

# Detonation temperature of high explosives from structural parameters

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## Abstract

A new scheme is introduced for calculating detonation temperature of different classes of high explosives. The ratio of oxygen to carbon and hydrogen to oxygen as well as specific structural parameters are the fundamental factors in the new method. An empirical new correlation is used to calculate detonation temperature of energetic compounds without considering heat contents of explosives and detonation products. Calculated detonation temperatures for both pure and explosive formulations show good agreement with respect to measured detonation temperatures and complicated computer code using BKWR and BKWS equations of state. Predicted detonation temperatures have root-mean-square (rms) percent deviation of 4.6, 14.2 and 4.6 from measured values for new method, BKWR and BKWS equations of state, respectively.

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## 1. Introduction

The development of theoretical methods as well as various empirical methods complemented the computer output for desk calculations would be needed because the expenditure connected with the development and synthesis of a new energetic material. Detonation temperature, heat of detonation, detonation velocity and detonation pressure are a variety of performance parameters for measuring the effectiveness of different explosives. Most of the work of an explosive in detonation is performed by the detonation reaction products because detonation reaction of an explosive is extremely fast and the heat liberated by detonation will raise the temperature of gases, which will in turn cause them to expand and work on surroundings.

The complicated computer codes and theoretical methods are convincing evidence of the utility of them for engineering calculations of detonation properties of explosives. Computer codes such as BKW [1], TIGER [2] and CHEETAH [3] (a C version of TIGER) with an appropriate empirical equation of state such as Becker–Kistiakosky–Wilson (BKW-EOS) [4]. It should be mentioned that the BKW-EOS in spite of its weak theoretical basis is used extensively to calculate detonation properties of high explosives so that the BKWC-EOS [3],

BKWR-EOS [5] and BKWS-EOS [6] are also three different parameterizations of the BKW-EOS. However, the BKWS-EOS is one of the best equations of states for predicting detonation temperatures. Empirical methods complemented the computer output for desk calculations can also be used to determine performance and various aspects of behavior of energetic compounds. Sikder et al. [7] reviewed some important correlations related to detonation velocity, Chapman–Jouguet (C–J) pressure, crystal density, oxygen balance and heat of formation along with structure–sensitivity relationships of CHNO energetic compounds. Some new correlations [8–24] have been recently introduced for simple evaluation performance and important aspects of properties of energetic compounds, e.g. impact sensitivity and Gurney velocity.

It can be assumed that heat of detonation of the explosive is entirely used to raise the temperature of products. If the quantities and the nature of the gaseous products as well as heat of detonation are known, detonation temperature can be calculated via molar heat capacities of detonation products. Some existing methods based on this procedure are reviewed elsewhere [25]. Condensed or gas phase heat of formation of explosive as well as some parameters can also be used for predicting detonation temperature [14,23].

The purpose of this work is to introduce the simplest method for calculating detonation temperature of high explosives only from elemental composition and some specific structural parameters without the use heat of formation and any experimental

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data of the explosive as well as detonation products. It is felt that the introduced procedure represents a significant advance in a priori computational or empirical methods of detonation temperature because there is no need to use heat content of pure explosive and energetic or non-energetic components in composite explosives. Another goal of this work is to provide insight to understanding the molecules, which are responsible for higher detonation temperature and which are not. The calculated detonation temperatures will also be tested with experimental data as well as computed results for well-known pure and composite explosives. The influence of chemical composition and structural parameters of explosive rather than detonation products for determining their detonation temperatures are of particular importance.

