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SENSITIVITY RELATIONSHIPS IN ENERGETIC MATERIALS

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In searching for new explosives one is most concerned with performance (detonation velocity and pressure), thermal properties, and sensitivity. Whether a new candidate explosive is ultimately widely used may well be determined by other factors, such as cost, toxicity, melting point, etc., but the initial research effort is guided by the trinity of performance, thermal stability, and sensitivity. This presents a difficult multifactoral problem in assessing the various molecular properties that contribute to each of these principal selection criteria. For instance, detonation velocity is affected by density, elemental composition, and heat of formation. These factors must be varied together in such a way as to maximize the combined effect on performance.

Sensitivity is a complex problem and there is no single useful definition. Tests of the sensitivity of an explosive are devised with the idea of judging the potential safety of use in a particular application. This immediately raises two questions: 1) How do different molecules rank within any given sensitivity test? 2) How do different sensitivity tests compare in ranking molecules?

An understanding of sensitivity is in large part a chemical problem. The ease with which a detectable reaction of any kind can be initiated in an explosive; the tendency of a small reaction, once established, to grow to destructive proportions; and the ease with which a high-order detonation can be established in an explosive all contribute to the materials response to the stimulus in a sensitivity test. These properties are a consequence of the kinetics and thermodynamics of the thermal decomposition of the explosive.

Weston et al. [1] have considered relationships among various shock sensitivity tests and Price [2-4] has considered a variety of factors important in shock sensitivity tests. Among the more sensitive explosives, correlations tend to be satisfactory between tests that rely on shock initiation. It is important to understand the critical factors in each test (small scale gap test, large scale gap test, radius of Extex primer in the minimum priming test, run distance to detonation in the wedge test (8.3 GPa), critical diameter for propagation in steady state detonation, critical flying plate kinetic energy fluence). In less sensitive explosives failure diameter effects appear to be the major problem in poor correlations.

Urizar et al. have considered the relations between four shock sensitivity tests [5] used at Los Alamos that initiate a detonation. These are the minimum priming charge, wedge, large scale gap and small scale gap tests. The tests reported in Ref. 5 were carried out on twenty one different materials made up under different conditions and in various compositions from seven pure explosives. They conclude "that the correlation is generally good, but that exceptions are numerous enough that no one test can be used with confidence as a measure of the detonation sensitivity of an explosive over a range of conditions of practical interest". Of the six possible cross-correlations among the four tests the poorest, surprisingly, was between the small-scale and large-scale gap tests

By far the most commonly used measure of an explosive's sensitivity is the drop-weight impact test. This is convenient, easy-to-run, and inexpensive. An important question is whether this test is indicative of the explosive's behavior under other circumstances, i.e., a shock stimulus. In a typical drop-weight impact test the time constant for reaction is in the range of 200-250 μs and the pressure is between 7-15 kbar. In a shock experiment the times range from 0.05-2.0 μs and the pressures range from 30-200 kbar. Is the mechanism of decomposition of the explosive at all similar under these rather different conditions?

A problem that one immediately encounters in approaching these questions is that only a limited number of compounds have been studied under well-controlled and defined conditions. For shock initiated studies the largest collection of information has been gathered by the Naval Surface Warfare Center (NSWC) using the Navy Small Scale Gap Test [6,7]. For drop-weight impact tests a large collection of consistent data is available from NSWC [8-12] and from the Los Alamos National Laboratory (LANL) [13-15].

In Table 1 we give the drop-weight impact sensitivity (h_{50},cm) and the shock sensitivity as measured by the NSWC small scale gap test (P_{90} the pressure in kbar required to initiate material pressed to 90% theoretical maximum density (TMD), P_{95} = 95% TMD, P_{98} = 98% TMD) for 21 explosives. The impact sensitivity given for TATB is estimated from oxygen balance correlations and will be discussed later.

If one selects from Table 1 a series of compounds that are closely related structurally, i.e. TNB, DIPAM, MATB, DATB, TATB, the correlation between the impact sensitivity and the shock sensitivity at 90% TMD ($h_{50} = 7.35P_{90}-27.44$, $R^2 = 0.99$) is excellent, Figure 1.

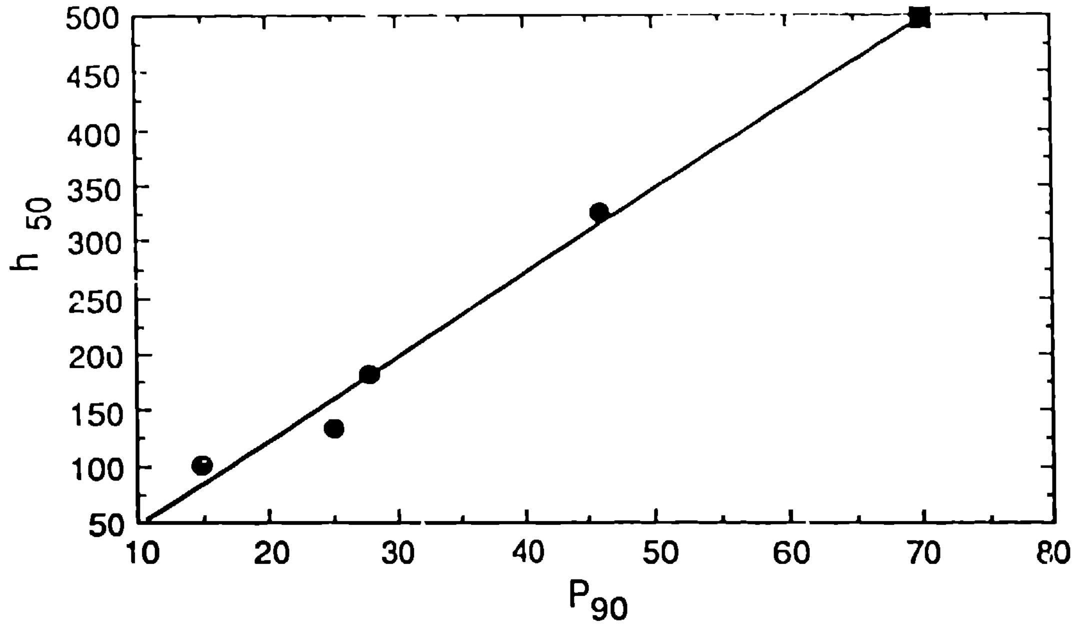

Figure 1. A plot of the drop-weight impact sensitivity (h_{50}) vs the NSWC small scale gap test shock sensitivity at 90% TMD for TNB, DIPAM, MATB, DATB, and TATB. Data from Table 1.

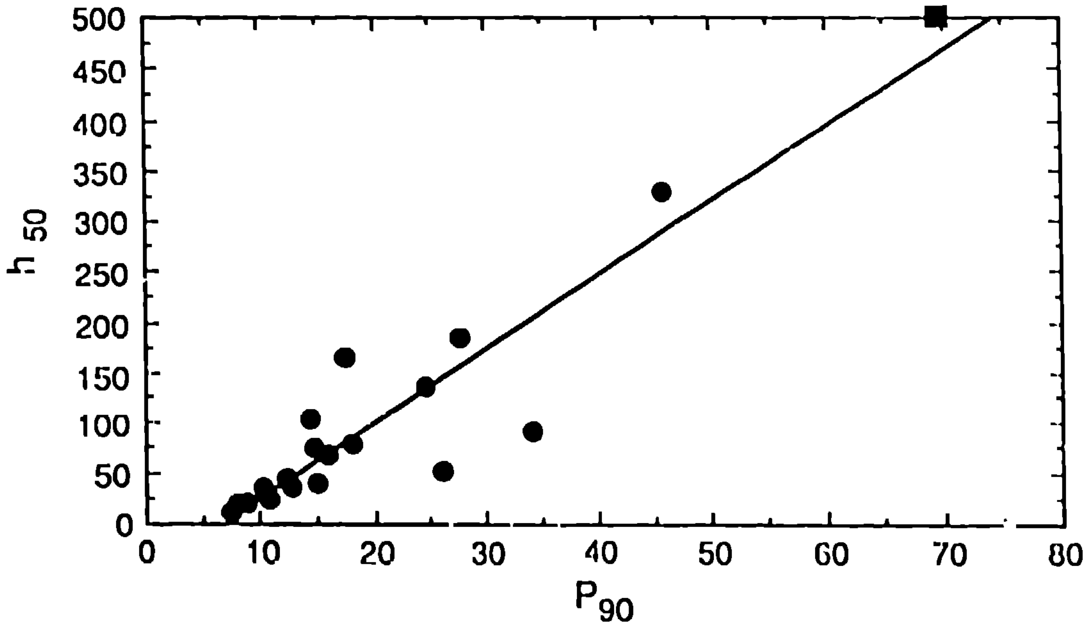

Figure 2. A plot of the drop weight impact sensitivity (h_{50}) vs the NSWC small scale gap test shock sensitivity at 90% TMD for the 21 explosives in Table 1.

TABLE 1. The impact and shock sensitivities of a variety of common explosives and their mixtures.

