Estimating Detonation Velocity and Detonation Pressure of C-H-N-O Explosives from Gas Coefficient

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New empirical equations are given for estimating detonation velocity and detonation pressure of C-H-N-O explosives ;

$D=(2630+990G)\rho+2330G+650$,

$P=(6.15+5.07G)^2\rho^2$,

where *D and P* are detonation velocity (m/s) and detonation pressure (kbar) respectively at density ρ (g/cm). *G* is Gas Coefficient and is dependent upon chemical structure and detonation products of the explosives. The absolute error for all 148 data points (70 explosives) is ±2.14% for detonation velocity ; the deviation between the calculated and exprimental detonation pressure values for 30 data points (18 exlosives) is ±4.32%.

1. INTRODUCTION

As detonation velocity(D)and detonation pressure(P)of explosives are important detonation parameters, acting in a close coordination with practical application of explosives, the calculation of detonation velocity and detonation pressure is of great theoretical and practical importance.

Urbanski[1] and Zhou Fa Qi[2] gave critical reviews on the methods of calculating parameters of detonation. The methods can be generally classified into two categories : derived from he hydrodynamic theory of detonation or based on empirical equations. Among the empirical methods, OB (oxygen balance) equation[1], NMQ equation (Kamlet-Jacobs method)[3], Nitrogen Equivalent equation (NE)[2] and Factor F equation (Rothestein-Petersen method)[9] etc. were recognized to be remarkable methods. In this paper, we propose a new empirical method of estimating detonation velocity and detonation pressure of C-H-N-O explosives.

2. GAS COEFFICIENT AND THE ESTIMATING EQUATIONS

Experiments show that detonation velocity of an explosive is dependent on structure, composition, charge density, detonation products and other factors. For an explosive, the detonation velocity over a wide range of density generally observes the following relatioship :

$$D=D_0+M(\rho-\rho_0) \quad (1)$$

where D, D_0 and ρ, ρ_0 are the detonation velocities and densities at their experimentally measured values respectively, M is a constant for a given explosive, Equation (1) can be alternatively expressed as

$$D=M\rho+A \quad (2)$$

The new equations of estimating detonation velocity and detonation pressure of C-H-N-O explosives are as follows :

$$D=(2630+990G)\rho+2330G+650 \quad (3)$$

$$P=(6.15+5.07G)^2\rho^2 \quad (4)$$

where *D*, P are detonation velocity (m/s) and detonation pressure (kbar) respectively at density ρ (g/cm), *G* is called Gas Coefficient, which is dependent structure, composition and explosion products.

G is defined as follows : in a mole of $C_aH_bN_cO_d$ explosive, effective nitrogens form nitrogen gas (N_2), effective oxygens first change hydrogen into water gas (H_2O), then the remaining effective oxygens change carbons into carbon dioxide gas (CO_2) (i.e., the H_2O-CO_2 decomposition), the mole number of gas formed is $(eN_2+fH_2O+gCO_2)$. For one mole of $C_aH_bN_cO_d$ explosive, if all of its nitrogens, hydrogens and carbons can change into nitrogen gas, water gas,

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and carbon gas, water gas and carbon dioxide gas. respectively, the mole number of gas would be ($c/2N_2 + b/2H_2O + aCO_2$), so G is expressed as

$$G=\frac{(eN_2+fH_2O+gCO_2)}{(c/2N_2+b/2H_2O+aCO_2)} \quad (5)$$

It is understandable that nitrogen or oxygen atoms in different groups do not have the same effectivity in the detonation reaction of an explosive, because of their different chemical structural environments. We assume that :

N and O of $-CNO_2$, $-NNO_2$, $-CNO$ and $-NNO$ groups are effective ;

N and O of $-C(NO_2)_2$ and $-C(NO_2)_3$ groups are effective with correction coefficients of 0.8 and 0.73 respectively ;

N doubly bonded directly to carbon or nitrogen as in $-C=N$, $-N=N$ and $-N_3$ are effective ;

