MONSANTO
CHEMICALS – PLASTICS

ORTHO-NITROBIPHENYL

Plasticizer & Chemical Intermediate

Monsanto Technical Bulletin No. O-78 July 30, 1951
Monsanto Chemical Company, Organic Chemicals Division, St. Louis, Mo.

Ortho-nitrobiphenyl (ONB) is a good general purpose plasticizer worthy of consideration in most types of plastic, lacquer and adhesive compositions where its low cost makes possible economies difficult to obtain with other primary plasticizers.

ONB is compatible with a wide variety of resins including cellulose esters and ethers, polyvinyl chloride and its copolymers, polyvinyl formal, polyvinyl butyral, polyvinyl acetate, polyvinyl alcohol, polystyrene, rosin, rosin esters, modified rosin esters, modified phenolic resins, oil soluble phenolic resins, alkyd resins and vegetable oils. This wide range of compatibility suggests the following uses:

Plasticizer in thermoplastic molding and extrusion compositions

Plasticizer in polystyrene latex paints

Plasticizer for polyvinyl chloride plastisols and organosols

Plasticizer in adhesives

Plasticizer in lacquer-type coatings

Camphor substitute in nitrocellulose compositions

ONB is also suggested as an intermediate for the manufacture of dyestuffs and it is valuable as a constituent in certain types of wood preserving formulations.

ORTHO-NITROBIPHENYL — Monsanto Technical Bulletin No. O-78 — July 30, 1951

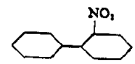
TABLE OF CONTENTS

0614287

PHYSICAL AND CHEMICAL PROPERTIES

PURE MATERIAL

Molecular Weight: 199.20

Formula: . . . . . 

COMMERCIAL PRODUCT

(approximate values — from typical analyses)

Appearance and Color:	Light yellow to reddish colored, liquid or crystalline solid
Odor:	Characteristic, sweet odor
Melting Point:	35°C. (supercools readily)
Boiling Point:	172°C. at 10 mm. Hg 330°C. at 760 mm. Hg
Vapor Pressure:	See chart on page 2
Refractive Index:	1.613 at 25°C.
Specific Gravity:	1.189 at 40°/15.5°C.
Weight per Gallon:	9.9 pounds
Viscosity:	38 centipoises at 25°C. (determined on supercooled material) 12 centipoises at 45°C.
Flash Point:	143°C.(289.5°F.)
Fire Point:	179°C.(354.5°F.)

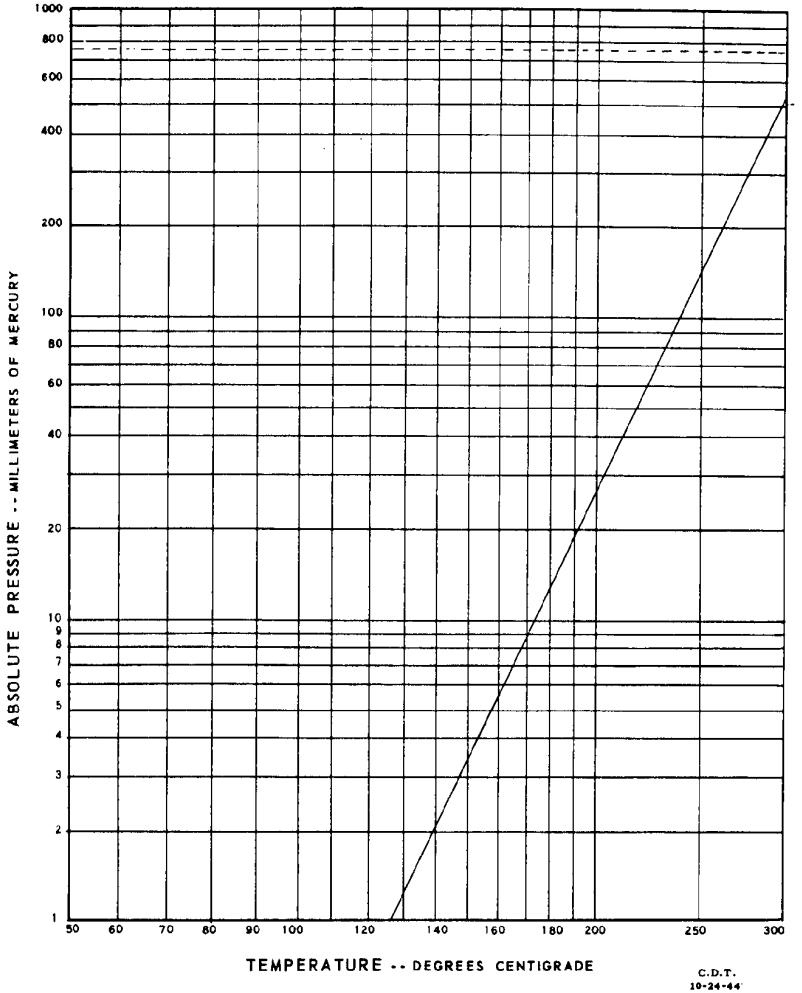
Solubility:

Practically insoluble in water (either hot or cold).

