-estimated heat of formation of DFTNB is 100% greater than that found by Amcel. If the Amcel value is correct, this would account for the relatively large deviations for this compound, recalling that for MFTNT a similar difference in the heat of formation used for input produced a 2.1% decrease in the computed value of D (using RDX parameters).

21. For TFTNB at $\rho_0 = 1.964$, the deviation from the DRI experimental value is +1.3%. Literature values for TNBTF, MFTNBTF, and DFTNBTF are listed in the Table, but NOL computations were not carried out at densities appropriate for comparison.

22. In the Amcel computations (results listed in Table 12) the older values of the equation of state parameters were used, and the carbon formed in the reaction was assumed incompressible. The resulting computed detonation properties may be useful for intercomparison of certain compounds, whether or not they are considered valid predictions of absolute values. Since the Amcel and NOL RUBY computations are based on different assumptions, the results necessarily disagree.

CONCLUSIONS

23. According to the computed results presented in this report, fluorination of C-H-N-O explosives promises improved performance in applications where relatively high detonation velocities and pressures are desirable but high energy is not required. (This is not consistent with the high energy outputs referred to in Ref. 1.) The RUBY computations for progressively fluorinated RDX, TWT, and DATB all show an increase in detonation velocity and Chapman-Jouguet pressure as the number of F atoms in the molecule is increased, with an accompanying decrease in the detonation energy (assuming each compound is at crystal density). For tetryl and TNBTF, the computations show an increase in P_j and D when RDX-type parameters are used, although when TNT-type parameters are used the computed values of these properties decrease on addition of the first F atom, with subsequent increase on additional fluorination. This suggests that the RDX-type parameters give the more valid results for these two series of compounds. The computations for the fluorinated TNB's show an irregular effect on P_j and D of progressive fluorination, but this may actually result from the difficulty of estimating heats of formation and densities. The computed $-\Delta E_{\text{chem}}$ for the fluorinated TNB's shows the usual steady decrease.

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24. The contract under which the present work was carried out (see paragraph 1) suggests that the most promising materials might be those with a stoichiometric balance to HF. If the results for the fluorinated RDX's (Figures 4-6) are examined from this standpoint, an apparent change in slope can be observed near the HF balance point (3 fluorine atoms in the molecule). This feature of the RDX curves, however, can be explained with equal validity as being related to the HF balance or as resulting from errors in the estimates of densities and heats of formation. The ranges of fluorination of the other series of compounds treated did not include the HF balance point.

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TABLE 1. DEFINITION OF NAMES USED FOR CHEMICAL COMPOUNDS

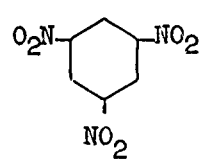
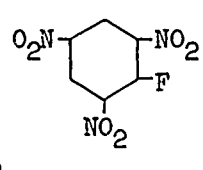
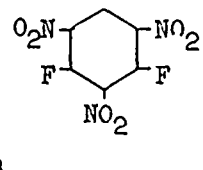
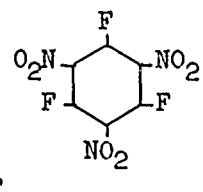
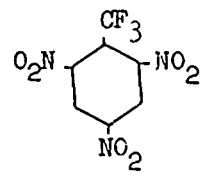
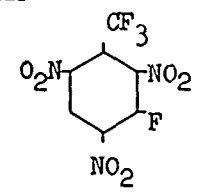
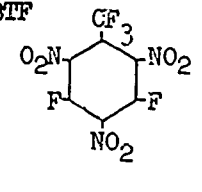
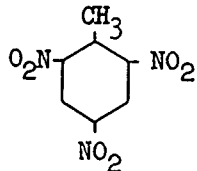
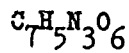
TNB		<p>Trinitrobenzene $C_6H_3N_3O_6$ MW = 213.11</p>
MFTNB		<p>Monofluorotrinitrobenzene $C_6H_2N_3O_6F$ MW = 231.10</p>
DFTNB		<p>Difluorotrinitrobenzene $C_6H_1N_3O_6F_2$ MW = 249.09</p>
TFTNB		<p>Trifluorotrinitrobenzene $C_6N_3O_6F_3$ MW = 267.08</p>
TNBTF		<p>Trinitrobenzotrifluoride $C_7H_2N_3O_6F_3$ MW = 281.11</p>
MFTNBTF		<p>Monofluorotrinitrobenzotrifluoride $C_7HN_3O_6F_4$ MW = 299.10</p>
DFTNBTF		<p>Difluorotrinitrobenzotrifluoride $C_7N_3O_6F_5$ MW = 317.09</p>

TABLE 1 Contd

TNT

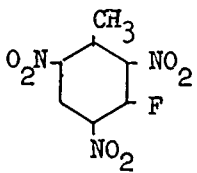


Trinitrotoluene

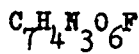


MW = 227.13

MFINT

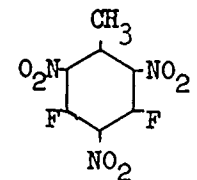


Monofluorotrinitrotoluene

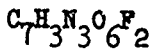


MW = 245.12

DFINT

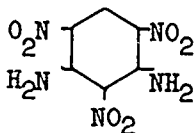


Difluorotrinitrotoluene

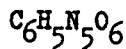


MW = 263.12

DATB

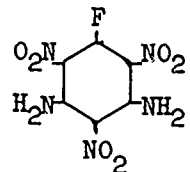


Diaminotrinitrobenzene

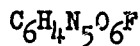


MW = 243.14

FDATB

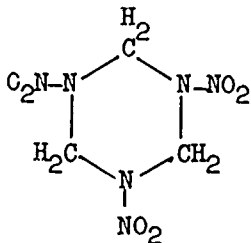


Fluorodiaminotrinitrobenzene

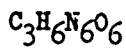


MW = 261.13

RDX



1,3,5-Trinitrohexahydro-s-triazine
(or Cyclotrimethylenetrinitramine)



MW = 222.12

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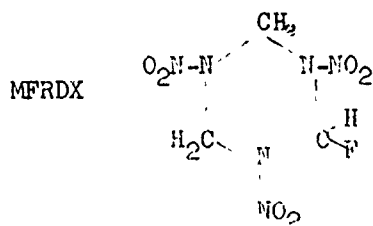
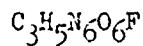


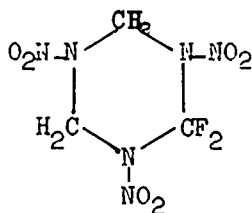
Table 1 Contd

2-Fluoro-1,3,5-trinitrohexahydro-s-triazine

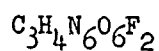


MW = 240.11

22DFRDX

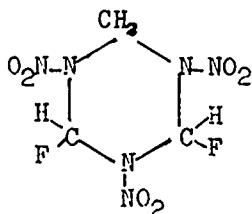


2,2-Difluoro-1,3,5-trinitrohexahydro-s-triazine

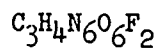


MW = 258.10

24DFRDX

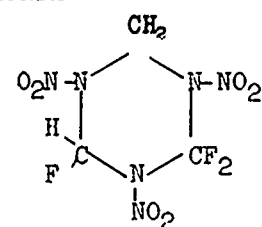


2,4-Difluoro-1,3,5-trinitrohexahydro-s-triazine

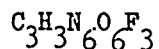


MW = 258.10

224TFRDX

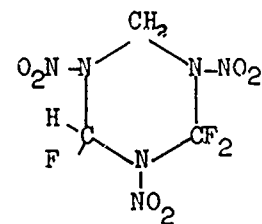


2,2,4-Trifluoro-1,3,5-trinitrohexahydro-s-triazine

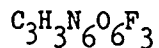


MW = 276.09

246TFRDX

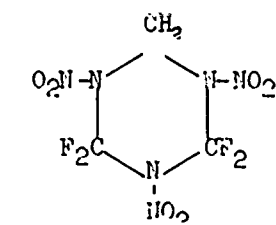


2,4,6-Trifluoro-1,3,5-trinitrohexahydro-s-triazine

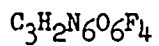


MW = 276.09

2244TFRDX



2,2,4,4-Tetrafluoro-1,3,5-trinitrohexahydro-s-triazine

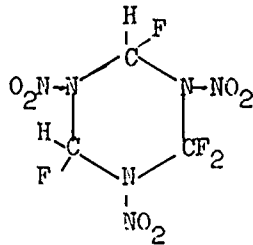


MW = 294.08

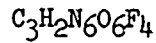
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Table 1 Contd

2246TTFRDX

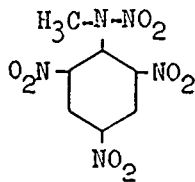


2,2,4,6-Tetrafluoro-1,3,5-trinitrohexahydro-
s-triazine

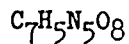


MW = 294.08

Tetryl



Trinitrophenylmethylnitramine

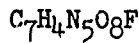


MW = 287.15

MFT

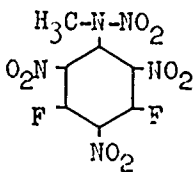


Monofluorotrinitrophenylmethylnitramine

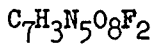


MW = 305.14

DFT

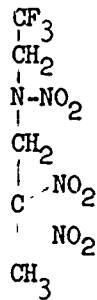


Difluorotrinitrophenylmethylnitramine

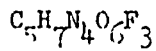


MW = 323.13

TFNA



1,1,1-Trifluoro-3,5,5-trinitro-3-azahexane



MW = 276.13

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Table 1 Contd

TFENA	$\begin{array}{c} \text{H-N-NO}_2 \\ \\ \text{C}_2\text{H}_2\text{F}_3 \end{array}$	Trifluoroethyl nitramine $\text{C}_2\text{H}_3\text{N}_2\text{O}_2\text{F}_3$ MW = 144.05
FDNP	$\begin{array}{c} \text{F} \\ \\ \text{O}_2\text{N-C-NO}_2 \\ \\ \text{CH}_2 \\ \\ \text{CH}_3 \end{array}$	Fluorodinitropropane $\text{C}_3\text{H}_5\text{N}_2\text{O}_4\text{F}$ MW = 152.05
FTNM	$\begin{array}{c} \text{F} \\ \\ \text{O}_2\text{N-C-NO}_2 \\ \\ \text{NO}_2 \end{array}$	Fluorotrinitromethane $\text{CN}_3\text{O}_6\text{F}$ MW = 169.03

TABLE 2. ESTIMATED HEATS OF FORMATION

HE	ΔH_f (Kcal/mole)	HE	ΔH_f (Kcal/mole)
MFINB	-58	MFRDX	-26
DFINB	-103	22DFRDX	-76
TFINB	-148	24DFRDX	-66
TNBTB	-171	224TFRDX	-116
MFINBTB	-216	246TFRDX	-106
DFINBTB	-262	2244TTFRDX	-166
MFINBT	-64	2246TTFRDX	-156
DFINBT	-109	MFT	-42
FDAITB	-76	DFT	-87

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TABLE 3. DENSITIES OF EXPLOSIVE MATERIALS USED FOR RUBY CALCULATIONS