N singly bonded directly to hydrogen or carbon as in $-NR$, where R can be $-H$, $-C$, etc., are non-effective for calculating detonation velocity, but effective when the compound has groups such as $-C(NO_2)_2$, $-C(NO_2)_3$ and $-ONO_2$;

O bonded directly to carbon in $-ONO_2$ are non-effective for calculating detonation velocity, but the correction coefficient 0.5 is given for calculating pressure ;

O in $-C=O$, $-COOR$, $-C-O-R$ where R can be $-H$ and $-C$ are non-effective other than having groups such as $-C(NO_2)_2$, $-C(NO_2)_3$ and $-ONO_2$ in the compound.

The computation of G from chemical composion and structure of an explosive is simple, as shown in the following examples.

① HMX, 1, 3, 5, 7-tetranitro-1, 3, 5, 7-tetraazacyclooctane molecular formula $C_4H_8N_8O_8$ all nitrogens and oxygens are effective

$a=4$, $b/2=4$, $c/2=4$, $e=4$, $f=4$, $g=2$

$G=(4+4+2)/(4+4+4)=0.833$

② HCO, 1, 3, 3, 5, 7, 7-hexanitro-1, 5-diazacyclooctane molecular formula $C_6H_8N_8O_{12}$ N and O of two $-C(NO_2)_2$ are needed for correction, the number of effective nitrogens is 7.2($2\times0.8\times2+4$) and the number of effective oxygens is 10.4($2\times0.80\times4+4$)

$a=6$, $b/2=4$, $c/2=4$, $e=3.6$, $f=4$, $g=3.2$

$G=(3.6+4+3.2)/(4+4+6)=0.771$,

③ PETN, pentaerythritol tetranitrate molecular formula $C_8H_8N_4O_{12}$

$a=5$, $b/2=4$, $c/2=2$, O bonded directly to cabon in nitrate group are needed for correction the number of effective oxygens is 8 (2×4) for calculating D($e=2$, $f=4$, $g=2$) and 10 for calculatingg P($e=2$, $f=4$, $g=3$)

$G=(2+4+2)/(2+4+5)=0.727$ for calculating D

$G=(2+4+3)/(2+4+5)=0.818$ for calculating P

3. RESULTS AND DISCUSSION

Table 1 collates the experimental detonation velocities together with the estimated values from equation (3). The experimental data are collected from recent literatures and books[1)4)5)6)7)8)]. The molecular formulas, chemical designations and data sources are listed in Table 2. The C-H-N-O explosives can be roughly classfied into four types according to their chemical structures. These are nitroaromatics. aliphatics, nitrate esters and azide compounds.

An analysis of the data in Table 1 shows that : (1) the absolute error for all 148 data points (70 explosives) is ±2.14%, (2) 121 of 148 calculated D values, 81.8%, lie within 3% of the experimental values, (3) 137 of 148 calculated D values, 92.6%, lie within 5% of the experimental values, (4) the largest deviation is ±8.81%, (5) the correlation coefficient for the linear regression plot of all 148 data is > 0.977, (6) the absolute error for 142 data points is ±1.58% (without 6 data points which deviated by > ±7%, one data for HNB, one for SORGUYL, four for NQ).The comparison of various methods for estimating detonation velocity are given in Table 3.

Equation (4) is similar to NMQ Equation and Nitrogen Equivalent Equation . P is linear plot of ρ^2 in all of these equations. Table 4 lists some experimental and calculated values of detonation pressure. The absolute error for all 30 data points (18 explosives) is ±4.82%. The results break down as follows : 17 calculated detonation pressures differ from measured values by ±0−3% ; 5, by ±3−6% ; 5, by ±6−10% ; 3, by > ±10%. The line correlation between exprimental and calculated detonation pressure by a least-squares fit is given by equation (6).

$$P_{exp}=1.029P_{cal}-6.4 \quad r=0.978 \quad n=30 \quad (6)$$

The comparision results of various methods for

Table 1 Experimental and Calculated Values of Detonation Velocity.

