

Reliable estimation of performance of explosives without considering their heat contents

Mohammad Hossein Keshavarz*

Department of Chemistry, Malek-ashtar University of Technology, Shahin-shahr, P.O. Box 83145/115, Islamic Republic of Iran

Received 18 December 2006; received in revised form 20 January 2007; accepted 22 January 2007

Available online 30 January 2007

Abstract

In this paper, a new approach is introduced to calculate detonation pressure of large class of explosives based elemental composition and specific structural groups rather than using their heats of formation. It is shown here how the loading density, atomic composition and some structural parameters can be integrated into an empirical formula for predicting the detonation pressure of pure and explosive formulations over a wide range of loading densities. The results show good agreement with experimental values so that the deviations are within about experimental errors. The calculated values of new method are also compared with the computed results obtained by complex computer code using BKWR and BKWS equations of state. Predicted detonation pressures have root-mean-square (rms) deviation for new method, BKWR and BKWS equations of state are 6.5, 11.7 and 7.4 kbar, respectively.

© 2007 Elsevier B.V. All rights reserved.

Keywords: Detonation pressure; Structural parameters; Performance; Loading density

1. Introduction

The calculated detonation properties of a notional energetic compound are 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. Moreover, determination of the performance of new energetic materials should be evaluated prior their actual synthesis because it reduces the costs associated with synthesis and test as well as evaluation of the materials. Predicting the performance of new energetic materials from a given molecular structure without using experimental measurement is very important to scientists. Since the difficulty of synthesis and the instability of energetic materials, the spending connected with the development and synthesis of new energetic materials also necessitates connected with the development of theoretical methods.

The pressure associated with the state of complete reaction has been regarded as one of the principal measures of performance of detonating explosive for many years. The determination of the time-independent state of chemical equilibrium,

which is defined in accordance with the Chapman–Jouguet (C–J), had historically special attention. It is reasonable to expect the calculated and experimental C–J pressures to differ by 10–20% because the nonsteady-state nature of the detonation wave [1]. It can be calculated either by some computer codes, such as RUBY [2] and latter's offspring TIGER [3] or CHEETAH [4] (a C Version of TIGER) with an appropriate empirical equation of state, such as Becker–Kistiakosky–Wilson (BKW-EOS) [5] or by empirical formulas [6]. Detonation pressure for ideal explosives can be evaluated by different pathways, such as heat of detonation at loading density greater than 1 g/cc [7–9] or any loading density [10], approximate detonation temperature [11–14] and gas phase heat of formation [15]. All of available methods require the heat of formation of energetic materials as one of the essential input parameter.

Simple reliable method is attractive to chemist for the expenditure connected with the development and synthesis of a new energetic material. The main focus thereafter will be on introducing the simplest method to calculate detonation pressure of high explosives only from elemental composition and some specific structural parameters without using heat of formation and any experimental data of the explosive as well as detonation products. It is felt that the introduced correlation represents a significant advance in a priori computational or empirical

* Tel.: +98 312 522 5071; fax: +98 312 522 5068.

E-mail addresses: mhkehavarz@mut-es.ac.ir, mhkir@yahoo.com.

Table 1
Comparison of detonation pressure (in kbar) of the new correlation, Eq. (2), as well as BKWS-EOS and BKWR-EOS with measured values [29]

