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NP Technical Data Sheet

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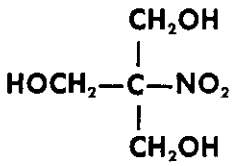
COMMERCIAL SOLVENTS CORPORATION · 245 PARK AVE., NEW YORK, N. Y. - 10017

TRIS NITRO® Brand of Tris(hydroxymethyl)nitromethane*



Introduction

Tris Nitro is a superior bactericide and slimicide for use in aqueous systems. It is also useful as a hardening agent for proteins and as a raw material for synthesis.

Tris Nitro is available in two forms: as a low-priced, 50% aqueous solution which is recommended for most industrial uses, and as a crystallized material.

Applications of Tris Nitro should be limited to inedible products unless it is intended to obtain clearance for using it in food processing from the Food and Drug Administration.

Properties

Tris Nitro is a white crystalline solid which is highly soluble in water and alcohols but practically insoluble in hydrocarbons. It is very stable when dry. Although Tris Nitro slowly decomposes at its melting point, the reaction is endothermic so there is no tendency for the decomposition to become self-sustaining. Tris Nitro is not considered as a flammable chemical.

Tris Nitro is quite stable in neutral solution. However, slight alkalinity such as might result from traces of salts of strong bases with weak acids causes slow decomposition. An increase in pH and/or temperature accelerates this reaction (Fig. 1) so Tris Nitro is, therefore, an unusually convenient formaldehyde donor characterized by lack of odor. The reaction rate can be easily controlled by pH and/or temperature so the working life can be varied from a few minutes to several months according to the conditions of use.

Solutions of Tris Nitro can be effectively stabilized by the addition of sodium bisulfite. For example, at pH 9.0 a solution containing 1% Tris Nitro showed marked decomposition after 24 hours at 60°C (approximately 62% of Tris Nitro had decomposed). Adding 1% sodium bisulfite protected the solution very appreciably for 6 days, though some decomposition did occur. Adding 2% sodium bisulfite protected the sample for a full six days, but it showed no bactericidal efficiency, whereas the sample containing 1% sodium bisulfite retained it. In another test, a 65% aqueous solution of Tris Nitro containing 2% sodium bisulfite showed stability for at least 30 days.

Our laboratories investigated a typical cutting oil concentrate containing about 10% sodium nitrite, 5% triethanolamine, and 1% Tris Nitro as the bactericide. Extensive decomposition of the Tris Nitro occurred in 24 hours at room temperature, but when 1% sodium bisulfite was added, it remained stable for at least 14 days with only slight discoloration. With 2% sodium bisulfite, complete stability was achieved but bactericidal properties diminished.

*Indexed by *Chemical Abstracts* as 2-hydroxymethyl-2-nitro-1,3-propanediol.

Typical Analyses

Crystalline	
Moisture	0.5% by wt
Free Formaldehyde	0.04% by wt
pH of 20% Aqueous Solution	3.5-6.5
Color of 20% Aqueous Solution (max.)	1 Gardner
Solution	
Tris Nitro	50% by wt
Water	50% by wt
Free Formaldehyde	<1% by wt
pH	4.0-5.1
Crystallization Point (approx.)	55°F
Specific Gravity at 20/20°C	1.222
Weight per Gallon at 68°F	10.15 lb

Physical Properties of Pure Material

Molecular Weight (calc.)	151.124
Melting Point*, approx.	175-176°C
pH of 0.1M Aqueous Solution at 20°C	5.0
Critical Humidity Point at 40°C	66% R. H.
Solubility in water, 20°C	220 g/100 ml

Very soluble in alcohols; insoluble in hydrocarbons such as heptane, diisobutylene, kerosene, styrene, mineral oil, benzene, toluene.

*Melts with decomposition

Bactericidal Uses

At a pH of 7.5 or over, there is a gradual release of formaldehyde that was once thought to be the

chief bactericidal agent. However, Tris Nitro has been demonstrated to be more effective than formaldehyde alone, and it is also effective at pH 6.0 and less where it is quite stable. Whatever the mechanism, Tris Nitro provides continuous protection for a prolonged period. There is at no time any detectable odor of formaldehyde.