No.	Explosive Abbr	G	Density g/cm³	D_{exp} m/s	D_{cal} m/s	$(D_{exp}-D_{cal})$	$(\Delta\%)_D$
1	DNB	0.444	1.47	6100	6197	−97	−1.59
2	PICAID	0.583	1.70	7350	7460	−110	−1.50
			1.60	7100	7139	−39	−0.55
			1.71	7260	7492	−232	−3.20
			1.71	7350	7492	−142	−1.93
			1.54	6899	6947	−48	−0.70
			1.00	5220	5216	4	0.08
			1.25	6070	6017	53	0.87
			1.667	7340	7355	−15	−0.20
3	XPLD	0.571	1.60	7150	7093	57	0.80
			1.55	6850	6932	−82	−1.20
4	DDNP	0.556	1.50	6600	6715	−115	−1.74
			1.58	6900	6969	−69	−1.00
5	ETPIC	0.481	1.55	6500	6585	−85	−1.31
6	TNAN	0.523	1.57	6800	6811	−11	−0.16
7	HNDP	0.569	1.60	7200	7085	115	1.60
			1.59	6993	7053	−60	−0.86
8	HNDPO	0.588	1.65	7180	7320	−140	−1.95
9	HNDS	0.556[a]	1.60	7000	7034	−34	−0.49
10	TACOT	0.500	1.64	7250	6953	310	4.28
			1.85	7250	7596	−346	−4.77
			1.63	6941	6909	32	0.46
11	TETRYL	0.646	1.71	7570	7746	−176	−2.32
			1.51	7150	7092	58	0.81
			1.60	7500	7386	114	1.52
			1.71	7850	7746	104	1.32
			1.70	7560	7713	−153	−2.02
			1.601	7319	7389	−70	−0.96
			1.70	7860	7713	147	1.87
			1.592	7284	7360	−76	−1.04
12	TNT	0.523	1.60	6900	6905	−5	−0.07
			0.95	4850	4859	−9	−0.35
			1.47	6480	6496	−16	−0.25
			1.64	6930	7031	−101	−1.65
			1.62	6970	6968	2	0.03
			1.64	6950	7031	−81	−1.17
			1.061	5254	5208	46	0.88
			1.595	6856	6889	−33	−0.48
			0.732	4200	4173	27	0.64
			1.63	6938	7000	−62	−0.89
			1.59	6950	6874	76	1.09
			1.637	6942	7021	−79	−1.14
			1.630	6940	7000	−60	−0.86
13	TATB	0.500	1.80	7350	7440	−90	−1.22
			1.88	7760	7690	70	0.90
			1.895	7860	7737	123	1.56
			1.847	7660	7587	73	0.95
14	TNA	0.550	1.72	7300	7397	−97	−1.33
			1.60	7000	7010	−10	−0.14
15	TNB	0.583	1.71	7300	7492	−192	−2.63
			1.662	7347	7339	8	0.11
16	TNC	0.523	1.62	6850	6968	−118	−1.63

(to be continued)

