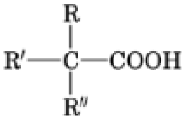
Kirk-Othmer Encyclopedia of Chemical Technology.

CARBOXYLIC ACIDS, TRIALKYLACETIC ACIDS

Trialkylacetic acids are characterized by the following structure:



$$\mathrm{R'}-\underset{\displaystyle \mathrm{R''}}{\overset{\displaystyle \mathrm{R}}{\mathrm{C}}}-\mathrm{COOH}$$

in which R, R′, and R″, are C_xH_{2x+1} with $x \geq 1$. The lowest member of the series ($\mathrm{R} = \mathrm{R'} = \mathrm{R''}$ CH_3) is the C_5 acid, trimethylacetic acid or 2,2-dimethylpropanoic acid (also, neopentanoic acid, pivalic acid). For higher members in the series, the products are typically mixtures of isomers, resulting from the use of mixed isomer feedstocks and the chemical rearrangements that occur in the manufacturing process.

Trialkylacetic acids have been produced commercially since the early 1960s, in the United States by Exxon and in Europe by Shell, and have been marketed as neo acids (Exxon) or as Versatic Acids (Shell). The principal commercial products are the C_5 acid and the C_{10} acid (neodecanoic acid, or Versatic 10), although smaller quantities of other carbon numbers, such as C_6, C_7, and C_9, are also produced.

The trialkylacetic acids have a number of uses in areas such as polymers, pharmaceuticals, agricultural chemicals, cosmetics, and metal-working fluids. Commercially important derivatives of these acids include acid chlorides, peroxyesters, metal salts, vinyl esters, and glycidyl esters.

1. Trimethylacetic Acid

1.1. Physical Properties

2,2-Dimethylpropionic acid [75-98-9], $(CH_3)_3CCOOH$, also referred to as neopentanoic acid or pivalic acid, is a solid at room temperature with a pungent odor typical of many lower molecular weight carboxylic acids. It is commercially available at a purity greater than 99.5%. Neopentanoic acid is a single isomer with a high degree of symmetry and, thus, has a relatively high melting point ($+34^\circ C$, compared to $-34.5^\circ C$ for *n*-pentanoic acid). Physical properties of a typical commercial sample are given in Table 1.

1.2. Chemical Properties

Neopentanoic acid [75-98-9] undergoes reactions typical of carboxylic acids. Reactions often proceed less readily than with straight-chain acids because of the steric hindrance around the carbonyl group. However, this steric hindrance at the α-carbon results in derivatives that are typically more resistant to hydrolysis and oxidation.

Table 1. Physical Properties of Commercially Available Neopentanoic Acid[a]

Property	Value
mp, °C	34.4
bp, °C	163–165
acid value, mg KOH/g	550
color, Pt/Co (Hazen) of molten material	50
specific gravity at 38/38°C	0.913
viscosity at 60°C, mm^2/s (=cSt)	1.7
flash point, °C (Tag closed cup)	63
water, wt %	0.05
vapor pressure, kPa[b] at 60°C	1.33
solubility in water, g 100 mL H_2O at 25°C	2.1
heat of vaporization, kJ/kg,[c] at the boiling point and 101.3 kPa[b]	423
ionization constant, $K_a \times 10^{-6}$ at 25°C	9.3

[a] Ref. 1.
[b] To convert kPa to mm Hg, multiply by 7.5.
[c] To convert kJ to kcal, divide by 4.184.

1.2.1. Acid Chloride Formation

Neopentanoic acid can be converted to neopentanoyl chloride [3282-30-2] by reaction with thionyl chloride (2), phosgene (3), phosphorus pentachloride, phosphorus trichloride, or by the reaction with benzotrichloride in the presence of Friedel-Crafts catalysts (4). A laboratory procedure using tetramethyl-α-halogenoenamines at room temperature has also been reported (5).

Commercially, neopentanoyl chloride is often the preferred starting material for the synthesis of peroxyesters, agricultural chemicals, pharmaceuticals, esters, and other fine chemicals because the reactivity of the acid halide is generally greater than that of the acid.