Readily Soluble In:

Acetone	Linseed Oil
Amyl Acetate	Methyl Alcohol
Benzene	Methyl Ethyl Ketone
Carbon Tetrachloride	Mineral Spirits
Corn Oil	Ortho-Dichlorobenzene
Ether	Perchlorethylene
Ethyl Acetate	Pine Oil
Ethyl Alcohol	Soya Bean Oil
Glacial Acetic Acid	Turpentine

VAPOR PRESSURE
(APPROXIMATE)
of
ORTHO-NITROBIPHENYL



C.D.T.
10-24-44

0614289

USES AS A PLASTICIZER

ONB is an economical primary plasticizer which plasticizes most resins, both synthetic and natural. The amount required to accomplish a particular job varies with the resin and the end properties desired. It is particularly useful in adhesives; polystyrene latex paints; polyvinyl chloride plastisols, organosols, extrusions and moldings; nitrocellulose lacquers and cellulose acetate molding compounds. The general utility of ONB in several plastics is indicated below:

Cellulose Nitrate (Plastics Grade)

ONB when used to plasticize cellulose nitrate gives properties very similar to a camphor plasticized film. It can be used in conjunction with camphor and in several cases these films have properties superior to films plasticized with camphor alone. ONB is generally used in the range of 30 to 40 parts per 100 parts of cellulose nitrate.

Cellulose Nitrate (Lacquer Grade)

In nitrocellulose lacquers, ONB produces hard, tough compositions. Solvent release is aided by using ONB. ONB raises the spew point of castor oil in cellulose nitrate coatings. A 50-50 blend of ONB-castor oil imparts better flex life than when castor oil is used alone. ONB has a volatility about equal to dibutyl phthalate though its efficiency is somewhat less.

Cellulose Acetate

When used in cellulose acetate, either in conjunction with other plasticizers or as the sole plasticizer, the use of ONB results in a lower volatility, lower water absorption and a lower percentage of soluble matter lost upon water immersion. 50 parts of ONB per 100 of cellulose acetate gives clear, transparent compositions of good molding properties and medium flexibility. Below are listed two formulations and test results of ONB and diethyl phthalate (DEP) in plasticized cellulose acetate compositions:

	Formulation Containing	
Composition	**DEP**	**ONB**
PM-3 Cellulose Acetate	100	100
Diethyl Phthalate	50	—
ONB	—	50
Test Results		
Volatility (% Plasticizer Loss, 74 hrs. at 84.5°C.)	33.0	30.8
% Water Absorbed	6.74	5.67
% Soluble Matter Lost	2.80	1.93

Cellulose Acetate Butyrate

ONB is compatible with cellulose acetate butyrate and produces hard, tough compositions suitable for molding. In cellulose acetate butyrate lacquers, ONB forms tough, durable films.

Polyvinyl Acetate

ONB is highly compatible with polyvinyl acetate. 40 to 50 parts of ONB per 100 of polyvinyl acetate gives very flexible, tacky compositions that make excellent emulsion adhesives. ONB is useful in polyvinyl acetate adhesives because it:

Has high compatibility with the resin

Increases water resistance

Imparts good solvent resistance

Imparts good tack

Is one of the few plasticizers that allows the preparation of rubbery, polyvinyl acetate adhesives

These properties suggest the use of ONB in polyvinyl acetate adhesives for wall tile mastic, cold padding cements for paper, tabbing cements for paper, and a general binding cement. It is also useful in general purpose, box and carton adhesives as well as wood cements for various types of woodwork. A suggested starting formula is listed below:

Polyvinyl acetate emulsion (50% solids)	100
ONB	20-25

Note: The ONB is melted and added slowly with moderate agitation to the polyvinyl acetate emulsion.

In cold climates, ONB will occasionally crystallize when used alone in polyvinyl acetate adhesives. This may be corrected by mixing ONB with other liquid, solvent plasticizers as dibutyl phthalate, tricresyl phosphate, etc.

Polyvinyl Formal (Formvar*)

In polyvinyl formal ONB imparts a better flexibility than it does in cellulose acetate. Temperatures of 150-160°C. are required for good flow characteristics in molding operations. The incorporation of 50 parts of ONB per 100 of resin results in twice the outdoor aging resistance over the unplasticized resin.