No.	Explosive Abbr	G	Density g/cm³	D_{exp} m/s	D_{cal} m/s	$(D_{exp}-D_{cal})$	$(\Delta\%)_D$
17	BTF	0.667	1.86	8490	8324	166	1.94
			1.859	8485	8321	164	1.93
			1.76	8262	7995	267	3.23
18	DBF	0.611	1.708	7584	7599	−15	−0.20
19	DATB	0.523	1.79	7520	7503	17	0.23
			1.788	7520	7497	23	0.31
			1.78	7600	7472	128	1.68
20	DIPAM	0.553	1.76	7400	7531	−131	−1.77
			1.79	7500	7626	−126	−1.68
21	HNAB	0.611	1.60	7311	7250	61	0.83
22	HNS	0.525	1.60	6800	6913	−113	−1.66
			1.70	7000	7228	−228	−3.26
			1.74	7130	7354	−224	−3.14
23	HNBiB	0.524	1.624	6888	6985	−97	−1.41
24	TNP	0.688	1.686	7645	7835	−190	−2.49
25	TENB	0.722	1.701	7836	8022	−186	−2.37
26	PNB	0.861	1.801	8593	8928	−335	−3.90
27	HNB	1.00	1.956	9300	10078	−730	−7.82
28	ABH	0.603	1.78	7600	7799	−199	−2.62
29	NONA	0.590	1.78	7560	7746	−186	−2.46
30	ONT	0.540	1.80	7330	7604	−274	−3.74
31	PYX	0.548	1.695	7254	7304	−50	−0.69
32	TPM	0.523	1.647	7083	7054	29	0.41
33	RDX	0.833	1.76	8750	8671	79	0.90
			1.77	8700	8706	−6	−0.07
			1.796	8741	8795	−54	−0.62
			1.786	8712	8716	−49	−0.56
			1.80	8754	8809	−55	−0.63
			1.60	8250	8118	132	1.60
			1.767	8639	8695	−56	−0.65
			1.00	5981	6046	−65	−1.09
34	DINGU	0.556	1.75	7580	7511	69	0.91
35	SORGUYL	0.944	1.95	9150	9800	−650	−7.10
			1.948	9205	9793	−588	−6.39
36	HMX	0.833	1.89	9110	9120	−10	−0.11
			1.90	9100	9155	−55	−0.60
			1.65	8410	8292	118	1.40
			1.75	8800	8637	163	1.85
			1.854	8917	8996	−79	−0.89
			1.877	9010	9076	−66	−0.73
37	TENSG	0.900	1.86	9050	9262	−246	−2.72
38	DNACP	0.688	1.622	7732	7624	108	1.40
39	DNATA	0.926	1.715	8893	8890	3	0.03
40	HCO	0.771	1.792	8520	8527	−7	−0.08
			1.845	8800	8707	93	1.06
41	TNCH	0.790	1.785	8852	8581	−29	−0.34
42	TMTN	0.667	1.49	7300	7107	193	2.64
			1.57	7800	7370	430	5.51
