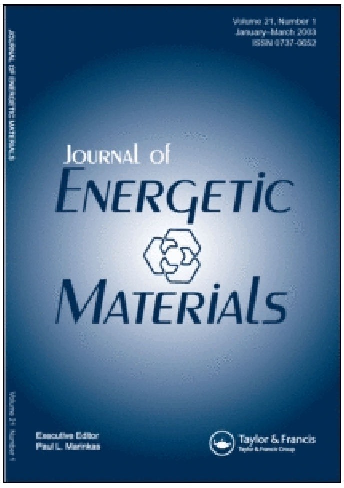

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A CORRELATION BETWEEN THE CHEMICAL AND PHYSICAL PROPERTIES OF C, H, N, O EXPLOSIVES

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SUMMARY

An attempt has been made to correlate the physical, chemical, and thermodynamic properties of C, H, N, O explosives and their reaction products.

INTRODUCTION

Any evaluation of the performance characteristics of explosive compounds depends on the evaluation criteria used. For example, the criterion for an explosive for shaped charge applications puts a premium on a high detonation pressure, while the criterion for a rock blasting explosive puts a premium on high explosion energy and expansion work at lower pressures. The criterion for a rocket propellant puts a premium on high energy and sonic velocity of the reaction products.

It is hoped that the presented correlations, and the deviations from the resulting normal curves, may throw some new light on

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the question: How do we find better performing explosives than those available today?

When reviewing and evaluating the thermodynamic properties of numerous organic C, H, N, O compounds as prospective explosives certain trends in the behavior of physical properties in concert with the chemical properties have been observed. This approach is not new of course, but it is hoped that some novel correlations can be documented, or saved from oblivion. Trends of impact sensitivity as a function of oxygen balance have been presented by Kamlet (1), and by Kamlet and Adolf (2), dependence of the response energy on initiation energy, and dependence of initiation energy on density has been studied by Petersen (3); Cady (4) has studied the relation between the chemical structure and density, so did Stine (5). Martin and Yallop (6) were predicting detonation velocities basing their calculations on modified oxygen balance. The important relationship between detonation velocity and the composition and structure of an explosive was given by Rothstein and Petersen (7), and by Rothstein (8), who included fluorinated explosives as well. Kamlet and Jacobs produced a very fundamental paper (9) in which detonation pressures and detonation velocities may be calculated by means of empirical equations containing chemical energy of detonation, the initial density of the explosive, and a set of fitting parameters. Results of the correlations correspond closely to the Kistiakowsky - Wilson equation of state. Kamlet and Ablard expanded this work by including explosives of low initial density (10), Kamlet and Dickinson (11) evaluated the CJ detonation pressures obtained from the empirical methods (9,10) comparing them to the available experimental information. Kamlet and Hurwitz (12) did the same with detonation velocities.

In this study, we have used the constant volume (15,16) explosion pressure P as a primary target variable, and we have attempted to find a correlation between P and several chemical, physical and thermodynamic parameters that are relatively easily determined without actual explosion experiments. We also attempted the back-calculation of densities for unknown cases, as well as for mixtures. Next step will be to use more sophisticated methods than the Taylor model (15), which is only the first step. Because of the use of this restrictive model, results can be compared only with each other, and not with the results of calculations done with more sophisticated methods such as the BKW- equation of state -code, or others. However, the present paper is avoiding the use of empirical parameters in the sense that Kamlet et al. do . The only fitting parameters without well founded physical meaning in use, are the 10^n additions or multiplications appearing in f_1 and in f_3. All these features make this systematization attempt different, not better of course, but different; and unalike correlations and backcalculations are being looked at, and proposed.

The calculations have been based on 33 solid organic compounds.

CALCULATION PROCEDURE

It has been observed that the more negative the heat of formation, the worse the explosive is. However, the higher the negative heat of combustion the better. Therefore, a factor

$$f_1 = 1 - (H_f-1000)/10H_c$$

where H_f and H_c are heats of formation and of combustion respectively. This value, although nondimensional, (1000 must have the same dimension as H_f), will depend on units used. Therefore, it is agreed to use KJ/mol units at all times.