HE	ρ (gm/cc)	Reference
MFNB	1.8383	1
DFNB	1.8564	1
TFNB	1.9477	1
TNBF	1.9	Estimated
MFNBIF	2.0	Estimated
DFNBIF	2.1	Estimated
MFNT	1.79	Estimated
DFNT	1.88	Estimated
FDATE	1.97	Estimated
MFRDX	1.90,1.87	Estimated
22DFRDX	2.00,1.94	Estimated
24DFRDX	2.00,1.94	Estimated
224TFRDX	2.09,2.00	Estimated
246TFRDX	2.09,2.00	Estimated
2244TTFRDX	2.17,2.05	Estimated
2246TTFRDX	2.17,2.05	Estimated
MFT	1.84	Estimated
DFT	1.92	Estimated
TFNA	1.692	5
TFENA	1.523	5
FDNP	1.35	12
FTNM	1.586	12

TABLE 4 COVOLUMES (k_1) USED IN THE RUBY COMPUTATIONS

Species	k_1 (cc/mole)	Species	k_1 (cc/mole)	Species	k_1 (cc/mole)
CF ₂	1330	CO ₂	600	N ₂	380
CF ₃	1330	COF ₂	1300	N ₂ O	600
CF ₄	1330	F	108	NH ₃	476
CH ₂ F ₂	1330	F ₂	387	NO	386
CH ₃ F	1920	H	76	NO ₂	600
CH ₄	528	H ₂	180	O	120
CHF ₃	1920	H ₂ O	250	O ₂	350
CO	390	HF	389	OH	413

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TABLE 5. COMPUTED DETONATION PROPERTIES FOR MFTNT, USING
DIFFERENT ΔH_f 's AND EQUATION-OF-STATE PARAMETERS

Property	Units	TNT	TNT	TNT	RDX	RDX	RDX
(Parameter Type)							
ΔH_f	kcal/mole	-50	-75	-100	-50	-75	-100
ρ_o	gms/cc	1.80	1.80	1.80	1.80	1.80	1.80
D	mm/ μ sec	7.292	7.186	7.079	7.668	7.588	7.510
P_J	megb	0.2465	0.2366	0.2266	0.2592	0.2500	0.2410
T_J	$^{\circ}$ K	2818.	2593.	2367.	2643.	2413.	2182.
ρ_J	gms/cc	2.425	2.414	2.404	2.384	2.372	2.360
γ		2.882	2.930	2.981	3.083	3.146	3.212
$E_J - E_o$	cal/gm HE	421.7	399.7	377.8	421.5	400.4	379.9
ΔE_{chem}	cal/gm HE	-1265.	-1166.	-1065.	-1267.	-1167.	-1066.
$S_J - S_o$	cal/ $^{\circ}$ K/gm/HE	0.05853	0.01639	-0.02947	0.06576	0.02199	-0.02596
Compo- sition of Product Mixture	CF_2	10^{-3} moles/ gm HE	*	*	*	*	*
	CF_3		*	*	*	*	*
	CF_4		0.9379	0.9544	0.9698	0.9651	0.9805
	CH_2F_2		*	*	*	*	*
	CH_3F		*	*	*	*	*
	CH_4		*	*	*	*	*
	CHF_3		*	*	*	*	*
	CO		0.3960	0.2422	0.1340	0.2488	0.1434
	CO_2		8.045	8.105	8.143	8.090	8.132
	COF_2		*	*	*	*	*
	F		*	*	*	*	*
	F_2		*	*	*	*	*
	H		*	*	*	*	*
	H_2		*	*	*	*	*
	H_2O		7.991	8.025	8.057	8.049	8.080
	HF		0.3272	0.2616	0.2004	0.2186	0.1574
	N_2		6.118	6.118	6.119	6.119	6.119
	N_2O		*	*	*	*	*
	NH_3		*	*	*	*	*
	NO		*	*	*	*	*
	NO_2		*	*	*	*	*
	O		*	*	*	*	*
	O_2		*	*	*	*	*
	OH		*	*	*	*	*
	C(graphite)		19.18	19.26	19.31	19.25	19.31
Σ moles gas	10^{-3} moles/ gm HE	23.82	23.71	23.62	23.69	23.60	23.54
V_g	cc/mole	14.18	14.29	14.39	14.58	14.70	14.81
V_s	cc/mole	3.892	3.913	3.936	3.847	3.864	3.881
*Mole fraction in gas mixture less than 10^{-4} .							

TABLE 6. COMPUTED DETONATION PROPERTIES FOR FLUORINATED RDX's
(Using RDX-Type Parameters)

Property	Units	RDX	MFRDX	22DFRDX	22DFRDX	24DFRDX	24DFRDX	224TFRDX	224TFRDX	224GTRDX	224GTRDX
ΔH_c	kcal/mole	+14.71	-26	-76	-66	-66	-66	-166	-166	-156	-156
ρ_0	gms/cc	1.802	2.00	1.94	2.00	1.94	2.00	2.17	2.05	2.17	2.05
D	m/sec	8.804	8.940	8.820	9.107	8.840	9.107	9.252	8.642	9.254	8.652
P _J	m ² /g	0.3442	0.3676	0.3886	0.3921	0.3641	0.3921	0.4056	0.3487	0.4089	0.3518
T _J	°K	2568.	2335.	2247.	2095.	2240.	2095.	1241.	1493.	1311.	1572.
ρ_J	gms/cc	2.391	2.507	2.615	2.619	2.553	2.619	2.776	2.655	2.782	2.660
γ		3.078	3.131	3.254	3.231	3.163	3.231	3.579	3.391	3.544	3.362
E_J-E_0	cal/gm HE	562.4	559.6	545.9	530.6	538.7	538.7	487.8	463.0	495.6	470.1
ΔF_{chem}	cal/gm HE	-1500.	-1424.	-1322.	-1360.	-1360.	-1360.	-1018.	-1020.	-1052.	-1054.
S_J-S_0	cal 'K gm HE	-0.2076	-0.2383	-0.2907	-0.2741	-0.2400	-0.2741	-0.4667	-0.3760	-0.4398	-0.3531
Compo- sition of Product Mixture	10^{-3} mole/gm HE	-	-	-	-	-	-	-	-	-	-
CF ₂		-	-	-	-	-	-	-	-	-	-
CF ₃		-	-	-	-	-	-	-	-	-	-
CF ₄		-	1.036	1.937	1.936	1.935	1.935	3.400	3.400	3.400	3.400
CH ₂ F ₂		-	-	-	-	-	-	-	-	-	-
CH ₃ F		-	-	-	-	-	-	-	-	-	-
CH ₄		-	*	*	*	*	*	*	*	*	*
CHF ₃		-	-	-	-	-	-	-	-	-	-
CO		0.1171	0.03237	0.004000	0.01190	0.006352	0.01771	*	*	*	*
CO ₂		6.694	7.277	7.748	7.747	7.743	7.743	6.801	6.801	6.801	6.801
COF ₂		-	-	-	-	-	-	-	-	-	-
F		-	*	*	*	*	*	*	*	*	*
F ₂		-	*	*	*	*	*	*	*	*	*
H		-	*	*	*	*	*	*	*	*	*
H ₂		-	*	*	*	*	*	*	*	*	*
H ₂ O		15.51	10.40	7.748	7.745	7.747	7.743	3.400	3.400	3.400	3.400
HF		-	0.01895	*	0.003405	0.01088	*	*	*	*	*
N ₂		13.51	12.49	11.62	11.62	11.62	11.62	9.596	9.731	9.592	9.726
N ₂ O		-	*	*	*	*	*	0.04965	0.04899	0.05910	0.05687
NH ₃		-	*	*	*	*	*	*	*	*	*
NO		-	*	*	*	*	*	*	*	*	*
NO ₂		-	*	*	*	*	*	*	*	*	*
O		-	-	-	-	-	-	-	-	-	-
O ₂		-	*	*	*	*	*	0.5636	0.8343	0.5697	0.8373
OH		-	-	-	-	-	-	-	-	-	-
C(graphite)		6.694	4.149	1.935	1.934	1.928	1.928	0.0	0.0	0.0	0.0
Σ moles gas	10^{-3} moles/gm HE	33.82	31.26	29.06	29.06	29.07	29.07	24.92	25.06	24.92	25.06
V _g	cc/mole	11.65	12.29	12.92	12.90	13.23	13.23	14.45	15.03	14.42	15.00
V _g	cc/mole	3.635	3.579	3.529	3.526	3.583	3.583	3.477	3.589	3.473	3.586

*Mole fraction in gas mixture less than 10^{-4}

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TABLE 7. COMPUTED DETONATION PROPERTIES FOR FLUORINATED TNB'S

Property	Units	TNB	MFNB	DFNB	TFNB	1,1-FNB	DFNB	TFNB	
(Parameter Type)		RDX	RDX	RDX	RDX	TNT	TNT	TNT	
ΔH_f	kcal/mole	-11.40	-58.	-103.	-148.	-58.	-103.	-148.	
ρ_o	gms/cc	1.688	1.8383	1.8564	1.9477	1.8383	1.8564	1.9477	
D	mm/usec	7.371	7.657	7.459	7.541	7.242	7.009	6.982	
P_J	megb	0.2299	0.2647	0.2525	0.2640	0.2500	0.2365	0.2418	
T_J	°K	2990.	2703.	2625.	2423.	2914.	2862	2723.	
ρ_J	gms/cc	2.253	2.437	2.457	2.557	2.482	2.506	2.613	
γ		2.989	3.071	3.090	3.196	2.856	2.856	2.926	
$E_J - E_o$	cal/gm HE	408.1	422.7	397.5	385.9	421.5	394.9	377.8	
ΔE_{chem}	cal/gm HE	-1340.	-1261.	-1188.	-1125.	-1257.	-1184.	-1122.	
$S_J - S_o$	cal/°K/gm HE	0.1464	0.07526	0.05387	0.00423	0.06991	0.05091	0.00652	
Composition of Product Mixture	CF ₂	10 ⁻³ mole/gm HE	-	*	*	*	*	*	
	CF ₃		-	*	*	*	*	*	
	CF ₄		-	1.050	1.987	2.808	1.030	1.970	2.808
	CH ₂ F ₂		-	*	*	-	*	*	
	CH ₃ F		-	*	*	-	*	*	
	CH ₄		*	*	*	-	*	*	
	CHF ₃		-	*	*	-	*	*	
	CO		1.005	0.2629	0.1865	0.06090	0.4609	0.3702	0.1847
	CO ₂		10.06	10.72	10.97	11.20	10.64	10.89	11.14
	COF ₂		-	*	*	*	*	*	
	F		-	*	*	*	*	*	
	F ₂		-	*	*	*	*	*	
	H		-	*	*	-	*	*	
	H ₂		-	*	*	-	*	*	
	H ₂ O		7.036	4.264	1.966	-	4.221	1.932	-
	HF		-	0.1257	0.08100	-	0.2069	0.1476	-
	N ₂		7.038	6.490	6.022	5.616	6.490	6.021	5.616
	N ₂ O		-	*	*	*	*	*	
	NH ₃		*	*	*	-	*	*	
	NO		-	*	*	*	*	*	
NO ₂		-	*	*	*	*	*		
O		-	*	*	*	*	*		
O ₂		-	*	*	*	*	*		
OH		-	*	*	-	*	*		
C(graphite)		17.09	13.93	10.95	8.394	13.83	10.85	8.332	
\bar{V} moles gas	10 ⁻³ moles/gm HE	25.14	22.91	21.21	19.69	23.05	21.34	19.49	
V_G	cc/mole	14.97	15.58	17.19	18.23	15.15	16.70	17.73	
V_S	cc/mole	3.953	3.833	3.866	3.824	3.886	3.925	3.902	