Compound	Composition	h_{50}[a] (cm)	P_{90}[b] (kbar)	P_{95}	P_{98}
PETN[c]	$C_5H_8N_4O_{12}$	12	7.47	10.76	13.69
Pentolite	50/50, PETN, TNT	18	8.21	11.73	15.18
TNETB[d]	$C_6H_6N_6O_{14}$	18	9.25	13.13	17.48
RDX[e]	$C_3H_6N_6O_6$	24	10.97	15.77	20.35
HMX[f]	$C_4H_8N_8O_8$	26	10.81	14.32	17.49
HNAB[g]	$C_{12}H_4N_8O_{12}$	32	12.77	18.11	22.48
Tetryl[h]	$C_7H_5N_5O_8$	32	10.64	15.14	19.42
Octol	75/25, HMX, TNT	42	12.62	19.23	25.98
Octol	65/35, HMX, TNT	42	12.30	18.50	26.02
HNS-I[i]	$C_{14}H_6N_6O_{12}$	47	26.26	30.15	32.90
HNS-II[j]	$C_{14}H_6N_6O_{12}$	39	15.03	20.29	24.70
Comp B	60/40, RDX, TNT	65	16.15	21.54	27.76
TNEDV[k]	$C_7H_9N_5O_{12}$	71	14.99	-----	-----
HNB[l]	$C_{12}H_4N_6O_{12}$	76	18.25	-----	-----
TACOT-z[m]	$C_{12}H_4N_8O_8$	85	34.43	41.26	-----
TNB[n]	$C_6H_3N_3O_6$	100	14.96	27.28	37.25
DIPAM[o]	$C_{12}H_6N_8O_{12}$	132	25.11	29.71	33.04
TNT[p]	$C_7H_5N_3O_6$	160	17.72	25.65	33.35
MATB[q]	$C_6H_4N_4O_6$	177	27.91	35.35	41.02
DATB[r]	$C_6H_5N_5O_6$	320	46.20	54.22	59.88
TATB[s]	$C_6H_6N_6O_6$	490[t]	70.38	121.92	164.86

a. The impact sensitivity (h_{50},cm) as measured at LANL and/or NSWC, using the Bruceton method, type 12 tools, 2.5 kg weight, 40 mg sample, 5/0 sandpaper, 25 trials. b. The shock sensitivity as measured by the NSWC small scale gap test, P_{90} the pressure in kbar required to initiate material pressed to 90% theoretical maximum density (TMD), P_{95}-95% TMD, P_{98}-98% TMD. c. Pentaerythritoltetranitrate. d. Trinitroethyltrinitrobutyrate. e. Cyclotrimethylenetrinitramine. f. Cyclotetramethylenetetranitramine. g. 2,2',4,4',6,6'-Hexanitroazobenzene. h. 2,4,6 Trinitrophenylmethylnitramine. i. Hexanitrostilbene (0.2 2 μ particle size). j. No particle size specification. k. Trinitroethyl 4,4 dinitrovalerate.

TABLE 1. (Continued)

l. 2,2',4,4,-6,6'-Hexanitrobiphenyl. m. 1,3,7,9-Tetranitrodibenzo-1,3a,4,6a-tetraazapentalene. n. Trinitrobenzene. o. 3,3'-Diamino-2,2',4,4',6,6'-Hexanitrobiphenyl. p. 2,4,6-Trinitrotoluene.
q. 2,4,6,-Trinitroaniline. r. 1,3-Diamino-2,4,6-trinitrobenzene.
s. 1,3,5-Triamino-2,4,6-trinitrobenzene. t. Estimated from oxygen balance of TNB, MATB, and DATB.

The correlation for this series between the shock sensitivity and 90% TMD and 95% TMD ($P_{95} = 1.74P_{90}-10.44$, $R^2 = 0.92$) is good and the correlation between the shock sensitivity at 95% TMD and 98% TMD ($P_{98} = 1.40P_{95}-7.79$, $R^2 = 0.99$) is excellent.

If one takes all 21 explosives listed in Table 1 and plots h_{50} vs P_{90} the correlation is not as good ($h_{50} = 7.23P_{90}-50.0$, $R^2 = 0.87$), as one might expect, Figure 2. There are three main outliers off of the principal regression line, HNS-I, TACOT, and TNT. HNS-I is a special grade of hexanitrostilbene that has a 0.2-2 μ particle size distribution. HNS-II, which has no particle size specification, lies close to the regression line. It is well accepted that a small particle size can reduce shock sensitivity at high density. TNT lies off of the regression in the other direction, i.e. it is somewhat more shock sensitive than its impact sensitivity would suggest. TNT has an unusually low melting point and it has been suggested that melting in the impact test makes it appear to be less sensitive. TACOT, the third extreme outlier is a zwitterionic heterocycle, has not been extensively characterized, and may be a true structural anomaly.

If these three outliers are removed the remaining 18 explosives give an excellent correlation ($h_{50} = 7.83P_{90}-54.25$, $R^2 = 0.99$), and this is the suggested regression for estimating the sensitivity of new materials. The shock sensitivity from 90% TMD to 95% TMD again correlates fairly well ($P_{95} = 1.55P_{90}-3.03$, $R^2 = 0.94$) and the correlation between 95% TMD and 98% TMD is excellent ($P_{98} = 1.33P_{95}-1.84$, $R^2 = 0.99$).

It is desireable to be able to estimate the sensitivity of proposed new materials. Even if only crude estimates can be made it is still useful for guidance for a synthetic effort. Kamlet [9-12] proposed a method for estimating impact sensitivity based on oxygen balance, which he defined as $OB_{100} = 100(2n_O-n_H-2n_C-2n_{COO})$/Molecular weight, where n_O, n_H, n_C, n_{COO} are the number of oxygen, hydrogen, carbon and carboxylate in the molecule. The problem has been considered by a number of other investigators [16-25]. Kamlet found reasonable correlations between OB_{100} and log h_{50} for broad classes of compounds, i.e. nitroaromatics, nitroaromatics with a ring methyl group, nitramines, nitroaliphatics, and dinitrofluoro compounds. It was pointed out that individual impact measurements have a large scatter, but that when a large number of measurements are averaged reasonably consistent results are obtained. The regressions reported by Kamlet and Adolph [9,12] for the various classes are:

1) Nitroaromatic, $\log h_{50} = 1.73-0.320B_{100}$
2) Nitroaromatic (alpha CH_3), $\log h_{50} = 1.33-0.260B_{100}$
3) Nitroaliphatic, $\log h_{50} = 1.74-0.230B_{100}$
4) Dinitrofluoro, $\log h_{50} = 2.14-0.300B_{100}$
5) Nitramine, $\log h_{50} = 1.37-0.170B_{100}$

Because of the multi-component nature of the sensitivity-performance problem in energetic materials it is highly desirable to have a system in which C,H,N,O explosives can be organized. Because the performance of an explosive is dependent only on relative composition, Stine [26] has proposed a system based on the geometric properties of a regular tetrahedron. The empirical formula for a $C_aH_bN_cO_d$ compound can be normalized so that:

$A+B+C+D=1$, where $A = a/n$, $B = b/n$, $C = c/n$, $D = d/n$, $n=a+b+c+d$ (Eq. 1).

This provides a convenient reference formula so different molecular compositions can be compared. 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 can arbitrarily be taken 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.

If the tetrahedron is centered at the origin of a cartesian coordinate system so that the four distances from any interior point to each of the four sides sum to unity, the coordinates on any interior point are: $X = \sqrt{2}(3D-1+C)/4$; $Y = \sqrt{6}(A-B)/4$; $Z = C-1/4$; where A,B,C, and D are as given in Eq. 1. Two oxygen balance planes can now be defined; one containing the normalized points for CO, H_2O, and N_2 and the other containing the points for CO_2, H_2O, and N_2. The two definitions of oxygen balance (balance to CO or CO_2) are then the perpendicular distances from the point to the respective plane. Illustrations of this tetrahedral representation are given in ref. 26.

We have chosen as an index of sensitivity the distance of a point from the CO oxygen-balance plane. This sensitivity index is then defined as $SI = 100(d-a-(b/2)-nCO)/5(a+b+c+d)$, where a,b,c,d are the coefficients of C,H,N,O, and nCO corresponds to the number of carbonyl groups in the molecule. This sensitivity index transforms to Kamlet's definition as $OBK = 0.8/SI-0.05$, $R^2 = 0.99$, for the 38 compounds in ref. 9.

In Tables 2-15 we have compiled the impact sensitivities for the compounds reported in Refs. 8-15. The compounds are grouped together by structural type. Table 2 reports nitroaromatic explosives (40 compounds); Table 3, nitroaromatic explosives with an alpha C-H linkage (17 compounds); Table 4, nitropyridine explosives (6 compounds); Table 5, nitroimidazole explosives (10 compounds); Table 6, nitropyrazole explosives (8 compounds); Table 7, nitrofurazan and nitrooxadiazole explosives (7 compounds); Table 8, nitro-1,2,4-triazole explosives (18 compounds); Table 9, nitro-1,2,3-triazole explosives (16 compounds); Table 10, nitropyrimidine explosives (4 compounds); Table 11, nitroaliphatic explosives (7 compounds); Table 12, nitroaliphatic explosives containing other functional groups (44 compounds); Table 13, nitramine explosives (61 compounds); Table 14, nitrate ester explosives (7 compounds); and Table 15, miscellaneous nitroheterocyclic explosives (13 compounds), providing impact sensitivity information on 258 pure explosives. Since the methods discussed here depend on having a close structural analogy, this wide variety of information is provided.

In Figure 3 the sensitivity index (SI) is plotted against the impact sensitivity (log h_{50}) for 40 nitroaromatic compounds from Table 2. This is very much the same result as obtained by Kamlet [9]. The correlation for the original set of nitroaromatics reported by Kamlet and Adolph [9] of OB_{100} vs log h_{50} is $R^2 = 0.866$; for the correlation of SI vs log h_{50} R^2 is 0.836, essentially the same. The overall regression for the 40 compounds in Table 2 is log $h_{50} = 1.72-0.19SI$, $R^2 = 0.639$.

If one considers groups of compounds that are structurally closely related the relation between impact sensitivity (log h_{50}) and SI are excellent. In Figure 4 we plot log h_{50} vs SI for TNB, MATB and DATB (Table 2, Nos. 5,12,15). This series gives an excellent correlation. If this is extrapolated to the SI of TATB (Tables 2-18) an impact sensitivity of 490 cm is predicted. This is the value used in Table 1 and in Figures 1 and 2. A similar value would be predicted from the h_{50} vs P_{90} plots in Figures 1 and 2.

Several of the families of compounds in Table 2 have excellent correlations between log h_{50} and SI, i.e.

polynitroanilines (2-4,9,12), log $h_{50} = 1.75-0.24SI$, $R^2 = 0.997$

polynitrobenzenes (2-1,3,5), log $h_{50} = 1.70-0.13SI$, $R^2 = 0.938$

polyaminopolynitrobenzenes (2-1,2,5), log $h_{50} = 0.58-0.84SI$, $R^2 = 0.998$

polynitrophenols (2-6,7,8,10,11,21,23,30,31), log $h_{50} = 1.72-0.28\ SI$, $R^2 = 0.895$.

The apparent scatter of points in Figure 3 is then the result of a series of families of crossing straight lines with rather different slopes and intercepts. If one wishes to estimate the impact sensitivity of a proposed explosive, and it is in any way related to known compounds, as closely related a series as possible should be chosen for interpolation or extrapolation to the appropriate SI value.

