LALP-83-64 March 1984

1 **DYNAMIC TESTING** | Los Alamos

Toward New Explosive Molecules

We have, in our supply of explosives, both the most energetic and the safest explosives ever used in the fabrication of nuclear weapons. Unfortunately, they are not both the same explosive. We can choose to build small, light weapons having reduced handling safety or larger, heavier weapons that are quite safe in handling. The need of safety in explosives coupled with high-energy output drives the effort in M Division for the synthesis of new explosive molecules.

You can think of an organic explosive molecule (generally containing atoms of carbon, hydrogen, oxygen, and nitrogen) as being composed of fuel, the hydrogen and carbon, and oxidizer, the oxygen. The nitrogen provides the atomic "insulation" that holds the oxygen close to, but separate from, the fuel. The fuel structure generally consists of the carbon, hydrogen, and sometimes nitrogen held close to one another. Such structures often have other, undesirable, groups of atoms clinging to them. The trick of synthesis, then, is to find ways to substitute oxygen, usually with its nitrogen insulation, onto the fuel structure in place of, or in addition to, the other groups of atoms already there.

In trying to synthesize very energetic explosives, the chemist first looks for highly compact fuel structures. The more compact fuels will result in higher than normal mass densities and, therefore, high performance. An exceptionally good mass density is 1.9 g/cm^3. For comparison, TNT (trinitrotoluene), a normal explosive, has a mass density of only 1.65 g/cm^3. We are working toward the synthesis of explosive molecules having predicted mass densities ranging from 1.9 to 2.1 g/cm^3. Explosives in this range are expected to be extremely powerful. Unfortunately, we have no reliable way of predicting their sensitivity, that is, susceptibility to detonation under the influences of heat, friction, and impact. They must be synthesized and tested in the laboratory.

PYX:* A Synthesis Success Story

The synthesis of explosive molecules tailored to specific needs is far from being an assured venture. Demanding a certain level of performance or degree of thermal stability is one matter; producing the material in the laboratory is another. Nevertheless, we have had some remarkable success. A particular high point at Los Alamos was the molecular sleuthing that led us to PYX, the most thermally stable high explosive known. Figure 1 shows the structural formula of the PYX molecule, and Table I shows some properties of both PYX and other explosive molecules that will be discussed later. The most notable property of PYX is its very high thermal stability temperature, 345°C. For comparison HMX** is stable only to 258°C. The measured performance of PYX is about 10% greater than that of TNT.

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*The acronym for 2,6-bis (picrylamino)-3,5-dinitropyridine, pronounced "PICKS."

**Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine high-melting explosive. HMX is one of our most energetic explosives.

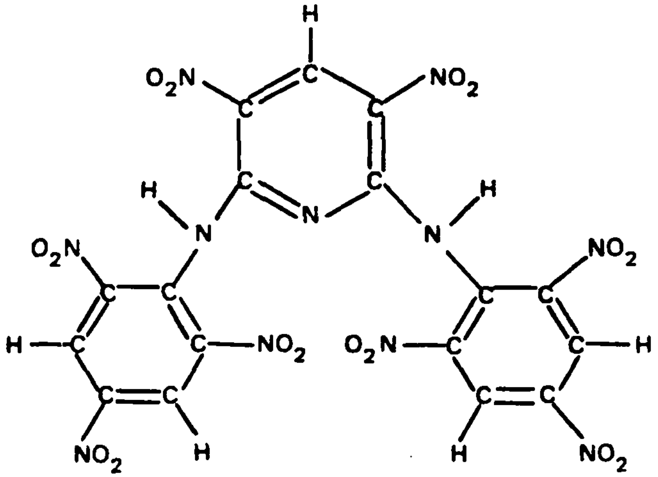


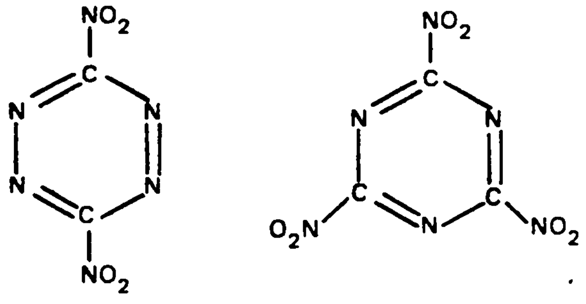
Fig. 1. PYX.

TABLE I. Properties of Explosives

	Density (g/cm^3)		Detonation Pressure (kbar)		Detonation Velocity (mm/µs)		Stability Temperature (°C)
	Actual	Predicted	Actual	Predicted	Actual	Predicted	
PYX ($C_{17}H_7N_{11}O_{16}$)	1.75[a]						345
3,6-dinitro-*s*-tetrazine		1.98		382		9.28	---
2,4,6-trinitro-*s*-triazine		1.97		342		9.146	---
HMX	1.9		390		9.11		258
3,4-dinitrofurazan		1.98		468		9.967	---
ONC		2.1		450		9.4	---
DINGU	1.98			368		8.9	204[b]

[a] Crystal density.

[b] Experimental.



(a) (b)

Fig. 2. Nitroheterocycles (a) 3,6-dinitro-*s*-tetrazine and (b) 2, 4, 6-trinitro-*s*-triazine.

PYX is produced for both DoD applications and industrial uses. The Air Force has qualified PYX as a thermally stable booster explosive, and Chemtronics, Inc., is producing PYX for stimulation of oil and gas wells.

