Asian Journal of Chemistry Vol. 19, No. 6 (2007), 4309-4314

Characterization and Calculation of Detonation Parameters of 2,6-Diamino-3,5-dinitropyrazine-1-oxide by BKW Codes

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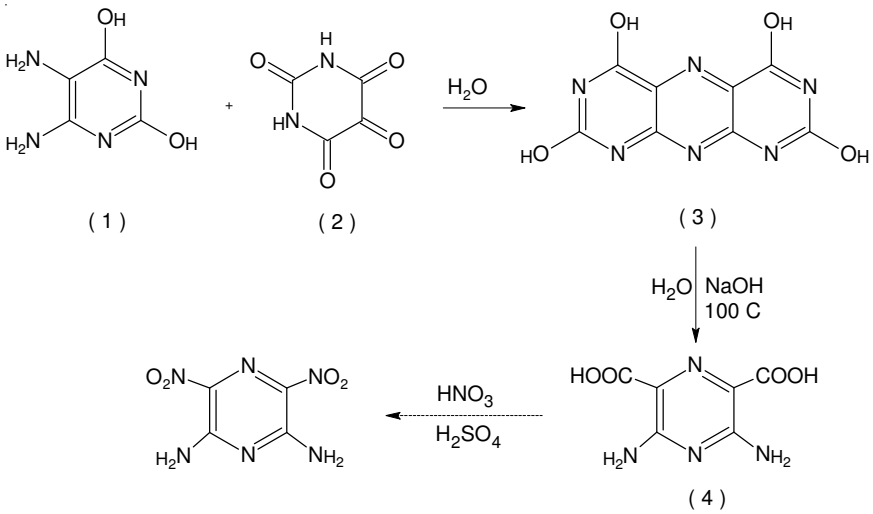
2,6-Diamino-3,5-dinitropyrazine-1-oxide (LLM-105) is a new molecules which shows performance and insensitivity between those of HMX and TATB. Its calculated energy content is about 85 % that of HMX and 15 % more than that of TATB. It is thermally stable, insensitive to shock, spark and friction and has impact insensitivity level approaching that of TATB. These combined properties make it a realistic high performance IHE material; attractive for applications that require moderate performance and insensitivity. In this article, the detonation parameters by BKW codes has been calculated and compared with the results of BKW for TATB, TNT, LLM-105, HMX.

Key Words: Explosive, Detonation parameters, BKW codes.

INTRODUCTION

Energetic heterocyclic compounds have interesting properties for last decade[1-3]. They have higher heat of formation, density and oxygen balance than carbonic compounds. Difficult synthesis of some of nitroaromatic systems is related to presence of low electrons in them. By addition of electron donor substitution, nitration of heteroaromatic systems is easily performed. One of heteroaromatic compound is LLM-105[4-8]. 2,6-Diamino-3,5-dinitropyrazine-1-oxide (LLM-105) was synthesized by Pagoria and co-workers[9,10]. They wanted to produce insensitive energetic materials that approach the energy of 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX). LLM-105 (**Scheme-I**) is a dense molecule (ρ =1.913 g/cc) with excellent physical properties, good safety characteristics and 30 % more energy than TNT. Pagoria *et al.*[9] synthesized 400 g of LLM-105. The synthesis had three steps reaction sequences. Tran *et al.*[11] was compared the physical properties and detonation spreading characteristics of LLM-105 to those of ultrafine TATB. The impact sensitivity (Drop hammer results) is sensitive to particle morphologies. Detonation spreading, spot-size tests on LLM-105 composition showed higher energy output and

superior divergence behaviour than is observed for ultrafine TATB. LlM-105 is insensitive to friction and spark and impact (Dh_{50} = 117 cm). This number is very close to insensitivity of TATB (> 177cm)[10,11].