TABLE 2. The drop-weight impact sensitivities of nitroaromatic explosives.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	Hexanitrobenzene	$C_6N_6O_{12}$	348	5.00	12	13
2	Benzotrifuroxan	$C_6N_6O_6$	252	0.00	50	13
3	1,2,4,5-Tetranitrobenzene	$C_6H_2N_4O_8$	258	1.00	27	13
4	2,3,4,5,6-Pentanitroaniline	$C_6H_2N_6O_{10}$	318	2.50	15	9
5	1,3,5-Trinitrobenzene	$C_6H_3N_3O_6$	213	-1.67	100	9
6	Picric acid	$C_6H_3N_3O_7$	229	-0.53	87	9
7	2,4,6-trinitroresorcinol	$C_6H_3N_3O_8$	245	0.50	43	9
8	2,4,6-Trinitrophloroglucinol	$C_6H_3N_3O_9$	261	1.43	27	9
9	2,3,4,6-tetranitroaniline	$C_6H_3N_5O_8$	273	0.45	41	9
10	2,4-Dinitroresorcinol	$C_6H_4N_2O_6$	200	-2.22	296	9
11	4,6-Dinitroresorcinol	$C_6H_4N_2O_6$	200	-2.22	>320	9
12	2,4,6-Trinitroaniline	$C_6H_4N_4O_6$	228	-2.00	177	9
13	2,4,6-Trinitro-3-aminophenol	$C_6H_4N_4O_7$	244	-0.95	138	9
14	2,3,4,6-Tetranitroaniline	$C_6H_4N_6O_8$	288	0.45	41	8
15	1,3-diamino-2,4,6-trinitrobenzene	$C_6H_5N_5O_6$	243	-2.27	320	9
16	1-Hydroxy-3,5-diamino-2,4,6-trinitrobenzene	$C_6H_5N_5O_7$	259	-1.30	120	8
17	Ammomium picrate	$C_6H_6N_4O_7$	246	-1.74	135	13
18	1,3,5-Triamino-2,4,6-trinitrobenzene	$C_6H_6N_6O_6$	258	-2.50	>320	8
19	2,4,6-Trinitrobenzonitrile	$C_7H_2N_4O_6$	238	-2.11	140	9
20	2,4,6-Trinitrobenzoic acid	$C_7H_3N_3O_8$	257	-1.43	109	9
21	2,4,6-Trinitroanisole	$C_7H_5N_3O_7$	243	-2.27	192	9
22	3-Methoxy-2,4,6-trinitroaniline	$C_7H_6N_4O_7$	258	-2.50	>320	9
23	1,3-Dimethoxy-2,4,6-trinitrobenzene	$C_8H_7N_3O_8$	273	-2.69	251	9
24	2',2',2'-Trinitroethyl-2,4,6-trinitrobenzoate	$C_9H_4N_6O_{14}$	420	1.21	24	9

TABLE 2. (Continued)

No.	Compound	Formula	Mol Wt.	SI	h_{50} (cm)	Ref.
25	2',2',2'-Trinitroethyl-3,5-dinitrobenzoate	$C_9H_5N_5O_{12}$	375	-0.32	73	9
26	2',2',2'-Trinitroethyl-3,5-dinitrosalicylate	$C_9H_5N_5O_3$	391	0.31	45	9
27	1,4,5,8-tetranitronapthalene	$C_{10}H_4N_4O_8$	308	-3.08	100	8
28	2',2'-Dinitropropyl-2,4,6-trinitrobenzoate	$C_{10}H_7N_5O_{12}$	389	-1.23	214	9
29	2,2',4,4',6,6'-Hexanitrobiphenyl	$C_{12}H_4N_6O_{12}$	424	-1.18	85	9
30	3-hydroxy-2,2',4,4',6,6'-hexanitrobiphenyl	$C_{12}H_4N_6O_{13}$	440	-0.57	42	9
31	3,3'-dihydroxy-2,2',4,4'-6,6'-hexanitrobiphenyl	$C_{12}H_4N_6O_{14}$	456	0.00	40	9
32	2,2',4,4',6,6'-Hexanitrodiphenylamine	$C_{12}H_5N_7O_{12}$	439	-1.09	48	9
33	3,3'-Diamino-2,2',4,4'-6,6'-hexanitrobiphenyl	$C_{12}H_6N_8O_{12}$	454	-1.58	132	9
34	2,2',4,4',6-Pentanitrobenzophenone	$C_{13}H_4N_5O_{11}$	407	-1.12	54	8
35	2,2',2",4,4',4",6,6',6"-nonanitro-m-terphenyl	$C_{18}H_5N_9O_{18}$	635	-1.00	39	8
36	2,2",4,4',4",6,6',6"-Octanitro-m-terphenyl	$C_{18}H_6N_8O_{16}$	590	-2.08	63	8
37	2,2',2",4,4",5',6,6"-Octanitro-p-terphenyl	$C_{18}H_6N_8O_{16}$	590	-2.08	40	8
38	2,2',2",4,4",6,6',6"-octanitro-p-terphenyl	$C_{18}H_6N_8O_{16}$	590	-2.08	59	8
39	Dodecanitroquaterphenyl	$C_{24}H_6N_{12}O_{24}$	846	-0.88	40	8
40	Azo-bis-2,2',4,4',6,6'-hexanitrobiphenyl	$C_{24}H_6N_{14}O_{24}$	874	-0.88	40	8

TABLE 3. The drop-weight impact sensitivities of nitroaromatic explosives with an alpha C-H linkage.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	2,4,6-Trinitrobenzaldehyde	$C_7H_3N_7O_7$	271	-2.08	36	9
2	2,4,6-Trinitrobenzaldoxime	$C_7H_4N_4O_7$	256	-1.82	42	9
3	2,4,6-Trinitrotoluene	$C_7H_5N_3O_6$	227	-4.09	160	9
4	1-Dinitromethyl-3-nitrobenzene	$C_7H_5N_3O_6$	227	-4.09	105	8
5	2,4,6-Trinitrobenzyl alcohol	$C_7H_5N_3O_7$	243	-2.27	52	9
6	2,4,6-Trinitro-m-cresol	$C_7H_5N_3O_7$	243	-2.27	191	9
7	1-(2,2,2-Trinitroethyl)-2,4,6-trinitrobenzene	$C_8H_4N_6O_{12}$	376	1.33	13	9
8	2,4,6-Trinitrostyrene	$C_8H_5N_3O_6$	239	-3.41	32	8
9	1-(2,2,2-Trinitroethyl)-2,4 dinitrobenzene	$C_8H_5N_5O_{10}$	331	-0.36	31	9
10	3,5-Dimethyl-2,4,6-trinitrophenol	$C_8H_7N_3O_7$	257	-3.60	77	9
11	1-(3,3,3 trinitropropyl)-2,4,6-trinitrobenzene	$C_9H_6N_6O_{12}$	390	0.00	21	9
12	1-(3,3,3-trinitropropyl)-2,4-dinitrobenzene	$C_9H_7N_5O_{10}$	345	-1.61	31	8
13	3-Methyl-2,2',4,4',6,6'-hexanitrobiphenyl	$C_{13}H_6N_6O_{12}$	438	-2.16	53	9
14	3-Methyl-2,2',4,4',6,-pentanitrobiphenyl	$C_{13}H_7N_5O_{10}$	393	-3.71	143	9
15	Hexanitrostilbene	$C_{14}H_6N_6O_{12}$	450	-2.63	39	8
16	2,2',4,4',6,6'-Hexanitrobibenzyl	$C_{14}H_8N_6O_{12}$	452	-3.00	114	9
17	3,3'-Dimethyl-2,2',4,4',6,6'-hexanitrobiphenyl	$C_{14}H_8N_6O_{14}$	452	-1.90	135	9

TABLE 4. The drop-weight impact sensitivities of nitropyridine explosives.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	2,4,6-Trinitropyridine-1-oxide	$C_5H_2N_4O_7$	230	1.11	20	13
2	3,3',5,5'-Tetranitro-2,2'-azopyridine	$C_{10}H_4N_8O_8$	364	-2.67	56	13
3	2,6-bis-(picrylazo)-3,5-dinitropyridine	$C_{17}H_5N_{13}O_{16}$	647	-1.37	33	13
4	2,6-bis-(picrylamino)-3,5-dinitropyridine	$C_{17}H_7N_{11}O_{16}$	621	-1.76	63	13
5	3,5-bis-(picrylamino)-2,6-dinitropyridine	$C_{17}H_7N_{11}O_{16}$	621	1.76	92	13
6	2,6-bis(picrylamino)-pyridine	$C_{17}H_9N_9O_{12}$	531	-4.04	192	13

TABLE 5. The drop-weight impact sensitivities of nitroimidazole explosives.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	2,4,5-Trinitro-imidazole	$C_3HN_5O_6$	203	3.33	68	13
2	2,7-Dinitroimidazole	$C_3H_2N_4O_4$	158	0.00	105	13
3	Ammonium-2,4,5-trinitroimidazole	$C_3H_4N_6O_6$	220	0.88	50	13
4	Ammonium-4,5-dinitroimidazole	$C_3H_5N_5O_4$	175	-1.76	77	13
5	4,4',5,5'-Tetranitro-biimidazole	$C_6H_2N_8O_8$	314	0.83	37	13
6	Diammonium-4,4',5,5'-tetranitrobiimidazolate	$C_6H_8N_{10}O_8$	348	-1.25	105	13
7	2,4-Dinitro-1-picryl-imidazole	$C_9H_3N_7O_{10}$	369	-0.34	46	13
8	2-Nitro-1-picryl-imidazole	$C_9H_4N_6O_8$	324	-2.22	112	13
9	4-Nitro 1-picryl-imidazole	$C_9H_4N_6O_8$	324	-2.22	161	13
10	1-Picrylimidazole	$C_9H_5N_5O_6$	279	4.40	314	13

TABLE 6. The drop-weight impact sensitivities of nitropyrazole explosives.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	Ammonium 3,5-dinitropyrazole	$C_3H_5N_5O_4$	175	-1.76	158	13
2	4-Nitro-1-picrylpyrazole	$C_9H_4N_6O_8$	324	-2.22	112	13
3	4-Nitro-3-picrylaminopyrazole	$C_9H_5N_7O_8$	339	-2.41	>320	13
4	3,5-Dinitro-1-methyl-4-picrylpyrazole	$C_{10}H_5N_7O_{10}$	383	-1.56	118	13
5	3,5-Dinitro-1-methyl-4-picrylaminopyrazole	$C_{10}H_6N_8O_{10}$	398	-1.76	274	13
6	1,4-Dipicrylpyrazole	$C_{15}H_6N_8O_{12}$	490	-2.93	314	13
7	4-Nitro-1-picryl-3-picrylaminopyrazole	$C_{15}H_6N_{10}O_{14}$	550	-1.78	149	13
8	5-Nitro-1-picryl-4-picrylaminopyrazole	$C_{15}H_6N_{10}O_{14}$	550	-1.78	>320	13