The bactericidal effectiveness of Tris Nitro against many organisms is indicated by the following spectrum. The test can be considered quite severe because the test plates received massive inoculations of the bacteria under optimum conditions for growth. Repeated plate transfers have been made with many of these bacteria, but they have shown no tendency to develop resistance.

Antibacterial Spectrum Of Tris Nitro

ture	*Gram Stain*	*Minimum Effective Concentration* Parts per million*
obacterium ranae	–	>1000
ococcus roseus	+	250-500
Micrococcus flavus	+	500-1000
Sarcina flava	–	>1000
Staphylococcus albus	+	250-500
Staphylococcus aureus	–	750-1000
Streptococcus fecalis	–	500-1000
Streptococcus hemolyticus	–	250-500
Streptococcus agalactiae	–	500-1000
Streptococcus erysipelatis	–	500-1000
Streptococcus viridans	–	500-1000
Aerobacter cloacae	–	>1000
Brucella abortus	–	>1000
Brucella bronchiseptica	–	500-1000
Eberthella typhosa	–	500-1000
Escherichia coli (NRRL 4348)	–	>1000
Escherichia coli (Waksman)	–	>1000
Klebsiella pneumoniae	–	>1000
Pasteurella pseudotuberculosis	–	500-1000
Proteus vulgaris	–	>1000
Pseudomonas aeruginosa	–	>1000
Salmonella enteritidis	–	500-1000
Salmonella pullorum	–	500-1000
Salmonella suipestifer	–	>1000
Shigella dysenteriae	–	500-1000
Bacillus subtilis	+	>1000
Lembeimers bacillus		>1000

*agar streak plate, pH 7.[illegible]

Molds appear to tolerate Tris Nitro better than bacteria, but a concentration of 1000 ppm will usually control them. As the solution ages and the Tris Nitro content falls, molds re-appear before bacteria. Where molds are especially troublesome, it is recommended that the Tris Nitro content be maintained. Green algae are quite tolerant of Tris Nitro as are many fungi. However, mushrooms and organisms associated with "athlete's foot" are reported to be sensitive to it. They apparently are exceptions.

Oil-in-Water Emulsions

One of the problems in metal working industries is the susceptibility of cutting oils (which are emulsions of oil in water) to bacterial attack. Were it not for bacterial contamination, the oil could be used for many months, but actually the bacterial growth shortens the working life of the oil considerably. Bacterial action may cause the emulsion to break and become acidic, thus causing corrosion problems. Some of the bacteria may be pathogenic which can cause skin infections and other industrial health problems. In addition, the mycelia can clog pumps and valves, and often a foul odor develops. In a large installation, frequent replacement of cutting oils is costly.

Studies have demonstrated that 0.1% Tris Nitro in a cutting oil formulation completely inhibited growth of bacterial flora in the oil for a period of over 60 days under conditions of optimum bacterial growth (1), and was more effective than over 200 compounds tested (2). Since publication of these papers, Tris Nitro has been widely employed with unparalleled success. The prevailing opinion among users is that it is outstanding in its effectiveness yet is less expensive than other bactericides. Also, unlike other bactericides, it creates no disposal problem.

Vapor Phase Disinfectant

Tris Nitro should be evaluated as a vapor-phase disinfectant in the packaging of inedible products that are liable to attack by micro-organisms. Dry tablets or wafers can be readily made with Tris Nitro and an alkaline reagent such as sodium carbonate or sodium acetate. Such a wafer can then be included in the package just before sealing. If the humidity within the package increases during shipment or storage, the alkaline reagent will promote the release of formaldehyde by the Tris Nitro in quantities lethal to microbiological organisms. In borderline conditions the dry mix can be made more effective by the incorporation of a hygroscopic agent.

According to Walker (3), 5 oz of formalin (the equivalent of 1.85 oz of pure formaldehyde) is sufficient to disinfect 1000 cu ft. One mole of Tris Nitro will release 2 moles of formaldehyde under alkaline conditions, so approximately 5 oz of Tris Nitro is theoretically sufficient to treat 1000 cu ft, provided the wafer contains the proper amount of alkaline reagent to cause complete decomposition.

Pulp and Paper Industry

Tris Nitro is of value for microbiological control in the paper and pulp industries. It is recommended for treatment of alkaline circuits for slime control. It should also be tested in non-protein sizing and adhesive solutions to prevent deterioration during storage.

