PATENT SPECIFICATION

Application Date: March 6, 1937. No. 555/37. 497,145

Complete Specification Accepted: Dec. 6, 1938.

COMPLETE SPECIFICATION

Improvements in Explosives

I, WILLIAM WARREN TRIGGS, of the firm of Marks & Clerk, 57 & 58, Lincoln's Inn Fields, London, W.C.2, a British subject, do hereby declare the nature of this invention (a communication to me from abroad by United States Powder Company, a corporation of the State of Nevada, United States of America, of 704, Market Street, San Francisco, State of California, United States of America,) and in what manner the same is to be performed, to be particularly described and ascertained in and by the following statement:—

This invention relates to improvements in nitro-compound explosives, and has for its objects a nitro-compound explosive and method of making the same, which explosive has greater brisance and shattering power than has heretofore been produced in nitro-compound explosives yet is economical to make and less dangerous to handle. Other objects and advantages will appear in the following description.

Broadly, this invention relates to the production of an explosive mixture and an improvement of nitro-compound explosives by the application of the principles of catalysis and utilization of the results of modern X-ray analysis of molecular structure, wherein my communicators have found that by adding a small quantity of an organic promoter of specific molecular length, together with a nitro-derivative of naphthalene, as later described, the brisance and the shattering power of explosives of the nitro-compound type is greatly increased, yet this improved explosive is economical to manufacture, and is safer and more effective in use than the conventional nitro-compound explosives heretofore made and used.

The invention consists in an explosive mixture comprising a nitro-compound and an oxidiser and having in addition a nitro-derivative of naphthalene and an organic promoter consisting of one or more aliphatic or aromatic compounds in which the "Molecular length" as hereinafter defined calculated from the values of atomic radii and bond angles herein specified is within 0.1 angstrom units of being equal to one of four characteristic molecular lengths of the naphthalene ring complex, namely 3.83, 4.19, 4.84 or 5.13 angstrom units.

In the accompanying drawing, the figure illustrates four characteristic atomic distances of the naphthalene ring complex with which this invention is concerned.

The nitro-compound may be any of the poly-nitro-compounds of benzene or its derivatives, examples being dinitrobenzene, trinitrobenzene, dinitrotoluene, trinitrotoluene, picric acid, styphnic acid. The oxidiser is desirably employed in sufficient quantity to produce substantially complete combustion and preferably is in the form of alkali, ammonium or alkaline earth nitrate but other oxidisers such as lead nitrate may be used. Such mixtures of a nitro-compound and an oxidiser have been known for many years and have found some commercial application.

My communicators have found that such mixtures, as above described, and which are well known, are rendered highly explosive by the incorporation therewith of a nitro derivative of naphthalene and a promoter, which consists of molecules whose length corresponds to or falls within the limits specified one of four characteristic distances in the naphthalene ring complex.

In the naphthalene ring complex, the four characteristic atomic distances with which this invention is concerned, are illustrated in the figure of the drawing by the dotted lines *a*, *b*, *c* and *d*, which extend between the opposite carbon atoms of each molecule. These distances are as follows:

a	- -	3.83 angstrom units
b	- -	4.19 ,, ,,
c	- -	4.84 ,, ,,
d	- -	513 ,, ,,

The nitro derivative of naphthalene used in this invention, may be mononitronaphthalene, dinitronaphthalene, trinitronaphthalene, or tetranitronaphthalene, is intimately mixed with the promoter, as described below.

In describing the promoter, the descrip-

[*Price* 1/-]

tive term " molecular length " means the equilibrium distance between the atoms, (exclusive of hydrogen atoms), which are farthest apart from each other in a molecule of either the aromatic or aliphatic type. Thus the molecular length of toluene is from its methyl-carbon atom to the fourth carbon atom of the benzene ring, or 4.33 angstrom units, while in lactic acid the molecular length is measured along the axis of the methyl-carbon atom to the hydroxy-oxygen atom of the carboxyl group and not from the oxygen atom of the alcohol group to the keto-oxygen atom of the carboxyl group.