TABLE 7. The drop-weight impact sensitivities of nitrofurazan and nitrooxadiazole explosives.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	3-Amino-4-nitrofurazan	$C_2H_2N_4O_3$	130	0.00	27	13
2	4,4'-Dinitro-3,3'-bifurazan	$C_4N_6O_6$	228	2.50	13	13
3	3-Nitro-4-picrylaminofurazan	$C_8H_3N_7O_9$	341	-0.37	60	13
4	3-Amino-4-picrylaminofurazan	$C_8H_5N_7O_7$	311	-2.59	120	13
5	2-5-Dipicryl-1,3,4-oxadiazole	$C_{14}H_4N_8O_{13}$	504	-1.54	20	8
6	3,4-Bis-(picrylamino)-furazan	$C_{14}H_6N_{10}O_{13}$	522	-1.86	71	13
7	3,5-Bis-(picrylamino)-1,2,4-oxadiazole	$C_{14}H_6N_{10}O_{13}$	522	1.86	95	13

TABLE 8. The drop-weight impact sensitivities of nitro-1,2,4- triazole explosives.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	3-Nitro-1,2,4-triazole	$C_2H_2N_4O_2$	114	-2.00	>320	13
2	3-Nitro-1,2,4-triazole-5-one	$C_2H_2N_4O_3$	130	1.82	291	14,15
3	Ammonium 3-nitro-1,2,4-triazolate	$C_2H_5N_5O_2$	131	-3.57	>320	13
4	Ammonium 3,5-dinitro-1,2,4-triazolate	$C_2H_4N_6O_4$	176	0.00	110	13
5	4-Methyl-3,5-dinitro-1,2,4-triazole	$C_3H_3N_5O_4$	173	-0.67	155	8
6	5,5'-Dinitro-3,3'-bi-1,2,4-triazole	$C_4H_2N_8O_4$	226	-1.11	153	13
7	4-(2-Nitroethyl)-3,5-dinitro-1,2,4-triazole	$C_4H_4N_6O_6$	232	0.00	35	8
8	3-Nitro-1-picryl-1,2,4-triazole	$C_8H_3N_7O_8$	325	-1.15	68	13
9	1-Picryl-1,2,4-triazole	$C_8H_5N_5O_{10}$	280	-3.33	>320	13
10	3,Picrylamino-1,2,4-triazole	$C_8H_5N_7O_6$	295	-3.46	>320	13
11	4-Picrylamino-1,2,4-triazole	$C_8H_5N_7O_6$	295	-3.46	314	13
12	3-Amino-5-picrylamino 1,2,4-triazole	$C_8H_6N_8O_6$	310	-3.57	230	13
13	4-(2,4-Dinitrobenzyl) 3,5-dinitro-1,2,4-triazole	$C_9H_5N_7O_8$	339	-2.41	96	8
14	4-(4-Nitrobenzyl)-3,5-dinitro-1,2,4-triazole	$C_9H_6N_6O_6$	294	-4.44	>320	8
15	2-Picryl-3 picrylamino-1,2,4-triazole	$C_{14}H_6N_{10}O_{12}$	506	2.38	>320	13
16	3,5-Bispicrylamino-1,2,4-triazole	$C_{14}H_7N_{11}O_{12}$	521	-2.50	240	13
17	N,N'Dipicryl-5,5'-dinitro-3,3'-bi-1,2,4-triazole	$C_{16}H_4N_{14}O_{16}$	648	-0.80	138	13
18	5,5'-Bispicrylamino-3,3'-bi-1,2,4-triazole	$C_{16}H_8N_{14}O_{12}$	588	1.20	>320	13

TABLE 9. The drop-weight impact sensitivities of nitro-1,2,3-triazoles.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	4-Nitro-1,2,3-triazole	$C_2H_2N_4O_2$	114	2.0	25	13
2	Ammonium 4-nitro-1,2,3-triazole	$C_2H_5N_5O_2$	131	-3.57	235	13
3	4-Nitro-1-picryl-1,2,3-triazole	$C_8H_3N_7O_8$	325	-1.15	9	13
4	4-Nitro-1-picryl-1,2,3-triazole	$C_8H_3N_7O_8$	325	-1.15	67	13
5	1-(3',5'-dinitrophenyl)-4-nitro-1,2,3-triazole	$C_8H_4N_6O_6$	280	-3.33	56	13
6	1-(3',4'-dinitrophenyl)-4-nitro-1,2,3-triazole	$C_8H_4N_6O_6$	280	-3.33	51	13
7	1-Picryl-1,2,3-triazole	$C_8H_4N_6O_6$	280	-3.33	10	13
8	2-Picryl-1,2,3-triazole	$C_8H_4N_6O_6$	280	-3.33	200	13
9	1-(3'-Amino-2',4',6'-trinitrophenyl)-1,2,3-triazole	$C_8H_5N_7O_6$	295	-3.46	31	13
10	4-Picrylamino-1,2,3-triazole	$C_8H_5N_7O_6$	295	-3.46	103	13
11	4,6-Dinitro-1-picryl-benzotriazole	$C_{12}H_4N_8O_{10}$	420	-2.35	40	13
12	5,6-Dinitro-1-picryl-benzotriazole	$C_{12}H_4N_8O_{10}$	420	-2.35	35	13
13	1-Picryl-4-picrylamino-1,2,3-triazole	$C_{14}H_6N_{10}O_{12}$	506	2.38	35	13
14	2,6-Dipicrylbenzo-[1,2-d:4,5-d']-bistriazole-4,8-dione	$C_{18}H_4N_{12}O_{14}$	612	3.33	95	13
15	1,7-dipicrylbenzo [1,2-d:4,5-d']-bistriazole	$C_{18}H_6N_{12}O_{12}$	582	3.75	38	13
16	1,5-Dipicrylbenzo-[1,2-d:4,5-d']-bistriazole	$C_{18}H_6N_{12}O_{12}$	582	-3.75	40	13

TABLE 10. The drop-weight impact sensitivities of nitropyrimidine explosives.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	2,4,6,2'2",4",6"-heptanitro-4',6'-diaza-m-terphenyl	$C_{16}H_5N_9O_{14}$	547	-2.05	58	8
2	2,4,6,4',2",4",6"-heptanitro-2',6'-diaza-m-terphenyl	$C_{16}H_5N_9O_{14}$	547	-2.05	58	8
3	1-picryl-2-picrylamino-1,2-dihydropyrimidine	$C_{16}H_7N_9O_{12}$	517	-3.41	106	13
4	5-Nitro-2,4,6-tris-(picrylamino)-pyrimidine	$C_{22}H_9N_{15}O_{20}$	803	-1.97	201	13

TABLE 11. The drop-weight impact sensitivities of nitroaliphatic explosives.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	1,1,1,3 tetranitrobutane	$C_4H_6N_4O_8$	238	0.91	33	10
2	1,1,1,3,5,5,5-heptanitropentane	$C_5H_5N_7O_{14}$	387	4.19	8	10
3	1,1,1,6,6,6-hexanitro-3-hexyne	$C_6H_4N_6O_{12}$	352	2.96	7	8
4	1,1,1,6,6,6-hexanitro-3-hexene	$C_6H_6N_6O_{12}$	354	2.00	17	8
5	3,3,4,4-tetranitro-hexane	$C_6H_{10}N_4O_8$	266	-2.14	80	10
6	2,2,4,4,6,6-hexanitroheptane	$C_7H_{10}N_6O_{12}$	370	0.00	29	10
7	2,2,4,6,6 pentanitroheptane	$C_7H_{11}N_5O_{10}$	325	-1.52	56	10

TABLE 12. The drop-weight impact sensitivities of nitroaliphatic explosives containing other functional groups

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	2,2,2-Trinitroethylcarbamate	$C_3H_4N_4O_8$	224	2.11	18	10
2	2,2-Dinitro-1,3-propanediol	$C_3H_6N_2O_6$	166	0.00	110	10
3	Methyl-2,2,2-trinitroethyl carbonate	$C_4H_5N_3O_9$	239	1.43	28	10
4	4,4,4-Trinitrobutyramide	$C_4H_6N_4O_7$	222	-0.95	40	8
5	Bis-(2,2,2-trinitroethyl)-carbonate	$C_5H_4N_6O_{15}$	388	4.67	16	10
6	Methylene-bis-N,N'-(2,2,2-trinitroacetamide)	$C_5H_4N_8O_{14}$	400	3.23	9	10
7	Bis-(trinitroethoxy)-methane	$C_5H_6N_6O_{14}$	374	3.87	17	8
8	N,N'-Bis-(2,2,2-trinitroethyl)-urea	$C_5H_6N_8O_{13}$	386	2.50	17	10
9	5,5,5-Trinitropentanone-2	$C_5H_7N_3O_7$	221	-2.27	125	10
10	Ethyl-2,2,2-trinitroethylcarbonate	$C_5H_7N_3O_9$	253	-0.42	81	10
11	N-(2-Propyl)-trinitroacetamide	$C_5H_8N_4O_7$	236	-2.50	112	8
12	Bis-(trinitroethyl)-oxalate	$C_6H_4N_6O_{16}$	416	3.75	15	8
13	2,2,2-Trinitroethyl-4,4,4-trinitrobutyrate	$C_6H_6N_6O_{14}$	386	2.50	18	10
14	Bis-(trinitroethyl) oxamide	$C_6H_6N_8O_{14}$	414	1.76	13	8
15	Trinitroethyl 2,2-dinitropropylcarbonate	$C_6H_7N_5O_{13}$	357	1.61	15	8
16	N-Trinitroethyl 4,4,4-trinitrobutyramide	$C_6H_7N_7O_{13}$	385	1.52	18	8
17	1,5-Bis-(trinitroethyl) biuret	$C_6H_7N_9O_{14}$	429	1.39	24	8
18	N-(t-Butyl) trinitroacetamide	$C_6H_{10}N_4O_7$	250	-3.70	110	8
19	Tris-(2,2,2-trinitroethyl) orthoformate	$C_7H_7N_9O_{21}$	553	4.77	7	10

TABLE 12. (Continued)