43	NIRDX	1.00	1.80	9000	9496	−496	−5.51
44	NIORDX	0.875	1.83	9020	9087	−67	−0.74
45	EDNA	0.786	1.62	8100	8003	97	1.19
			1.35	7130	7083	47	0.66
			1.25	6800	6742	58	0.85

(to be continued)

No.	Explosive Abbr	G	Density g/cm³	D_{exp} m/s	D_{cal} m/s	$(D_{exp}-D_{cal})$	$(\Delta\%)_D$
46	NQ	0.60	1.71	8200	7561	639	7.79
			1.55	7650	7045	605	7.91
			1.62	7930	7271	699	8.81
			1.629	7980	7303	677	8.48
47	DNDMOA	0.611	1.48	7100	6862	238	3.35
48	MN	0.75	1.138	6290	6235	55	0.87
			1.128	6290	6202	88	1.40
49	TMN	0.35[b]	1.60	6400	6229	171	2.67
			1.64	6360	6348	12	0.19
50	NTNEMA	0.818	1.787	8732	8703	29	0.33
51	BTENED	0.838	1.842	8970	8975	−5	−0.06
52	BTNEU	0.756	1.733	8400	8266	134	1.60
			1.62	8000	7885	115	1.44
53	TNEAE	0.829	1.805	8740	8810	−70	−0.80
54	NTNATE	0.778	1.708	8490	8270	220	2.59
55	BTNDATA	0.738	1.69	8227	8049	178	2.16
56	DEGN	0.611	1.38	6600	6538	62	0.94
57	DNPEN	0.519	1.58	6800	6826	−26	−0.38
58	TNPON	0.615	1.65	7600	7427	173	2.28
59	NG	0.821	1.59	7600	8037	−437	−5.75
			1.59	7650	8037	−387	−5.06
			1.60	7700	8071	−371	−4.82
60	PETN	0.727	1.70	8400	8039	361	4.30
			1.60	7900	7704	196	2.48
			1.76	8260	8239	21	0.25
			1.67	7980	7938	42	0.53
			1.77	8300	8273	27	0.32
			1.45	7275	7201	74	1.02
			1.723	8083	8115	−32	−0.40
			1.765	8160	8256	−96	−1.18
			1.67	7975	7938	37	0.46
61	TMPTN	0.558	1.48	6440	6660	−220	−3.42
62	MNT	0.75	1.217	6300	6502	−202	−3.21
63	ENT	0.65	1.10	5800	5763	15	0.26
64	EGDN	0.80	1.48	7300	7578	−278	−3.81
65	FIVONITE	0.559	1.55	7040	6887	153	2.10
66	ISBDN	0.545	1.08	5300	5343	−43	−0.81
67	CUTA	0.667	1.02	5500	5559	−59	−1.07
			1.15	5600	5988	−388	−6.93
68	TATAB	0.75	1.74	8576	8267	309	3.60
69	DATNH	0.786	1.61	8100	7969	131	1.62
			1.65	8300	8105	195	2.35
70	DATEN	0.794	1.563	7724	7839	−115	−1.49