1.2.2. Esterification

Esters of neopentanoic acid can be prepared either from the chloride or directly from the acid and alcohol. An example of the former reaction is that between neopentanoyl chloride and *tert*-butyl hydroperoxide to give *tert*-butyl peroxyneopentanoate [927-07-1], which is used as a free-radical initiator in polymerizations. For direct esterification, acid catalysts, such as sulfuric acid or toluene sulfonic acid, are used, although higher catalyst concentrations are generally required because of the lower reactivity of the acid. Methyl neopentanoate [598-98-1] has been prepared using an acid catalyst (6) or sulfonic acid cation-exchange resin (7); aromatic neopentanoate esters can be made by standard esterification procedures (8). Vinyl neopentanoate [3377-92-2] is prepared from neopentanoic acid and acetylene using zinc neopentanoate [15827-10-8] as catalyst and zinc chloride as cocatalyst (9). It can also be prepared from the acid and vinyl acetate [108-05-4] using ruthenium carbonyl as the catalyst (10). The glycol monoester can be prepared in high yields, essentially free of the diester, by reaction of the acid with ethylene oxide using an hydroxyalkylamine as the catalyst (11).

The neo acids are generally less reactive than their straight-chain counterparts. For example, neopentanoic acid reacts approximately 15 times slower than *n*-pentanoic acid (12). Greater steric hindrance, as brought about by ethyl groups, for example, results in even slower esterification rates. Once formed, however, the esters of neopentanoic acid are more resistant to hydrolysis than the corresponding linear acid esters. For example, under basic conditions, hexyl neopentanoate [5434-57-1] is hydrolyzed approximately 20 times more slowly than hexyl valerate [1117-59-5]. Under acid conditions, the difference in hydrolysis rate is a factor of 160 (13).

1.2.3. Reduction

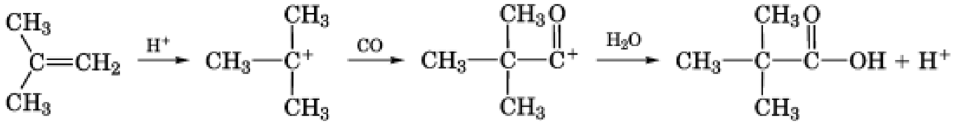
2,2-Dimethylpropanal [630-19-3] can be prepared by the reduction of neopentanoic acid using various catalysts, such as iron (14), tin or zirconium oxides (15, 16), iron–chromium (17), and other reagents (18, 19). The reduction of neopentanoic acid to 2,2-dimethylpropanol [75-84-3] (neopentyl alcohol) has been accomplished using supported osmium and rhenium (20), copper–zinc or nickel (21), metal oxides (22), or sodium borohydride (23). Reduction to the alkane, 2,2-dimethylpropane [463-82-1] (neopentane), has been claimed using a copper oxide–zinc oxide catalyst (24).

1.2.4. Other Reactions

The anhydride of neopentanoic acid, neopentanoyl anhydride [1538-75-6], can be made by the reaction of neopentanoic acid with acetic anhydride (25). The reaction of neopentanoic acid with acetone using various catalysts, such as titanium dioxide (26) or zirconium oxide (27), gives 3,3-dimethyl-2-butanone [75-97-8], commonly referred to as pinacolone. Other routes to pinacolone include the reaction of pivaloyl chloride [3282-30-2] with Grignard reagents (28) and the condensation of neopentanoic acid with acetic acid using a rare-earth oxide catalyst (29). Amides of neopentanoic acid can be prepared directly from the acid, from the acid chloride, or from esters, using primary or secondary amines.

1.3. Manufacture

Trialkylacetic acids are prepared using variants of the Koch reaction (30), a two-stage reaction for the preparation of carboxylic acids. In the first stage, olefin, carbon monoxide, and a strong acid catalyst react to give what is commonly referred to as the complex. In the second stage, the complex is hydrolyzed to give the carboxylic acid and to regenerate the catalyst. A number of Brønsted acid catalysts have been used, including H_2SO_4, H_3PO_4, HF, and Lewis acids such as BF_3. Temperatures used depend on the choice of catalyst, and can range from -20 to $+80^\circ C$, pressures used can be as high as 10 MPa (100 atm). Koch reactions have been reviewed (31). The mechanism of reaction is believed to proceed by the formation of a carbenium ion from the olefin, followed by addition of carbon monoxide to give an acylium cation. The acylium cation then reacts with water to give the carboxylic acid. This is illustrated using isobutylene [115-11-7] as the olefin, which gives neopentanoic acid as the product.



$$(CH_3)_2C{=}CH_2 \xrightarrow{H^+} (CH_3)_3C^+ \xrightarrow{CO} (CH_3)_3C{-}C^+{=}O \xrightarrow{H_2O} (CH_3)_3C{-}C({=}O){-}OH + H^+$$

Neopentanoic acid has also been produced commercially from diisobutylene [18923-87-0], in which the first step in the reaction sequence is a cracking or depolymerization of the olefin to give isobutylene.