*Mole fraction in gas mixture less than 10⁻⁴

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TABLE 8. COMPUTED DETONATION PROPERTIES FOR FLUORINATED TETRYLS

Property	Units	Tetryl	MFT	DFT	MFT	DFT	
(Parameter Type)		RDX	RDX	RDX	TNT	TNT	
ΔH_P	kcal/mole	+4.67	-42.	-87.	-42.	-87.	
ρ_0	gms/cc	1.73	1.84	1.92	1.84	1.92	
D	mm/ μ sec	7.817	8.031	8.129	7.596	7.599	
P_J	megb	0.2644	0.2927	0.3065	0.2765	0.2852	
T_J	$^{\circ}$ K	2971.	2734.	2543.	2964.	2831.	
ρ_J	gms/cc	2.307	2.442	2.532	2.488	2.585	
γ		2.999	3.055	3.139	2.839	2.887	
$E_{J-\infty}$	cal/gm HE	456.7	468.8	460.9	467.8	456.7	
ΔE_{chem}	cal/gm HE	-1422.	-1355.	-1295.	-1351.	-1292.	
$S_{J-\infty}$	cal/ $^{\circ}$ K/gm HE	+0.07156	+0.02059	-0.01841	+0.01466	-0.01905	
Composition of Product Mixture	CF ₂	10 ⁻³ moles/gm HE	-	*	*	*	*
	CF ₃		-	*	*	*	*
	CF ₄		-	0.7902	1.536	0.7684	1.520
	CH ₂ F ₂		-	*	*	*	*
	CH ₃ F		-	*	*	*	*
	CH ₄		*	*	*	*	*
	CHF ₃		-	*	*	*	*
	CO		0.7063	0.2461	0.09655	0.4537	0.2502
	CO ₂		9.225	9.738	10.02	9.657	9.961
	COF ₂		-	*	*	*	*
	F		-	*	*	*	*
	F ₂		-	*	*	*	*
	H		-	*	*	*	*
	H ₂		-	*	*	*	*
	H ₂ O		8.705	6.496	4.619	6.449	4.585
	HF		-	0.1157	0.04515	0.2028	0.1104
	N ₂		8.706	8.193	7.737	8.191	7.736
	N ₂ O		-	*	*	*	*
	NH ₃		*	*	*	*	*
	NO		-	*	*	*	*
NO ₂		-	*	*	*	*	
O		-	*	*	*	*	
O ₂		-	*	*	*	*	
OH		-	*	*	*	*	
C(graphite)		14.45	12.17	10.01	12.06	9.932	
Σ moles gas	10 ⁻³ moles/gm HE	27.34	25.58	24.06	25.73	24.16	
V_g	cc/mole	13.82	14.22	14.87	13.84	14.45	
V_s	cc/mole	3.846	3.760	3.718	3.811	3.783	

*Mole fraction in gas mixture less than 10⁻⁴

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TABLE 9. COMPUTED DETONATION PROPERTIES FOR FLUORINATED TNT'S AND DATB

Property	Units	TNT	MFNT	DFINB	MFINT	DFINT	DATB	FDATB	FDATB
(Parameter Type)		TNT	TNT	TNT	RDX	RDX	TNT	TNT	RDX
ΔH_f	kcal/mole	-17.81	-64.	-109.	-64.	-109.	-29.23	-76.	-76.
ρ_0	gms/cc	1.651	1.79	1.88	1.79	1.88	1.837	1.97	1.97
D	mm/ μ sec	7.000	7.204	7.208	7.586	7.695	7.661	7.823	8.498
P_J	megb	0.2071	0.2303	0.2466	0.2527	0.2644	0.2679	0.2953	0.3256
T_J	$^{\circ}$ K	2884.	2704.	2568.	2529.	2339.	2373.	2151.	1843.
ρ_J	gms/cc	2.219	2.408	2.515	2.367	2.466	2.444	2.609	2.555
γ		2.907	2.898	2.961	3.104	3.210	3.025	3.082	3.370
$E_J - E_0$	cal/gm HE	383.7	408.1	395.7	408.2	399.2	432.9	438.8	451.9
ΔE_{chem}	cal/gm HE	-1280.	-1209.	-1144.	-1211.	-1146.	-1165.	-1096.	-1096.
$S_J - S_0$	cal/ $^{\circ}$ K/gm HE	+0.09679	+0.03903	-0.00105	0.04574	0.000085	-0.1204	-0.1789	-0.1904
Compo- sition of Product Mixture	10^{-3} moles/gm HE								
CF ₂		-	*	*	*	*	-	*	*
CF ₃		-	*	*	*	*	-	*	*
CF ₄		-	0.9419	1.862	0.9694	1.883	-	0.9507	0.9564
CH ₂ F ₂		-	*	*	*	*	-	*	*
CH ₃ F		-	*	*	*	*	-	*	*
CH ₄		*	*	*	*	*	*	*	*
CHF ₃		-	*	*	*	*	-	*	*
CO		0.8523	0.3233	0.1582	0.1941	0.06625	0.1058	0.02596	0.003553
CO ₂		7.282	8.077	8.511	8.113	8.536	7.145	7.653	7.658
COF ₂		-	*	*	*	*	-	*	*
F		-	*	*	*	*	-	*	*
F ₂		-	*	*	*	*	-	*	*
H		-	*	*	*	*	-	*	*
H ₂		-	*	*	*	*	-	*	*
H ₂ O		11.00	7.999	5.623	8.057	5.666	10.28	7.645	7.657
HF		-	0.3116	0.1515	0.2018	0.06982	-	0.02670	0.004118
H ₂		6.602	6.118	5.700	6.119	5.701	10.28	9.574	9.574
N ₂ O		-	*	*	*	*	-	*	*
NH ₃		0.003797	*	*	*	*	*	*	*
NO		-	*	*	*	*	-	*	*
NO ₂		-	*	*	*	*	-	*	*
O		-	*	*	*	*	-	*	*
O ₂		-	*	*	*	*	-	*	*
OH		-	*	*	*	*	-	*	*
C(graphite)		22.68	19.21	16.07	19.28	16.12	17.43	14.35	14.36
V_g moles gas	10^{-3} moles/gm HE	25.74	23.77	22.01	23.66	21.92	27.81	25.88	25.85
V_g	cc/mole	13.96	14.31	15.23	14.71	15.69	12.32	12.74	13.11
V_s	cc/mole	4.028	3.913	3.881	3.866	3.819	3.811	3.731	3.64

*mole fraction in gas mixture less than 10^{-4}

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TABLE 10. COMPUTED DETONATION PROPERTIES FOR RING-FLUORINATED TNBTF'S

Property	Units	TNBTF	MFINBTF	DFINBTF	TNBTF	MFINBTF	DFINBTF
(Parameter Type)		RDX	RDX	RDX	TNT	TNT	TNT
ΔH_f	kcal/mole	-171.	-216.	-261.	-171.	-216.	-261.
ρ_0	gms/cc	1.9	2.0	2.1	1.9	2.0	2.1
D	mm/usec	7.506	7.696	7.911	6.956	7.010	7.070
P_J	megs	0.2507	0.2707	0.2931	0.2303	0.2425	0.2557
T_J	°K	2115.	1909.	1699.	2372.	2233.	2094.
ρ_J	gms/cc	2.481	2.593	2.703	2.535	2.655	2.776
γ		3.271	3.375	3.485	2.992	3.052	3.104
E_J-E_0	cal/gm HE	369.2	369.7	371.9	362.8	357.5	354.6
ΔE_{chem}	cal/gm HE	-1027.	-979.4	-936.8	-1026.	-979.0	-936.6
S_J-S_0	cal/°K/gm HE	-0.04528	-0.09342	-0.1453	-0.04165	-0.08129	-0.1228
Compo- sition of Product Mixture	10^{-3} mole/gm HE	*	*	*	*	*	*
CF ₂		*	*	*	*	*	*
CF ₃		*	*	*	*	*	*
CF ₄		2.660	3.342	3.942	2.646	3.337	3.942
CH ₂ F ₂		*	*	-	*	*	-
CH ₃ F		*	*	-	*	*	-
CH ₄		*	*	-	*	*	-
CHF ₃		*	*	-	*	*	-
CO		0.02367	0.004256	*	0.08013	0.03019	0.009924
CO ₂		8.889	9.193	9.461	8.876	9.186	9.456
COF ₂		*	*	*	*	*	*
F		*	*	*	*	*	*
F ₂		*	*	*	*	*	*
H		*	*	-	*	*	-
H ₂		*	*	-	*	*	-
H ₂ O		3.542	1.670	-	3.511	1.659	-
HF		0.03083	0.004286		0.08948	0.02495	-
N ₂		5.336	5.015	4.731	5.336	5.015	4.731
N ₂ O		*	*	*	*	*	*
NH ₃		*	*	-	*	*	-
NO		*	*	*	*	*	*
NO ₂		*	*	*	*	*	*
O		*	*	*	*	*	*
O ₂		*	*	*	*	*	*
OH		*	*	-	*	*	-
C(graphite)		13.33	10.86	8.672	13.30	10.85	8.668
Σ moles gas	10^{-3} moles/gm HE	20.48	19.23	18.13	20.54	19.25	18.14
V_g	cc/mole	17.17	17.92	18.63	16.67	17.38	18.02
V_s	cc/mole	3.849	3.785	3.719	3.924	3.879	3.834

*Mole fraction in gas mixture less than 10^{-4}

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TABLE 11. COMPUTED DETONATION PROPERTIES FOR FDNP/FINM MIXTURES
 (Using RDX-Type Parameters)

Property	Units	FDNP	FDNP/FINM 55.0/45.0	FDNP/FINM 50.3/49.7	FDNP/FINM 45.0/55.0	FINM	
ΔH_f	cal/gm	-528.7	-390.1	-375.6	-359.3	-220.7	
ΔH_f	kcal/mole	-80.4	-	-	-	-37.3	
ρ_0	gms/cc	1.35	1.4469	1.4578	1.4703	1.586	
D	mm/ μ sec	6.848	7.258	7.211	7.108	6.089	
P_J	megb	0.1809	0.2160	0.2165	0.2103	0.1416	
T_J	$^{\circ}$ K	2817.	3417.	3614.	3414.	1289.	
ρ_J	gms/cc	1.890	2.019	2.041	2.051	2.089	
γ		2.500	2.528	2.501	2.532	3.152	
E_J-E_0	cal/gm HE	457.5	505.7	506.9	484.0	257.1	
ΔE_{chem}	cal/gm HE	-1253.	-1455.	-1508.	-1409.	-531.7	
S_J-S_0	cal/ $^{\circ}$ K/gm HE	-0.02247	+0.05126	+0.04768	+0.02622	-0.3784	
Composition of Product Mixture	CF ₂	10 ⁻³ moles/gm HE	*	*	*	*	*
	CF ₃		*	*	*	*	*
	CF ₄		0.8976	1.129	1.084	1.122	1.479
	CF ₂ F ₂		*	*	*	*	-
	CH ₃ F		*	*	*	*	-
	CH ₄		*	*	*	*	-
	CHF ₃		*	*	*	*	-
	CO		1.115	2.480	0.2557	0.02987	*
	CO ₂		5.128	9.901	11.52	10.98	4.437
	COF ₂		*	*	*	*	*
	F		0.003654	0.01543	0.08283	0.1190	*
	F ₂		*	*	0.005129	0.01535	*
	H		*	*	*	*	-
	H ₂		0.008791	0.007511	*	*	-
	H ₂ O		14.93	8.153	7.359	6.610	-
	HF		2.981	1.743	1.816	1.573	-
	N ₂		6.572	7.605	7.664	7.587	8.635
	N ₂ O		*	*	0.008053	0.03166	*
	NH ₃		0.005459	0.004899	*	*	-
	NO		*	0.003636	0.08568	0.3190	0.003748
NO ₂		*	*	0.006171	0.1230	0.4710	
O		*	*	*	*	*	
O ₂		*	*	0.05269	1.082	12.84	
OH		*	*	*	*	-	
C(graphite)		12.58	0.	0.	0.	0.	
Σ moles gas	10 ⁻³ moles/gm HE	31.64	31.05	29.94	29.59	27.87	
V_g	cc/mole	15.08	15.95	16.36	16.48	17.18	
V_s	cc/mole	4.128	4.021	4.029	4.042	4.228	