## 2. A simple method for predicting detonation temperature

Detonation temperature as well as the other detonation parameters of a notional explosive compound is recognized to be cost-effective, environmentally desirable and time saving in the decision to whether it is worth the effort to attempt a new or complex synthesis. Detonation temperature is not well-resolved measurements in contrast to detonation velocity [1]. High explosives produce detonation products at high pressures and temperatures simultaneously which covers a wide range of pressures,  $\sim 1$ –100 GPa, and temperatures,  $\sim 1000$ –5000 K [26]. Detonation temperature is one of the detonation parameters with least information in the C-J state which is measured experimentally from the brightness of the detonation front as it proceeds toward detector. Moreover, its measurement is difficult and is usually done by the brightness of the detonation front interacting with a detector with absolute accuracies estimated to be  $\pm 100$  K for liquid explosives and  $\pm 200$  K for solid explosives. However, there is some uncertainty for determination of radiation in measurement of detonation temperature because it is not known how much it is absorbed from detonation products by the shocked and partially decomposed explosive between the detector and the end of the reaction zone. Density discontinuities free system such as a liquid or a single crystal is to be useful for measurement of the detonation temperature because any voids or density discontinuities can lead to measurements of the brightness of the shocked air or shocked detonation products rather than the C-J detonation products. Since nitromethane is transparent, its measured detonation temperature is better known than for any other explosives so that its detonation temperature results lie between 3300 and 3500 K [27]. In contrast, detonation velocities are measured at various charge diameters and extrapolated to an “infinite diameter” for comparing with equilibrium calculations. However, detonation velocities can typically be measured to within a few percent. Detonation pressures determined by indirect method span a range of 10–20% that nonequilibrium effects in reaction zones may contribute to large uncertainty [1]. The measurement can be taken behind the von Neumann spike and in front of C-J plane so that the measured pressures may be higher than equilibrium calculations.

The computation of detonation parameters by computer codes in spite of its complexity usually requires measured condensed heat of formation of the explosive. It should be noted that the accuracy of predictive methods are not necessarily enhanced by greater complexity. Moreover, the heat content of explosive is also one of the essential parameter for determining detonation temperature via the other theoretical methods [14,23,25]. The solid and liquid phase heats of formation for the systems under consideration can be obtained as the difference between gas phase values and sublimation or vaporization enthalpies [7]. Two well-known group additivity and quantum mechanical methods can be used to provide gas phase heat of formation of energetic compounds. Rice et al. [28,29] have developed a computational method for predicting condensed phase heat of formation as well as heat of detonation of energetic materials from quantum mechanical calculations of the isolated molecules. They used the 6-31G\* basis set [30] and the hybrid density B3LYP [31,32] density functional for computation of heat of formation. However, since time and computer limitations, they did not perform an extensive search of the global minimum energy conformation for each molecule. Some theoretical methods have also been recently developed for calculating condensed phase heat of formation of some classes of energetic compounds [33–35].

It can be assumed that all the chemical bonds present in the reacting molecules are broken so that monatomic species appear. Subsequently, reactive species recombine to form stable products. The ratio of oxygen, as oxidizer, to carbon and hydrogen, as fuels, are important for obtaining high or low detonation temperature. Some structural parameters such as specific functional groups may also affect the value of detonation temperature. The study of detonation temperatures for various well-known pure and composite explosives shows that elemental composition as well as some structural parameters can affect their values. To find a good correlation, finding reliable data would be needed. Since experimental data of detonation temperature are rare, comparison of results with some theoretical predictions would be needed. The BKWS-EOS is one of the best equations of state for reliable prediction of detonation temperature. However, their predictions of detonation temperature are better than the BKWR-EOS. To create detonation temperature as a function of mentioned parameters, suitable general equation would be needed. The results showed that the following equation can supply the suitable pathway for predicting detonation temperature:

$$T(/K) = w_1 + w_2a + w_3b + w_4c + w_5d + w_6r_{O/C} + w_7r_{H/O} + \sum_{i=8} w_i SP_i \quad (1)$$

where  $a$ ,  $b$ ,  $c$  and  $d$  are the number carbon, hydrogen, nitrogen and oxygen in chemical formula,  $r_{H/O}$  and  $r_{O/C}$  the ratio of hydrogen to oxygen and oxygen to carbon, respectively, and  $SP_i$  is the number of specific structural parameters in the molecular structure of energetic compounds. The results also showed that the numbers of  $-NH_2$  and  $NH_4^+$  specific structural parameters in the energetic compounds have predominant effect in conducting correlation for reliable prediction of detonation temperature.