Polyvinyl Butyral (Butvar*)

40 parts of ONB per 100 of polyvinyl butyral results in a flexible composition with a flow temperature of 120-130°C. At 50 parts of ONB per 100 of resin the film is flexible but somewhat tacky.

*Reg. U.S. Pat. Off.

Polyvinyl Chloride

ONB is compatible with polyvinyl chloride and is particularly useful in plastisols, organosols and extrusions. It is generally used in conjunction with one or more other plasticizers such as Santicizer*107, Santicizer 141, Santicizer 160, tricresyl phosphate or dibutyl phthalate. ONB is compatible in vinyls up to at least 40 parts per 100 of polyvinyl chloride. The low temperature properties and volatility of ONB, compared to dibutyl phthalate (DBP) and dioctyl phthalate (DOP), are listed below:

	% Plasticizer (wt.)	T_F (°C.)	% Plasticizer Lost
ONB	30	+ 2.5	20.2
ONB	40	−12.2	38.0
DBP	30	−13.7	21.2
DBP	40	−42.0	40.5
DOP	30	−15.0	3.4
DOP	40	−36.0	3.2

ONB plasticized plastisols have good viscosity stability during storage. This property suggests its use in such end products as glove, rack and other dip applications as well as vinyl strip coatings. Other uses suggested are miscellaneous fabric and paper coatings. A typical low cost starting formula for dipping applications is listed below:

P.V.C. resin (plastisol type)	100
Santicizer 107	25
ONB	20
Aroclor*1254	15
Filler	20
Stabilizer	1-4
Pigment	0-3

In thick or semirigid extrusions or moldings ONB improves flow characteristics and gloss. A suggested starting formula that illustrates the use of ONB in extrusion compounds is listed below:

P.V.C. resin	100
Santicizer 160	20
Santicizer 140	10
ONB	15
Low temperature plasticizer (dioctyl adipate or fatty acid type)	10
Filler	15
Stabilizer	2-5
Pigment	0-3

*Reg. U.S. Pat. Off.

The physical and electrical properties of polyvinyl chloride plasticized with ONB, dioctyl phthalate and tricresyl phosphate (TCP), respectively, are listed below:

Property	Formulation Containing		
	ONB	DOP	TCP
Tensile	2000	1930	2650
Elongation, %	290	290	290
Low Temp. Flex. (1)	−17°C.	−38°C.	−12°C.
Durometer	85	83	87
Power Factor	0.052	0.027	0.033
SIC	13.1	7.83	9.68
Loss Factor	0.681	0.211	0.322
Ins. Res., 10^{12}ohms/cm³.	0.117	0.649	0.203

(1) Clash & Berg Method

In all polyvinyl chloride applications, where light stability is a factor, the total amount of ONB should not exceed 30% of the total plasticizer as ONB has a tendency to darken on exposure.

Polystyrene

ONB is highly compatible with polystyrene and imparts flexibility without causing undue softening and tackiness usually encountered with other plasticizers. It is an excellent solvent for polystyrene and increases the amount of non-compatible material that can be incorporated in a formulation by serving as a mutual solvent for the polystyrene and the incompatible material. Recent work has indicated that advantage of this property can be taken in preparing plasticized polystyrene emulsion paints. As an example, a plasticizer blend consisting of 25% ONB, 75% Panflex BN-1, by weight, may be used to replace less available materials. Such an emulsion paint has good flow characertistics, good emulsion stability, good adhesion, good initial color, excellent washability and no appreciable odor. Aroclors, particularly 1254 and 1262, may be used to replace Panflex BN-1 in this formulation to improve the light stability.

A suggested starting formula, utilizing ONB in conjunction with two Monsanto Plastics Division Products, Lustrex* 820 and Lustrex 601-40, is detailed below:

Components

"A"	258	lbs.	TiO_2 (Rayox R-610 or similar)
	64	"	water ground mica, 200/325 mesh
	278	"	water
	31	"	Lustrex 820 (alkali-soluble protective colloid)
"B"	10	lbs.	glyceryl monoricinoleate (or other defoamer)
	9.4	"	conc. ammonium hydroxide (27-28% NH_3)

*Reg. U.S. Pat. Off.

"C"	18.75	lbs.	ONB
	56.25	"	Panflex BN-1
"D"	16	lbs.	water
	294	"	Lustrex 601-40 (polystyrene emulsion)
"E"	7	lbs.	5% wetting agent solution (Sterox*SK, Areosol OT or similar)
	0-30	"	thickening solution (12.5% solution sodium polyacrylate)
	100	gals. (approx. total)	

Process

A change-can mixer is charged with "A" and stirred for 30-60 minutes.