One potential application for PYX is in the area of geothermal well logging. The Laboratory is developing a Hot Dry Rock geothermal reservoir in the Valles Caldera, where temperatures approach 350°C at depths of 12 000-15 000 ft. Geologists require measurements of wave speeds and exact knowledge of the locations of bore holes at the maximum hole depth. Explosive devices are convenient sources of pressure pulses that can be used for well logging. PYX may be the only explosive usable under these temperature conditions.

Toward New Explosive Molecules

Current Research

Recall that we are after explosives with potentially high performance and satisfactory sensitivity properties. The direction in which we are heading is toward synthesizing hydrogen-free molecules containing only carbon, nitrogen, and oxygen. Such molecules have improved densities, and high density generally means compact fuel/oxidizer systems and high performance.

We are interested in pursuing two classes of hydrogen-free molecules: nitroheterocycles and nitrated "cage" compounds. Two of the target nitroheterocycles are 2,4,6,-trinitro-*s*-triazine and 3,6-dinitro-*s*-tetrazine (Fig. 2). We may have already made 3,6-dinitro-*s*-tetrazine. We are not sure. All we were able to isolate were fragments. If we really did succeed in synthesizing this compound, the nitro groups must have destabilized the ring, causing it to rupture. Conversely, if our attempts at synthesis were unsuccessful, then the compound could well be stable. Only continued work can provide an answer.

If the results of our efforts to make 3,6-dinitro-*s*-tetrazine are equivocal, those for 3-amino-4-nitrofurazan shown in Fig. 3 are not. This molecule has been synthesized. The only remaining task is to replace the second amino group with a nitro group to get the desired dinitro structure. We are also trying to synthesize another hydrogen-free heterocycle, 3,4-dintrofurazan (Fig. 3). The predicted properties of this compound are substantially better than the known properties of HMX.

The last hydrogen-free molecule we will discuss here, octanitrocubane (ONC), is very interesting because its predicted performance is very good. The molecule is one of the "strained cages," so-called because of the shape of the fuel part. In ONC the fuel is a cube of carbon atoms with a nitro group at

(a) (b)

Fig. 3. Hydrogen-free heterocycles (a) 3,4-dinitrofurazan and (b) 3-amino-4-nitrofurazan.

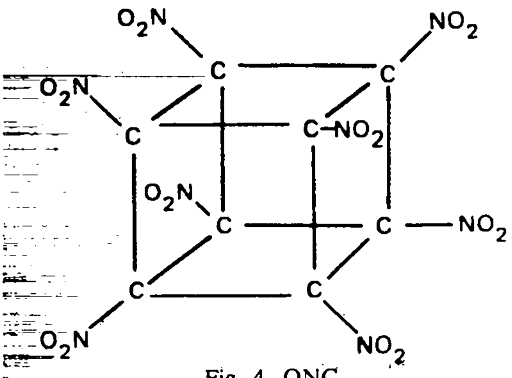


Fig. 4. ONC.

each corner (Fig. 4). Groups M-1 (Explosives Technology) and T-14 (Detonation Theory and Application) at Los Alamos are collaborating in an effort to achieve a synthesis route to ONC. Dinitrocubane, a doubly nitrated cubane, has been synthesized at the University of Chicago.

We should emphasize that synthesizing any new molecule that will detonate is not a particularly difficult task. Hundreds of organic explosives that have various undesirable properties have been synthesized already or will be synthesized in the future as part of ongoing synthesis research. All of these useless molecules add to our knowledge of both synthesis chemistry and the behavior of explosives. Many point to new molecules that might be synthesized and to routes whereby the synthesis could be attained.

New Looks at Old Materials

In the business of providing explosives for the many tasks that require them, we look to all sources of potentially useful materials. One recent example of an external find is DINGU.* The French orginally proposed DINGU as a candidate Insensitive High Explosive and had done some characterization of the material. Our resultant interests in this material (Fig. 5, Table I) have generated a small-scale pilot-plant production capability for DINGU that allows us to prepare enough of this material for evaluation at Los Alamos.

Preliminary work indicates that a PBX (plastic bonded explosive) based on DINGU can be formulated at near-100% TMD (theoretical maximum density). This PBX is extremely insensitive to shock wave initiation, and tests are under way at lower percentage TMDs to find a DINGU-based PBX with appropriate shock wave characteristics. Some of the initial concerns that DINGU might be very thermally unstable have been re-examined in the light of carefully produced material of relatively high purity. We have found the thermal stability of our material to be satisfactory for many of the usual applications.

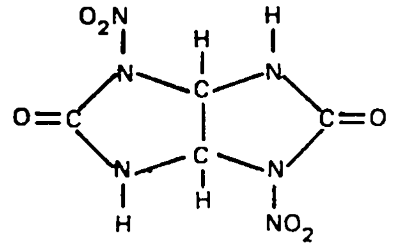


Fig. 5. DINGU.

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*DINGU is the acronym for dinitroglycoluril.

This brief news note on explosive synthesis at Los Alamos has been provided to give an insight into this very interesting and challenging research area. If you have questions or would like more information on this subject please contact Mike Coburn (M-1, 7-7996), Mary Stinecipher (M-1, 7-4962), Kien-Yin Lee (M-1, 7-7131), or Jim Ritchie (T-14, 7-8205). Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36. The Laboratory is an affirmative action/equal opportunity employer.