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
20	1,1,1,7,7,7-Hexanitroheptanone-4	$C_7H_8N_6O_{13}$	384	0.59	34	10
21	Methylene-bis-(trinitroethyl)-carbamate	$C_7H_8N_8O_{16}$	460	1.54	27	8
22	2,2-Dinitropropyl-trinitrobutyrate	$C_7H_9N_5O_{12}$	355	-0.30	151	8
23	2,2,2-Trinitroethyl-4,4-dinitrovalerate	$C_7H_9N_5O_{12}$	355	-0.30	70	10
24	Bis-(2,2-dinitropropyl)-carbonate	$C_7H_{10}N_4O_{11}$	326	-1.25	300	10
25	2,2 Dinitropropyl-4,4,4-trinitrobutyramide	$C_7H_{10}N_6O_{11}$	354	-1.18	72	10
26	Bis-(trinitropropyl)-urea	$C_7H_{10}N_8O_{13}$	414	0.00	23	8
27	Bis-(1,1,1-trintro-2-propyl)-urea	$C_7H_{10}N_8O_{13}$	414	0.00	19	8
28	Bis-(trinitroethyl)-fumarate	$C_8H_6N_6O_{16}$	442	1.67	14	8
29	Trinitroethyl-bis-(trinitroethoxy)-acetate	$C_8H_7N_9O_{22}$	581	4.13	6	8
30	4,4,4-Trinitrobutyric anhydride	$C_8H_8N_6O_{15}$	428	0.54	30	10
31	Bis-(2,2,2-trinitroethyl)-succinate	$C_8H_8N_6O_{16}$	444	1.05	30	10
32	Bis-(2,2-dinitropropyl)-oxalate	$C_8H_{10}N_4O_{12}$	354	-1.76	227	10
33	N,N'-Bis-(3,3,3-trinitropropyl)-oxamide	$C_8H_{10}N_8O_{14}$	442	-0.50	45	10
34	2,2,2-Trinitroethyl-4,4-dinitrohexanoate	$C_8H_{11}N_5O_{12}$	369	-1.39	138	10
35	2,2-Dinitrobutyl-4,4,4-trinitrobutyramide	$C_8H_{11}N_5O_{12}$	369	-1.39	101	10
36	2,2-dinitropropyl-4,4-dinitrovalerate	$C_8H_{12}N_4O_{10}$	324	-2.94	>320	10
37	Nitroisobutyl-4,4,4-trinitrobutyrate	$C_8H_{12}N_4O_{10}$	324	-2.94	279	10
38	Tetrakis-(2,2,2-trinitroethyl)-orthocarbonate	$C_9H_8N_{12}O_{28}$	732	5.26	7	10
39	Methylene-bis-(4,4,4-trinitrobutyramide)	$C_9H_{12}N_8O_{14}$	456	1.40	113	10
40	Ethylene-bis-(4,4,4-trinitrobutyrate)	$C_{10}H_{12}N_6O_{16}$	472	0.91	120	10
41	N,N-Bis-(2,2-dinitropropyl)-4,4,4-trinitrobutyramide	$C_{10}H_{14}N_8O_{15}$	486	1.28	72	10

TABLE 12. (Continued)

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
42	Bis-(2,2,2-trinitroethyl)-4,4-dinitroheptanedioate	$C_{11}H_{12}N_8O_{20}$	576	0.39	68	10
43	2,2-Dinitropropane-1,3-1,3-diol-bis-(4,4,4-trinitrobutyrate)	$C_{11}H_{12}N_8O_{20}$	576	0.39	50	10
44	Bis-(2,2,2 Trinitroethyl)-4,4,6,6,8,8-hexanitro-undecanedioate	$C_{15}H_{16}N_{12}O_{28}$	812	0.85	32	10

TABLE 13. The drop-weight impact sensitivities of nitramine explosives.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	N,N'-Dintiro-methanediamine	$CH_4N_4O_4$	136	1.54	13	10
2	N-Nitro-N-methyl-formamide	$C_2H_4N_2O_3$	104	-3.64	320	13
3	N,N'-Dinitro-1,2-ethanediamine	$C_2H_6N_4O_4$	150	-1.25	34	10
4	Methyl-2,2,2-trinitro-ethylnitramine	$C_3H_5N_5O_8$	239	2.38	9	10
5	Trinitroethyl-nitroguanidine	$C_3H_5N_7O_8$	267	2.17	15	8
6	Cyclotrimethylene-trinitramine	$C_3H_6N_6O_6$	222	0.00	26	10
7	N-Methyl-N,N'-dinitro-1,2-ethanediamine	$C_3H_8N_4O_4$	164	-3.16	114	10
8	Trinitroethyl-cyanomethylnitramine	$C_4H_4N_6O_8$	264	1.82	11	8
9	Bis-(2,2,2-trinitro-ethyl)-nitramine	$C_4H_4N_8O_{14}$	388	5.33	5	10
10	N-Methyl-N-nitro-(trinitroethyl)-carbamate	$C_4H_5N_5O_{10}$	283	2.08	17	8
11	N,N'-dimethyl-N,N'-dinitrooxamide	$C_4H_6N_4O_6$	206	-3.00	79	8
12	N-Nitro-N-(trinitro-ethyl)-glycinamide	$C_4H_6N_6O_9$	282	0.80	17	8
13	Cyclotetramethylene-tetranitramine	$C_4H_8N_8O_8$	296	0.00	29	10
14	N,N'-Dinitro-N-[2-(nitroamino)ethyl]-1,2-ethanediamine	$C_4H_{10}N_6O_6$	238	-2.31	39	10
15	1,3,3,5,5-Pentanitro-piperidine	$C_5H_6N_6O_{10}$	310	1.48	14	10
16	2,2,2-Trinitroethyl-3',3',3'-trinitropropyl-nitramine	$C_5H_6N_8O_{14}$	402	3.64	6	10
17	N,N'-Bis-2,2,2-trinitro-ethyl)-N,N'-dinitro-methanediamine	$C_5H_6N_{10}O_{16}$	462	4.32	5	10
18	Trinitroethyl-N-ethyl-N-nitro-carbamate	$C_5H_7N_5O_{10}$	297	0.37	19	8
19	Trinitroethyl-2-methoxy-ethylnitramine	$C_5H_9N_5O_9$	28[illegible]	-0.36	42	8

TABLE 13. (Continued)

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
20	N-methyl-N'-trinitroethyl-N,N'-dinitro-1,2,-ethanediamine	$C_5H_9N_7O_{10}$	327	0.32	11	10
21	N,N'-3,3-Tetranitro-1,5-pentanediamine	$C_5H_{10}N_6O_8$	282	-1.38	35	10
22	N-nitro-N-(3,3,3-trinitropropyl)-2,2,2-trinitroethyl carbamate	$C_6H_6N_8O_{16}$	446	3.33	9	10
23	2,2,2-Trinitroethyl-N-(2,2,2-trinitroethyl)-nitramino acetate	$C_6H_6N_8O_{16}$	446	3.33	9	10
24	2,2,2-trinitroethyl-4-nitrazavalerate	$C_6H_9N_5O_{10}$	311	-1.00	35	10
25	Trinitropropyl-(2,2 dinitropropyl)-nitramine	$C_6H_9N_7O_{12}$	371	0.88	17	8
26	2',2',2'-Trinitroethyl-2,5-dinitrazahexanoate	$C_6H_9N_7O_{12}$	371	0.29	15	10
27	2,2,2-trinitroethyl-3,3-dinitrobutyl nitramine	$C_6H_9N_7O_{12}$	371	0.88	20	10
28	N-(2,2-Dinitropropyl)-N,2,2-trinitro-1-propanamine	$C_6H_{10}N_6O_{10}$	326	-0.63	29	10
29	1,7-dimethoxy-2,4,6-trinitrazaheptane	$C_6H_{14}N_6O_8$	298	-2.94	166	8
30	N,N'-Dinitro-N,N'-bis [2-(nitroamino)ethyl]-1,2-ethanediamine	$C_6H_{14}N_8O_8$	326	-2.78	53	10
31	Bis-(trinitroethyl)-2,4-dinitrazapentanedioate	$C_7H_5N_{10}O_{20}$	550	3.72	10	8
32	2,2-dinitropropyl-5,5,5-trinitro-2-nitrazapentanoate	$C_7H_9N_7O_{14}$	415	0.81	16	8
33	Trinitroethyl-5,5-dinitro-3-nitrazahexanoate	$C_7H_9N_7O_{14}$	415	0.81	25	8
34	2,2,2-Trinitroethyl-2,5,5-trinitro-2-azahexanoate	$C_7H_9N_7O_{14}$	415	0.81	22	10
35	N-nitro-N,N'-bis-(trinitropropyl)-urea	$C_7H_9N_9O_{15}$	459	1.25	21	8
36	2,2,2-Trinitroethyl-2,4,6,6-tetranitro-2,4-diazaheptaneoate	$C_7H_9N_9O_{16}$	475	1.71	18	10
37	Bis-(2,2,2-trinitroethyl) 3-nitrazaglutarate	$C_8H_8N_8O_{18}$	504	1.90	14	10
38	N,N'-Dinitro N,N'-bis-3,3,3-trinitropropyl)-oxamide	$C_8H_8N_{10}O_{18}$	532	1.82	9	10

TABLE 13. (Continued)