Table 1

Comparison of detonation temperature (in K) of the new correlation, Eq. (2), as well as BKWS- and BKWR-EOS with measured values [6]

Name <sup>a</sup>	$\rho_0$ (g/cc)	$T_{exp}$	$T_{new}$	%Dev new	$T_{BKWR-EOS}$	%Dev BKWR-EOS	$T_{BKWS-EOS}$	%Dev BKWS-EOS
HMX	1.6	4300	4406	2.5	3470	−19.3	4270	−0.7
NG	1.6	4260	4180	−1.9	3750	−12.0	4550	6.8
NM	1.13	3430	3206	−6.5	3220	−6.1	3580	4.4
PETN	1.6	4400	4393	−0.2	3520	−20.0	4390	−0.2
TETRYL	1.61	4200	4319	2.8	3590	−14.5	4270	1.7
	1.4	4130	4319	4.6	3750	−9.2	4350	5.3
	1.2	4300	4319	0.5	3840	−10.7	4380	1.9
	1	4390	4319	−1.6	3840	−12.5	4340	−1.1
TNM	1.64	2800	2869	2.5	2180	−22.1	2860	2.1
TNT	1	3400	3778	11.1	3410	0.3	3750	10.3
rms percent deviation				4.6		14.2		4.6

<sup>a</sup> See Appendix A for glossary of compound names.

However, the optimized correlation can be given as follows:

$$T(/K) = 5136 - 190.1a - 56.4b + 115.9c + 148.4d - 466.0r_{O/C} - 700.8r_{H/O} - 282.9n_{NH_x} \quad (2)$$

where  $-NH_x$  is the number of  $-NH_2$  and  $NH_4^+$  in the energetic compounds. Due to large uncertainty in detonation temperature data,  $R$ -squared value or the coefficient of determination of this correlation is 0.93 [36]. This equation provides the simplest empirical procedure for estimation of detonation temperature of pure and composite explosives, which require as input information only the elemental composition and the number  $-NH_2$  and  $NH_4^+$  in the explosive. Calculated detonation temperatures for underoxidized and overoxidized pure as well as mixed explosives are given in Tables 1 and 2. They are compared with corresponding measured values and computed results of BKWR- and BKWS-EOS. Predicted and experimental detonation temperatures using the new method, BKWR- and BKWS-EOS computations as well as the percent error, [(predicted – measured)/measured]  $\times$  100, are also given in Table 1. However, as seen in Tables 1 and 2, the introduced simple hand calculated empirical correlation for determining detonation temperatures show surprisingly very good agreement with experimental values as well as the computed detonation temperatures by BKWR- and BKWS-EOS which may be taken as appropriate validation test of the new method with pure and mixed  $C_aH_bN_cO_d$  explosives. The calculated detonation temperatures for some pure and mixed explosives where experimental data were not available are given in Table 2. As seen, the results of new correlation are close to computed predictions of BKWS-EOS. To very approximate guess of detonation temperature of CHNOF and CHNOCIF explosives, Eq. (2) can also be used for mentioned compounds. There is no need to use the contribution of Cl and F in Eq. (2) for these energetic compounds. The results are shown in Table 3 and compared with corresponding computed values by BKWS-EOS and BKWR-EOR. Since by considering large percent deviations generally attributed to experimental measurements of detonation temperature, the agreement between calculated values with measured and BKWS-EOS outputs are also satisfactory. As seen from Table 1, the root-mean-square (rms) deviation for new method,

Table 2

Comparison of detonation temperature (in K) of the new correlation, Eq. (2), BKWR- and BKWS-EOS [6]

Name <sup>a</sup>	$\rho_0$ (g/cc)	$T_{new}$	$T_{BKWR-EOS}$	$T_{BKWS-EOS}$
ABH	1.64	4778	3960	4710
COMP A-3	1.64	3541	3090	3670
COM B	1.72	3944	3230	3950
COM B-3	1.72	3984	3260	4000
COM C-3	1.6	3872	3150	3790
COM C-4	1.66	3617	3120	3760
CYCLOTOL-78/22	1.76	3939	3240	4070
CYCLOTOL-77/23	1.74	3941	3260	4070
CYCLOTOL-75/25	1.76	3948	3240	4050
CYCLOTOL-75/25	1.62	3948	3400	4130
CYCLOTOL-70/30	1.73	3965	3270	4040
CYCLOTOL-65/35	1.72	3977	3270	4030
CYCLOTOL-60/40	1.74	3988	3240	3990
CYCLOTOL-60/40	1.72	3988	3260	4000
CYCLOTOL-50/50	1.63	4001	3340	4000
DATB	1.8	3568	2860	3550
	1.78	3568	2870	3550
DEGN	1.38	3579	3240	3690
DIPM	1.76	3842	3310	4040
EXP D	1.55	3732	2840	3360
	1.48	3732	2890	3380
HMX	1.89	4406	3090	4070
	1.4	4406	3680	4380
	1.2	4406	3830	4450
	1	4406	3900	4480
	0.75	4406	4000	4440
HNAB	1.6	4638	3900	4620
HNS	1.6	3863	3580	4150
	1.7	3863	3500	4120
LX-01	1.24	3525	3670	4230
LX-14	1.84	3792	3030	3910
MEN-2	1.02	2663	2520	2720
NONA	1.7	4486	3780	4510
NQ	1.78	2864	2090	2740
	1.72	2864	2130	2760
	1.62	2864	2210	2790
	1.55	2864	2260	2830
OCTOL-78/22	1.82	3945	3160	4020
OCTOL-76/23	1.81	3945	3170	4020
OCTOL-75/25	1.81	3948	3170	4010