a sulphur is treated to form SO_2 gas in the H_2O-CO_2 decomposition.
b correction coeffcient 0.175 is given.

estimating detonation pressure are shown in Table 5.

The characterstic of the method discribed in this paper is that factors affecting detonation velocity and detonation pressure are divided into density and Gas Coefficient G. G values are derived from molecular formulas and chemical structures. The method does not require any measured or estimated thermochemical properties such as the heat of formation of unreacted explosive. The method is also an empirical method, but is more simple and more direct than other methods in the literature.

Effectivity of nitrogen or oxygen atoms and correction coefficient of a group may be qualitatively explained by considering the heat of formation and structural factors. It is apparent that that different kinds of groups or bonds have different contribution

Table 2 Chemicial Designations and Data Sources

No.	Abbrev.	Chemical designation	Molecular formula	Ref.
1	DNB	m-dinitrobenzene	$C_6H_4N_2O_4$	(4)
2	PICAID	2, 4, 6-trinitrophenol	$C_6H_3N_3O_7$	(4) (5) (8)
3	XPLD	ammonium picrate	$C_6H_6N_4O_7$	(4) (5)
4	DDNP	diazodinitrophenol	$C_6H_2N_4O_5$	(1) (4)
5	ETPIC	ethylpicrate	$C_8H_7N_3O_7$	(4)
6	TNAN	2,4,6-trinitroanisole	$C_7H_5N_3O_7$	(4)
7	HNDP	2 2',4,4' -hexanitrodiphenylamine	$C_{12}H_5N_7O_{12}$	(4) (6)
8	HNDPO	2,2',4,4' ,6,6' -hexanitrodiphenyloxide	$C_{12}H_4N_6O_{13}$	(4)
9	HNDS	2 2',4,4',6,6' -hexanitrodiphenylsulfide	$C_{12}H_4N_6O_{12}S$	(4)
10	TACOT	tetranitrodibenzotetrapentalene	$C_{12}H_4N_8O_8$	(4) (5) (6)
11	TETRYL	N,2,4,6-tetranitro-N-methylaniline	$C_7H_5N_5O_8$	(4) (5) (6) (7)
12	TNT	2,4,6-trinitrotoluene	$C_7H_5N_3O_6$	(4) (5) (6) (7) (8)
13	TATB	1,3,5-triamino-2, 4, 6-tritrobenzene	$C_6H_6N_6O_6$	(4) (5) (7) (8)
14	TNA	2,4,6-trinitroaniline	$C_5H_4N_4O_6$	(4)
15	TNB	1,3,5-trinitrobenzene	$C_6H_3N_3O_6$	(4) (6)
16	TNC	2,4,6-trinitrocresol	$C_7H_5N_3O_7$	(4)
17	BTF	benzotrifuroxane	$C_6N_6O_6$	(5) (7)
18	DBF	4,6-dinitrobenzofuroxane	$C_6H_2N_4O_6$	(6)
19	DATB	1,3diamino2,4,6trinitrobenzene	$C_6H_5N_5O_6$	(5) (7) (8)
20	DIPAM	3,3' -diamino-2,2' ,4,4' ,6,6' -hexanitrodiphenyl	$C_{12}H_6N_8O_{12}$	(5) (7)
21	HNAB	2,2' ,4,4' ,6,6' -hexanitrobenzene	$C_{12}H_4N_8O_{12}$	(7)
22	HNS	2,2' ,4,4' ,6,6' -hexanitrostilbene	$C_6H_6N_6O_{12}$	(5) (7)
23	HNBiB	2,2' ,4,4' ,6,6' -hexanitrobibenzyl	$C_{14}H_8N_6O_{12}$	(5) (7)
24	TNP	2,4,6-trinitropyridine	$C_5H_2N_4O_6$	(6)
25	TENB	1,2,3,5-tetranitrobenzene	$C_6H_2N_4O_8$	(6)
26	PNB	pentanitrobenzene	$C_6HN_5O_{10}$	(6)
27	HNB	hexanitrobenzene	$C_6N_6O_{12}$	(6)
28	ABH	azo-bis(2, 2' , 4, 4' , 6, 6' -hexanitrobiphenyl)	$C_{24}H_6N_{14}O_{24}$	(7)
29	NONA	2, 2, ' 2", 4, 4' , 4", 6, 6' , 6"-nonanitro-m-terphenyl	$C_{18}H_5N_9O_{18}$	(7)
30	ONT	2, 2' , 4, 4' , 4", 6, 6' , 6"-ocatanitro-m-terphenyl	$C_{18}H_6N_8O_{16}$	(7)
31	PYX	2, 6-bis(picrylamino)-3, 5-dinitropyridine	$C_{17}H_7N_{11}O_{16}$	(6)
32	TPM	2,4,6-tripicryl-s-melamine	$C_{21}H_9N_{15}O_{18}$(6)	
33	RDX	1,3,5-trinitro-1,3,5-triazacyclohexane	$C_3H_6N_6O_6$	(4)(5)(6)(7)(8)
34	DINGU	dinitroglycolurile	$C_4H_4N_6O_6$	(4)
35	SORGUYL	tetranitroglycolurine	$C_4H_2N_8O_{10}$	(4)(6)
36	HMX	1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane	C_4H_8N8O8	(5)(6)(7)
37	TENS	2,4,6,8-tetranitro-2,4,6,8-Gtetraazabicyclo(3,3,0)octanone-3	$C_4H_4N_8O_9$	(6)
38	DNACP	1,3-dinitro-1,3-diazacyclopentane	$C_3H_6N_4O_4$	(6)
39	DNATA	3,6-dinitramine-1,2,4,5-tetrazine	$C_2H_2N_8O_4$	(6)
40	HCO	1,3,3,5,7,7-hexanitro-1,5-diazacyclooctane	$C_6H_6N_8O_{12}$	(6)

(to be continued)