Name ^a	ρ_0 (g/cc)	P_{exp}	P_{new}	%Dev new	$P_{BKWR-EOS}$	%Dev BKWR-EOS	$P_{BKWS-EOS}$	%Dev BKWS-EOS
COM B	1.72	295	285	-3.4	302	2.4	276	-6.4
COM B-3	1.72	287	285	-0.8	299	4.2	273	-4.9
CYCLOTOL-78/22	1.76	317	304	-4.1	329	3.8	302	-4.7
CYCLOTOL-77/23	1.74	313	296	-5.3	320	2.2	294	-6.1
CYCLOTOL-75/25	1.76	316	303	-4.0	327	3.5	300	-5.1
CYCLOTOL-75/25	1.62	265	254	-4.1	271	2.3	249	-6.0
CYCLOTOL-65/35	1.72	292	286	-2.0	303	3.8	277	-5.1
CYCLOTOL-50/50	1.63	231	251	8.6	257	11.3	235	1.7
DATB	1.8	251	253	0.6	292	16.3	258	2.8
	1.78	251	245	-2.3	280	11.6	250	-0.4
HMX	1.89	390	378	-3.0	405	3.8	374	-4.1
	1.6	280	273	-2.5	281	0.4	259	-7.5
	1.4	210	211	0.2	213	1.4	199	-5.2
	1.2	160	156	-2.2	160	0.0	151	-5.6
	1	110	111	0.6	117	6.4	110	0.0
	0.75	60	65	8.5	69	15.0	64	6.7
HNAB	1.6	205	215	5.0	222	8.3	204	-0.5
LX-14	1.84	370	337	-9.0	377	1.9	345	-6.8
NG	1.6	253	268	5.8	260	2.8	250	-1.2
NM	1.13	125	110	-11.8	134	7.2	130	4.0
NQ	1.72	245	276	12.7	292	19.2	250	2.0
OCTOL-78/22	1.82	342	326	-4.7	355	3.8	326	-4.7
OCTOL-76/23	1.81	338	322	-4.7	350	3.6	321	-5.0
OCTOL-60/40	1.8	320	314	-1.8	332	3.8	304	-5.0
PBX-9011	1.77	324	306	-5.4	337	4.0	307	-5.2
PENTOLITE	1.68	251	266	5.8	267	6.4	248	-1.2
PETN	1.76	337	318	-5.7	298	-11.6	312	-7.4
	1.7	307	296	-3.5	279	-9.1	289	-5.9
	1.6	266	262	-1.6	251	-5.6	254	-4.5
	1.45	208	214	3.0	215	3.4	208	0.0
	1.23	139	153	10.0	161	15.8	153	10.1
	0.99	87	98	12.1	104	19.5	100	14.9
	0.88	68	76	11.9	82	20.6	78	14.7
	0.48	24	20	-18.7	28	16.7	26	8.3
RDX	1.8	341	336	-1.3	364	6.7	334	-2.1
	1.77	338	325	-3.8	351	3.8	322	-4.7
	1.72	313	307	-1.9	329	5.1	302	-3.5
	1.6	263	266	1.0	281	6.8	260	-1.1
	1.46	211	221	4.8	232	10.0	216	2.4
	1.4	213	203	-4.6	214	0.5	199	-6.6
	1.29	166	173	3.9	183	10.2	172	3.6
	1.2	152	149	-1.9	160	5.3	152	0.0
	1.1	122	125	2.7	138	13.1	130	6.6
	1	89	103	16.2	117	31.5	110	23.6
	0.95	96	93	-2.8	107	11.5	100	4.2
	0.7	48	50	4.9	60	25.0	57	18.8
	0.56	32	32	0.0	41	28.1	38	18.8
TATB	1.85	259	251	-2.9	314	21.2	271	4.6
TETRYL	1.68	239	257	7.4	260	8.8	239	0.0
	1.61	226	233	2.9	237	4.9	218	-3.5
	1.36	142	155	9.4	168	18.3	157	10.6
TNT	1.64	210	221	5.0	223	6.2	203	-3.3
	1.45	144	160	10.8	167	16.0	153	6.3
	1.36	124	133	7.4	145	16.9	134	8.1
BTF	1.86	360	338	-6.0	343	-4.7	336	-6.7
TNM	1.64	159	159	0.0	150	-5.7	150	-5.7
rms deviation (kbar)				6.5		11.7		7.4

^a See Appendix A for glossary of compound name.

methods of detonation pressure because there is no need to use heat content of pure explosive and energetic or nonenergetic components in composite explosives. Another goal of this work is to provide insight to understanding the molecules which are responsible for higher detonation pressure and which are not. The calculated detonation pressures will also be tested with experimental data as well as computed results for well-known pure and composite explosives over a wide range of loading densities.