It has been observed that the more equal the number of H, O, and N atoms are, the higher the performance of the explosive, (Note: RDX has H = N = O = 6, HMX has H = N = O = 8). Here, C, H, N, O, are numbers of corresponding atoms in a molecule. Therefore, a "symmetry factor" has been devised:

$$H*O*N/0.3333^3(H+O+N) = H*O*N/0.03704(H+O+N) = f_2$$

Factor f_2 maximizes when H=N=O; it has been normalized to its highest value equal to 0.3333^2 = 0.03704. For RDX and HMX , f_2 = 1, for TNT 0.887, for $C_{10}H_{14}N_4O_7$ it is 0.678, and for $C_{20}H_{44}NClO_4$ 0.0404 .

Factor f_3 tries to embrace the influence of the ratio of nitrogen atoms to the total number of atoms in the molecule in question $N/\sum m$, the negative influence of a high molecular weight, and the beneficial influence of a low negative, or a positive oxygen balance:

$f_3 = 1400.67N(1-Mw/1000)/\sum m(100 - B_O)$;

where oxygen balance is

$B_O = -100(2C + 0.5H - O)*15.994/Mw$;

Mw is molar weight in grams per mole, $\sum m$ is the sum of all atoms in the molecule, 15.9994 and 14.0067 are atomic weights of oxygen and nitrogen respectively. It should be stressed however that there is a sensitivity limit on B_O (2). Factor f_3 certainly needs some tune-up; the reason is that low molecular weight of an explosive tends to position the corresponding point below, and a high Mw, above, the statistically best fit curve on Fig 1. The influence of Carbon atoms is perhaps not explicit, but it is clear that it is built-in into the heat of combustion H_C and into the oxygen balance B_O.

Density in the second power (13,14) is an important contributing factor, and, therefore

$f_4 = d^2$

The total contributing factor is

$f = f_1 * f_2 * f_3 * f_4$

For reasons of making the numerical correlation between the X and the Y axes more handy we shall take a logarithm of f, where log f = F, and where

$$F = \log\left(1 - \frac{H_f - 1000}{10H_c}\right)\left(\frac{H*O*N}{0.03704(H+O+N)^3}\right)\left(\frac{1400.67\ N\left(1-\frac{M_w}{1000}\right)}{\sum_m(100-B_O)}\right) + 2\log d \qquad /1/$$

The factor f_4 related to density has been separated for the benefit of further discussion.

RESULTS

Figure 1 has been plotted on basis of data pertaining to thirty-three C,H,N,O, compounds listed in Table I. The F values have been calculated from data contained in Encyclopedia of Explosives (17), Rudolf Meyer's (18) Explosives, CRC Handbook of Chemistry and Physics (19), Eugene Domalski's Selected Values (20), Stull's, Westrum's and Sinke's (21) Chemical Thermodynamics of Organic Compounds, Pedley's, Naylor's and Kirby's Thermochemical Data of Organic Compounds (22), K.Toedheide (23), M.Sanesi et al. (24), Molten Salts Handbook by Janz (25), International Critical Tables (26), Bichowsky and Rossini (27), Cingolani et al.(28), Coker, Ambrose and Janz (29), Gordon (30,31,32), and Gordon and SubbaRao (33), Mellor's VIII volume (34), Wagman's et al.Selected Values (35), and LLNL Explosives Handbook by Dobratz and Crawford (36). Densities not found in the quoted literature were estimated using Cady's method (4) for compound #19, and Stine's method (5) for compounds ##18, 22, and for other compounds not directly included into constructing the F-curve. Missing heat of combustion data, or heat of formation data were calculated where necessary: according to Janz (37), or CRC Handbook (19), or according to Domalski (20).

Organic perchlorates show a different behavior than other compounds (probably due to certain assumptions built-in in the computer code (16), and concerning the reactions of chlorine), and as such, have not been included into the calculation.

The best fit curves obtained are, line I:

$Y = P(atm) = A_0 + A_1 EXP(B_1 * X)$ /2/

where X is identical with the parameter F; line II:

$Z = V*Mw/1000T\ (\ell\ K^{-1}mol^{-1}) = A_{00} + A_{11} EXP(B_{11} * X)$ /3/

and line III:

$YZ = P*V*Mw/1000T\ (\ell\ atmK^{-1}mol^{-1}) = A_0 A_{00} +$
$A_0 A_{11} EXP(B_{11} * X) + A_{00} A_1 EXP(B_1 * X) +$
$A_1 A_{11} EXP(B_1 * X + B_{11} * X);$ /4/

Line I has a positive slope, line II has a negative slope, and line III exhibits a minimum at X = F = -0.3 .