Table 2 (Continued)

Name <sup>a</sup>	$\rho_0$ (g/cc)	$T_{\text{new}}$	$T_{\text{BKWR-EOS}}$	$T_{\text{BKWS-EOS}}$
OCTOL-60/40	1.8	3988	3160	3950
PBX-9007	1.64	3722	3190	3810
PBX-9011	1.77	3742	2980	3720
PBX-9205	1.67	3756	3190	3870
PBX-9501	1.84	3798	3070	3970
PENTOLITE	1.71	4031	3290	3990
	1.7	4031	3300	4000
	1.68	4031	3320	4010
	1.64	4031	3360	4030
PETN	1.76	4393	3330	4280
	1.7	4393	3400	4320
	1.45	4393	3710	4490
	1.23	4393	3940	4600
PETN	0.99	4393	4150	4640
	0.88	4393	4240	4640
	0.48	4393	4460	4560
	0.3	4393	4470	4450
	0.25	4393	4460	4400
PICRATOL	1.63	3855	2990	3520
PICRIC ACID	1.76	4086	3280	4010
	1.71	4086	3330	4030
	1.6	4086	3420	4080
RDX	1.8	4180	3220	4140
	1.77	4180	3260	4160
	1.72	4180	3330	4200
	1.66	4180	3400	4230
	1.6	4180	3480	4280
	1.46	4180	3630	4360
	1.4	4180	3690	4390
	1.29	4180	3780	4430
	1.2	4180	3840	4460
	1.1	4180	3890	4480
	1	4180	3920	4490
	0.95	4180	3920	4490
	0.7	4180	4060	4450
	0.56	4180	4180	4450
TACOT	1.85	4083	3330	4040
TATB	1.88	3227	2550	3250
	1.85	3227	2580	3260
TETRYL	1.73	4319	3460	4210
	1.71	4319	3480	4220
	1.68	4319	3520	4240
	1.36	4319	3780	4360
TNT	1.64	3778	3210	3720
	1.45	3778	3330	3780
	1.36	3778	3380	3790
	0.8	3778	3330	3610
BTF	1.86	5115	4590	5570
	1.76	5115	4700	5600
HNB	1.97	5540	4360	5470
TNTAB	1.74	5811	4600	5640

<sup>a</sup> See Appendix A for glossary of compound names.

Table 3

Comparison of detonation temperature (in K) of the new correlation, Eq. (2), BKWR- and BKWS-EOS [6] for CHNOF and CHNOCIF explosives

Name <sup>a</sup>	$\rho_0$ (g/cc)	$T_{\text{new}}$	$T_{\text{BKWR-EOS}}$	$T_{\text{BKWS-EOS}}$
FEFO	1.59	4442	3520	4390
LX-04	1.86	3826	2940	3840
LX-07	1.87	3828	2990	3920
LX-09	1.84	3821	3120	4050
LX-10	1.86	3827	3070	4010
LX-11	1.87	3810	2860	3750
LX-15	1.58	4262	–	4210
LX-17	1.91	3209	–	3361
PBX-9010	1.78	3852	–	4250
PBX-9404	1.84	3618	–	3910
PBX-9407	1.6	3829	–	4170
PBX-9502	1.9	3196	–	3320
PBX-9503	1.9	3321	–	3450

<sup>a</sup> See Appendix A for glossary of compound name.