Water Treatment

Tris Nitro is effective for inhibition of microbiological growth such as slimes in industrial water systems. Since the conditions of use would vary greatly, no specific recommendations can be given, but it is effective in protecting drilling muds and would be expected to be useful in such applications as oilfield flooding where the growth of sulfate reducing bacteria is a serious problem in corrosion and formation plugging. Laboratory tests indicate that concentrations of 50-100 ppm are sufficient to inhibit these bacteria.

Other Uses

In addition to the bactericidal uses of Tris Nitro, this product has been employed in a number of

applications. The following examples are taken in part from the patent and technical literature.

Embalming and Preservative Fluids

Solutions of Tris Nitro make very effective preservative and embalming fluids. The slow liberation of the formaldehyde permits super-penetration of the tissues before hardening and the specimen retains a flexible texture with a life-like appearance. Lack of formaldehyde odor is a very great advantage in this use. This product would seem to offer considerable value for the preservation of biological and anatomical specimens and should be evaluated for this use.

Pre-Vulcanization Inhibitor

Premature vulcanization of an accelerated rubber stock with subsequent failure to flow and fill the mold can be avoided by incorporating Tris Nitro into the stock at a concentration of 5% by weight of the rubber. The rubber can be cured in a two temperature operation. At the lower temperature, the stock flows to fill the mold and the Tris Nitro retards vulcanization, while at the upper temperature, the retarding effect of Tris Nitro disappears and the stock cures. Perfect moldings were obtained by use of Tris Nitro.

Formaldehyde-Type Resins

When Tris Nitro is used to replace some of the formaldehyde in the preparation of phenol-formaldehyde resins, the resin becomes much more resilient than is normally the case. Manufacturers of such resins should evaluate this "plasticizing" effect of Tris Nitro wherever a more flexible resilient product is desired.

Hardening Agent for Polyvinyl Alcohol and Esters

Tris Nitro is an excellent hardening or cross-linking agent for polyvinyl alcohol and esters. It is superior to other hardening materials because there is no risk of gelation of the polyvinyl alcohol solution prior to use. The hardening or cross-linking effect is obtained by heating the dried film at 110-120°C for 30 minutes.

Polyurethane Foams

Because of Tris Nitro's three active hydroxy groups, it would appear to be useful as a cross-linking agent for polyurethane foams.