Scheme-I ANPZ synthesis using commercial reagents

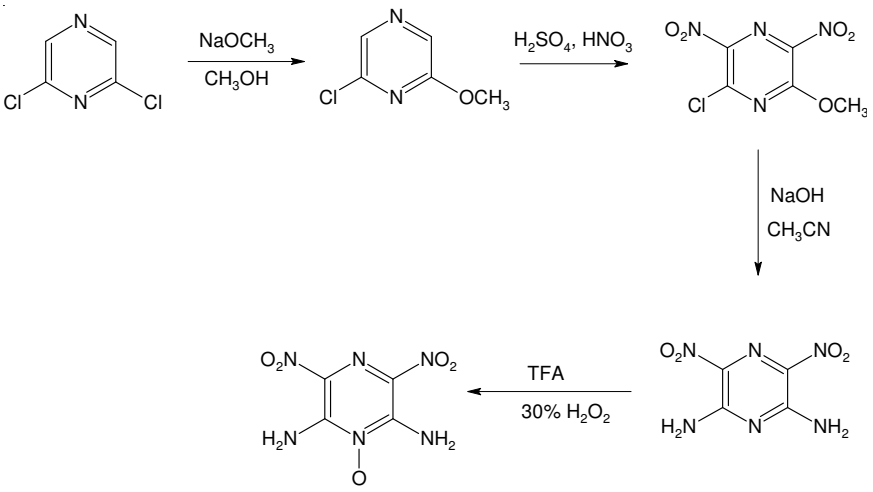
EXPERIMENTAL

Synthesis of LLM-105

LLM-105 was prepared by oxidation of 2,6,diamino-3,5-dinitropyrazine (ANPZ) by using trifluoroacetic acid in ambient temperature. In this way, diaminomaleo nitryl with diiminosuccinonitril in trifuoroaceticacid tetracyanopyrazine condensed and in reaction with ammonia and hydrolysis the pyrazine dicarboxylic acid was obtained. The product then nitrated by mixture of nitric and sulfuric acid to prepare ANPZ[12,13].

Pagoria *et al.*[9,10] synthesized LLM-105 in 400 g (with efficiency 31 %) with 2,6-dichloro pyrazine (**Scheme-II**).

The LLM-105 particle morphology and chemical purity depend on its synthetic and processing history. Collaborative development between synthesis and characterization efforts have yielded several materials with a range of particle sizes and morphologies. Pure LLM-105 plastic bonded composites and an inert binder have a range of safety and processing characteristics. Current interest has been on alternative IHE booster materials with energy approaching that of HMX (type 3 in Table-1) was studied extensively. Its physical morphologies most resembles that of ultrafine TATB (UF-TATB) (Table-2), *i.e.* granular shapes with low aspect ratio and some fines[1].



Scheme-II Synthesis of LLM-105 using 2,6-dichloro pyrazine

TABLE-1
PROPERTIES OF LLM-105 PARTICLES AND SELECTED DATA

LLM-105 type	Preparation method	Morphology (average size-micron)	Drop hammer Dh_{50} (cm)
0	Uncrystallized (original)	(80)	115-120
1	Slow recrystallization from DMSO/water	Sharp needles (60)	105
2	Crash participitates from DMSO/cold water	Small particles (2)	60
3	Crash participitates from butrylacetone/xylene solution	Rounded granules and small fines (40 + 2)	55
4	Type 1 materials subjected to milling for 22 h	Fractured granules (2)	80

Pagoria *et al.*[9] synthesized 400 g of LLM-105 with the 81 % the energy of HMX and excellent thermal stability. The synthesis has three steps and the starting material is 2,6-dichloropyrazine, with overall yield of 36 %[2].

Calculation of detonation parameters using BKW codes

The efficiency of LLM-105 using BKW, the detonation parameter of LLM-105 was calculated and compared with those of TATB, TNT, HMX.