2. New procedure for determining the performance

Loading density and condensed phase heat of formation of an energetic molecule are two important parameters to screen potential explosives. Since suitable energetic materials must combine good performance with low vulnerability (whose high safety is obtained as the expense of the performance), the performance of a new energetic material can be evaluated prior its actual synthesis. Since well-known group additivity and quantum mechanical methods provide gas phase heat of formation, 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 [16]. To predict condensed phase heats of formation of energetic materials from quantum mechanical calculations of the isolated molecules, Rice et al. [17] have developed a computational method. Their quantum mechanical computations are based on the 6-31G* basis set [18] and the hybrid density B3LYP [19,20] density functional for computation of heat of formation. Later, Rice and Hare [21] has also used quantum mechanical predictions heat of formation of explosives to calculate their heats of detonation. They did not perform an extensive search of the global minimum energy conformation for each molecule because time and computer limitations. Moreover, some improvements have been recently developed to evaluate condensed phase heat of formation of some class of energetic compounds [22–24].

The study of detonation pressure 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 correlation between molecular properties and measured data, finding reliable data would be needed. To establish detonation pressure as a function of mentioned parameters, suitable general equation would be needed. Since pressure is proportional to ρ_0^2 which is adapted to experimentally measured values of detonation pressure [25,26], this condition should be considered in the new model. The results showed that of different combinations of mentioned parameters, the following model can provide the suitable pathway to obtain prediction of detonation pressure:

$$P \text{ (kbar)} = y_1 + y_2 \rho_0^2 + y_3 a + y_4 b + y_5 c + y_6 d + \sum_{i=7} y_i SP_i \quad (1)$$

where a , b , c and d are the number carbon, hydrogen, nitrogen and oxygen in chemical formula, ρ_0 the loading density, y_i the

adjustable parameters and SP_i is the number of specific structural parameters in the molecular structure of energetic compounds. To establish kind of specific functional groups that can affect the values of detonation pressure, various functional groups were examined. The results showed that the numbers of $-NH_2$ and NH_4^+ in the energetic compounds have predominant effect in conducting correlation for reliable prediction of detonation pressure. To find adjustable parameters, experimental data of various pure explosives, which are listed in Table 1, were used. The following correlation (R^2 -value or the coefficient of determination

Table 2
Comparison of detonation pressure (in kbar) of the new correlation, Eq. (2), BKWR-EOS and BKWS-EOS [29]

Name ^a	ρ_0 (g/cc)	P_{new}	$P_{\text{BKWR-EOS}}$	$P_{\text{BKWS-EOS}}$
ABH	1.64	193	230	211
COMP A-3	1.64	257	287	266
COM C-3	1.6	245	253	230
COM C-4	1.66	265	296	273
CYCLOTOL-70/30	1.73	291	311	285
CYCLOTOL-60/40	1.74	292	307	281
CYCLOTOL-60/40	1.72	285	299	273
DEGN	1.38	166	189	183
DIPM	1.76	220	266	239
EXP D	1.55	187	195	176
	1.48	165	175	158
HNS	1.6	178	206	187
	1.7	213	236	214
LX-01	1.24	142	172	165
MEN-2	1.02	74	95	94
NONA	1.7	221	241	221
NQ	1.78	298	317	272
	1.62	241	252	217
	1.55	218	227	198
OCTOL-75/25	1.81	322	349	320
PBX-9007	1.64	256	279	256
PBX-9205	1.67	269	295	271
PBX-9501	1.84	337	379	348
PENTOLITE	1.71	276	277	258
	1.7	273	274	255
	1.64	252	253	235
PICRATOL	1.63	230	221	200
PA	1.76	260	259	237
	1.71	242	243	222
	1.6	204	210	192
RDX	1.66	286	304	279
TACOT	1.85	283	288	233
TATB	1.88	263	328	285
TETRYL	1.73	274	277	255
	1.71	267	270	248
	1.4	167	178	165
	1.2	113	133	127
	1	67	97	95
BTF	1.76	301	307	302
HNB	1.97	415	382	329
TNTAB	1.74	327	321	312

^a See Appendix A for glossary of compound name.