The A_0, ...etc, B_1...etc parameters have following values obtained from the curve fitting:

Curve I: Y vs X or P vs F : $A_0 = 23850$; $A_1 = 39493$; $B_1 = +1.674$; Standard deviation: absolute 16841.5; standard deviation of nat.logarithmic fit = 0.2781 .

Curve II: Z vs X or V*Mw/1000T vs F: $A_{00} = 0.022200$; $A_{11} = 0.031855$; $B_{11} = -1.242462$ Standard deviation: absolute 0.01358; standard deviation of nat.logarithmic fit = 0.7301.

The solid C, H, N, O, compounds involved in the correlation calculation are: [1]-1,3,5,-Trinitrobenzene,

[2]-EthyltripropylAPic, [3]-PentylAPic, [4]-ButylAPic, [5]-Iso-ButylAPic, [6]-DiethylAPic, [7]-MethylEthylAPic, [8]-DimethylAPic, [9]-DimethylAN, [10]-EthylAN, [11]-TNT, [12]-Ortho-Dinitrobenzene, [13]-Styphnic Acid, [14]-N-Methyl-N-2,4,6-Tetranitroaniline, [15]-Tetryl, [16]-Trinitroaniline, [17]-HMX, [18]-5-Methoxytetrazole, [19]-NN'-Dinitroethylenediamine, [20]-RDX, [21]-HNAB, [22]-1,1,1,Trinitroethane, [23]-DIPAM, [24]-DATB, [25]-TetrapropylAPic, [26]- 4-Nitroaniline, [27]-HeptylAPic, [28]-HNS, [29]- Trinitrometacresol, [30]-TATB, [31]-TACOT, [32]-EDD, and [33]-DIPEHN. Here "APic" signifies Ammonium Picrate, and "AN" Ammonium Nitrate. MethylAN and NQ,although not included into the calculation have been plotted on Fig.1 for reasons of comparison. Each triangular point on Curve II corresponds to a circular point on Curve I; in other words, each explosive is represented by two points (on two different curves).

Figure 2 is derived from Figure 1. Here, the curve I is identical to that in Fig.1, but curve IV (with a negative slope) represents the dependence of pressure P on V*Mw/1000T without any involvement of X = F. (Corresponding F can be found from Curve I when P, which is common for both curves, is known). The term V*Mw/1000T has the dimension of R/P, and as such, curve IV should be, and is,asymptotic to both axes.

Ideally, one should be able to calculate the density, or the H_f/H_c ratio, density given, if F is known statistically from Figure 2. Let us try two examples:

a) 1,1,1-Trinitroethane exhibits constant volume pressure P = 180120 atm which corresponds to F = 0.82; H_f = -130.3, H_C = -1541.6 KJ/mol, Mw = 165.068; hence 0.82 - log(0.8989*0.8438*2.6337) = 2log d, where from d = 1.818, as compared to 1.71 in the literature, or 1.82 as calculated by Stine (5).

b) HMX exhibits a constant volume pressure of P = 227427 atm (only constant volume pressures can be used with these, statistically obtained F curves, as all calculations in this study are based on the Taylor model. The better known value for HMX pressure equal to P=390000 atm cannot be used here). The pressure 227427 atm corresponds to F = 0.97; hence f_1 = 0.96465; f_2 = 1.0; f_3 = 2.3160 for this explosive, as H_f = 75.06 and H_C = -2626.3 KJ/mol; B_0 = -21.606, Mw = 296.2 and $N/\Sigma m$ = 0.2857. Therefore: 0.97 - log(0.9645*1.0*2.3160) = 2log d = 0.621; d = 2.04 g/cm^3, which is almost 8% too high.

However it should be emphasized that the F parameter is arbitrary, it is only expressing proportionality and not determining an absolute value. We are not sure if f_4 should be equal to d in second power or in 2.5 power or still another power. We are not yet sure if f_3 should be proportional to exactly 1-Mw/1000 since only explosives with Mw 200 to 300 lie close to the line obtained by the best fit correlation. Therefore, any uncritical backcalculation of otherwise measurable physical or thermodynamic properties is risky, especially if the explosive is expected to lie away from the best-fit curve. Perhaps in the future one could collect enough data, to tune-up the f_1....to f_4 factors, so that all explosives lie rigorously on one physically meaningful line. Backcalculation of properties would then become risk-free and more useful in rechecking the H_f/H_c ratios, as well as densities.