### 3. Conclusions

One of the important conclusions regarding the applicability of the new approach to detonation temperature estimation is that the results are very promising. The new method can develop systematic and scientific formulations of appropriate futuristic target molecules having desired detonation temperature. Moreover, there is no need to assume detonation products that is usually done by complicated computer codes. The results of Eq. (2) are remarkable because it has the same reliance on their answers as one could attach to the more complex computer code without considering heat content of explosives and detonation products.

Reported experimental data for detonation temperatures are rare because difficulty of measurement of detonation temperature. However, the new method can estimate detonation temperature only by the chemical formula of a real or hypothetical pure or mixture of explosives. The introduced correlation requires no prior knowledge of any measured properties of explosive and assumed detonation products.

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### Appendix A. Glossary of compound names

1. ABH: azobis(2,2',4,4',6,6'-hexanitrobisphenyl) ( $\text{C}_{24}\text{H}_6\text{N}_{14}\text{O}_{24}$ )
2. COMP A-3: 91/9 RDX/wax ( $\text{C}_{1.87}\text{H}_{3.74}\text{N}_{2.46}\text{O}_{2.46}$ )
3. COMP B: 63/36/1 RDX/TNT/wax ( $\text{C}_{2.03}\text{H}_{2.64}\text{N}_{2.18}\text{O}_{2.67}$ )
4. COMP B-3: 60/40 RDX/TNT ( $\text{C}_{2.04}\text{H}_{2.50}\text{N}_{2.15}\text{O}_{2.68}$ )
5. COMP C-3: 77/4/10/5/1/3 RDX/TNT/DNT/MNT/NC/TETRYL ( $\text{C}_{1.90}\text{H}_{2.83}\text{N}_{2.34}\text{O}_{2.60}$ )

BKWR and BKWS equations of state are 4.6, 14.2 and 4.6 K, respectively. The average deviations in Table 1 for new, BKWR- and BKWS-EOS methods are also 3.4, 12.7 and 3.5 K, respectively.