[27] 0.987) can be found:

$$P(\text{kbar}) = -22.3207 + 104.0393\rho_0^2 - 10.9781a - 1.9967b \\ + 5.5619c + 5.5392d - 23.6834n_{-\text{NH}_x} \\ - 154.0862n_1^0 \quad (2)$$

where $-\text{NH}_x$ is the number of $-\text{NH}_2$ and NH_4^+ in the energetic compounds and n_1^0 has the value one for an energetic compound that follows condition $d > 3(a+b)$ and for the other situations has zero value.

3. Comparison of the results of the new method with outputs of complex computer computations

Predicted and experimental detonation pressures using the new method, BKWR-EOS [28] and BKWS-EOS [29] computations as well as the percent error, [(predicted – measured)/measured] \times 100, are given in Table 1. 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 [4], BKWR-EOS [28] and BKWS-EOS [29] are also three different parameterizations of the BKW-EOS. The BKWS-EOS predictions of detonation pressure are better than the BKWR-EOS predictions. The BKWS-EOS was calibrated over the entire density range meanwhile the BKWR-EOS was calibrated with explosives with initial densities greater than 1 g/cc. Therefore, the BKWR-EOS performs well at higher densities but the BKWS-EOS tends to perform better than the BKWR-EOS over the intermediate and low density ranges. As seen in Table 1, calculated detonation pressures of well-known pure and composite explosives are compared with experimental data as well as computed values of BKWS-EOS and BKWR-EOS. The results of the new method show surprisingly very good agreement with experimental data over a wide range of loading densities as compared to the outputs of complicated computation. It should be emphasized that comparison of the calculated results with experimental data may be taken as appropriate validation test of the introduced simple correlation for overoxydized and underoxydized explosives.

As indicated in Table 1, the results are in good agreement with values obtained from computational methods. The rms deviation of the new method from experiment is 6.5 kbar, but the rms deviation of the computed values for BKWR-EOS and BKWS-EOS are 11.7 and 7.4 kbar, respectively. The average deviations in Table 1 for new, BKWR-EOS and BKWS-EOS methods are 5.1, 9.1 and 5.7 kbar, respectively. The estimated detonation pressure by this new approach is within 5 kbar of the reported values for 37 explosive compounds, within 5–10 kbar for 12 explosive compounds, and more than 10 kbar for remainder 7 explosive compounds.

One of the important conclusions regarding the applicability of the new approach to detonation pressure estimation is that the results are very promising. A total 56 experimental data of well-known CHNO explosives containing nitramines, nitro and nitrate energetic compounds were considered in the new approach. The explosives of Table 1 cover a wide range in oxygen balance and are considered to be representative of the entire class of CHNO pure and composite explosives. Since the lower accuracy generally attributed to the experimental measurements of the C-J pressure, the agreement between calculated and measured pressures is also satisfactory. Considering wide range heat of formation of explosives, e.g. +116 kcal/mol for ABH and -90.8 kcal/mol for NG [29], it is found that the overall agreement of the new approach with reported detonation pressure without using heat of formation is quite good.

Since there is no need to have experimental or calculated data of any proposed explosives, the new method can provide the simplest available approach to calculate detonation performance. It is very important for explosive chemists to develop explosives with higher performance than HMX. The compound 2,4,6-trinitro-1,3,5-triazine [30,31] is a high-energy density material so that there is no method reported for its synthesis [31]. Two different calculated crystal densities 1.98 [30] and 2.10 g/cc [31] were reported for this compound, hence, their calculated detonation pressures by new method give 419 and 470 kbar, respectively. These values consistent with recent theoretical per-

Table 3
Comparison of detonation pressure (in kbar) of the new correlation, Eq. (2), as well as BKWR-EOS and BKWS-EOS with measured values [29] for CHNOF and CHNOCIF explosives