No.	Abbrev.	Chemical designation	Molecular formula	Ref.
41	TNCH	1, 3, 5, 5-tetranitro-1, 3-diazacyclohexane	$C_4H_6N_6O_8$	(6)
42	TMTN	1, 3, 5-triaza-1, 3, 5-trinitrosocyclohexane	$C_3H_6N_6O_3$	(4)
43	NIRDX	6-nitroimino-1, 3, 5-trinitro-1, 3, 5-triazacyclohexane	$C_3H_4N_8O_8$	(6)
44	NIORDX	2-nitroimino-1, 3-dinitro-diaza-5-oxacyclohexane	$C_3H_4N_6O_7$	(6)
45	EDNA	ethylenedinitramine	C2H6N4O4	(1) (6)
46	NQ	nitroguanidine	$CH_4N_4O_2$	(4) (5) (7)
47	DNDMOA	dinitrodimethyloxamide	$C_4H_6N_4O_6$	(4)
48	NM	nitromethane	CH_3NO_2	(4) (5) (7)
49	TNM	tetranitromethane	CN_4O_8	(4) (7)
50	NTNEMA	N-nitro-N-trinitroethylmethylamine	$C_3H_5N_5O_8$	(6)
51	BTENED	bis(trinitroethyl)ethylene dinitramine	$C_6H_8N_{10}O_{16}$	(6)
52	BTNEU	bis(trinitroethyl)urea	$C_5H_6N_8O_{13}$	(1) (6)
53	TNEAE	N-nitro-N-trinitroethylaminoethanol nitrate	$C_4H_6N_6O_{15}$	(6)
54	NTNATE	N-nitro-N-trinitroethylaminotriazol	$C_4H_4N_8O_6$	(6)
55	BTNDATA	3, 6-bis(trinitroethylemino)-1, 2, 4, 5-tetrazine	$C_6H_6N_{12}O_{12}$	(6)
56	DEGN	diethyleneglycoldinitrate	$C_4H_8N_2O_7$	(4)
57	DNPEN	2, 4-dinitrophenoxyethylnitrate	$C_8H_7N_3O_8$	(4)
58	TNPON	2, 4, 6-trinitrophenoxyethylnitrate	$C_8H_6N_4O_{10}$	(4)
59	NG	nitroglycerin	$C_3H_5N_3O_9$	(4) (5)
60	PETN	pentaerythritol tetranitrate	$C_5H_8N_4O_{12}$	(4) (5) (6) (7) (8)
61	TMPTN	trimethylolethymethane trinitrate	$C_6H_{11}N_3O_9$	(4)
62	MNT	methylnitrate	CH_3NO_3	(4)
63	ENT	ethylnitrate	$C_2H_5NO_3$	(4)
64	EGDN	ethyleneglycol dinitrate	$C_2H_4N_2O_6$	(4)
65	FIVONITE	tetramethylcyclopentanon tetranitrate	$C_9H_{12}N_4O_{13}$	(4)
66	ISBDN	isosorbitol dinitrate	$C_6H_8N_2O_8$	(4)
67	CUTA	cyanuric triazide	C_3N12	(4) (7)
68	TATAB	1, 3, 5-triazido-2, 4, 6-trinitrobenzene	$C_6N_{12}O_6$	(7)
69	DATNH	1, 7-diazido-2, 4, 6-trinitro-2, 4, 6-triazaheptane	$C_4H_8N_{12}O_6$	(6)
70	DATEN	1, 9-diazido-2, 4, 6, 8-tetranitro-2, 4, 6, 8-tetraazanonane	$C_5H_{10}N_{14}O_8$	(6)

to the heat of formation of the explosive which decide the heat of detonation. We can say that nitrogen or oxygen atoms in the molecule of an explosive vary in their energy potential according to their bonding and chemical structural environments. Therefore, certain suitable correction coefficients are needed for some groups in the molecule of an explosive for extimating detonation paramters. However, the present correction coefficients are given empirically and arbitrarily.

From the defination of G and equation (3), we can see that G is a measure of forming gaseous detonation products in th H_2O–CO_2 decomposition assumption for an explosive. These gaseous detonation products are connected with the heat released in detonation process, therefor, G is an index of energy in an explosive. G would be related to other detonation parameters of an explosive.