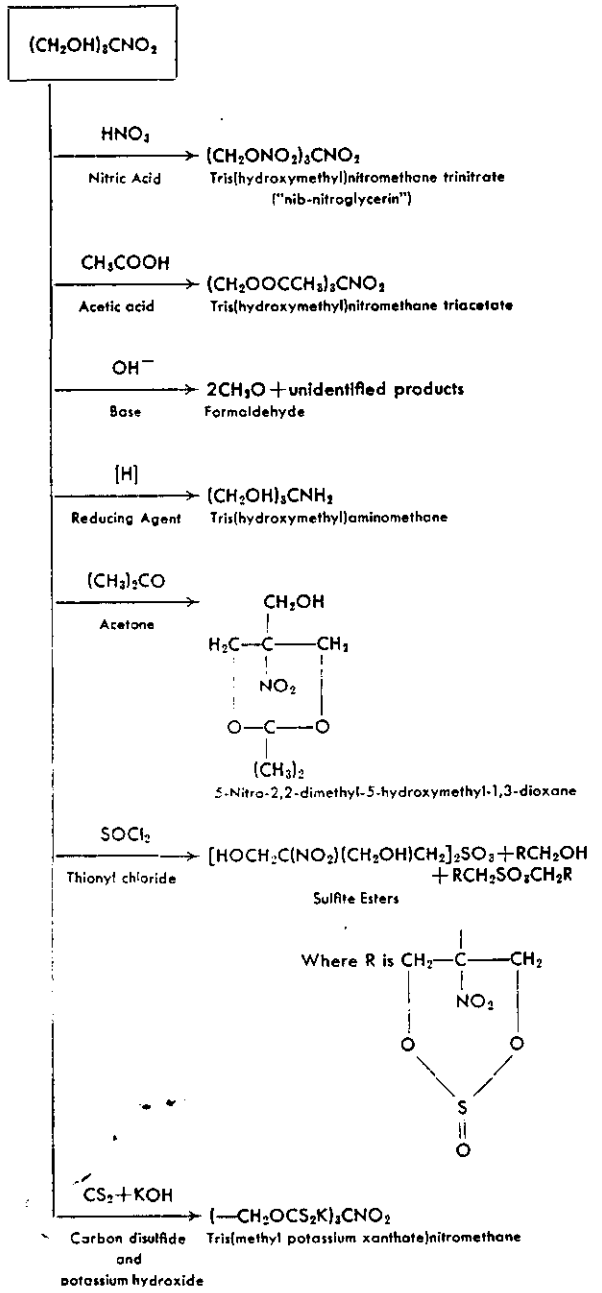
Adhesives and Coatings

Since Tris Nitro is a formaldehyde donor under conditions which can be easily controlled, there are many possible uses in hardening of protein-based adhesives and coatings such as casein and gelatin emulsions. By adding the Tris Nitro just before use (and adjustment of the pH of the emulsion if necessary), the formulator can achieve a controllable hardening time for his coating or adhesive and still maintain an excellent shelf life for the uncombined product.

Explosive Synthesis

Tris(hydroxymethyl)nitromethane trinitrate can be made by treating Tris Nitro with nitric acid in the presence of sulfuric acid. This product, also known as "nib-nitrogylcerin", is a powerful explosive and has the advantage over nitroglycerin of better stability and a lower melting point. Although known for many years, it has never been widely used. Now that Tris Nitro is readily available at a moderate price it is suggested that explosive manufacturers review the properties of this excellent explosive.

Chemical Reactions



Toxicity

The toxicology of Tris Nitro was investigated by Machle, Scott, and Treon (4). They found that the minimum lethal dose for rats by oral administration is 0.5-1.0 g/kg. The following data were obtained on mice in the toxicology laboratories of CSC:

	Oral	*Intraperitoneal*
LD_0	1.00 g/kg	1.00 g/kg
LD_{50}	1.90 ± 0.35	1.85 ± 0.34
LD_{100}	3.00	3.00

On the basis of these results, Tris Nitro would be considered only slightly toxic according to the rating method of Hodge and Sterner (5).

The effect on the skin (4) was tested by applying the material to the clipped abdominal skin of a rabbit and rubbing it in. After 4 hours, it was washed off with soap and water. Although the treatments were repeated daily for 5 days, no sign of damage was observed. This test was followed by a series of 48-hour patch tests conducted by an independent dermatologist on 25 human subjects using Tris Nitro at concentrations of 0.3% and 0.6% in some typical cutting oil emulsions. Another group was exposed to the cutting oil alone without Tris Nitro. The tests were severe in that they were conducted with concentrations of Tris Nitro considerably higher than any that have been found necessary to protect the emulsions from bacterial contamination. Both the closed and open methods of application were employed. The closed method insures maximal contact of the preparation with the skin and minimal loss by evaporation or wiping on the subject's clothing. There was absolutely no skin irritation in either the open or closed tests on any of the 25 subjects.

In order to check on the sensitizing potential of aged cutting oil emulsions containing Tris Nitro, a series of human patch tests were conducted by an independent organization different from the one mentioned above. The subjects were housewives, 30-65 years of age. The tests consisted of three successive patch exposures of 24 hours duration with 24 hours or more between exposures. The three compositions employed consisted of a typical cutting oil emulsion without Tris Nitro, the same emulsion to which 0.5% Tris Nitro had been added just before use in the test, and the third sample consisted of the same emulsion to which 0.5% Tris Nitro had been added some time previously so that aging effects would have had ample opportunity to develop.

The results of this test showed that addition of 0.5% Tris Nitro (five to ten times as much as normally used) caused no increase in irritating effect whether it was added just before use or sometime previously. The dermatologist concluded that normal users of the emulsions would not be expected to exhibit any evidence of primary irritation under the usual conditions of use.

These findings are ample evidence that Tris Nitro is not a primary irritant and the sensitizing potential is minimal. This product has been manufactured by CSC for over 20 years and there has never been a case of irritation or dermatitis among plant workers that could be attributed to its action. A small but significant proportion of workers exposed to cutting oils in the metal working industry experience dermatitis from several diverse causes. Some cutting oils containing Tris Nitro may be involved in a fraction of these cases due to some chemical reaction which is not understood, but which may occur over a long period of time.