Commercial production of these acids essentially follows the mechanistic steps given. This is most clearly seen in the Exxon process of Figure 1 (32). In the reactor, catalyst, olefin, and CO react to give the complex. After degassing, hydrolysis of this complex takes place. The acid and catalyst are then separated, and the trialkylacetic acid is purified in the distillation section. The process postulated to be used by Shell (Fig. 2) is similar, with additional steps prior to distillation being used. In 1980, the conditions used were described as ca 40–70°C and 7–10 MPa (70–100 bar) carbon monoxide pressure with H_3PO_4–BF_3–H_2O in the ratio 1:1:1 (Shell) or with $BF_3 \cdot 2H_2O$ (Enjay) as catalyst (33).

Work on the process for the production of these acids has continued in recent years. One patent discloses the use of zeolite catalysts (34) for the synthesis of neopentanoic acid from isobutylene. The use of a copper catalyst in a strong acid, such as sulfuric acid, operating at lower pressures, has also been claimed (35).

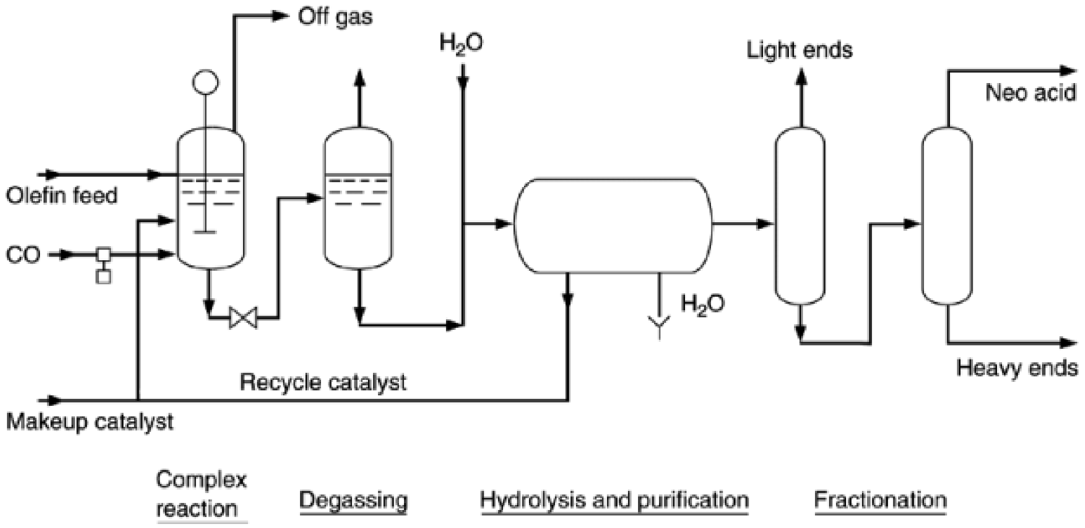


Fig. 1. Neo acid production schematic (32).(Courtesy of *Hydrocarbon Processing*.)

1.4. Economic Aspects and Shipment

Production worldwide of neopentanoic acid is estimated at 15 thousand metric tons per year. Both Shell (36) and Exxon (37) have announced expansions in capacity. Neopentanoic acid is shipped in heated tank cars, heated tank trucks, and drums.

1.5. Health and Safety Factors

Neopentanoic acid possesses low toxicity, either by ingestion (oral LD_{50} in rats is 2.0 g/kg) or by skin absorption (dermal LD_{50} in rabbits is 3.16 g/kg). The principal hazards associated with neopentanoic acid at ambient temperatures are from eye and skin irritation. At elevated temperatures, where concentrations of the vapor are significant, irritation of the respiratory tract can also occur. Contact with the material should be avoided.

Eye contact should be followed by flushing the eyes with large amounts of water. If irritation persists, medical attention should be obtained. Skin contact should be followed by flushing with water, using soap if available. Neopentanoic acid is combustible and will burn. Fire should be extinguished with foam, dry chemical, or water spray.

1.6. Uses

1.6.1. Polymers and Resins

tert-Butyl peroxyneopentanoate and other peroxyesters of neopentanoic acid can be used as free-radical initiators for the polymerization of vinyl chloride [75-01-4] (38) or of ethylene [74-85-1]. These peresters have also been used in the preparation of ethylene–vinyl acetate copolymers [24937-78-8] (39), modified polyester granules (40), graft polymers of aminoalkyl acrylates with vinyl chloride resins (41), and copolymers of *N*-vinyl-pyrrolidinone [88-12-0] and vinyl acetate [108-05-4] (42). They can also be used as curing agents for unsaturated polyesters (43).