Name ^a	ρ_0 (g/cc)	P_{exp}	P_{new}	%Dev new	$P_{\text{BKWR-EOS}}$	% Dev BKWR-EOS	$P_{\text{BKWS-EOS}}$	%Dev BKWS-EOS
FEFO	1.59	250	251	0.6	234	-6.4	211	-15.6
LX-04	1.86	350	341	-2.6	342	-2.3	304	-13.1
LX-07	1.87		347		364		327	
LX-09	1.84	377	338	-10.3	377	0.0	347	-8.0
LX-10	1.86	375	345	-7.9	376	0.3	342	-8.8
LX-11	1.87		343		328		288	
LX-15	1.58		222				181	
LX-17	1.91		286				289	
PBX-9010	1.78	328	314	-4.3			307	-6.4
PBX-9404	1.84	375	330	-12.1			341	-9.1
PBX-9407	1.6	287	252	-12.1			248	-13.6
PBX-9502	1.9		280				287	
PBX-9503	1.9		293				300	

^a See Appendix A for glossary of compound name.

formance study of this highly interesting energetic compound [32].

The calculated detonation pressures 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 BKWR-EOS and BKWS-EOS. The new correlation can also be used for CHNOF and CHNOCIF pure and mixed explosive, which is shown in Table 3. There is no need to use the contribution of Cl and F in Eq. (2) for mentioned energetic compounds.

One of the useful hydrodynamic relations is given as follows [1]:

$$P = \frac{\rho_0 D^2}{\Gamma + 1} \quad (3)$$

where D and Γ are detonation velocity and the adiabatic exponent, respectively, at given loading density. The following correlation [33] can be used to estimate detonation velocity via Eq. (3):

$$\Gamma = 1.819 - \frac{0.196}{\rho_0} + 0.712\rho_0 \quad (4)$$

As representative example, calculated detonation velocity for HMX via calculated detonation pressure at $\rho_0 = 1.89$ g/cc ($P_{\text{cal, Eq. (2)}} = 378$ kbar) is 9.01 km/s which is close to measured value, i.e. 9.11 km/s [29].

4. Conclusions

The main aim of this work was to introduce the simplest method for calculating detonation pressure of pure and composite explosives over a wide range of initial densities only from elemental composition and structural parameters of explosives without the use of heat of formation of explosives and detonation products. This work has also provided insight to understanding suitable mixture of high explosives which are responsible for higher detonation pressure and which are not. The influence of chemical composition rather than detonation products for determining their detonation pressures are of particular importance. The new correlation requires no prior knowledge of any measured, estimated or calculated physical, chemical or thermochemical properties of explosive and assumed detonation products.

In brief, the new approach is the simplest method for reliable quick estimation of detonation pressure and at the same time gives results that are comparable with computed values obtained from complex computer codes.

Acknowledgements

I would like to thank the research committee of Malek-ashtar University of Technology (MUT) for supporting this work. This research was supported in part by Institute of Chemical and Science Technology-Tehran-Iran Research Council Grant (No. ICST-8103-2132).