The product curve III on Fig.1 represents energy per mole and degree Kelvin. Unexpectedly, it shows a minimum, saying that perhaps there might exist high-energy explosives in the negative F range as well. It is, however, very doubtful if such explosives, even if their total energy per mole and degree Kelvin is high, (but P and T low), could produce sufficient detonation velocities. Therefore the ascending branch, or in other words the positive F region of Curve III is much more important: it represents the true high pressure- and high-temperature regions. The apparently high values of molar energy of the descending branch (or of the negative F region) are produced merely by high volumes and high molecular weights, instead.

Table I presents data for each of the 33 explosives. The numbering of explosives is identical to that in figure 1, and to that above in the text.

The Product-curve $F = YZ = PVMw/1000T$ shown on Fig.1 can also be thought of as $F = YZ = zRMw/1000$ where R is the ideal gas constant, and z is the deviation from ideality. As expected, z is lowest at the low pressure region, specifically for the case of compounds ## 4,27,25,2,and 3, which all belong to the same

TABLE I

Data for 33 explosives. Their numbering corresponds to the numbering in [ ] brackets in the text, Column A: # of explosive; Column B: Values of F; Column C: P(atm); Column D: $V*M^{W}/1000T$(/K mol); Columns D and E are calculated according to (15) and (16).

A	B	C	D
[1.]	0.4303	111359	0.0306
[2.]	-0.9649	34916	0.13453
[3.]	-0.3497	43873	0.07887
[4.]	-0.2131	48564	0.07030
[5.]	-0.2071	49192	0.07000
[6.]	-0.1859	50871	0.06930
[7.]	0.0149	58235	0.06130
[8.]	0.0627	63156	0.05520
[9.]	-0.1506	40518	0.04520
[10.]	-0.0455	52707	0.04700
[11.]	0.2177	69459	0.04020
[12.]	0.1894	72850	0.02800
[13.]	0.4190	126355	0.03720
[14.]	0.4784	106170	0.04440
[15.]	0.5627	136713	0.04140
[16.]	0.5926	124595	0.03560
[17.]	0.9020	227427	0.04890
[18.]	0.5686	135079	0.03280
[19.]	0.7621	145835	0.03280
[20.]	0.9018	197992	0.03680
[21.]	0.4126	143332	0.05627
[22.]	0.8206	180120	0.02290
[23.]	0.4670	136722	0.06430
[24.]	0.6734	131183	0.04170
[25.]	-1.0629	32721	0.14510
[26.]	-0.1185	40220	0.03770
[27.]	-0.5796	38948	0.09660
[28.]	0.2518	112858	0.06140
[29.]	0.3067	94842	0.04100
[30.]	0.7804	173829	0.04841
[31.]	0.5182	131283	0.05094
[32.]	0.4575	80916	0.05933
[33.]	0.0523	112270	0.09573

(picrate) homologous series. It seems that the energy (per mole) of a chemical compound of this series comes mainly from the volume and molecular weight, and, as stated above, this is not what a good explosive should derive its energy from. Average values of z are encountered for compounds #16 and #23 (Trinitroaniline and DIPAM respectively), and, z is highest in the high pressure region, especially in the case of HMX, 5-Methoxytetrazole and RDX (compounds 17,18 and 20 respectively).

There is another way of finding densities for pure explosive substances if their molecular weight is roughly between 200 and 300, as well as for mixtures of explosives, provided the properties of their pure components lie close to the best fit curve. For the sake of example we shall use known substances (instead, as we should, substances, the density of which is not known too well). Let's take Styphnic Acid which is #13 and Dimethylammonium Picrate #8. One can find a curve for each of these explosives, which, with changing density will give different values of P and of V*Mw/1000T, as in Fig.2 and Tables II and III:

TABLE II

Curve #13 Styphnic Acid

Density	Pressure	$\frac{V\,M_w}{T\,1000}$	Point on Fig. 2
1.25	52452	0.05032	f
1.50	77627	0.04311	g
1.75	112355	0.03722	h
1.95	152253	0.03604	i

This curve 13 intersects Curve IV at point where d = 1.83, P =126355 and V*Mw/1000T = 0.03722. Indeed the density of the Styphnic Acid is 1.83.