*Mole fraction in gas mixture less than 10⁻⁴

TABLE 12. LITERATURE VALUES FOR DETONATION VELOCITIES

HE	ρ_0 (gm/cc)	NOL (Calculated)		Literature		
		ΔH_f (Kcal/mole)	D[RDX/TNT] (mm/ μ sec)	Ref.	ΔH_f (Kcal/mole)	D (mm/ μ sec)
DFTNB	1.695	-103.	6.924	a		7.190
	1.768	-103.	7.155	a		7.415
	1.841	-103.	7.404	a		7.636
	1.855(extrap)			a		7.750
	1.84			b		7.474
	1.855			c(Expt)		7.618
	1.873			c(Calc)	-51.3	7.618
	1.8564	-103.	7.459/7.009			
DFTNBTF	1.937			c(Calc)	(sic)225.0	6.799
	2.1	-261.	7.911/7.070			
MFTNB	1.512	-58.	6.659	a		6.650
	1.615	-58.	6.936	a		7.050
	1.802	-58.	7.526	a		7.515
	1.80			b		7.182
	1.83			c(Expt)		7.655
	1.802			c(Calc)	-47.1	7.766
	1.8383	-58.	7.657/7.242			
MFTNBTF	1.887			c(Calc)	-184.2	7.050
	2.0	-216.	7.696/7.010			
TFTNB	1.964	-148.	7.603	a		7.502
	1.920			c(Calc)	-135.1	7.085
	1.9477	-148.	7.541/6.982			
TNBTF	1.82			a		7.170
	1.82			b		6.919
	1.805			c(Expt)		7.185
	1.816			c(Calc)	-142.2	7.249
	1.9	-171.	7.506/6.956			

References:
 a. Denver Research Institute (Ref. 1)
 b. Picatinny Arsenal (Ref. 13)
 c. Amcel Propulsion Company (Ref. 14)