Appendix A. Glossary of compound names

1. ABH: Azobis(2,2',4,4',6,6'-hexanitrobisphenyl) ($C_{24}H_6N_{14}O_{24}$)
2. COMP A-3: 91/9 RDX/wax ($C_{1.87}H_{3.74}N_{2.46}O_{2.46}$)
3. COMP B: 63/36/1 RDX/TNT/wax ($C_{2.03}H_{2.64}N_{2.18}O_{2.67}$)
4. COMP B-3: 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
5. COMP C-3: 77/4/10/5/1/3 RDX/TNT/DNT/MNT/NC/TETRYL ($C_{1.90}H_{2.83}N_{2.34}O_{2.60}$)
6. COMP C-4: 91/5.3/2.1/1.6 RDX/di(2-ethylhexyl)sebacato/polyisobutylene/motor oil ($C_{1.82}H_{3.54}N_{2.46}O_{2.51}$)
7. CYCLOTOL-78/22: 78/22 RDX/TNT ($C_{1.73}H_{2.59}N_{2.40}O_{2.69}$)
8. CYCLOTOL -77/23: 77/23 RDX/TNT ($C_{1.75}H_{2.59}N_{2.38}O_{2.69}$)
9. CYCLOTOL -75/25: 75/25 RDX/TNT ($C_{1.78}H_{2.58}N_{2.36}O_{2.69}$)
10. CYCLOTOL-70/30: 70/30 RDX/TNT ($C_{1.87}H_{2.56}N_{2.29}O_{2.68}$)
11. CYCLOTOL-65/35: 65/35 RDX/TNT ($C_{1.96}H_{2.53}N_{2.22}O_{2.68}$)
12. CYCLOTOL-60/40: 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
13. CYCLOTOL-50/50: 50/50 RDX/TNT ($C_{2.22}H_{2.45}N_{2.01}O_{2.67}$)
14. DATB: 1,3-Diamino-2,4,6-trinitrobenzene ($C_6H_5N_5O_6$)
15. DEGN: Diethyleneglycol dinitrate ($C_4H_8N_2O_7$)
16. DIPM: Dipiramide ($C_{12}H_6N_8O_{12}$)
17. EXP D: Ammonium picrate ($C_6H_6N_4O_7$)
18. HMX: Cyclotetramethylenetetranitramine ($C_4H_8N_8O_8$)
19. HNAB: 2,2',4,4',6,6'-Hexanitroazobenzene ($C_{12}H_4N_8O_{12}$)
20. HNS: 2,2',4,4',6,6'-Hexanitrostilbene ($C_{14}H_6N_6O_{12}$)
21. LX-01: 51.7/33.2/15.5 NM/TNM/1-nitropropane ($C_{1.52}H_{3.73}N_{1.69}O_{3.39}$)
22. LX-14: 95.5/4.5 HMX/estane 5702-F1 ($C_{1.52}H_{2.92}N_{2.59}O_{2.66}$)
23. MEN-II: 72.2/23.4/4.4 Nitromethane/methanol/ethylene diamine ($C_{2.06}H_{7.06}N_{1.33}O_{3.10}$)
24. NG: Nitroglycerine ($C_3H_5N_3O_9$)
25. NM: Nitromethane (CH_3NO_2)
26. NONA: 2,2',2'',4,4',4'',6,6',6''Nonanitroterphenyl ($C_{18}H_5N_9O_{18}$)
27. NQ: Nitroguanidine ($CH_4N_4O_2$)
28. OCTOL-78/22: 77.6/22.4 HMX/TNT ($C_{1.74}H_{2.59}N_{2.39}O_{2.69}$)
29. OCTOL-76/23: 76.3/23.7 HMX/TNT ($C_{1.76}H_{2.58}N_{2.37}O_{2.69}$)
30. OCTOL -75/25: 75/25 HMX/TNT ($C_{1.78}H_{2.58}N_{2.36}O_{2.69}$)
31. OCTOL -60/40: 60/40 HMX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
32. PBX-9007: 90/9.1/0.5/0.4 RDX/polystyrene/DOP/rosin ($C_{1.97}H_{3.22}N_{2.43}O_{2.44}$)
33. PBX-9011: 90/10 HMX/estane ($C_{1.73}H_{3.18}N_{2.45}O_{2.61}$)
34. PBX-9205: 92/6/2 RDX/polystyrene/DOP ($C_{1.83}H_{3.14}N_{2.49}O_{2.51}$)
35. PBX-9501: 95/2.5/2.5 HMX/estane/EDNPA-F ($C_{1.47}H_{2.86}N_{2.60}O_{2.69}$)
36. PENTOLITE: 50/50 TNT/PETN ($C_{2.33}H_{2.37}N_{1.29}O_{3.22}$)