6. COMP C-4: 91/5.3/2.1/1.6 RDX/di(2-thylhexyl)sebacato/polyisobutylene/motor oil (C<sub>1.82</sub>H<sub>3.54</sub>N<sub>2.46</sub>O<sub>2.51</sub>)
7. CYCLOTOL-78/22: 78/22 RDX/TNT (C<sub>1.73</sub>H<sub>2.59</sub>N<sub>2.40</sub>-O<sub>2.69</sub>)
8. CYCLOTOL-77/23: 77/23 RDX/TNT (C<sub>1.75</sub>H<sub>2.59</sub>N<sub>2.38</sub>-O<sub>2.69</sub>)
9. CYCLOTOL-75/25: 75/25 RDX/TNT (C<sub>1.78</sub>H<sub>2.58</sub>N<sub>2.36</sub>-O<sub>2.69</sub>)
10. CYCLOTOL-70/30: 70/30 RDX/TNT (C<sub>1.87</sub>H<sub>2.56</sub>N<sub>2.29</sub>-O<sub>2.68</sub>)
11. CYCLOTOL-65/35: 65/35 RDX/TNT (C<sub>1.96</sub>H<sub>2.53</sub>N<sub>2.22</sub>-O<sub>2.68</sub>)
12. CYCLOTOL-60/40: 60/40 RDX/TNT (C<sub>2.04</sub>H<sub>2.50</sub>N<sub>2.15</sub>-O<sub>2.68</sub>)
13. CYCLOTOL-50/50: 50/50 RDX/TNT (C<sub>2.22</sub>H<sub>2.45</sub>N<sub>2.01</sub>-O<sub>2.67</sub>)
14. DATB: 1,3-diamino-2,4,6-trinitrobenzene (C<sub>6</sub>H<sub>5</sub>N<sub>5</sub>O<sub>6</sub>)
15. DEGN: diethyleneglycol dinitrate (C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>7</sub>)
16. DIPM: dipiramide (C<sub>12</sub>H<sub>6</sub>N<sub>8</sub>O<sub>12</sub>)
17. EXP D: ammonium picrate (C<sub>6</sub>H<sub>6</sub>N<sub>4</sub>O<sub>7</sub>)
18. HMX: cyclotetramethylenetetranitramine (C<sub>4</sub>H<sub>8</sub>N<sub>8</sub>O<sub>8</sub>)
19. HNAB: 2,2',4,4',6,6'-hexanitroazobenzene (C<sub>12</sub>H<sub>4</sub>N<sub>8</sub>O<sub>12</sub>)
20. HNS: 2,2',4,4',6,6'-hexanitrostilbene (C<sub>14</sub>H<sub>6</sub>N<sub>6</sub>O<sub>12</sub>)
21. LX-01: 51.7/33.2/15.5 NM/TNM/1-nitropropane (C<sub>1.52</sub>-H<sub>3.73</sub>N<sub>1.69</sub>O<sub>3.39</sub>)
22. LX-14: 95.5/4.5 HMX/estane 5702-F1 (C<sub>1.52</sub>H<sub>2.92</sub>N<sub>2.59</sub>-O<sub>2.66</sub>)
23. MEN-II: 72.2/23.4/4.4 nitromethane/methanol/ethylene diamine (C<sub>2.06</sub>H<sub>7.06</sub>N<sub>1.33</sub>O<sub>3.10</sub>)
24. NG: nitroglycerine (C<sub>3</sub>H<sub>5</sub>N<sub>3</sub>O<sub>9</sub>)
25. NM: nitromethane (CH<sub>3</sub>NO<sub>2</sub>)
26. NONA: 2,2',2'',4,4',4'',6,6',6''-nonanitroterphenyl (C<sub>18</sub>-H<sub>5</sub>N<sub>9</sub>O<sub>18</sub>)
27. NQ: nitroguanidine (CH<sub>4</sub>N<sub>4</sub>O<sub>2</sub>)
28. OCTOL-78/22: 77.6/22.4 HMX/TNT (C<sub>1.74</sub>H<sub>2.59</sub>N<sub>2.39</sub>-O<sub>2.69</sub>)
29. OCTOL-76/23: 76.3/23.7 HMX/TNT (C<sub>1.76</sub>H<sub>2.58</sub>N<sub>2.37</sub>-O<sub>2.69</sub>)
30. OCTOL-75/25: 75/25 HMX/TNT (C<sub>1.78</sub>H<sub>2.58</sub>N<sub>2.36</sub>O<sub>2.69</sub>)
31. OCTOL-60/40: 60/40 HMX/TNT (C<sub>2.04</sub>H<sub>2.50</sub>N<sub>2.15</sub>O<sub>2.68</sub>)
32. PBX-9007: 90/9.1/0.5/0.4 RDX/polystyrene/DOP/rosin (C<sub>1.97</sub>H<sub>3.22</sub>N<sub>2.43</sub>O<sub>2.44</sub>)
33. PBX-9011: 90/10 HMX/estane (C<sub>1.73</sub>H<sub>3.18</sub>N<sub>2.45</sub>O<sub>2.61</sub>)
34. PBX-9205: 92/6/2 RDX/polystyrene/DOP (C<sub>1.83</sub>H<sub>3.14</sub>-N<sub>2.49</sub>O<sub>2.51</sub>)