4. ACKNOWLEDGMENTS

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Table 3 A Comparison of the Detnation Velocities Calculated by Various Methods

Type of explosive	Corrected OB[a] $(\pm\Delta\%)_D$ (data)		NMQ[a] $(\pm\Delta\%)_D$ (data)		Corrected NE[a] $(\pm\Delta\%)_D$ (data)		F formula[b] $(\pm\Delta\%)_D$ (data)		This paper $(\pm\Delta\%)_D$ (data)	
Aromatics	39 (256)	2.38	23 (236)	1.80	39 (256)	1.90	27	2.63	32 (75)	1.50
Aliphatis	66 (202)	3.09	25 (162)	2.30	83 (237)	1.54	13	1.42	23 (46)	2.16
Nitrate esters	22 (96)	3.98	15 (94)	4.50	25 (105)	2.57	12	2.42	11 (21)	2.08
Azides	4 (9)	2.42	3 (8)	7.45	4 (9)	2.89	1	5.0	4 (6)	2.84
Total	159 (563)	2.99	66 (500)	3.67	151 (607)	2.09	53	2.58	70 (148)	2.14

a Result of Ref. (2), b Result calculated from Ref. (9)

Table 4 Experimental and Calculated Detonation Pressure

Explosive	G	Density g/cm³	Pexp Kbar	Pcal Kbar	Pexp−Pcal	$(\Delta\%)_p$	Ref.
TACOT	0.500	1.85	263	259	4	1.52	(1)
TETRYL	0.646	1.614	226.4	231	−4.6	−2.03	(8)
TNT	0.523	1.637	189.1	207	−17.9	−9.46	(8)
		1.63	210	206	4	1.90	(5)
		1.64	190	208	−18	−9.47	(7)
TNTB	0.500	1.895	315	271	44	13.97	(7)
		1.50	175	170	5	2.86	(8)
		1.847	259	259	0	0.00	(8)
TNB	0.585	1.64	219	223	−4	−1.83	(6)
BTF	0.667	1.859	360	314	46	14.65	(5)
DATB	0.523	1.78	251	246	5	1.99	(5)
		1.788	259	248	11	4.25	(7)
HNAB	0.611	1.60	205	219	−14	−6.83	(5)
TENB	0.722	1.68	260	271	−11	−4.23	(6)
PNB	0.861	1.799	345	358	−13	−3.77	(6)
RDX	0.833	1.767	338	337	1	0.30	(5)
		1.773	337	337	0	0.00	(6)
		1.80	347	348	−1	−0.29	(7)
HMX	0.833	1.90	393	388	5	1.27	(7)
		1.90	395	388	7	1.77	(8)
		1.89	390	384	6	1.54	(5)
HCO	0.771	1.781	336	321	15	4.46	(6)
NM	0.75	1.128	141	127	14	9.93	(7)
		1.135	125	128	−3	−2.4	(5)
TMN	0.35	1.64	159	169	−10	−6.29	(7)
TNEAE	0.854	1.819	364	364	0	0.00	(6)
NG	0.929	1.59	253	295	−42	−16.60	(5)
PETN	0.818	1.67	300	296	4	1.33	(7)
		1.77	335	332	3	0.90	(7)
		1.67	310	296	14	4.52	(8)

Table 5 A Comaprison of the Detonation Pressure Calculated by Various Methods

Method	NMQ[a]	Corre. NE[a]	F formula[b]	this paper
Explosive	17	18	11	18
Data Point	112	114		30
± (Δ%) $_p$	6.91	6.70	10.5	4.33

a Results of Ref. (2), b Ref. (9).

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気体係数によるC-H-N-O系爆薬の爆速と爆轟圧力の計算

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C-H-N-O系爆薬の爆速と爆轟圧力の計算の新しい経験式を提出した。

$D = (2630+990G)\rho+2330G+650$

$P = (6.15+5.07G)^2\rho^2$

D と P は密度ρ (g/cm³) における爆速 (m/s) と爆轟圧力 (kbar) である。Gは爆薬の化学構造と爆轟生成気体によって決まる気体係数である。計算結果を実験結果と比較すると，爆速に対しては，148のデータ値 (70種の爆薬) についての誤差が±2.14%である；爆轟圧力に対しては，30のデータ値 (18種の爆薬) についての誤差が±4.32%であった。

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