TABLE III

Curve #8 Dimethylammonium Picrate

Density	Pressure	$\frac{V\ M_w}{T\ 1000}$	Point of Fig. 2
1.00	35211	0.06824	k
1.25	50133	0.05943	l
1.50	77629	0.05237	m
1.75	120301	0.04891	n

Here curve 8 intersects Curve IV at a point p where d =1.37, P = 63156, and VMw/1000T = 0.05522 . The density of DimethylAPic is indeed 1.37.

It is evident that explosives with lower P's and higher V*Mw/1000T ratios are more amenable to this procedure, as Curve IV asymptotically approaches the horizontal axis; there the points of intersection can be defined much easier.

As far as mixtures of explosives are concerned, points a,b,c on Fig.2 represent 33%, 50% , and 66% mixtures of explosive #13 and #8 respectively, their average molar weights calculated in a simple manner. Point d represents a 50/50 mixture if density were assumed equal to that of compound 8, point e, if density were assumed equal to that of compound 13; point b, which lies at the intersection with Curve IV, corresponds indeed to the average density 1.567, and to the average molar weight 258.830. This way, those explosives which lie close to the best-fit line can have the density of their mixtures estimated from the graph, the same way point b was calculated. A more universal fit embracing all explosives is being contemplated, to make full use of such techniques.

CONCLUSIONS

Further search for better fitting parameters is necessary. Those parameters must continue to maintain a well founded physical meaning.

Possibility of the existence of stronger explosives than HMX and RDX cannot be excluded. High value of F for Nitroguanidine (NQ in Fig.1) is intriguing, as well as the existence of a minimum at F = -0.3 for the energy-per- degree Kelvin-and-mole curve (Curve III).

DATB (2.4.6-Trinitro 1,3-Benzene Diamine #24) has almost identical properties to Tetryl (#15) in terms of the Taylor model (Table I). The same applies in lesser degree to points ## 11 and 12 (TNT and o-Dinitrobenzene) in Fig.1.

Techniques for rechecking or calculating densities, or H_f/H_c ratios can be improved to become generally useful and risk-free. The next step would be to apply the BKW model and the energy density concept to this type of systematization of explosives, as well as to compare the results with other methods of evaluation.