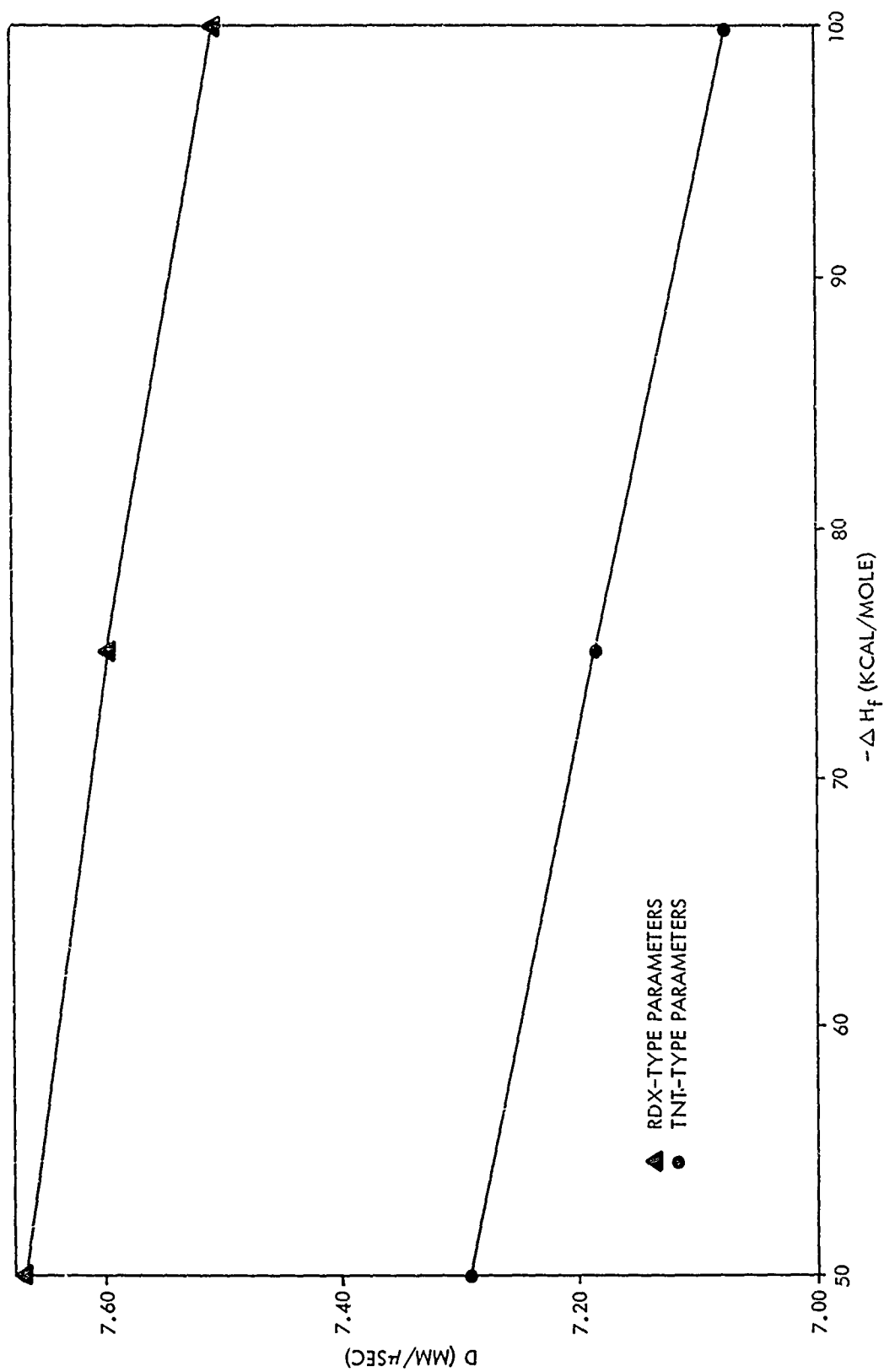


FIG. 1 COMPUTED D FOR MFTNT, VARYING ΔH_f AND EQUATION OF STATE PARAMETERS

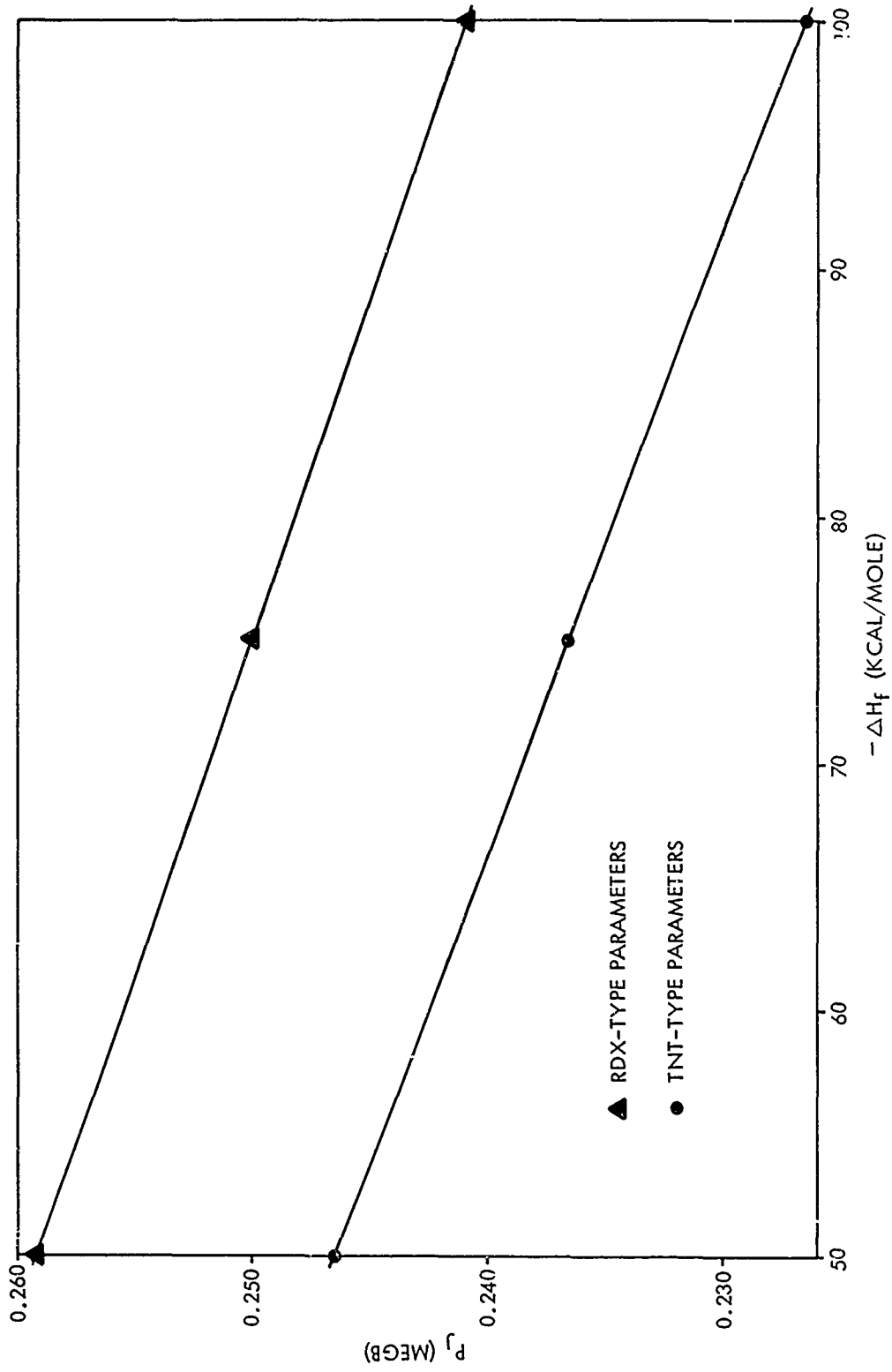


FIG. 2 COMPUTED P_j FOR MFNT, VARYING ΔH_f AND EQUATION OF STATE PARAMETERS

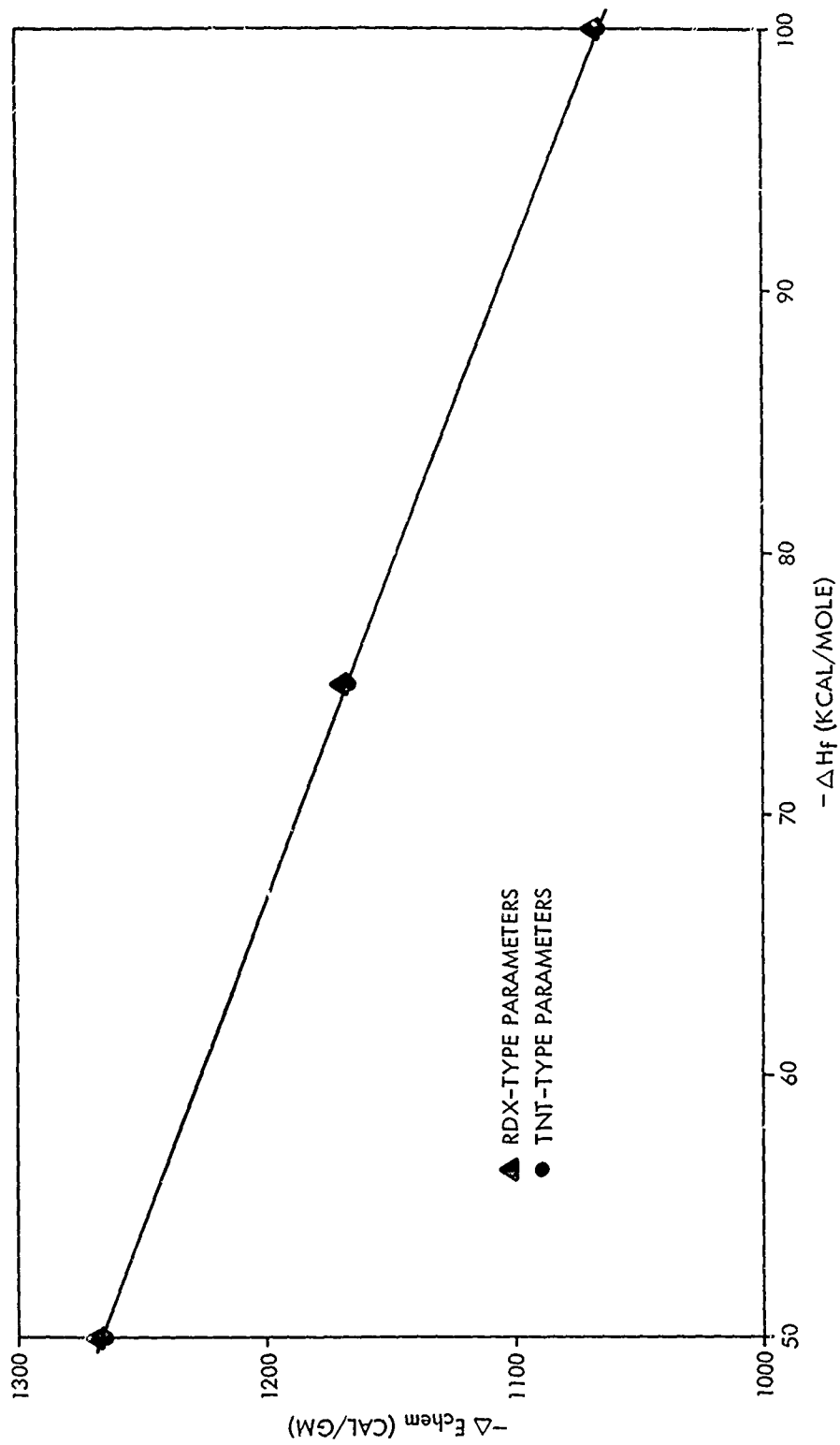


FIG. 3 COMPUTED ΔE_{chem} FOR MFTNT, VARYING ΔH_f AND EQUATION OF STATE PARAMETERS

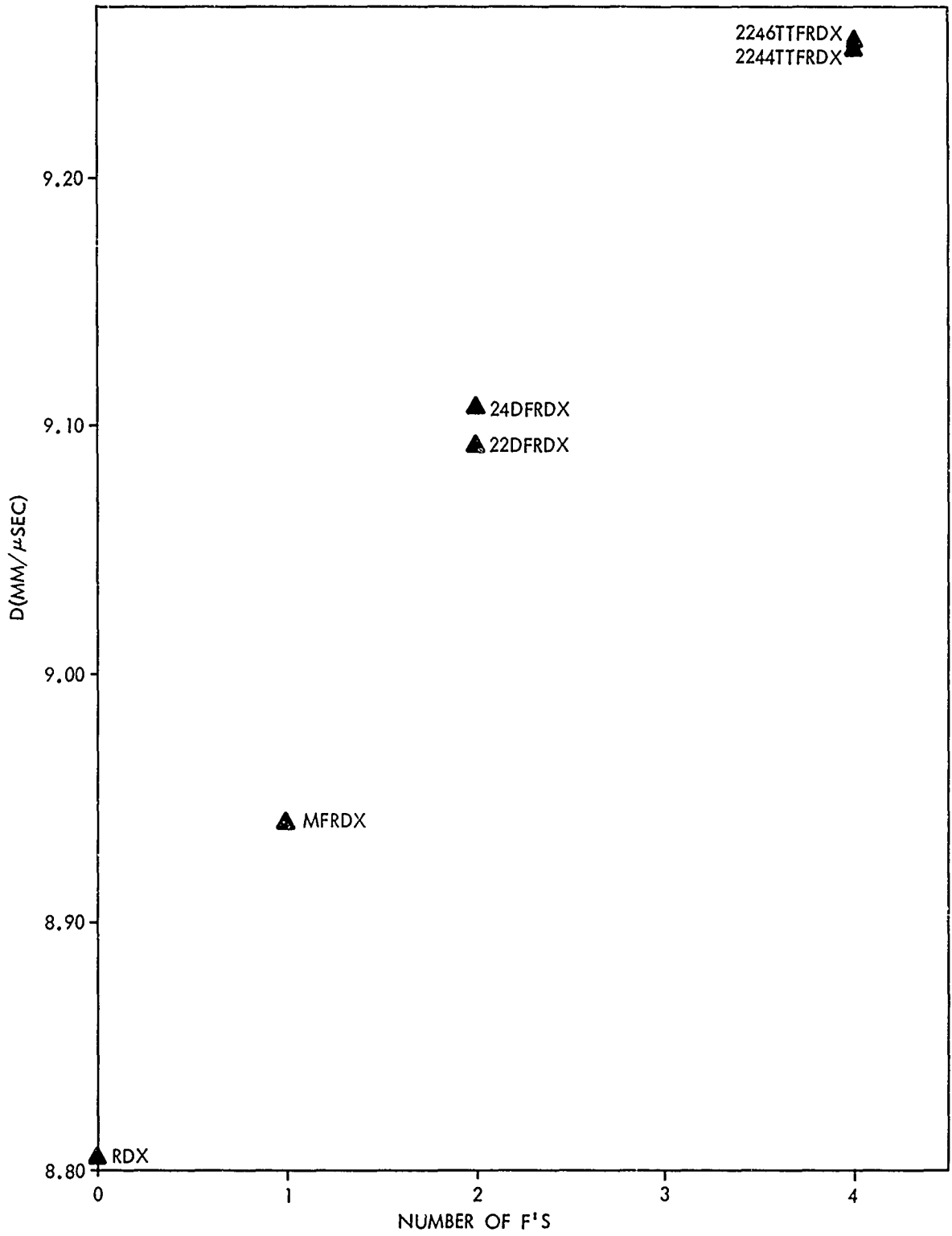


FIG. 4 COMPUTED DETONATION VELOCITY VS. NUMBER OF FLUORINE ATOMS FOR FLUORINATED RDX'S

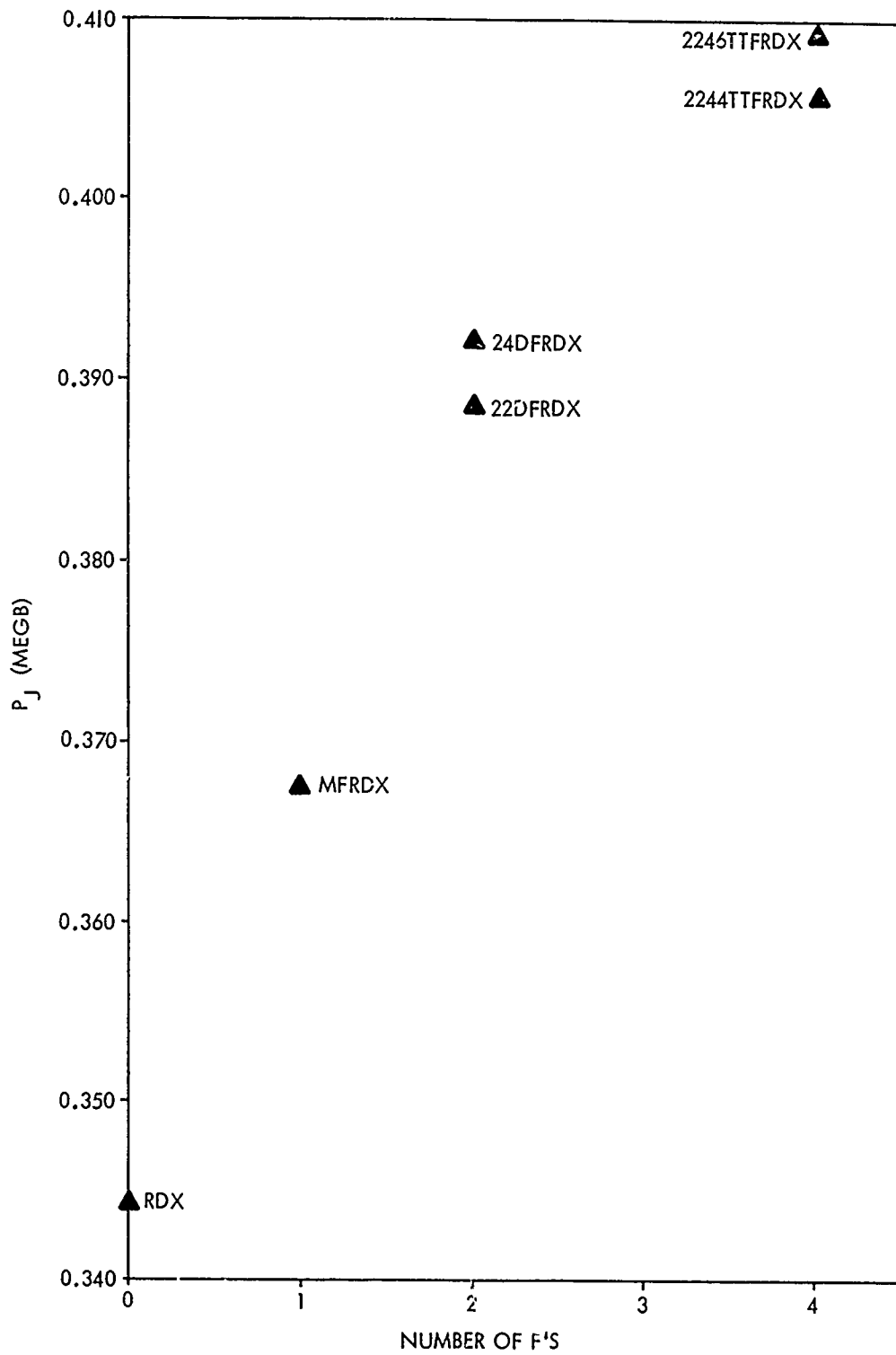


FIG. 5 COMPUTED CJ PRESSURE VS NUMBER OF FLUORINE ATOMS FOR FLUORINATED RDX'S

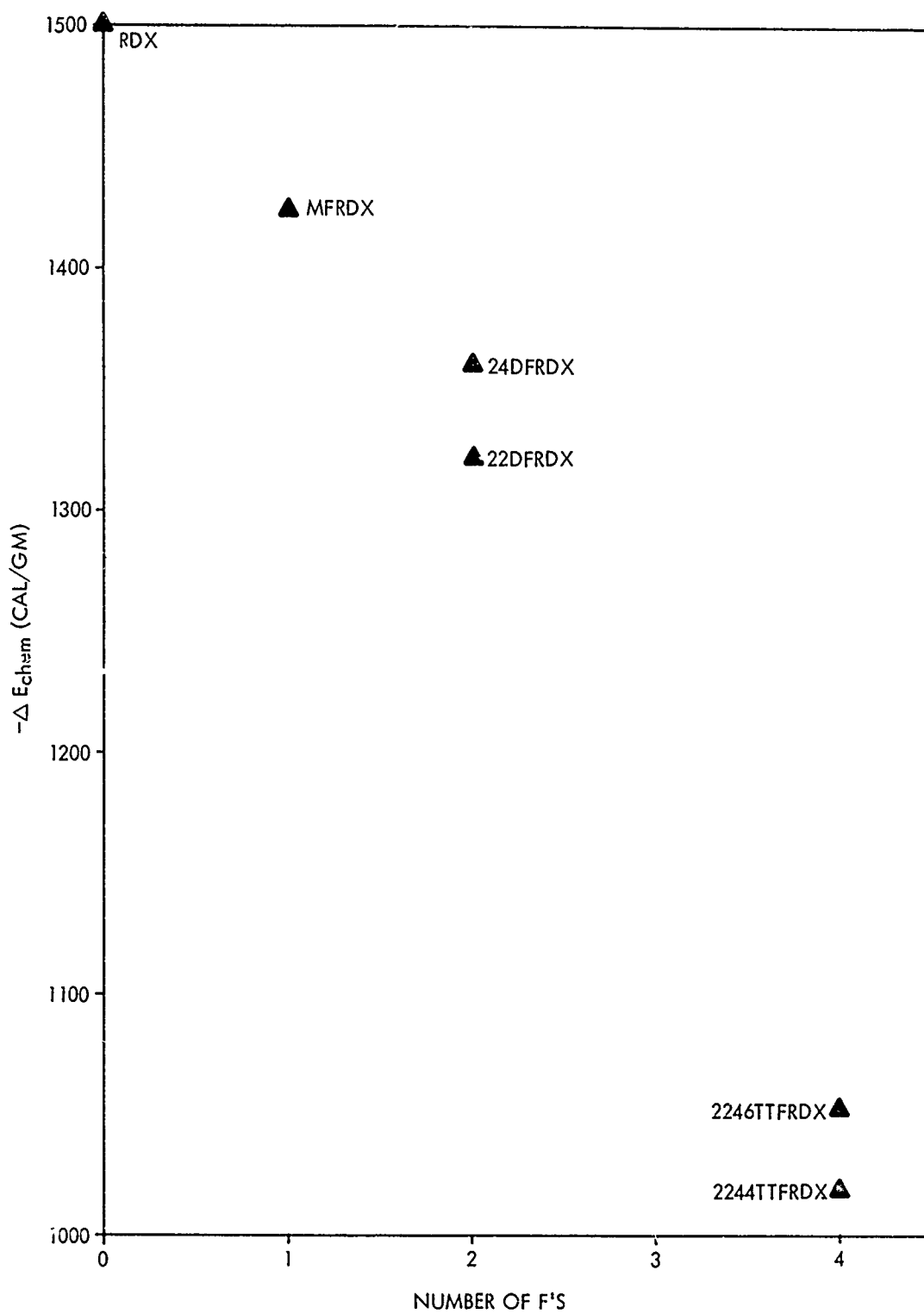


FIG. 6 COMPUTED CHEMICAL ENERGY VS. NUMBER OF FLUORINE ATOMS FOR FLUORINATED RDX'S

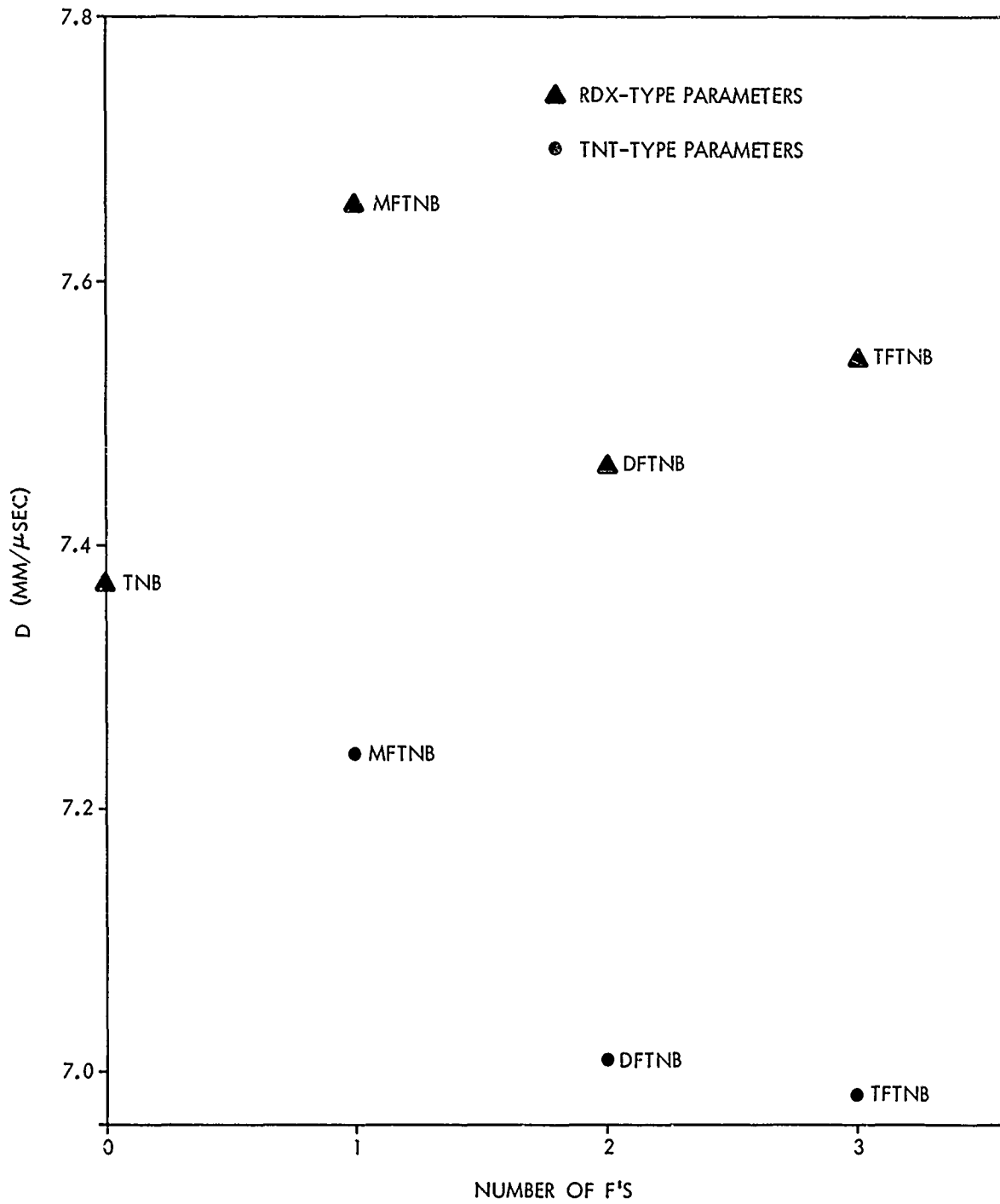


FIG. 7 COMPUTED DETONATION VELOCITY VS. NUMBER OF FLUORINE ATOMS FOR FLUORINATED TNB'S

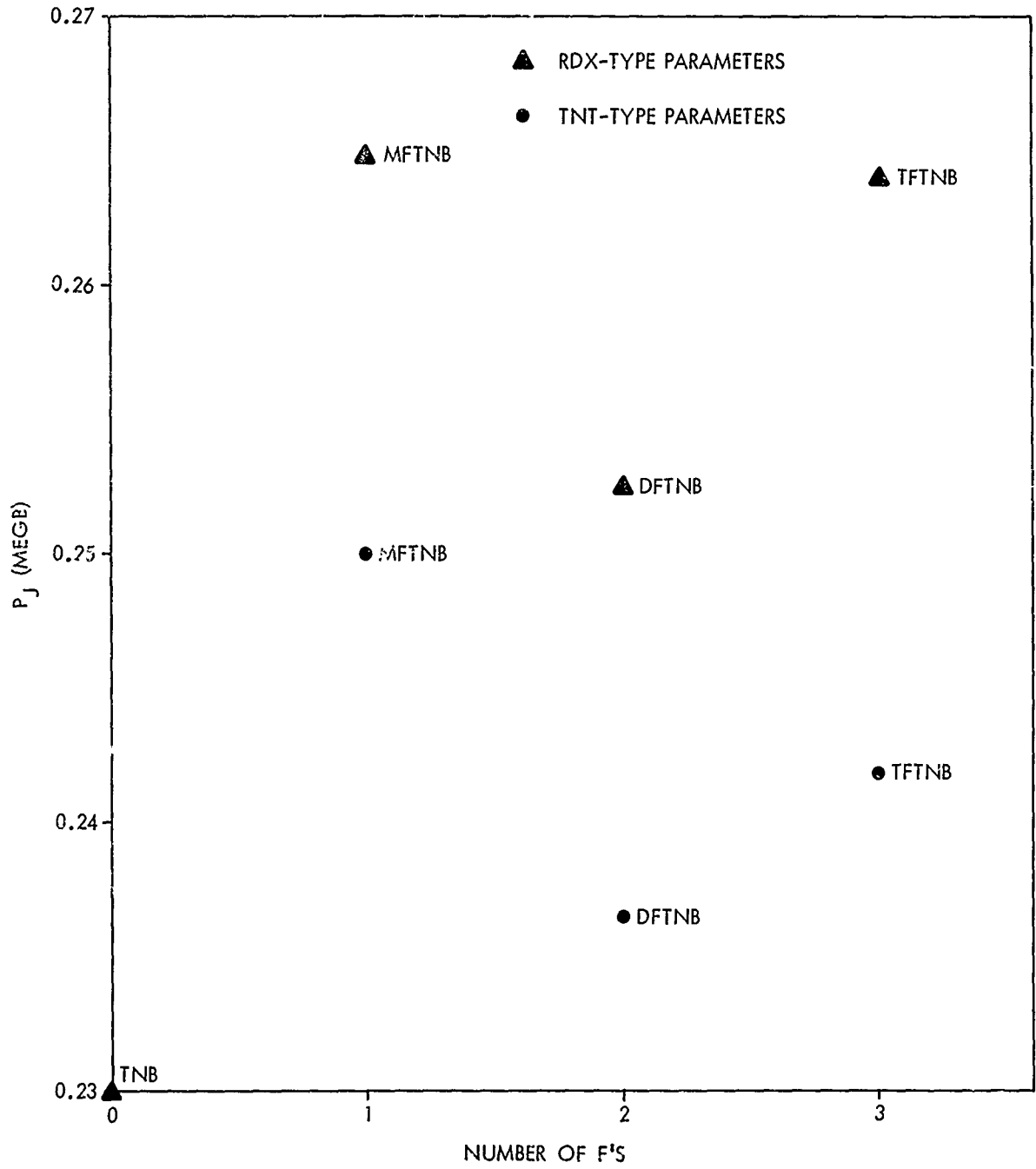


FIG. 8 COMPUTED CJ PRESSURE VS. NUMBER OF FLUORINE ATOMS FOR FLUORINATED TNB'S

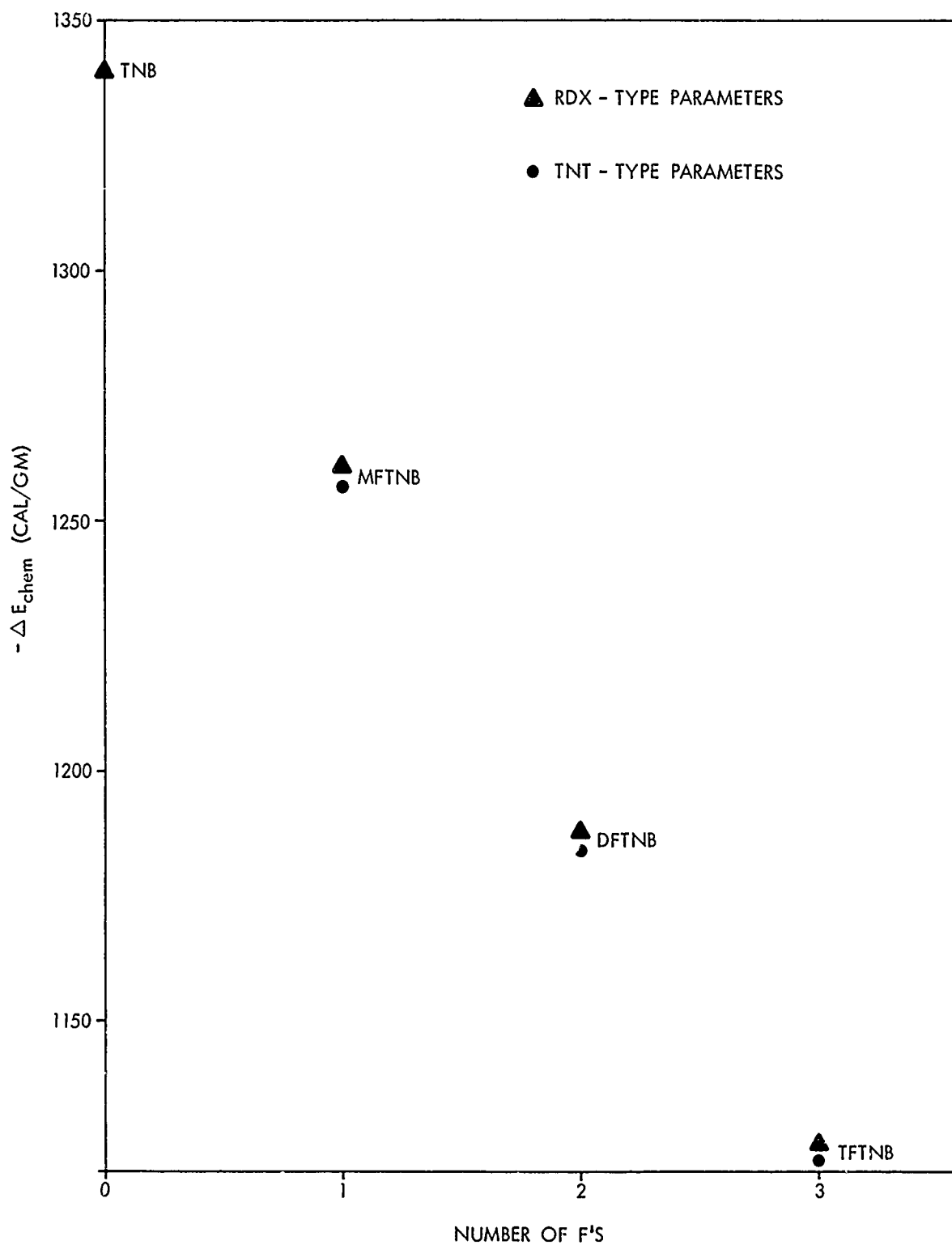


FIG. 9 COMPUTED CHEMICAL ENERGY VS. NUMBER OF FLUORINE ATOMS FOR FLUORINATED TNB'S

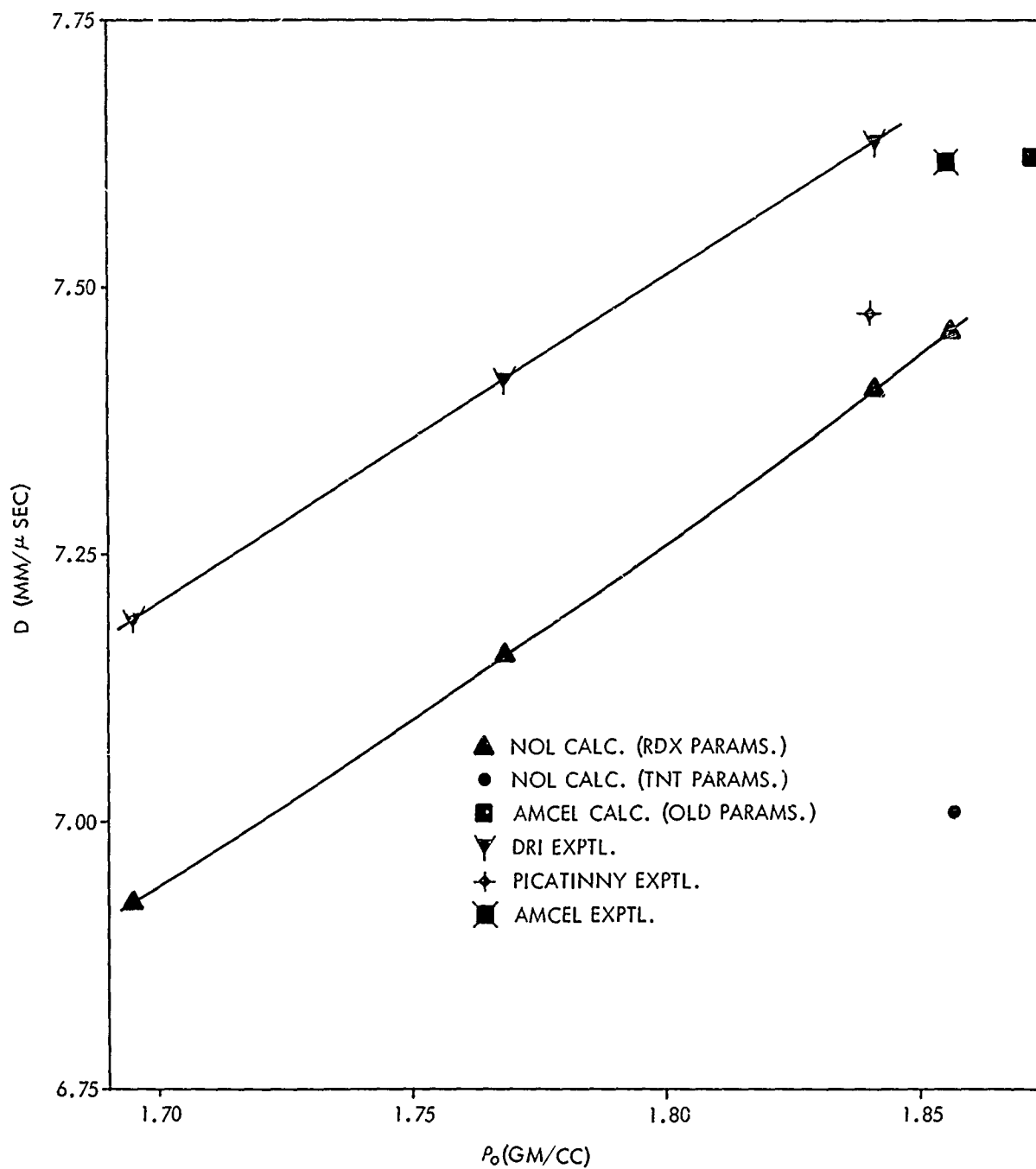


FIG. 10. DETONATION VELOCITIES FOR DFTNB, FROM NOL AND OTHER SOURCES

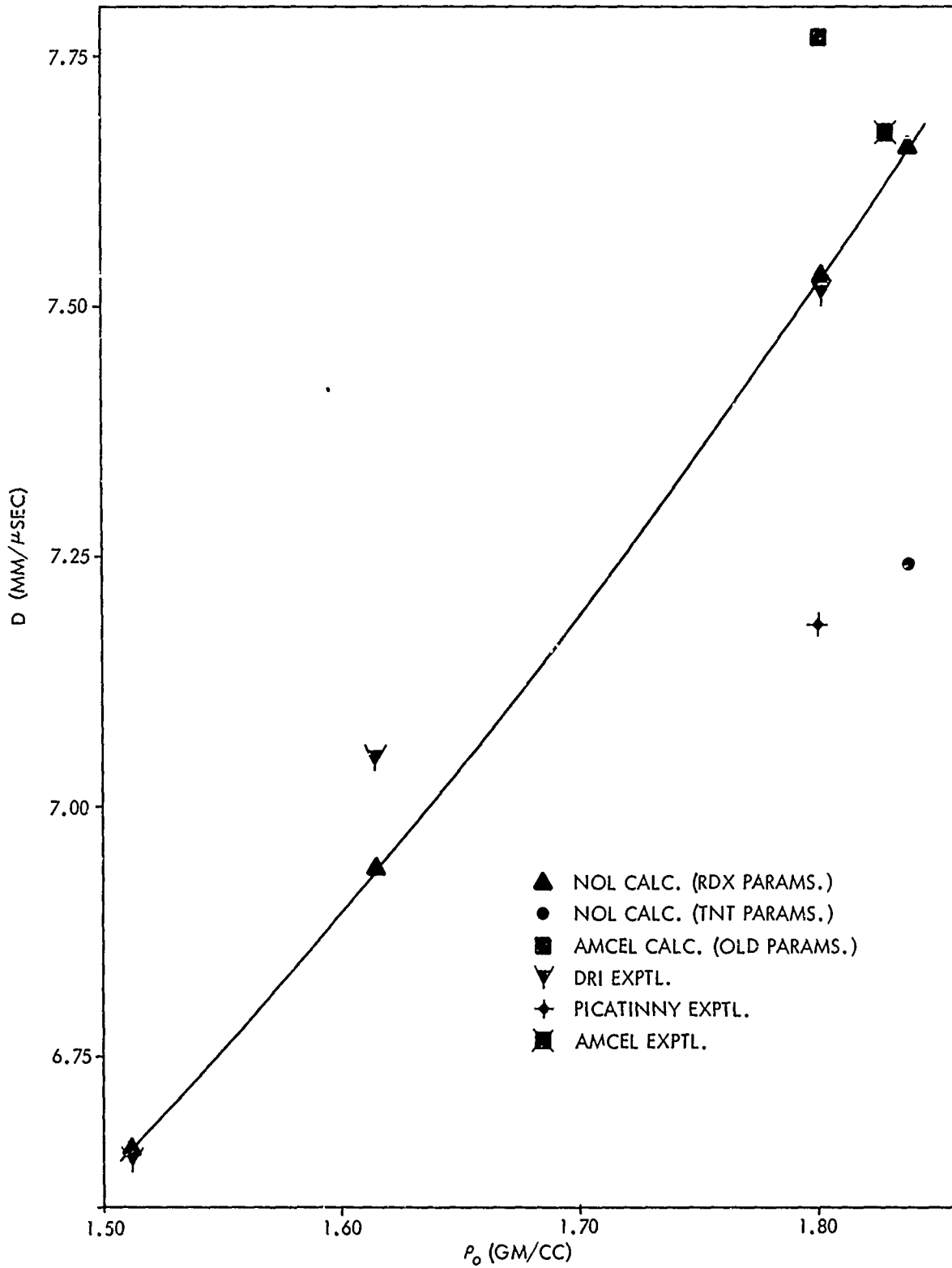


FIG. 11. DETONATION VELOCITIES FOR MFTNB, FROM NOL AND OTHER SOURCES

