Detonation performance of high-dense BTF charges

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Abstract. New experimental data on detonation wave parameters and explosive performance for benzotrifuroxan are presented. Optical pyrometry was applied in order to measure the temperature and pressure of BTF detonation products. Chapman-Jouguet temperature was obtained as 3990 - 4170 K (charge densities 1.82 - 1.84 g/cc). The heat of explosion and the acceleration ability were measured also. It is also considered the hypothesis of formation of nanodiamond particles in detonation products directly behind the detonation front and influence of these processes on the temperature-time history in detonation products.

1. Introduction

BTF, benzotrifuroxan (C₆N₆O₆), is a powerful hydrogen-free HE with single-crystal density ρ = 1.903 g/cc [1] and enthalpy of formation 2.31 MJ/kg [2]; detonation parameters are the following detonation velocity D = 8.49 km/s (ρ₀ = 1.85 - 1.86 g/cc); failure diameter dₖ = 0.5 – 1.0 mm; C-J pressure pC-J = 33.0 – 36.0 GPa (ρ₀ = 1.85 - 1.86 g/cc) [3], while there are significant differences in the calculated temperatures of detonation products (DPs) T = 3700 – 5100 K [4-6]. BTF properties determine the specific areas of its application, in particular, in synthesis of detonation diamonds of special droplet shape, formation of which is ascribed to extremely high temperature. The analysis of the published data on BTF shows that, in spite of the high interest to DP-performance of BTF, there is no data on DPs state in the front of detonation wave. In this paper, there are given experimental results on DP-performance of BTF, as well as the data on the heat of explosion and the acceleration ability.

2. Experimental

Two-channel optical pyrometer (wavelengths 627 and 420 nm) was used to measure temperature time-histories T(t) and pressure p(t) (so-called “window” and “indicator” techniques [7,8]). Brightness temperatures were measured at the interface between BTF charge and the window (LiF or glycerol). Radiation emitted from the shock front spreading in liquid indicator (CHBr₃ or CCl₄) poured on the BTF charge served as peculiar gauge to obtain p(t). To prevent the influence of a luminescence of DPs the surface of charges was covered by a layer of a black varnish. In some shots the thin aluminum plate was located between BTF charge and the indicator. The charges were initiated by plane-wave generator of 40-mm diameter through the booster charge, both made of RDX with wax. The experimental assemblies used were very much alike those sketched in [9]. There were tested pressed charges both 30 mm of height and diameter with density ρ = 1.82 g/cc or ρ = 1.84 g/cc. The error was estimated to be ±150 K for T and ±1 GPa for p.
Bomb calorimeter (internal volume 1.7 L) was used in order to measure the heat of explosion. The error was estimated to be 1%, for detail see [2]. The technique T-20 (the analog of cylinder test) was used to measure the acceleration ability [10]. The error of casing velocity measurement was 1%. Detonation velocity was also measured in the test with an accuracy of 0.5%.

Brightness DP-temperatures measured at two wavelengths do not differ within the measurement error. \( T(t) \)-curves averaged over the wavelengths are shown in figure 1, where \( T(t) \)-curves for TNT, BTNEN, and TNT with 1% of carbon black are given for a comparison. For the LiF-window used, \( T(t) \)-records obtained for HMX [9] and BTNEN [11] differ from \( T(t) \) for BTF. Form of \( T(t) \) is very much alike that measured for TNT, both are characterized by “temperature plateau” within first microsecond; which was not observed for any other HE tested. \( T(t) \)-records measured with the help of two windows of different compressibility makes it possible to obtain DP-temperature in the C-J point \( (T_{C-J}) \) [9]. Using Mi-Gruneisen EOS of DPs and assuming \( \Gamma/V = \text{const} \), one can deduce the expression:

\[
T_i = T_{C-J} \exp \left\{ \frac{\Gamma}{V} \left( V_{C-J} - V_i \right) \right\},
\]

where \( T_i \) – DP-temperature measured in the isentrope or double shock; \( V_{C-J} \) and \( V_i \) – specific volumes in the C-J and reflected waves states respectively. Basing on values \( T_1 \) and \( T_2 \) corresponding to the states with experimental pressures \( p_1 \) and \( p_2 \), one can calculate \( T_{C-J} \).