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
39	Bis-(trinitroethyl)-2,4,6-trinitraza-heptanedioate	$C_8H_8N_{12}O_{22}$	624	3.20	13	8
40	2,2,6,9,9-Pentanitro-4-oxa-5-oxo-6-azadecane	$C_8H_{12}N_6O_{12}$	384	-1.58	47	10
41	1,1,1,3,6,9,11,11,11-nonanitro-3,6,9-triazaundecane	$C_8H_{12}N_{12}O_{18}$	564	1.60	12	10
42	N-(2-2-Dinitrobutyl)-N-2,2-trinitro-1-butanamine	$C_8H_{14}N_6O_{10}$	354	-2.63	80	10
43	N,N'-Dinitro-N,N'-bis-(3-nitrazabutyl)-oxamide	$C_8H_{14}N_8O_{10}$	382	-3.50	90	10
44	2,2,4,7,9,9,hexanitro-4,7-diazadecane	$C_8H_{14}N_8O_{12}$	414	-1.43	72	10
45	N,N'-dinitromethylene-bis-(4,4,4-trinitro)-butyramide	$C_9H_{10}N_{10}O_{18}$	546	0.85	13	8
46	1,1,1,5,7,10,14,14,14-Nonanitro-3-12-dioxa-4,11-dioxo-5,7,10-triazatetradecane	$C_9H_{10}N_{12}O_{22}$	638	2.26	11	10
47	Bis-(5,5,5-trinitro-3-nitrazapentanoyl)-methylenedinitramine	$C_9H_{10}N_{14}O_{22}$	666	2 18	15	8
48	1,1,1,4,6,6,8,11,11,11-Decanitro-4,8-diazaundecane	$C_9H_{12}N_{12}O_{20}$	608	1.89	11	10
49	1,1,1,3,6,6,9,11,11,11 Decanitro-3,9-diazaundecane	$C_9H_{12}N_{12}O_{20}$	608	1.89	10	10
50	Bis-(2,2,2-trinitroethyl)-4-nitraza-1,7-heptanedioate	$C_{10}H_{12}N_8O_{18}$	532	0.00	29	10
51	Bis-(2,2,2-trinitroethyl)-3,6-dinitraza-1,8-octanedioate	$C_{10}H_{12}N_{10}O_{20}$	592	0.77	29	10
52	Bis-(trinitroethyl)-2,5,8-trinitrazanonanedioate	$C_{10}H_{12}N_{12}O_{22}$	652	1.43	17	8
53	N,N'-Dinitro-N,N'-bis-(3,3-dinitrobutyl)-oxamide-triazatetradecane	$C_{10}H_{14}N_8O_{14}$	470	-2.17	37	10
54	1,1,1,3,6,9,12,14,14,14-Decanitro-3,6,9,12-tetraza-tetradecane	$C_{10}H_{16}N_{14}O_{20}$	652	0.67	19	10
55	Bis-(trinitroethyl)-5,5-dinitro-2,8-dinitraza-nonanedioate	$C_{11}H_{12}N_{12}O_{24}$	696	1.69	12	8

TABLE 13. (Continued)

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
56	2,2,4,7,7,10,12,12-Octanitro-4,10-diazatridecane	$C_{11}H_{18}N_{10}O_{16}$	546	-1.45	44	10
57	2,2,5,7,7,9,12,12-Octanitro-5,9-diazatridecane	$C_{11}H_{18}N_{10}O_{16}$	546	-1.45	37	10
58	1,4-Bis-(5,5,5-trinitro-2-nitrazapentanoate)-2-butyne	$C_{12}H_{12}N_{10}O_{20}$	616	0.00	16	8
59	1,1,1,18,18,18-Hexanitro 3,16-dioxa-4,15-dioxo-5,8, 11,14-tetranitrazaoctadecane	$C_{12}H_{16}N_{14}O_{24}$	740	0.61	19	10
60	1,1,1,3,6,6,8,10,10,13, 15,15,15-tridecanitro-3,8,13,-triazapentadecane	$C_{12}H_{16}N_{16}O_{26}$	800	1.71	23	10
61	2,2-Dinitropropanediol-bis-(5,5-dinitro-2-nitraza-hexanoate)	$C_{13}H_{18}N_{10}O_{20}$	634	-1.31	138	8

TABLE 14. The drop-weight impact sensitivities of nitrate ester explosives.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	1,2,3-Propanetriol trinitrate	$C_3H_5N_3O_9$	227	3.50	20	13
2	N-(2,2,2-Trinitroethyl)-nitraminoethyl nitrate	$C_4H_6N_6O_{11}$	314	2.96	7	10
3	2,2-Bis(nitroxymethyl)-1,3-propanediol dinitrate	$C_5H_8N_4O_{12}$	316	2.07	13	13
4	3-[N-(2,2,2-Trinitroethyl) nitramino]-propyl nitrate	$C_5H_8N_6O_{11}$	328	1.33	12	10
5	3,5,5-Trinitro-3-azahexyl nitrate	$C_5H_9N_5O_9$	283	0.36	21	10
6	1,9-Dinitrato-2,4,6,8-tetranitrazanonane	$C_5H_{10}N_{10}O_{14}$	434	2.05	10	8
7	4,4,8,8-Tetranitro-1,11-dinitrato-6-nitraza undecane	$C_{10}H_{16}N_8O_{16}$	504	-0.80	87	10

TABLE 15. The drop-weight impact sensitivities of miscellaneous nitroheterocyclic explosives.

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
1	Ammonium 5-Nitro-tetrazolate	$CH_4N_6O_2$	132	-1.54	30	13
2	Ethylenediammonium di-5-nitrotetrazolate	$C_4H_{10}N_{12}O_4$	290	-3.33	42	13
3	3,5-Dinitroisoxazole	$C_3H\ N_3O_5$	159	2.50	29	13
4	1,4-Dinitroglycoluril	$C_4H_4N_6O_6$	232	-2.0	100	13
5	1-Nitro-2,5-bis-(trinitromethyl)-pyrrolidine	$C_6H_6N_8O_{14}$	414	2.94	6	8
6	5-Picrylaminotetrazole	$C_7H_4N_8O_6$	296	-2.40	36	13
7	3,3,9,9-Tetranitro-1,5,7,11-Tetraoxaspiro-(5.5)-undecane	$C_7H_8N_4O_{12}$	340	0.65	66	10
8	N-(2,2,2-Trinitroethyl)-3,3,5,5-tetranitro-piperidine	$C_7H_8N_8O_{14}$	428	1.62	18	10
9	N (Trinitropropyl) 3,3,5,5-tetranitro piperdine	$C_8H_{10}N_8O_{14}$	442	0.50	29	8

TABLE 15. (Continued)

No.	Compound	Formula	Mol. Wt.	SI	h_{50} (cm)	Ref.
10	1,3,7,9-Tetranitrodibenzo-1,3a,4,6a-tetraazapentalene	$C_{12}H_4N_8O_8$	388	-3.75	85	8
11	3-6-Bis-(picrylamino)-s-tetrazine	$C_{14}H_6N_{12}O_{12}$	534	-2.27	61	13
12	1,3,5-Tris(1-oxo-5,5,5-trinitro-3-nitrazapentyl) s-triazacyclohexane	$C_{15}H_{18}N_{18}O_{27}$	882	0.00	13	8
13	Tripicryl-s-triazene	$C_{21}H_6N_{12}O_{18}$	714	-2.11	85	8

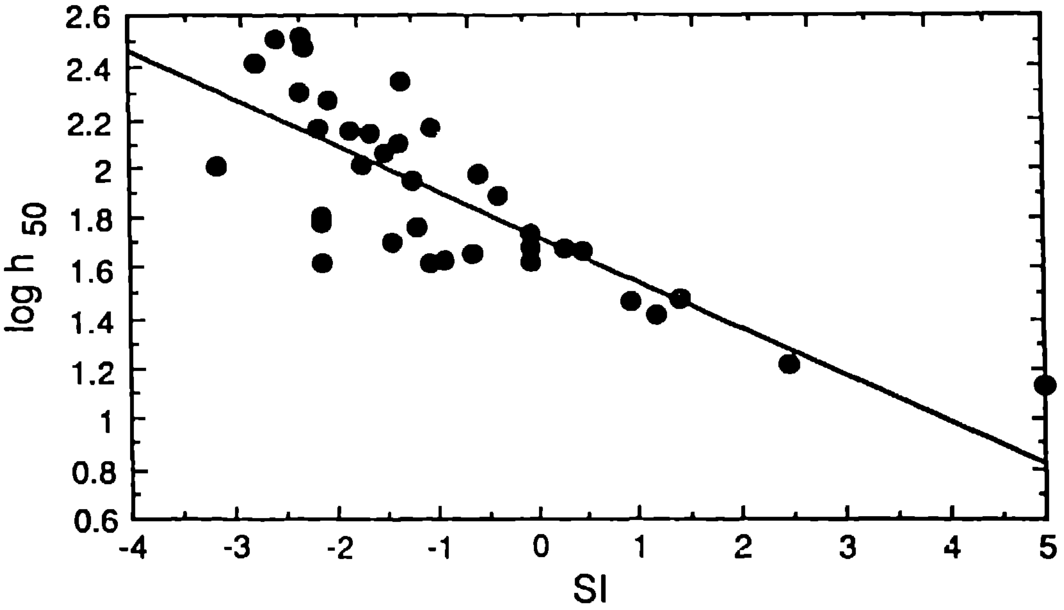

Figure 3. A plot of the impact sensitivity (log h_{50}, cm) of the 40 nitroaromatic explosives in Table 2 vs the sensitivity index (SI). The regression is log h_{50} = 1.70-0.20 SI, R^2 = 0.605.

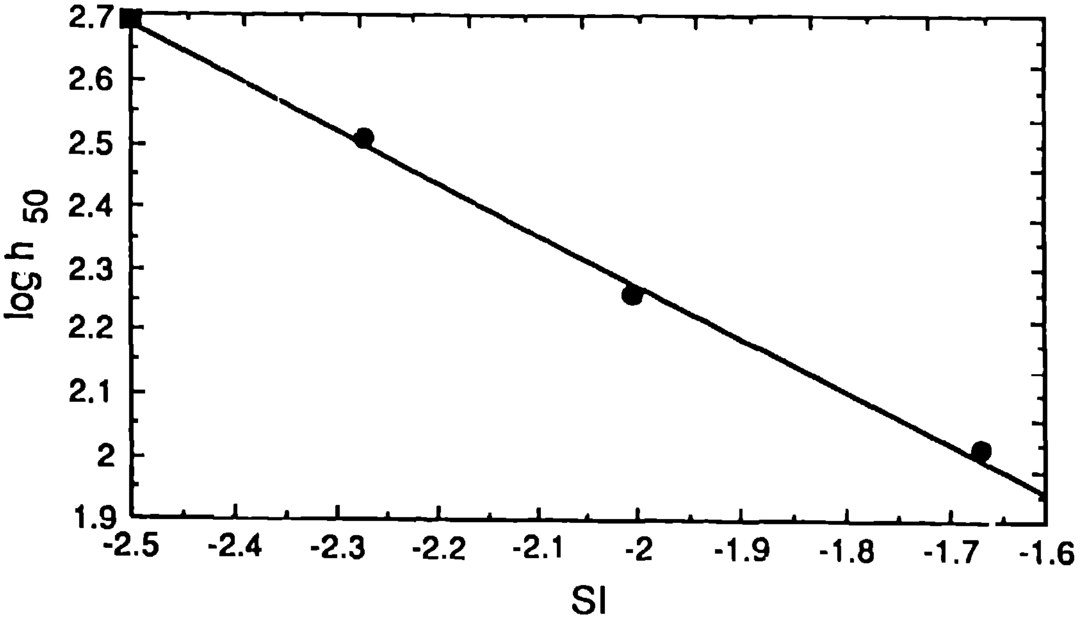

Figure 4. A plot of the impact sensitivity (log h_{50}, cm) of TNB, MATB, and DATB vs the sensitivity index (SI), extrapolated to TATB. The regression is log h_{50} = 0.59-0.84SI, R^2 = 0.998. See Table 2 5,12,15,18 for values plotted.