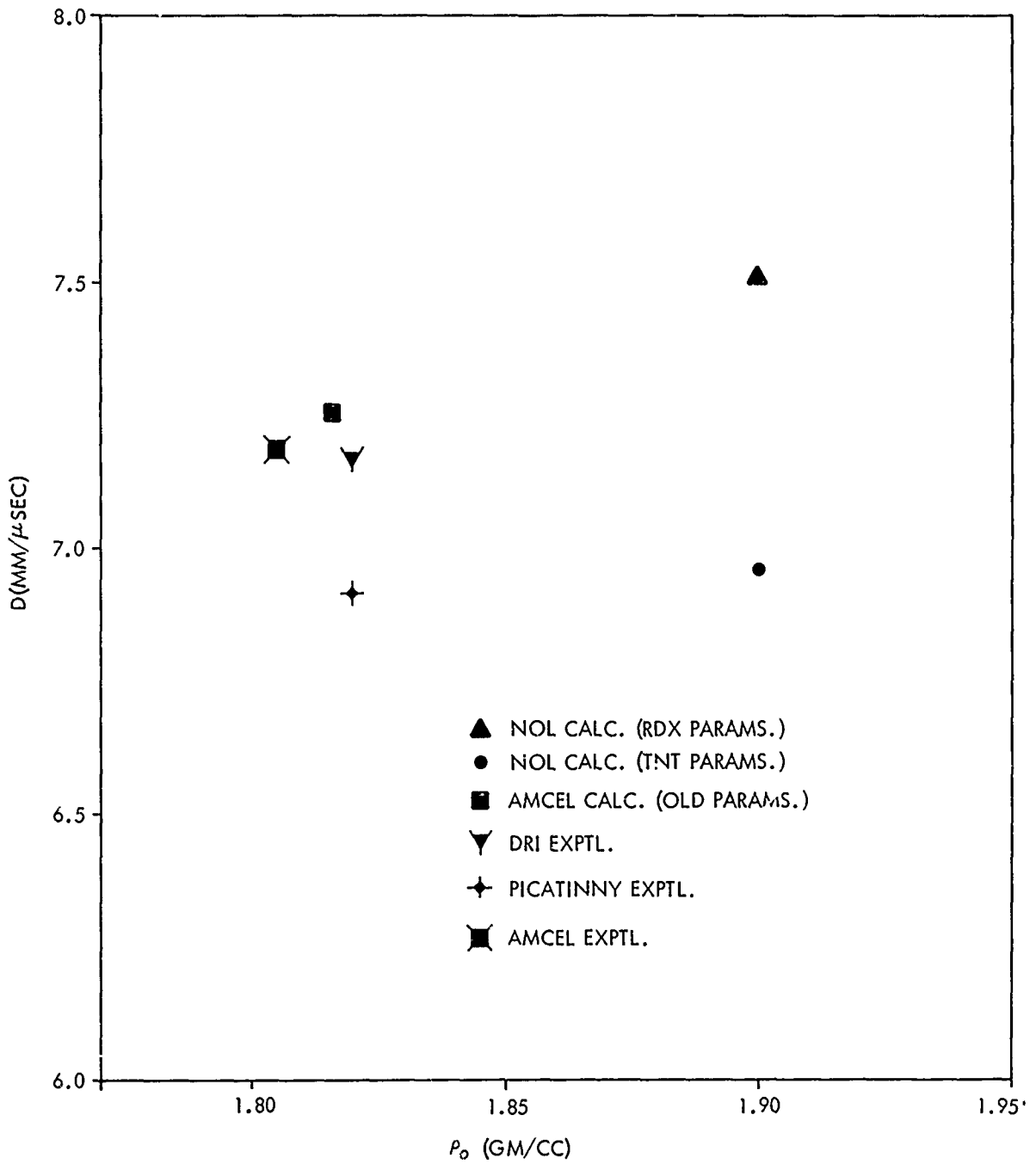


FIG. 12. DETONATION VELOCITIES FOR TNBTF, FROM NOL AND OTHER SOURCES

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APPENDIX

ESTIMATION OF HEATS OF FORMATION (ΔH_f)

	ΔH_f (kcal/mole)	Reference
MFTNB	$C_6H_5F(l)$	15
	$C_6H_6(l)$	16
	(Fluoro-)	-46.5 (Difference)
	TNB(s)	-11.4
	MFTNB(s)	-57.9 (Sum)
DFTNB	$m-C_6H_4F_2(l)$	17
	$C_6H_6(l)$	16
	(Difluoro-)	-91.36 (Difference)
	TNB(s)	-11.40
	DFTNB(s)	-102.76 (Sum)
TFTNB	$m-C_6H_4F_2(l)$	17
	$C_6H_5F(l)$	15
	(Fluoro-)	-44.8 (Difference)
	DFTNB(s)	-103.0
	TFTNB(s)	-148.0 (Sum)
TNBTF	TNB(s)	4
	$C_6H_6(l)$	16
	(Trinitro)	-23.12 (Difference)
	$C_6H_5CF_3(l)$	-147.8
	TNBTF(s)	-170.9 (Sum)
MFTNBTF	TNB(s)	4
	$C_6H_6(l)$	16
	(Trinitro-)	-23.12 (Difference)
	$m-FC_6H_4CF_3(l)$	-193.2
	MFTNBTF(s)	-216.3 (Sum)

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	ΔH_f (kcal/mole)	Reference
DFINBTF		
MFINBTF(s)	-216.3 (Estimated)	
TNBTF(s)	-170.9 (Estimated)	
(Fluoro-)	-45.4 (Difference)	
MFINBTF(s)	-216.3	
DFINBTF(s)	-261.7 (Sum)	
MFINBTF		
TNT(s)	-17.81	4
$C_6H_5CH_3(l)$	+2.867	16
(Trinitro-)	-20.68 (Difference)	
p- $FC_6H_4CH_3(l)$	-43.43	17
MFINBTF(s)	-64.11 (Sum)	
DFINBTF		
MFINBTF(s)	-64 (Estimated)	
MFINB(s)	-58 (Estimated)	
(Methyl-)	-6 (Difference)	
DFINB(s)	-103 (Estimated)	
DFINBTF(s)	-109 (Sum)	
FDATE		