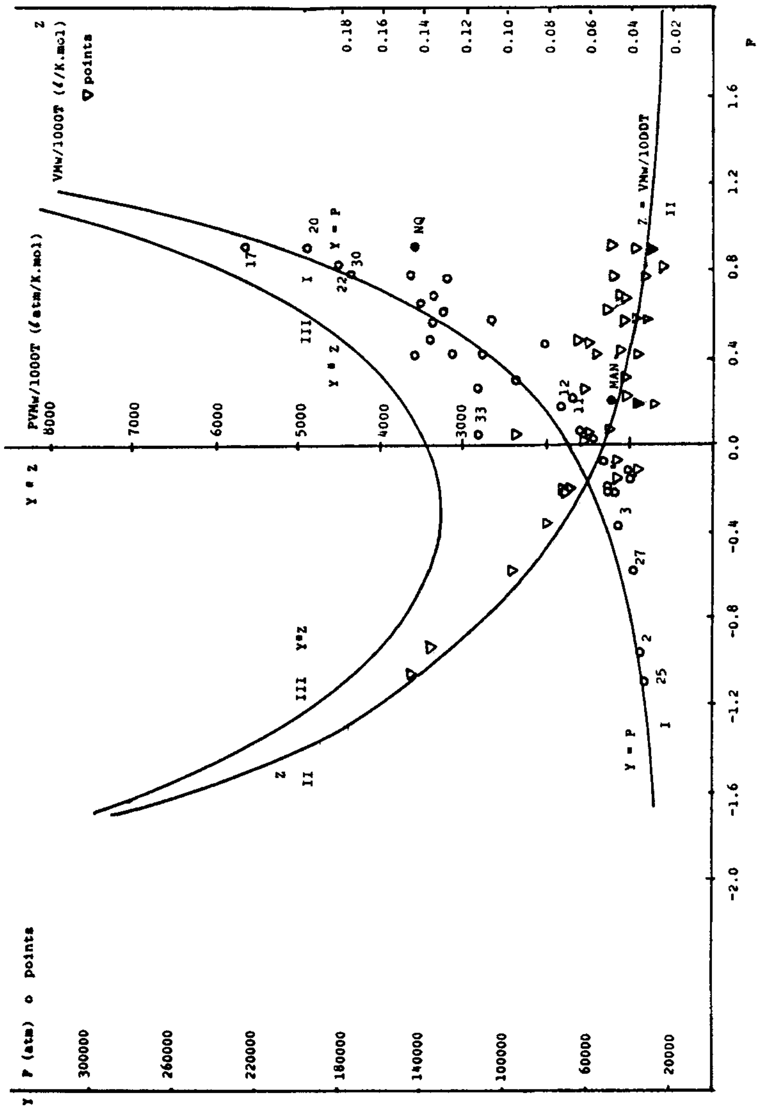

Fig.1 : Curve I: Presure vs F; Curve II: V*Mw/1000T ratio vs F; Curve III is the product of I*II plotted vs. parameter F. The thermodynamic values P,V, and T are from the Taylor (15,16) model. For reasons of clarity, only some points are numbered; their numbers correspond to Column A in Table I, and to the numbers in [] brackets in the text.

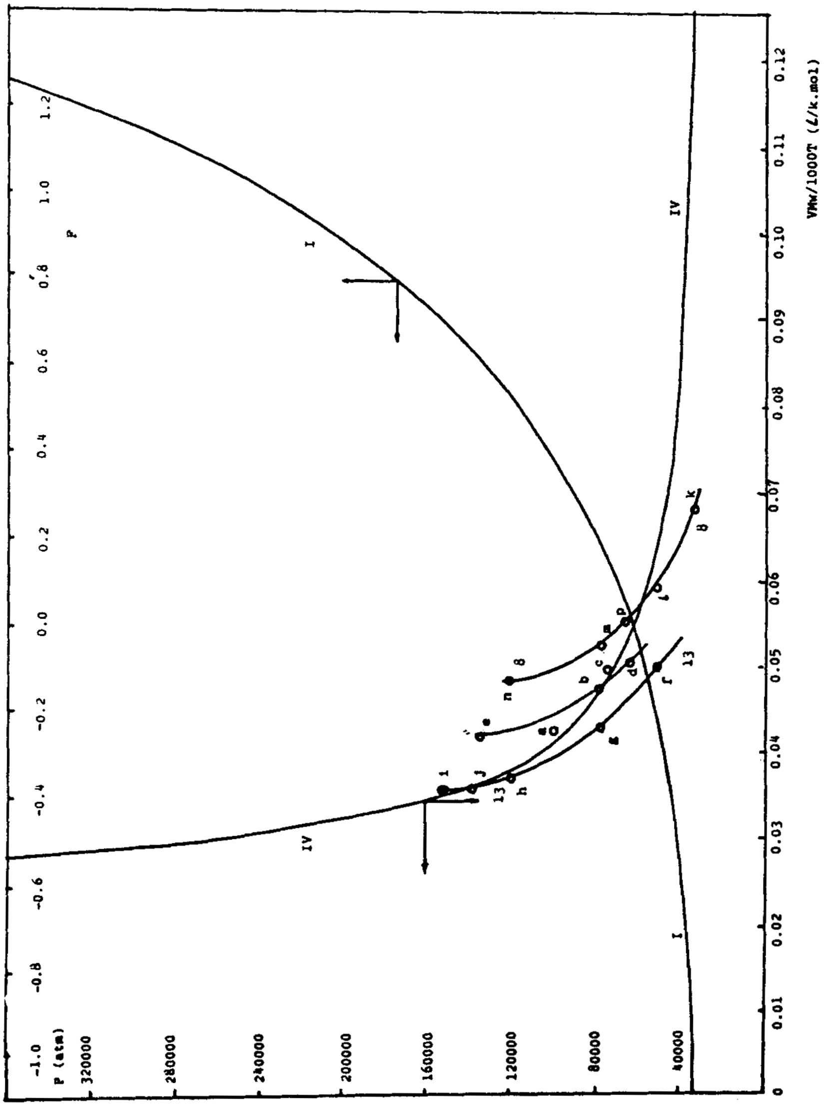

Fig.2 : Pressure plotted vs parameter F (Curve I), and vs the V*Mw/1000T ratio (Curve IV); P,V,T calculated from Taylor (15,16) model. Curves 8 and 13 help estimating densities for compounds #8 and #13, as well as for their mixtures.

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