An example of the use of the different families is given in Figure 5. Here we plot compounds 1,2,3,5,12,15,18,29 and 33 from Table 2, providing examples of the polynitrobenzene series, the polyaminotrinitrobenzene series and benzotrifuroxan. To estimate the sensitivity of 5,7-diamino-4,6-dinitrobenzofuroxan (DADNBF) a tie-line between TATB and BTF is used, log h_{50} = 1.70-0.40SI. This family relationship suggests a sensitivity of 268 cm for DADNBF. To estimate the impact sensitivity of 7-amino-4,6-dinitrobenzofuroxan (ADNBF) a tie line is constructed between DATB and BTF, log h_{50} = 1.70-0.36SI. This estimates an impact sensitivity for ADBNF of 174 cm.

In Figure 6 we plot the impact sensitivity of the 18 1,2,4-triazoles given in Table 8. The 1,2,4-triazoles that have no other sensitive functional group generally lie above the regression observed for nitroaromatic explosives and thus form an inherently less-sensitive class of explosives.

The 1,2,3-triazoles also provide some interesting examples, Table 9. The very large difference in the impact sensitivities of 1-picryl-1,2,3-triazole compared to 2-picryl-1,2,3-trazole and 4-nitro-1-picryl-1,2,3-triazole compared to 4-nitro-2-picryl-1,2,3-triazole have been commented on previously [19]. Recent consideration of the problem [27] has ascribed the large difference in sensitivity to the facile loss of nitrogen in the 1-picryl isomers. This illustrates another use of the correlations, large exceptions point out important structural factors. This in turn suggests molecules that are interesting for detailed calculations and provides clues as to decomposition mechanisms.

Among explosives chemists the belief is widely held that ammonium salts are "unusually stable". When an acid is converted to its ammonium salt three extra hydrogens are added and the ammonium salt will certainly be more stable (i.e. less sensitive) than the parent acid. In Figure 7 we plot the SI vs log h_{50} for a variety of ammonium salts. The numbers in the figure refer to the table from which the data are taken. The solid line represents the general nitroaromatic regression and is for reference. The two extreme deviations in the sensitive direction (15-1,2) are nitrotetrazoles, an inherently sensitive class of materials. Seven of the ten ammonium salts follow the general nitroaromatic regression reasonably well. Ammonium 3,5-dinitro-1,2,4-triazolate appears to be rather more insensitive than expected. It has already been pointed out (Figure 6) that 1,2,4-triazoles are as a class less sensitive. It appears that an ammonium counter-ion provides no special "insensitivity".

In any energetic material one is pursuing a compromise between energy content and metastability. When a hot spot is formed it will grow if the rate of heat production is greater than the rate of heat loss [28,29]. In general as more nitro groups are added the available heat per molecule (Q) increases. For a homologous series, as a

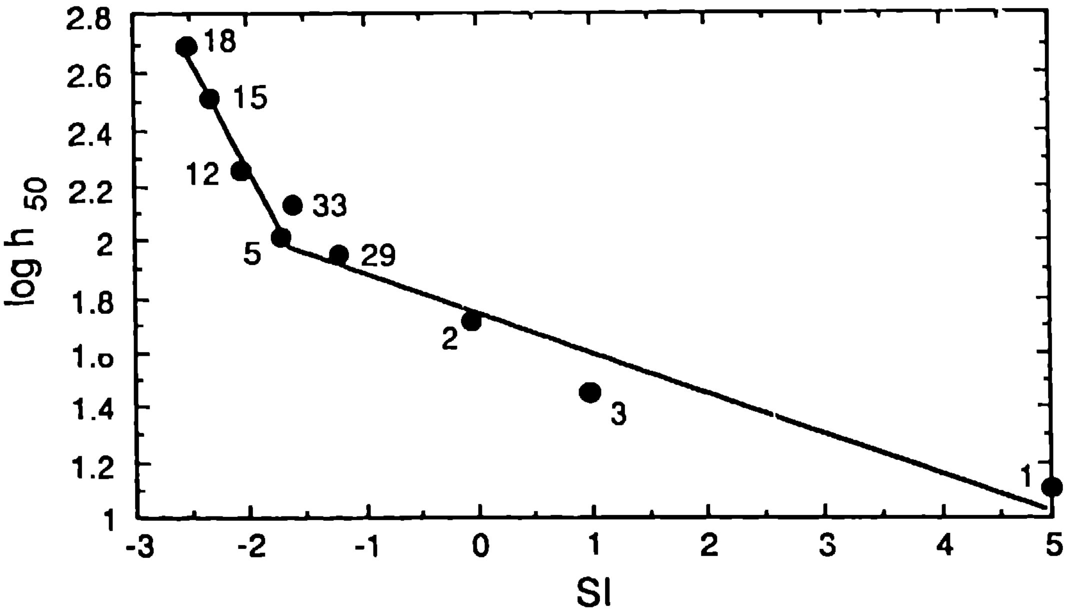

Figure 5. A plot of the impact sensitivity (log h_{50}, cm) of compounds 1,2,3,5,12,15,18,29 and 33 from Table 2 vs the sensitivity index (SI).

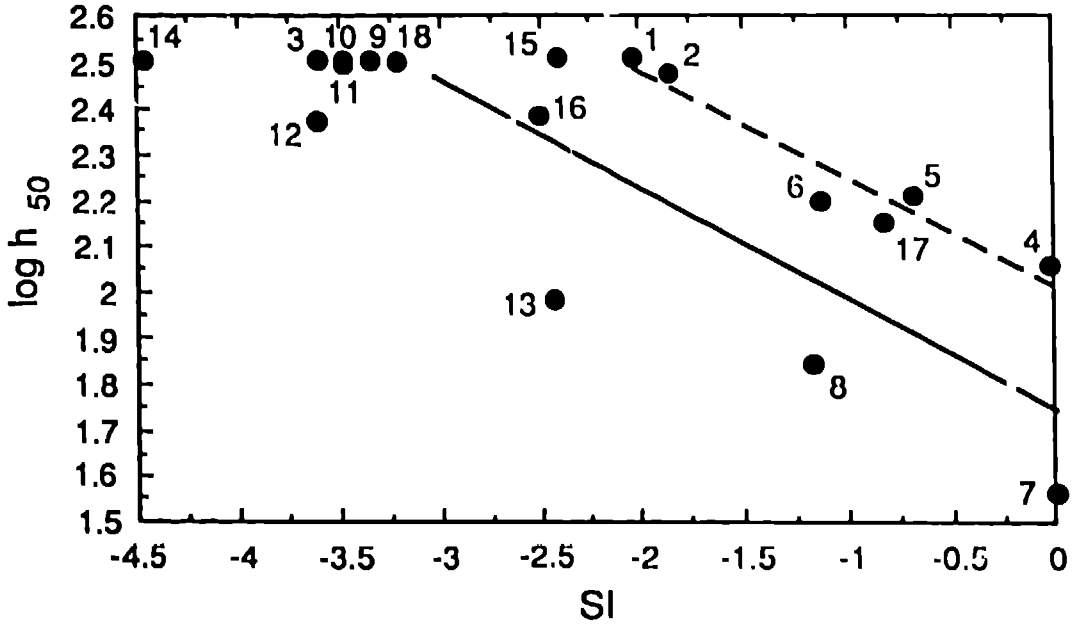

Figure 6. A plot of the impact sensitivity (log h_{50}, cm) of the 18 nitro-1,2,4-triazoles in Table 8 vs the sensitivity index (SI). The regression for points 1,2,4,5,6,17 is $\log h_{50} = 2.00 - 2.4SI$, $R^2 = 0.929$. The solid line is the regression for nitroaromatics from Table 2 and is for a reference comparison.

reaction becomes more exothermic the transition state leading to the products becomes lower (Hammond postulate) [30]. This leads to an increased rate of energy release at a given temperature. It is commonly observed in linear free energy relationships in homologous series that rate constants (k) and equilibrium constants (K) have linear relationships. So it is not surprising that the sensitivity index (an oxygen balance related number) relates in a systematic way to the impact sensitivity.

Based on an examination of the properties of various explosives tested for impact and/or shock sensitivity it would be desireable to identify the most important factors contributing to the decomposition. Kamlet and Adolph [12] suggested in 1981 "that impact sensitivities of explosives depend on the rates of thermal decomposition reactions which occur at the temperatures generated under the impact hammer, with the rate determining step usually being the homolytic cleavage of the weakest atom linkage (referred to as the "trigger linkage")." Their proposal was based in part on earlier work by Wenograd [31] which demonstrated that the time delay to explosion for most organic explosives could be described by $\tau = A\exp(B/RT)$, where τ is the delay time, T the absolute temperature, and A and B constants. This led Wenograd [31] to suggest that the important parameter in impact sensitivity is the temperature reached during the 250 μs confinement interval under the impact hammer.

An explosive has a characteristic critical temperature, i.e. the lowest constant surface temperature at which a specific material of a specific size and shape will self-heat catastrophically. Below the critical temperature, energetic materials still decompose, but they fail to generate sufficient heat to become self-sustaining.

The critical temperature for the thermal explosion of an explosive may be calculated from the Frank-Kamenetskii equation [32]:

$$\frac{E}{Tm} = R\ln\frac{a^2\rho QZE}{Tm^2\lambda\delta R} ,$$

where R is the gas constant (1.99 cal $mol^{-1}K^{-1}$), a is the radius of a sphere or cylinder or the half-thickness of a slab, ρ is the density (g cm^{-3}), Q is the heat of explosion (cal g^{-1}), Z is the pre-exponential (s^{-1}) and E the activation energy (kcal mol^{-1}) from the Arrhenius expression, λ is the thermal conductivity (cal $cm^{-1}sec^{-1}K^{-1}$), and δ is a shape factor (0.88 for infinite slabs, 2.00 for infinite cylinders, and 3.22 for spheres). Rogers [32,33] has determined the kinetics constants for a variety of explosives (PETN, TETRYL, RDX, HMX, DIPAM, TNT, HNS, DATB, TACOT, TATB) for which shock sensitivity and impact sensitivity data are also available (Table 1). Using the kinetics constants and physical properties reported by Rogers [32,33], the heats of explosion given by Zeman et al. [34], and the cylindrical dimensions of the NSWC small scale gap test [6] we calculate the critical temperatures for these explosives as given in Table 16.