My communicators have found that compounds consisting of molecules having a molecular length coming within ±0.1 angstrom units of any one of the four characteristic atomic distances of the naphthalene ring complex, namely, *a*, *b*, *c*, *d*, or 3.83, 4.19, 4.84, 5.13 angstrom units, act as effective promoters in breaking the ring structure and thus initiate disruption of the nitronaphthalene compound. Hence any compound whose molecules have a length falling between 3.73 to 3.93; 4.09 to 4.29; 4.74 to 4.94; or 5.03 to 5.23 angstrom units may be used as a promoter together with a nitro-derivative of naphthalene in an explosive mixture comprising a nitro-compound and an oxidiser for accomplishing the desired results of this invention.

In further explanation, as has been established, glycine, propionic acid or its alpha-derivatives such as lactic acid, alanine, propanol or its alpha-derivatives or beta-derivatives, all have a molecular length that comes within 0.1 angstrom units of being equal to 3.83 angstrom units, or length *a* in the figure of the drawing, and when any of these compounds are added in small quantities to a suitable explosive mixture containing nitro-naphthalene or its di-, tri-, or tetra-nitro-derivatives, it produces a very good brisance and great shattering power.

Similarly, my communicators have found that 1.2-dichloroethylene has a molecular length that comes within 0.1 angstrom units of being equal to 4.19 angstrom units, or length *b* in the figure of the drawing, and therefore acts as a good promoter in seting off mixtures containing nitronaphthalene.

Compounds, such as butanol, alpha-derivatives of butanol, beta-derivatives of butanol, gamma-derivatives of butanol, butyric aldehyde, alpha-derivatives of butyric aldehyde, beta-derivatives of butyric aldehyde, butyric acid, alpha-derivatives of butyric acid, beta-derivatives of butyric acid, ethyl acetate, methyl propionate, provided that in the derivatives the side chain is never longer than the main chain so that the longest axis is always between 4.74 and 4.94 angstrom units, all have a molecular length coming within 0.1 angstrom units of being equal to 4.84 angstrom units or length *c* in the figure of the drawing, and are good promoters.

Benzyl alcohol, benzaldehyde, benzoic acid, salicylic acid, or benzylamine, all have a molecular length coming within 0.1 angstrom units of being equal to 5.13 angstrom units, or length *d* in the figure of the drawing, hence act as excellent promoters in an explosive mixture containing a nitro-derivative of naphthalene. Also any of the derivatives of any of the above-named ingredients whose distance between opposite end atoms (exclusive of hydrogen) taken in the direction of the longest axis of the molecule is between 5.03 to 5.23 angstrom units, are good promoters, since their molecular length falls within 0.1 angstrom units of being equal to 5.13 angstrom units.

In general, the amount of promoter added to the nitro-naphthalene is from .005% to 2% by weight of the entire explosive mixture. However, we do not wish to restrict the invention to these exact limits.

In making the improved explosive, the organic substances are mixed together as by melting together the nitronaphthalene and the nitro-compound such as trinitrobenzene or trinitrotoluene. To the molten mass is added the promoter and the necessary moisture which moisture is generally in the form of a 50% calcium nitrate or aluminium nitrate solution, and finally the powdered and warmed nitrate is incorporated in the mixture so that the particles of nitrate are coated with the organic explosive mixture. To produce a plastic powder, an additional quantity of a suitable mixture containing generally tetranitronaphthalene, dinitrotoluene and the promoter is added to the mixed explosive. This mixture, whether in granular form or in plastic form, can now be exploded by an ordinary detonating cap.

The following are several examples of satisfactory formulas, which are not exclusive, but show the use of trinitrobenzene or trinitrotoluene, it being obvious from the description of the invention that the promoters specifically designated can be interchanged in the several formulas, or any two or more of the named promoters can be used in any one of the formulas, the essential feature being that the molecules of the promoter used have the physical dimensional characteristic of the molecular length or lengths coming

within 0.1 angstrom units of the distances *a*, *b*, *c*, *d*, as set out specifically in angstrom units in this description of the invention. Also in the following formulas, a mixture of trinitrobenzene and trinitrotoluene can be substituted for either trinitrobenzene alone or trinitrotoluene alone, and picric acid or other nitro-compound explosive can be substituted for trinitrobenzene, or trinitrotoluene.