$C_6H_5F(l)$	-34.8	15
$C_6H_6(l)$	+11.7	16
(Fluoro-)	-46.5 (Difference)	
DATE(s)	-29.2	4
FDATE(s)	-75.7 (Sum)	
MFRDX		
RDX	+14.71	4
*	-40.4	(See Ref. 18)
MFRDX	-25.7 (Sum)	

*Heats of formation of the fluorinated RDX's were estimated by using the increments for substitution of a fluorine atom for a hydrogen atom in aliphatic hydrocarbons given by Good et al in reference 18. The increments vary with the number of other fluorines attached to the same carbon atom and are therefore listed separately in this table.

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	ΔH_p (kcal/mole)	Reference
22DFRDX		
RDX	+14.71	4
*	<u>-40.4</u>	(See Ref. 18)
MFRDX	-25.7 (Sum)	
22DFRDX		
RDX	+14.71	4
*	<u>-90.4</u>	(See Ref. 18)
22DFRDX	-75.7 (Sum)	
24DFRDX		
RDX	+14.71	4
*	<u>2(-40.4)</u>	(See Ref. 18)
24DFRDX	-66.1 (Sum)	
224TFRDX		
RDX	+14.71	4
*	<u>-90.4</u> <u>-40.4</u>	(See Ref. 18)
224TFRDX	-116.1 (Sum)	
246TFRDX		
RDX	+14.71	4
*	<u>3(-40.4)</u>	(See Ref. 18)
246TFRDX	-106.5 (Sum)	
2244TIFRDX		
RDX	+14.71	4
*	<u>2(-90.4)</u>	(See Ref. 18)
2244TIFRDX	-166.1 (Sum)	
2246TIFRDX		
RDX	+14.71	4
*	<u>-90.4</u>	(See Ref. 18)
2246TIFRDX	-156.5 (Sum)	

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	ΔH_f (kcal/mole)	Reference
MFT		
C_6H_5F (l)	-34.8	15
C_6H_6 (l)	+11.7	16
(Fluoro-) Tetryl(s)	<u>-46.5</u> +4.7	(Difference) 4