Handling and Storage

Tris Nitro has a high melting point and can be easily handled in the plant. It is somewhat hygroscopic (see Fig. 2) and therefore should be stored in a closed container in a dry place. Even when dry, however, Tris Nitro tends to cake during storage, probably as a result of "cold flow." Caked Tris Nitro can be broken up with shovel, mallet, etc. Tris Nitro tends to slowly decompose in the presence of alkaline materials so it should be protected from vapors of ammonia and amines during handling and storage to prevent deterioration of quality.

Crystalline Tris Nitro performs well in tableting machines. It is readily compacted and requires no binder. The finished tablets are free from dusting and possess good mechanical strength assuring freedom from breakage due to rough handling.

Shipping Containers

	Net Weight, lb	
	Crystalline	*Solution*
1-gal. fiber drum with liner	5	
5-gal. fiber drum with liner	25	
38½-gal. fiber drum with liner	200	
55-gal. coated steel drum		57

Literature Cited

(1) H. O. Wheeler and E. O. Bennett, *Applied Microbiol.*, 4, 122-126 (1956).

(2) E. O. Bennett, *Soap and Chemical Specialties* 32, 47-49 (October 1956); 46-48 (November 1956).

(3) J. F. Walker, "Formaldehyde", 3rd Edition, ACS Monograph No. 159, Reinhold Publishing Corp., New York, 1964, p. 572.

(4) W. Machle, E. W. Scott, and J. Treon, *J. Ind. Hyg. Toxicol.* 22, 315-332 (1940).

(5) H. C. Hodge and J. H. Sterner, *Am. Ind. Hyg. Assoc. Quart.* 10 [4], 93-96 (1949).

The information and data contained herein are believed to be correct. However, we do not warrant either expressly or by implication the accuracy thereof. In presenting uses for this product, no attempt has been made to investigate or discuss any patent situations which may be involved.