FORMULA A (by weight)

0.005% to 2% water
0.005% to 2% organic promoter of molecular length 3.83; 4.19; 4.84; or 5.13 angstrom units or any combination of promoters of said molecular lengths.
4% to 15% mononitronaphthalene, or the di-, tri- or tetranitro-derivatives, or any combination thereof.
5% to 55% nitrocompound, such as trinitrobenzene or any combination of nitrocompounds.
40% to 95% oxidizer, such as the alkali nitrates, alkaline earth nitrates or ammonium nitrate.

FORMULA B

0.1% butanol
4.7% mono-nitronaphthalene
14.2% trinitrotoluene
80 % ammonium nitrate
1 % water

FORMULA C

1 % benzoic acid
4 % di-nitronaphthalene
22 % trinitrobenzene
72 % sodium nitrate
1 % water

FORMULA D

1 % benzaldehyde
6 % trinitronaphthalene
30 % trinitrotoluene
62 % sodium nitrate
1 % water

FORMULA E

0.1 % salicylic acid
6.75% tetranitronaphthalene
11.75% trinitrotoluene
79 % ammonium nitrate
2.4 % of 50% calcium nitrate solution to furnish 1.2% water.

FORMULA F

0.1% salicylic acid
4 % tetranitronaphthalene
5.7% trinitrotoluene
88 % ammonium nitrate
2.2% of a 50% aluminium nitrate solution to furnish 1.1% water.

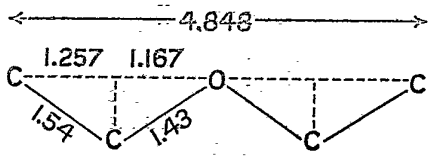
A simple method of calculating molecular length is as follows:—

1. Aliphatic compounds exist in their crystalline state as molecules with one main axis along which the atoms are arranged in a zig-zag line. For short molecules a plane surface is reasonably accurate for representing this zig-zag line, for very long molecules (like stearic acid) there is a shortening of the zig-zag line due to a slight twisting of the plane in a spiral form, so that the real distance of C—C of 1.54 angstroms appears to become 1.51 angstroms. However as the problem at hand deals only with the calculation of short molecules, having from 4 to 6 atoms in line, this shortening of the molecule may be ignored. The following are the atomic radii and bond angles employed in calculating molecular length in accordance with the invention:

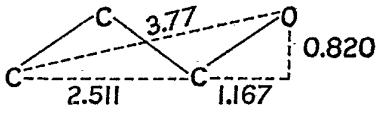
Atomic radii (for single bonds)	C	0.77	angstroms
	N	0.70	,,
	O	0.66	,,
	S	1.04	,,
	Cl	0.99	,,
(for double bonds)	C	0.69	,,
	N	0.63	,,
	O	0.59	,,
Atomic radii (for triple bonds)	C	0.61	,,
	N	0.55	,,
	O	0.52	,,
(for resonating single-double bonds)	C	0.71	,,
	N	0.66	,,
	O	0.62	,,

Bond angles for single bonds C – C—C is 110°
double bonds C = C—C is 125°
triple bond C ≡ C—C is 180°

For atoms other than carbon, the same bond angles are used. For instance in order to calculate the molecular length of solid ethyl ether, the following dimensions are calculated from atomic radii and bond angles:



The hypothenuse of each triangle is the interatomic distance, obtained by adding the atomic radii, thus for C–C 1.54 and for C–O 1.43 angstroms. The base of the C–C triangle becomes 1.257 and of the C–O triangle 1.167 angstroms; adding these four base lengths together gives 4.848 angstroms as the length of the molecule. Naturally in even numbered atoms per molecule the molecular length is not obtained merely by adding the base lengths, but must be obtained by a further calculation of the hypothenuse of the triangle with determined base and height; as for example in propanol:

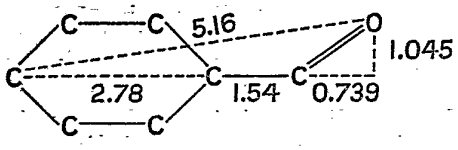


where the base is 3.678, the height 0.82, hence the length of the first carbon atom to the oxygen 3.77 angstrom units.