37. PETN: Pentaerythritol tetranitrate ($C_5H_8N_4O_{12}$)
38. PICRATOL: 52/48 EXP D/TNT ($C_{2.75}H_{2.33}N_{1.48}O_{2.75}$)
39. PA: Picric acid ($C_6H_3N_3O_7$)
40. RDX: Cyclomethylene trinitramine ($C_3H_6N_6O_6$)
41. TACOT: 2,4,8,10-Tetranitro-5H-benzotriazol[2,1,a]-benzotriazol-6-ium, hydroxide, inner salt ($C_{12}H_4N_8O_8$)
42. TATB: 1,3,5-Triamino-2,4,6-trinitrobenzene ($C_6H_6N_6O_6$)
43. TETRYL: *N*-Methyl-*N*-nitro-2,4,6-trinitroaniline ($C_7H_5N_5O_8$)
44. TNT: 2,4,6-Trinitrotoluene ($C_7H_5N_3O_6$)
45. BTF: Benzotris [1,2,5] oxadiazole, 1,4,7-trioxide ($C_6N_6O_6$)
46. HNB: Hexanitrobenzene ($C_6N_6O_{12}$)
47. TNM: Tetranitromethane ($C_1N_4O_8$)
48. TNTAB: Trinitrotriazidobenzene ($C_6N_{12}O_6$)
49. FEFO: 1,1'-[Methylenebis(oxy)]bis[2-fluoro-2,2-dinitroethane] ($C_5H_6N_4O_{10}F_2$)
50. LX-04: 85/15 HMX/viton A ($C_{1.55}H_{2.58}N_{2.30}O_{2.30}F_{0.52}$)
51. LX-07: 90/10 HMX/viton A ($C_{1.48}H_{2.62}N_{2.43}O_{2.30}F_{0.35}$)
52. LX-09: 93/4.6/2.4 HMX/pDNPA/FEFO ($C_{1.43}H_{2.74}N_{2.59}O_{2.72}F_{0.02}$)
53. LX-10: 95/5 HMX/viton A ($C_{1.42}H_{2.66}N_{2.57}O_{2.57}F_{0.17}$)
54. LX-11: 80/20 HMX/viton A ($C_{1.62}H_{2.54}N_{2.16}O_{2.16}F_{0.70}$)
55. LX-15: 95/5 HNS/KEL ($C_{3.05}H_{1.29}N_{1.27}O_{2.53}Cl_{0.04}F_{0.13}$)
56. LX-17: 92.5/7.5 TATB/KEL ($C_{2.30}H_{2.19}N_{2.15}O_{2.15}Cl_{0.05}F_{0.2}$)
57. PBX-9010: 90/10 RDX/KEL ($C_{1.41}H_{2.48}N_{2.43}O_{2.43}Cl_{0.27}F_{0.26}$)
58. PBX-9404: 94/3/3 HMX/NC/CEF ($C_{1.40}H_{2.75}N_{2.57}O_{2.69}Cl_{0.03}P_{0.01}$)
59. PBX-9407: 94/6 RDX/Exon 461 ($C_{1.41}H_{2.66}N_{2.54}O_{2.69}Cl_{0.07}F_{0.09}$)
60. PBX-9502: 95/5 TATB/KEL ($C_{2.31}H_{2.23}N_{2.21}O_{2.21}Cl_{0.04}F_{0.13}$)
61. PBX-9503: 80/15/5 TATB/HMX/KEL ($C_{2.16}H_{2.29}N_{2.27}O_{2.27}Cl_{0.04}F_{0.13}$)