MFT(s)	-41.8	(Sum)
DFT		
m- $C_6H_4F_2$ (l)	-79.6	17
C_6H_6 (l)	+11.7	16
(Difluoro-) Tetryl(s)	<u>-91.3</u> +4.7	(Difference) 4
DFT(s)	-86.6	(Sum)

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1 ORIGINATING ACTIVITY (Corporate author) U. S. Naval Ordnance Laboratory White Oak, Silver Spring, Maryland		2a REPORT SECURITY CLASSIFICATION Confidential
		2b GROUP 4
3 REPORT TITLE Computation of Detonation Properties of Fluoroexplosives (U)		
4 DESCRIPTIVE NOTES (Type of report and inclusive dates)		
5 AUTHOR(S) (Last name, first name, initial) Hurwitz, Harold		
6. REPORT DATE 10 June 1966	7a TOTAL NO OF PAGES 41	7b NO OF REFS 18
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d		
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11 SUPPLEMENTARY NOTES	12 SPONSORING MILITARY ACTIVITY U. S. Air Force Eglin AFB, Fla.	
13. ABSTRACT The RUBY code has been used to compute detonation properties for a number of fluorinated explosives. Results are given for fluorinated TNB, RDX, tetryl, TNT, DATB, and trinitrobenzotrifluoride, and for fluorodinitropropane and fluorodinitromethane. When necessary densities and heats of formation of the explosives were estimated for input to RUBY.		

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14. KEY WORDS	LINK A		LINK B		LINK C	
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