Figure 1. Brightness temperatures time-histories of detonation products: a) LiF-window: 1 – BTF, \( \rho_0 = 1.82 \text{ g/cc} \); 1a – BTNEN, \( \rho_0 = 1.88 \text{ g/cc} \). Glycerol-window: 2 – BTF, \( \rho_0 = 1.82 \text{ g/cc} \); b) LiF-window: 1 – TNT, \( \rho_0 = 1.62 \text{ g/cc} \); 2 – TNT with 1% of carbon black, \( \rho_0 = 1.62 \text{ g/cc} \)

Figure 2. Pressure-time histories in indicators for BTF charges (1.82 g/cc)

Pressure histories \( p(t) \) in CHBr\(_3\) and CCl\(_4\) are shown in figure 2. Assuming that parts of \( p(t) \)-curve, shown by arrows, correspond to the von Neumann peak, one can estimate the duration of detonation zone as \( \tau = 60-75 \text{ ns} \).

Using results of the tests, there were calculated \( p-u \)-states of DPs, see figure 3. The calculations were made basing on the Hugoniots of the materials and \( D(p) \)-relation for BTF: \( D = 4.265+2.27p \) [3].
Obtained $p$-$u$-states give the best fitting points for the polytrope with exponent $n = 2.8$. The values of $p$ and $T$ are given in table 1, in which the data [7] for HMX and RDX are also shown. Temperature of DPs of BTF, $4100 \pm 150$ K, is $500 – 1000$ K less than the most of calculated values published.

The measured value of the heat of explosion ($Q$) for BTF is given in table 2, the data for HMX are shown for comparison. The Ornellas data [12] are given in the last column, where the charge density is shown in brackets. The number of moles of gaseous DPs ($N_\rho$) was calculated according to the procedure described in [13]. Taking into account $Q(\rho)$-relation, one can conclude that the measured $Q$ values are close to those given in [12]. BTF herewith slightly surpasses HMX in the heat of explosion. Nevertheless, HMX has the advantage in a number of moles of gases, and this, in general, provides better conditions for energy transformation into the work of expanding DPs.

### Table 1. Temperature and pressure of DPs.

| HE   | $\rho_0$, g/cc | Window  | $p_i$, GPa | $T_i$, K | $p_{C-J}$, GPa | $T_{C-J}$, K |
|------|----------------|---------|------------|----------|----------------|--------------|
| BTF  | 1.82           | LiF     | 38.6       | 4060     | 33.8           | 3990         |
|      |                | Glycerol| 25.2       | 3840     |                |              |
| BTF  | 1.84           | LiF     | 39.2       | 4250     | 34.5           | 4170         |
|      |                | Glycerol| 25.6       | 4000     |                |              |
| RDX  | 1.71           | LiF     | 37.5       | 3850     | 31.4           | 3740         |
|      |                | H2O     | 20.3       | 3450     |                |              |
| HMX  | 1.80           | LiF     | 42.0       | 3800     | 36.1           | 3700         |
|      |                | H2O     | 22.6       | 3380     |                |              |

### Table 2. Heat of explosion and number of moles of gaseous DPs.

| HE   | $\rho_0$, g/cc | $Q$, MJ/kg | $Q_\rho 10^{-3}$, MJ/m$^3$ | $N_\rho 10^{-3}$, mole/m$^3$ | $Q$, MJ/kg [11] |
|------|----------------|------------|---------------------------|-----------------------------|----------------|
| BTF  | 1.82           | 5.80       | 10.56                     | 55.9                        | 5.90 (1.86)    |
| HMX  | 1.81           | 5.61       | 10.15                     | 67.6                        | 5.71 (1.89)    |

### Table 3. Casing velocity and Gurney energy.

| HE   | $D$, km/s | $R-R_{0}$, mm |
|------|-----------|----------------|
|      |           | 4   | 5   | 7   | 10  | 12  | 15  |
| BTF  | 8.41      | $W$, km/s        | 1.53 | 1.60 | 1.67 | 1.73 | 1.77 | 1.81 |
|      |           | $W_1$, km/s      | 1.58 | 1.64 | 1.70 | 1.75 | 1.78 | 1.81 |
|      |           | $E_{Gn}$, MJ/kg  | 3.32 | 3.58 | 3.83 | 4.06 | 4.18 | 4.34 |
| HMX  | 8.78      | $W$, km/s        | 1.59 | 1.65 | 1.72 | 1.77 | 1.80 | 1.83 |
|      |           | $W_1$, km/s      | 1.64 | 1.69 | 1.75 | 1.79 | 1.81 | 1.83 |
|      |           | $E_{Gn}$, MJ/kg  | 3.60 | 3.83 | 4.08 | 4.27 | 4.36 | 4.47 |

Experimental data obtained in the frame of “T-20” technique (velocity of external surface of the casing ($W$) versus radii increment ($R-R_0$) and detonation velocity ($D$), are given in table 3. The $W$ is referred to the central part of the casing and it is obtained basing on the $W$ value being recalculated according to the procedure [10]. $E_{Gn}$ values were calculated using the $W_1$ values. Despite the fact that BTF is superior to HMX in $Q$, HMX surpasses BTF in acceleration ability, and this is evidence for more efficient transformation of chemical energy to kinetic one in the case of HMX.