The language of program was Fortran 4 and was able to work on compounds that having CHNO, Al, S, Cl, F, B, Si, Na, P elements. Ruby, Arpeg and Tiger codes also written on bases on equation of states. BKW code, is workable by PC in Malekashtar university, that data are given. An

TABLE-2
LIST OF SEVERAL FORMULATIONS CONTAINING UF-TATB, LLM-105 AND A BINDER

Formulation	LLM-105 type	Weight percent (%)				TMD (g/cc)	Max. density pressed	
		UF-TATB	LLM-105	Viton A	Kel-F		g/cc	TMD (%)
UF-TATB		100				1.938	1.857	96
LLM-105			100			1.913		
RX-55-AA	1		95	5		1.910		
RX-55-AB (LX-17)	1		92.4		7.6	1.921	1.856	97
RX-55-AE	2		97.5	2.5		1.911	1.676	88
RX-55-AE2	3		97.5	2.5		1.911	1.76	92
RX-55-AF	2		22.5	2.5		1.926	1.857	96

entrance file should be introduced. If the composition, density and heat of formation of propellant or explosive was known, Chapman-Jougut (C-J) pressure and width percent of products in C-J (equilibrium), detonation velocity, gamma C-J and temperature was obtained.

Virial equation is a equation of state that are used for this equation:

$$Z = \frac{PV_m}{RT} = 1 + \frac{B(T)}{V_m} + \frac{C(T)}{V_m^2}$$

$$y = \frac{B(T)}{V_m}$$

$$Z = 1 + y + y\beta^2 \cong 1 + ye^{\beta y}$$

In this equation α, β, K are as below:

$$\beta = \frac{K}{(T+\theta)^{\alpha}} \text{ and } \alpha = \frac{3}{n} \text{ and } K = A \propto A^{\frac{3}{n}}$$

So, BKW equation was obtained for mix of gases as below:

$$Z = 1 + ye^{\beta\upsilon} \qquad y = \frac{k\sum x_i k_i}{V_m (t+\theta)^{\alpha}}$$

K_i and X_i are common volum and mole fraction of ith sample in mixture. α, β and K are experimental constant that are earn by standard tables as CRC.

RESULTS AND DISCUSSION

In present studies, the detonation velocity, C-J gammas and temperature for detonation of LLM-105 have been calculated. For comparison the detonation parameters of HMX and TNT are available (Table-3).

TABLE-3
DETONATION PARAMETERS OF DIFFERENT COMPOUNDS CALCULATED USING BKW CODES

Explosive	C-J Parameters	Experimental	BKW (RDX parameters)	BKW (TNT parameters)
TATB	D (mm/μs)	7860	8411	7848
ρ = 1.895	P (kbar)	315	326	297
$C_6H_6N_6O_6$	T (k)	–	1887	2128
E_0 = -17.0	γ	2.72	3.11	2.92
TNT	D	6950	7197	6950
ρ = 1.64	P	190	213	206
$C_7H_5N_3O_6$	T	–	2829	2937
E_0 = -1.44	γ	3.16	2.98	2.85
LLM-105	D	–	8600	–
ρ = 1.913	P	–	341	–
$C_4H_4N_6O_5$	T	–	1851	–
E_0 = -3.1	γ	–	3.14	–
HMX	D	9100	9159	–
ρ = 1.90	P	393	395	–
$C_4H_8N_8O_8$	T	–	2364	–
E_0 = 43.46	γ	3	3.03	–

In Table-4. Number of moles of species in detonation exhaust gas was shown. These are calculated by BKW codes too.

TABLE-4
NUMBER OF MOLES OF DETONATION EXHAUST GAS

Species	H_2O	CO_2	N_2
No. of moles	1.999982E+00	1.499673E+00	3.000000E+00
Species	H_2	O_2	CO
No. of moles	1.810471E-05	1.214611E-08	6.719837E-04
Species	NH_3	H	NO
No. of moles	1.263201E-07	1.000000E-08	1.800759E-07
Species	OH	CH_4	Solid C
No. of moles	1.000000E-08	1.000000E-08	2.499655E+00

The results show that LLM-105 is a good explosive between HMX and TATB. The velocity and detonation power 95 and 85 % of HMX and TATB, respectively but it has better detonation parameters than TATB.

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(*Received*: 24 April 2006; *Accepted*: 12 April 2007) AJC-5556