FIG. 1

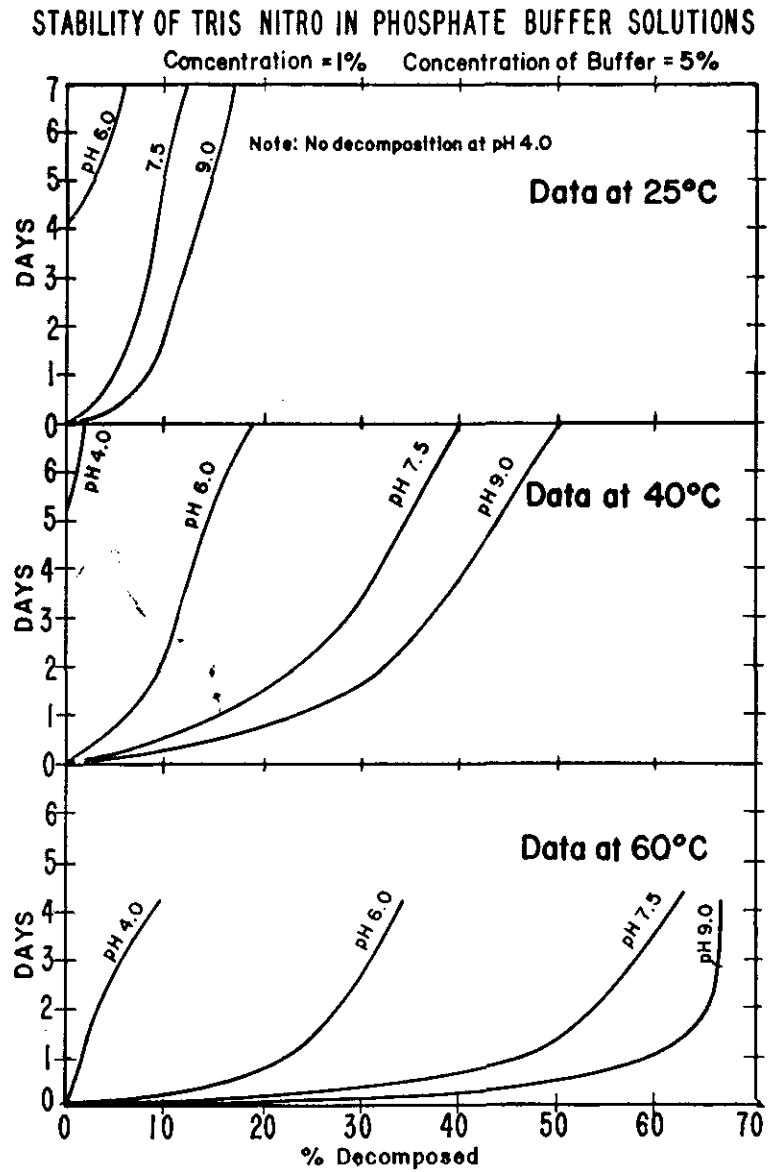
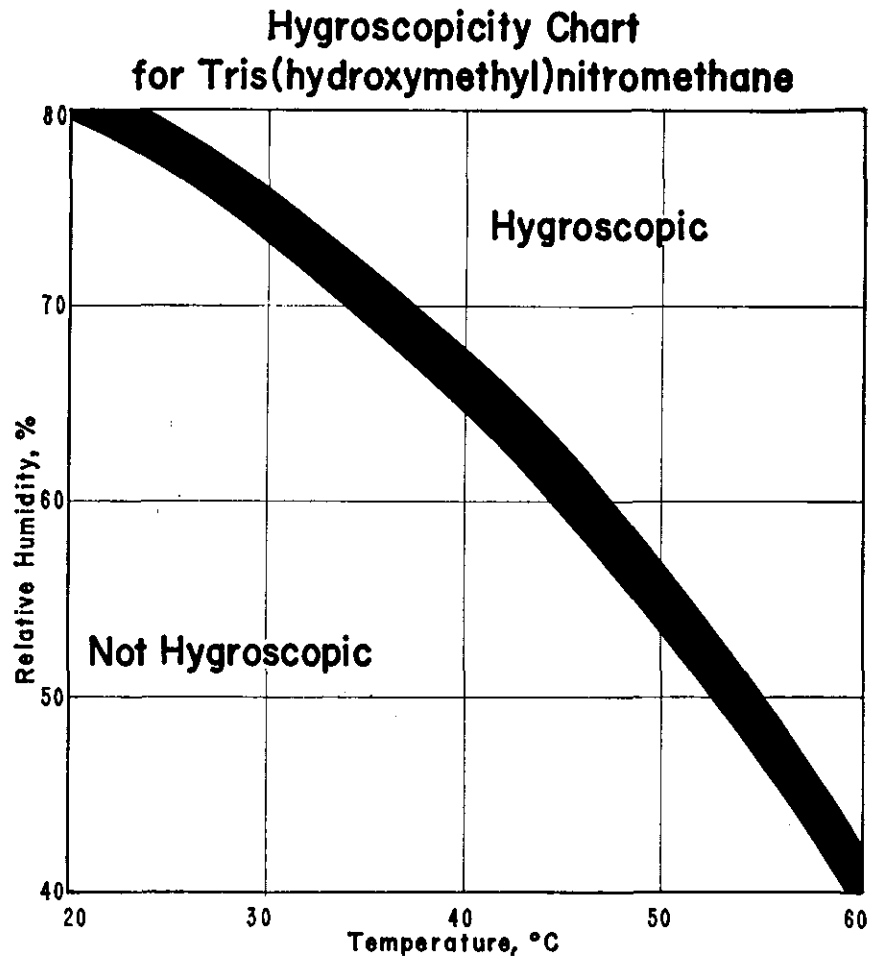

STABILITY OF TRIS NITRO IN PHOSPHATE BUFFER SOLUTIONS
Concentration = 1%
Concentration of Buffer = 5%
Note: No decomposition at pH 4.0
Data at 25°C
Data at 40°C
Data at 60°C
pH 4.0
pH 6.0
pH 7.5
pH 9.0
DAYS
% Decomposed

FIG. 2


Hygroscopicity Chart
for Tris(hydroxymethyl)nitromethane
Hygroscopic
Not Hygroscopic
Relative Humidity, %
Temperature, °C

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