Add "B" and stir 15 minutes.

Add "C" and stir one hour.

Add "D" and stir one to three hours, depending on mixer efficiency.

Add the wetting agent solution and stir 20 minutes.

Thickener can then be added, if desired, and the whole product mixed another few minutes.

Ethyl Cellulose

The compatibility of ONB in 48% ethoxy, 100 cps., ethyl cellulose is approximately 45% by weight. This produces compositions which age about twice as well as the unplasticized material. The volatility of ONB is slightly higher than dibutyl phthalate in ethyl cellulose.

Rubber (Natural and Synthetic)

The use of ONB alone and in conjunction with Dutrex is suggested as a processing aid for both natural and synthetic rubbers.

ONB is useful in rubber-based adhesives. A suggested starting formula illustrating this use is:

Chlorinated rubber	20
Aroclor 5460	20
ONB	10
Dibutyl phthalate	10
Solvent (aromatic & aliphatic hydrocarbons)	40

*Reg. U.S. Pat. Off.

OTHER USES

Dyestuffs

The chemical structure of ONB is such as to suggest its use in the manufacture of dyestuffs.

Anti-Blooming Agent in Wood Preservatives

ONB has some value as an anti-blooming agent in paintable type Santophen*20 (Monsanto's technical grade of pentachlorophenol, commonly known as PENTA) formulations for the preservation of wood products.

HANDLING INFORMATION

ONB possesses some degree of toxicity, but this makes it by no means unique when plasticizers and solvents are considered in general. The lethal dose (LD_{50}), per kilogram of body weight, of ortho-nitrobiphenyl, when administered orally at one time to rabbits as a 25% preparation in olive oil, is 1.58 grams. The corresponding lethal dose administered in a similar manner to rats is 1.23 grams. This toxicity is of the same order as that of tricresyl phosphate and triphenyl phosphate. Patch tests indicate that ONB is neither a primary irritant nor a sensitizing agent. The breathing of concentrated vapors or continuous breathing of lesser concentrations of ONB must be avoided by providing either adequate ventilation or respirators. Additional toxicity data is available upon request.

In cold weather ONB crystallizes making it necessary to melt the material so that it can be easily removed from the drum. One method commonly employed is to wrap a steam line around the drum and thus slowly melt the ONB. If a heated room or oven is available, it can be used for this purpose. Direct heating by gas flame or electric plates is not recommended.

*Reg. U.S. Pat. Off.

SUPPLIERS OF MATERIALS LISTED IN SUGGESTED FORMULATIONS

PRODUCT	SUPPLIER
Aerosol OT	American Cyanamid Company New York, New York
Aroclor 1254	Monsanto Chemical Company St. Louis, Missouri
Aroclor 1262	Monsanto Chemical Company St. Louis, Missouri
Aroclor 5460	Monsanto Chemical Company St. Louis, Missouri
Butvar	Shawinigan Resins Corporation Springfield, Massachusetts
Dutrex	Shell Chemical Company San Francisco, California
Formvar	Shawinigan Resins Corporation Springfield, Massachusetts
Lustrex 820	Monsanto Chemical Company Springfield, Massachusetts
Lustrex 601-40	Monsanto Chemical Company Springfield, Massachusetts
Panflex BN-1	Pan American Chemical Div. Pan American Refining Corp. New York, New York
Rayox R-610	R. T. Vanderbilt Co., Inc. New York, New York
Santicizer 107	Monsanto Chemical Company St. Louis, Missouri

SUPPLIERS OF MATERIALS LISTED IN SUGGESTED FORMULATIONS

PRODUCT	SUPPLIER
Santicizer 140	Monsanto Chemical Company St. Louis, Missouri
Santicizer 160	Monsanto Chemical Company St. Louis, Missouri
Santophen 20	Monsanto Chemical Company St. Louis, Missouri
Sterox SK	Monsanto Chemical Company St. Louis, Missouri

For further information about Ortho-Nitrobiphenyl,

contact the nearest Monsanto office.

MONSANTO CHEMICAL COMPANY

ST. LOUIS

AKRON • BIRMINGHAM • BOSTON • CHARLOTTE • CHICAGO
CINCINNATI • CLEVELAND • DETROIT • HOUSTON • LOS ANGELES
NEW YORK • PHILADELPHIA • PORTLAND (Ore.) • SAN FRANCISCO
SEATTLE

MONSANTO CHEMICALS LTD.
London

MONSANTO (CANADA) LTD.
Montreal, Toronto, Vancouver

MONSANTO CHEMICALS (AUSTRALIA) LTD.
Melbourne

Representatives in the Principal Cities of the World

0614298