2. Aromatic compounds depend upon the benzene ring whose dimensions can be projected upon a plane surface as a hexagon with angles of 120°. The following are the atomic distances within this ring:

C–C	1.39 angstroms	(radius of hexagon)
C–C–C	2.41 ,,	(width of hexagon)
C–C–C–C	2.78 ,,	(diameter of hexagon)

Molecular length of derivatives are calculated similar to those of aliphatic compounds. Thus for benzaldehyde, the dimensions are:



where the bond angle C–C=O is 125° and the distance of the para-carbon atom to the oxygen is the hypothenuse (5.16 angstroms) of the base 2.78+1.54+0.739 =5.059 angstroms.

Having now particularly described and ascertained the nature of my said invention and in what manner the same is to be performed, I declare that what I claim is:—

1. An explosive mixture comprising a nitro-compound and an oxidiser and having in addition a nitro-derivative of naphthalene and an organic promoter consisting of one or more aliphatic or aromatic compounds in which the "molecular length" as hereinbefore defined calculated from the values of atomic radii and bond angles hereinbefore specified is within 0.1 angstrom unit of being equal to 3.83, 4.19, 4.84 or 5.13 angstrom units.

2. An explosive mixture comprising a nitro-compound and an oxidiser and having in addition a nitro-derivative of naphthalene and an organic promoter consisting of one or more of the compounds ethyl acetate, methyl propionate, propanol, butanol, propionic acid, lactic acid, butyric acid, alanine, butyric aldehyde, benzyl alcohol, benzyl-amine, benzaldehyde, benzoic acid, salicylic acid, 1.2–dichlorethylene, or glycine.

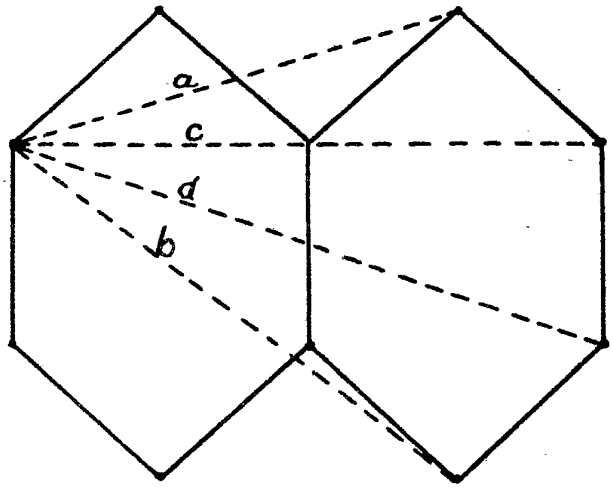
3. An explosive mixture as claimed in Claim 1 or 2 wherein the nitro derivative of naphthalene is mononitronaphthalene, dinitro-naphthalene, trinitro-naphthalene or tetranitro-naphthalene.

4. A nitro-compound explosive mixture comprising, by weight:

5% to 55%	trinitrobenzene or other nitro-compound or any combination of nitro-compounds.
40% to 95%	oxidizer in the form of an alkali nitrate, alkali nitrates, alkaline earth nitrates, or ammonium nitrate.
5% to 15%	one of the members of the group, mononitronaphthalene, dinitronaphthalene, trinitronaphthalene, tetranitronaphthalene or any combination of said members.
0.005% to 2%	organic promoter consisting of one or more aliphatic or aromatic compounds in which the "molecular length" as hereinbefore defined calculated from the values of atomic radii and bond angles hereinbefore specified is within 0.1 angstrom unit of being equal to one of the distances 3.83; 4.19; 4.84; 5.13 angstrom units.
0.005% to 2%	water.

Dated the 7th day of January, 1937.
MARKS & CLERK.

Leamington Spa: Printed for His Majesty's Stationery Office, by the Courier Press.—1939.



Malby & Sons, Photo-Litho.