References

- [1] C.L. Mader, Numerical Modeling of Explosives and Propellants, second ed., CRC Press, 1998.
- [2] H.B. Levine, R.E. Sharples, Operator's Manual for RUBY, Lawrence Livermore Laboratory Report UCRL-6815, Livermore, CA, 1962.
- [3] M. Cowperthwaite, W.H. Zwisler, TIGER Computer Program Documentation, Stanford Research Institute, 1973 (SRI publication number 2106).
- [4] L.E. Fried, W.M. Howard, P.C. Souers, CHEETAH 2. 0 User's Manual, Lawrence Livermore National Laboratory, Livermore, CA, 1998.
- [5] C.L. Mader, Detonation properties of condensed explosives computed using the Becker–Kistiakosky–Wilson equation of state, Los Alamos Scientific Laboratory Report LA-2900, New Mexico, 1963.
- [6] M.H. Keshavarz, A simple theoretical prediction of detonation velocities of non-ideal explosives only from elemental composition, in: P.B. Waley (Ed.), New Research on Hazardous Materials, Nova Science Publishers, Inc., 2006 (Chapter 8).
- [7] M.J. Kamlet, S.J. Jacobs, J. Chem. Phys. 48 (1968) 23.
- [8] M.J. Kamlet, J.E. Ablard, J. Chem. Phys. 48 (1968) 36.
- [9] M.J. Kamlet, C. Dickinson, J. Chem. Phys. 48 (1968) 43.
- [10] M.H. Keshavarz, H.R. Pouretedal, Thermochim. Acta 414 (2004) 203.
- [11] M.H. Keshavarz, M. Oftadeh, High Temp. High Pressure 34 (2002) 495.
- [12] M.H. Keshavarz, M. Oftadeh, Bull. Korean Chem. Soc. 24 (2003) 19.
- [13] M.H. Keshavarz, M. Oftadeh, Indian J. Eng. Mater. Sci. 10 (2003) 236.
- [14] M.H. Keshavarz, H.R. Pouretedal, J. Chin. Inst. Eng. 29 (2006) 145.
- [15] M.H. Keshavarz, J. Hazard. Mater. A 119 (2005) 25.
- [16] A.K. Sikder, G. Maddala, J.P. Agrawal, H. Singh, J. Hazard. Mater. A 84 (2001) 1.
- [17] B.M. Rice, S.V. Pai, J. Hare, Combust. Flame 118 (1999) 445.
- [18] W.J. Hehre, L. Rdom, P.V.R. Schleyer, J.A. Pople, Ab Initio Molecular Orbital Theory, Wiley, New York, 1986, p. 271, 298.
- [19] A.D. Becke, J. Chem. Phys. 98 (1993) 5648.
- [20] C. Lee, W. Yang, R.G. Parr, Phys. Rev. B 37 (1998) 785.
- [21] B.M. Rice, J. Hare, Therochem. Acta 384 (2002) 377.
- [22] M.H. Keshavarz, M. Oftadeh, High Temp. High Press. 35/36 (2003/2006) 499.
- [23] M.H. Keshavarz, J. Hazard. Mater. A 136 (2006) 145.
- [24] M.H. Keshavarz, J. Hazard. Mater. A 136 (2006) 425.
- [25] C.H. Johansson, P.A. Persson, Detonics of High Explosives, Academic Press, New York, 1970, p. 34.
- [26] R. Chirat, G. Pittion-Rossillon, J. Chem. Phys. 74 (1981) 4634.
- [27] W.J. Palm III, Matlab for Engineering Applications, WBC/McGraw-Hill, 1999, p. 334.
- [28] M. Fringer, E. Lee, F.H. Helm, B. Hayes, H. Hornig, R. McGuire, M. Kahara, M. Gudiry, Proceedings of the Sixth Symposium (International) on Detonation, Coronads, CA, Washington, DC, Office of the Chief of Naval Operations, 1976.
- [29] M.L. Hobbs, M.R. Baer, Calibrating the BKW-EOS with a large product species database and measured C-J properties, in: 10th Symposium (International) on Detonation, Boston, MA, 1993.
- [30] R.E. Kirk, D.F. Othmer, Encyclopedia of Chemical Technology, vol. 10, fourth ed., Jhon Wiley & Sons, 1993, pp. 54–55.
- [31] A.A. Korkin, R.J. Bartlett, J. Am. Chem. Soc. 118 (1996) 12244.
- [32] M.H. Keshavarz, M. Oftadeh, Asian J. Chem. 17 (2005) 663.
- [33] M.H. Keshavarz, H.R. Pouretedal, Indian J. Eng. Mater. Sci. 13 (2006) 259.