35. PBX-9501: 95/2.5/2.5 HMX/estane/EDNPA-F (C<sub>1.47</sub>H<sub>2.86</sub>-N<sub>2.60</sub>O<sub>2.69</sub>)
36. PENTOLITE: 50/50 TNT/PETN (C<sub>2.33</sub>H<sub>2.37</sub>N<sub>1.29</sub>O<sub>3.22</sub>)
37. PETN: pentaerythritol tetranitrate (C<sub>5</sub>H<sub>8</sub>N<sub>4</sub>O<sub>12</sub>)
38. PICRATOL: 52/48 EXP D/TNT (C<sub>2.75</sub>H<sub>2.33</sub>N<sub>1.48</sub>O<sub>2.75</sub>)
39. PA: picric acid (C<sub>6</sub>H<sub>3</sub>N<sub>3</sub>O<sub>7</sub>)
40. RDX: cyclomethylene trinitramine (C<sub>3</sub>H<sub>6</sub>N<sub>6</sub>O<sub>6</sub>)
41. TACOT: 2,4,8,10-tetranitro-5H-benzotriazol[2,1-a]benzotriazol-6-ium, hydroxide, inner salt (C<sub>12</sub>H<sub>4</sub>N<sub>8</sub>O<sub>8</sub>)
42. TATB: 1,3,5-triamino-2,4,6-trinitrobenzene (C<sub>6</sub>H<sub>6</sub>N<sub>6</sub>O<sub>6</sub>)
43. TETRYL: *N*-methyl-*N*-nitro-2,4,6-trinitroaniline (C<sub>7</sub>H<sub>5</sub>-N<sub>5</sub>O<sub>8</sub>)
44. TNT: 2,4,6-trinitrotoluene (C<sub>7</sub>H<sub>5</sub>N<sub>3</sub>O<sub>6</sub>)
45. BTF: benzotris [1,2,5] oxadiazole, 1,4,7-trioxide (C<sub>6</sub>N<sub>6</sub>O<sub>6</sub>)
46. HNB: hexanitrobenzene (C<sub>6</sub>N<sub>6</sub>O<sub>12</sub>)
47. TNM: tetranitromethane (C<sub>1</sub>N<sub>4</sub>O<sub>8</sub>)
48. TNTAB: trinitrotriazidobenzene (C<sub>6</sub>N<sub>12</sub>O<sub>6</sub>)
49. FEFO: 1,1'-[methylenebis(oxy)]bis[2-fluoro-2,2-dinitroethane] (C<sub>5</sub>H<sub>6</sub>N<sub>4</sub>O<sub>10</sub>F<sub>2</sub>)
50. LX-04: 85/15 HMX/Viton A (C<sub>1.55</sub>H<sub>2.58</sub>N<sub>2.30</sub>O<sub>2.30</sub>F<sub>0.52</sub>)
51. LX-07: 90/10 HMX/Viton A (C<sub>1.48</sub>H<sub>2.62</sub>N<sub>2.43</sub>O<sub>2.30</sub>F<sub>0.35</sub>)
52. LX-09: 93/4.6/2.4 HMX/pDNPA/FEFO (C<sub>1.43</sub>H<sub>2.74</sub>-N<sub>2.59</sub>O<sub>2.72</sub>F<sub>0.02</sub>)
53. LX-10: 95/5 HMX/Viton A (C<sub>1.42</sub>H<sub>2.66</sub>N<sub>2.57</sub>O<sub>2.57</sub>F<sub>0.17</sub>)
54. LX-11: 80/20 HMX/Viton A (C<sub>1.62</sub>H<sub>2.54</sub>N<sub>2.16</sub>O<sub>2.16</sub>F<sub>0.70</sub>)
55. LX-15: 95/5 HNS/KEL (C<sub>3.05</sub>H<sub>1.29</sub>N<sub>1.27</sub>O<sub>2.53</sub>Cl<sub>0.04</sub>F<sub>0.13</sub>)
56. LX-17: 92.5/7.5 TATB/KEL (C<sub>2.30</sub>H<sub>2.19</sub>N<sub>2.15</sub>O<sub>2.15</sub>-Cl<sub>0.05</sub>F<sub>0.2</sub>)
57. PBX-9010: 90/10 RDX/KEL (C<sub>1.41</sub>H<sub>2.48</sub>N<sub>2.43</sub>O<sub>2.43</sub>Cl<sub>0.27</sub>-F<sub>0.26</sub>)
58. PBX-9404: 94/3/3 HMX/NC/CEF (C<sub>1.40</sub>H<sub>2.75</sub>N<sub>2.57</sub>O<sub>2.69</sub>-Cl<sub>0.03</sub>P<sub>0.01</sub>)
59. PBX-9407: 94/6 RDX/Exon 461 (C<sub>1.41</sub>H<sub>2.66</sub>N<sub>2.54</sub>O<sub>2.69</sub>-Cl<sub>0.07</sub>F<sub>0.09</sub>)
60. PBX-9502: 95/5 TATB/KEL (C<sub>2.31</sub>H<sub>2.23</sub>N<sub>2.21</sub>O<sub>2.21</sub>Cl<sub>0.04</sub>-F<sub>0.13</sub>)
61. PBX-9503: 80/15/5 TATB/HMX/KEL (C<sub>2.16</sub>H<sub>2.29</sub>N<sub>2.27</sub>-O<sub>2.27</sub>Cl<sub>0.04</sub>F<sub>0.13</sub>)

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