### Discussion

The data on C-J states of DPs of BTF and $T(t)$ recorded with LiF window permits one to consider carbon phase in the DPs in a new fashion. The possibility of nanodiamonds formation correlates with determination of the DP-states as well as equilibrium lines in the carbon phase diagram, of special interest here are the phase diagrams built for carbon nanoparticles (see figure 4). Calculations [5] show
that nanodiamond particles about 5 nm in a size are formed in TNT, RDX, RDX/TNT and HMX products. Comparison of the results [5] with the phase diagram of nanocarbon shows that CJ-states for TNT, RDX, RDX/TNT and HMX lie near and over the equilibrium line graphite - diamond of 5-nm nanoparticles. BTF CJ-states lie in the region of higher temperatures near the melting line of 5-nm size nanodiamond. This is the region of the stability liquid nanocarbon droplets, which could be formed in the DPs of BTF. Nanodiamond formation was found near the detonation front of HE [14]. For BTF, particle size was estimated as 6 nm in 0.5 µs, 22 nm in 1.0 µs, and 70 nm in 4 µs; while for RDX/TNT it was 5 nm in 0.5 µs, 6 nm in 1.0 µs, and 4 nm 70 µs. Processes of coagulation and agglomeration (growth) can be accompanied by a small energy release. This assumption correlates with plateau temperature profile for DPs of BTF and TNT within the first microsecond. One may assume that nucleation and consequent growth of nanodiamonds, if it be, would affect on DP-temperature history.

![Image of C-J-states diagram](image.png)

**Figure 4.** C-J-states of HEs in carbon phase diagram.

1 – TNT mixed with HMX or RDX; 2 – BTF [15]; 3 – TNT; 4 – TNT/RDX (50/50); 5,6 – RDX; 7 – HMX [7]; 8 – BTF [16]; 9 – BTF (data of present work). Carbon phase diagrams:

10 – ultrafine (2 nm); 11– ultrafine (5 nm); 12 – [5]; 13 – bulk carbon; 14 –ultrafine (2 nm); 15– ultrafine (5 nm) [17].

4. Conclusion

There were obtained experimental data on BTF detonation performance and explosive ones. The C-J parameters were obtained as following: 33.8 GPa and 3990 K; 34.5 GPa and 4170 K for charge density ranged from 1.82 to 1.84 g/cc respectively, the polytropic exponent of DPs was estimated as 2.8. The heat of explosion of BTF is slightly greater than that of HMX. However HMX surpasses BTF in the acceleration ability and this is evidence for more efficient transformation of chemical energy to kinetic one in the case of HMX. BTF as a whole is close to HMX in explosive performance.

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References

[1] Condensed energy system. A short encyclopedic dictionary 2000 ed. B Zhukov (Moscow: Janus-K)
[2] Pepekin V, Makhov M and Lebedev Y 1977 Doklady Akademii Nauk. 232 852
[3] Dobratz B 1981 LLNL Explosives Handbook Properties of Chemical Explosives and Explosive Simulants (LLNL)
[4] Finger M, et al. 1976 Proc. 6-th Int. Detonation Symposium 710
[5] Victorov S, et al. 2005 Khimicheskaya Fizika 24 (12) 22
[6] Tolochko B, et al. 2005 Physico-chemical model of the detonation nanodiamond synthesis (Novosibirsk: Budker INPh)
[7] Gogulya M and Brazhnikov M 1995 Chem. Phys. Reports 13 (1) 81
[8] Gogulya M and Dolgoborodov A 1995 Chem. Phys. Reports 13 (12) 2059
[9] Gogulya M, et al. 1998 Proc. 11-th Int. Detonation Symposium 979
[10] Gogulya M, et al. 2012 Russian J. of Physical Chemistry B 6 730
[11] Gogulya M, et al. 2002 Proc. 12-th Int. Detonation Symposium 249
[12] Ornellas D 1974 Combustion and Flame 23 37
[13] Makhov M and Pepekin V 1981 Polish J. of Chemistry 55 1381
[14] Titov V, et al. 2011 Combustion, Explosion, and Shock Waves 47 (6) 3
[15] Anisichkin V, Dolgushin D and Petrov E 1995 Combustion, Explosion, and Shock Waves 31 (1) 106
[16] Kondrikov B and Sumin A 1987 Combustion, Explosion, and Shock Waves 23 (1) 105
[17] Yang C, Li S 2008 J. Phys. Chem. C 112 1423