In Figure 8 the calculated critical temperature (Tm) for the diverse set of explosives in Table 16 is plotted against the shock initiation pressure ($\log P_{90}$) taken from Table 1. The regression is $\log P_{90} = 0.007Tm-2.03$, $R^2 = 0.848$. For these same explosives Tm plotted against the sensitivity index provides a R^2 correlation of 0.554, impact sensitivity ($\log h_{50}$) plotted against the sensitivity index for this series of explosives provides a R^2 correlation of 0.512. The critical temperature-shock sensitivity relationship is about as satisfactory at 95% TMD ($\log P_{95} = 0.007Tm-1.87$, $R^2=0.823$) and at 98% TMD ($\log P_{98} = 0.007Tm-1.76$, $R^2=0.808$). This relationship of calculated critical temperature and shock sensitivity is consistent with the hypothesis of Wenograd [31] and of Kamlet and Adolf [12] that the rate of thermal decomposition is a critical factor in shock and impact sensitivity.

A great deal of attention has been focussed on the notion of a critical "trigger linkage" in explosives. If such a bond could be identified, and avoided, less sensitive materials could be designed [12]. In more sensitive explosives it is likely that a single early dominant step can be identified. A detailed analysis of a series of picryl-1,2,3-triazoles has been made [27]. In less sensitive explosives complex chemistry is likely to preceed a rate determining step and the insensitivity of the explosive is in fact the consequence of the chemistry preceeding the rate determining step.

A good example is TATB. The thermal decomposition of TATB has been reported to consist of a slow endothermic stage followed by two slow exothermic stages, culminating in an explosive reaction above the critical temperature [35]. Sharma et al. [36] have observed the formation of furazans in impacted TATB and suggest that this is an important early decomposition step for the reaction of TATB. The heat of formation of TATB is 37 kcal/mole and for BTF it is 145 kcal/mole [37]. On converting an ortho-nitroamino functionality to a furoxan the ΔH is increased on average by 61 kcal/mole. The value for a furazan would be somewhat less, but still a substantial positive change. Thus the elimination of water (58 kcal/mole) to form a furazan functionality is nearly a thermochemically neutral reaction. During the early stages of hot spot existance there is little early energy release to drive growth. This provides a favorable effect on sensitiveness (ease of initiating a reaction center) and on explosiveness (ease of transition to a violent explosion). Since the safety of an explosive is approximately the reciprocal of the product of these factors [38], TATB is a rather safe material (for an explosive) to work with. The inherent insensitive nature of the material resides in the themochemically neutral chemistry required before exothermic decomposition ensues. It is difficult, in this scheme, to identify a "trigger linkage."

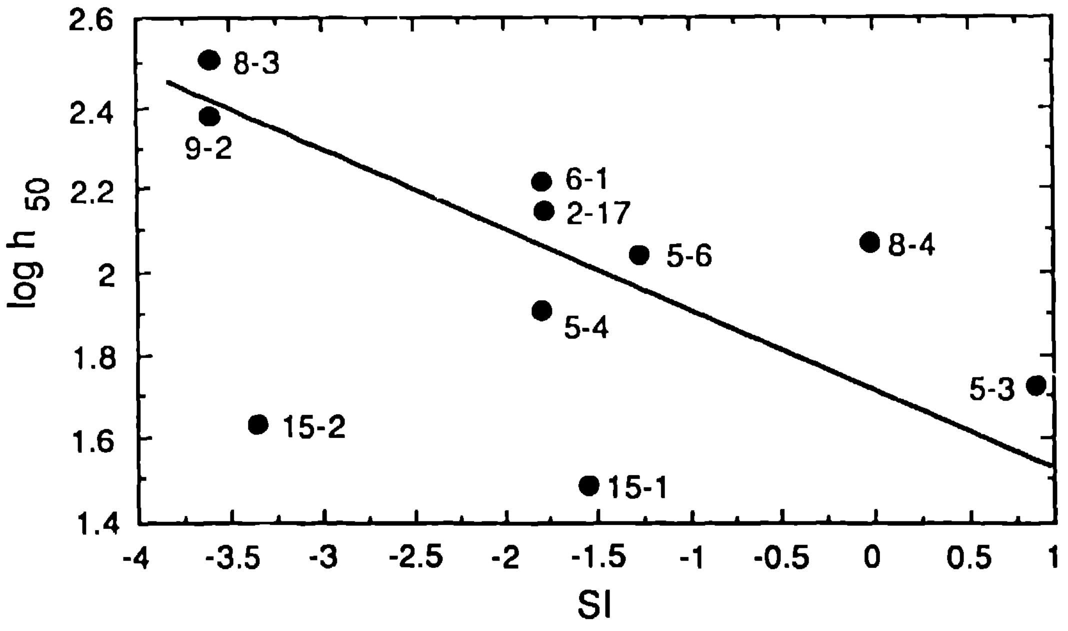

Figure 7. A plot of the impact sensitivity (log h_{50}) for nine ammonium salts of nitroazole explosives and ammonium picrate. The numbers on the graph refer to the Table which is the source of the data. The solid line is the nitroaromatic regression (Table 2) and is for reference

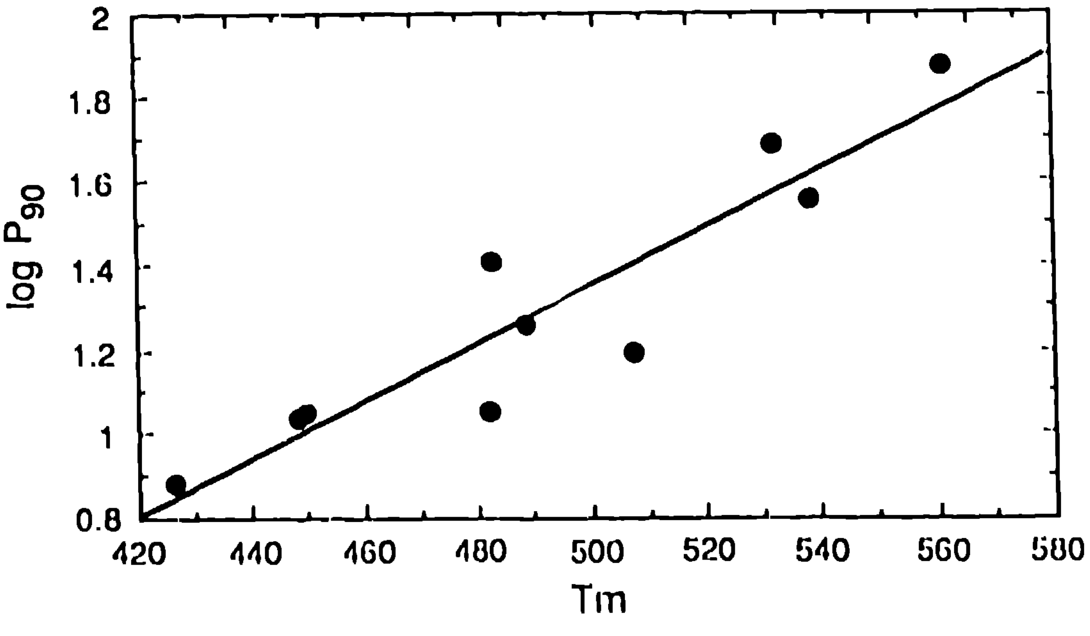

Figure 8. A plot of the calculated critical temperatures (Tm) vs the shock sensitivities (log P_{90}) for the diverse set of explosives in Table 16
The shock sensitivities are from Table 1.

TABLE 16. The critical temperatures calculated from the Frank-Kamenetskii equation for a diverse set of explosives.

Compound[a]	Tm(K)	Compound	Tm(K)
PETN	427	TNT	491
TETRYL	449	HNS	508
RDX	450	DATB	533
HMX	483	TACOT	539
DIPAM	484	TATB	562

a. See Table I for abbreviations.

Nitromethane is another interesting case. Engelke et al. [39] have provided a variety of evidence that the early critical intermediate in nitromethane decomposition is the aci ion ($CH_2NO_2^-$). In pure nitromethane the driving force at high pressure is the electrostriction effect of the formation of the $CH_3NO_2H^+$-$CH_2NO_2^-$ ion pair. If this has a ΔV of -20 cc/mole one can very crudely estimate aci ion concentrations of 10^{-7} to 10^{-10} M at pressure conditions adequate to initiate homogeneous nitromethane. The aci ion is a very reactive species. It is known to be a good nucleophile, a precursor to fulminic acid, and a facile electron transfer agent. If these very small amounts of an intermediate are kinetically competent to bring about the violent exothermic decomposition of nitromethane it must indeed be very reactive. This is the basis for the arguments related to the amine sensitization of nitromethane [39]. Does one then view the C-H bond in nitromethane as the trigger linkage?

A third example is the dramatic difference in the impact sensitivity of 1-picryl-1,2,3-triazole and 2-picryl-1,2,3-triazole, as mentioned earlier in this article. An extensive structural and theoretical analyses [27] has been carried out on these isomers. It was concluded that the 1-picryl-1,2,3-triazole isomer loses nitrogen by a low activation energy, exothermic, process. This drives the propagation of the hot spot. In this case the N_2 loss is certainly a "trigger linkage".

We have shown a relationship between impact and shock sensitivity and illustrated how a sensitivity index based on oxygen balance can be used to estimate sensitivity in closely related series of molecules. It is shown that the critical temperature of an explosive calculated by the Frank Kamenetskii equation correlates fairly well with the shock sensitivity of the material. This supports the idea that the shock or impact initiation of an explosive is primarily a thermal event and not dominated by pressure driven chemistry. The concept of the "trigger linkage" in explosives is discussed and it is pointed out that insensitive explosives will require early chemistry that is thermochemically neutral or endothermic and leads to the build up of later strongly exothermic chemistry.

ACKNOWLEDGEMENT

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