Vinyl neopentanoate is used in the preparation of adhesives and binders (44–46), optical materials for plastic lenses (47), gas permeable membranes for oxygen enrichment (48), and in coating applications (49, 50).

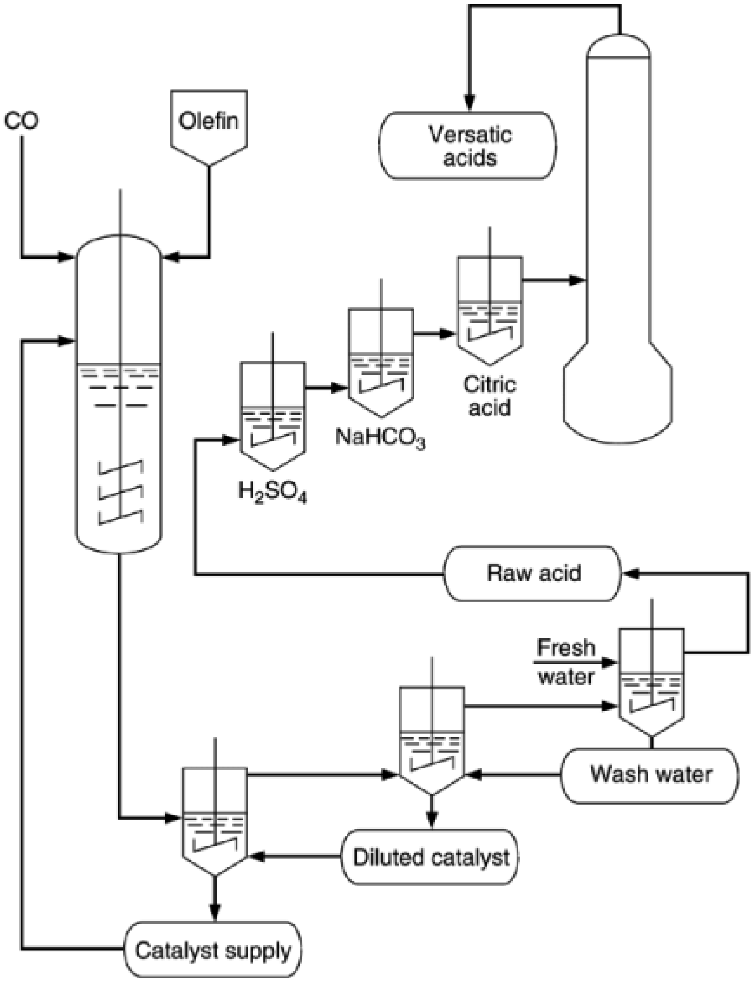


Fig. 2. Flow sheet of Shell Versatic Acid unit (33).

1.6.2. Pharmaceuticals

Neopentanoic acid derivatives are widely used in the preparation of pharmaceuticals, eg, as a means of introducing the *tert*-butyl group into a molecule. More frequently, however, derivatives have been prepared that exploit the enhanced hydrolytic stability of the neopentanoate group. For example, when salmon calcitonin is treated with *N*-hydroxysuccinimide pivalate [42014-50-6], the resulting derivative retains the biological activity of the precursor, but gives an extended duration of activity (51).

Chloromethyl 2,2-dimethylpropionate [18997-19-8] has also been used to prepare a number of ester derivatives with improved properties compared to the nonderivatized compound. The pivaloyloxymethyl ester derivative of piperacillin [61477-96-1] is an orally administrable antibiotic agent (52) (see Antibiotics, β-lactams). The pivaloyloxymethyl ester [77372-61-3] of 2-propylpentanoic acid [99-66-1] shows comparable anti-epileptic and anticonvulsant activity to the acid, but is more rapidly and uniformly absorbed in the intestinal tract than the acid itself (53). The pivaloyloxymethyl ester of 2-anilinonicotinic acid retains the analgesic and anti-inflammatory activity without the ulcerogenic activity of the free acid (54). Similarly, pivaloyloxymethyl salicylate [66195-29-7], prepared from sodium salicylate and chloromethyl pivalate, has all the favorable properties of aspirin without undesirable gastric irritation (55).

Neopentanoyl chloride has been used in the preparation of AZT (56), which is used in the treatment of acquired immune deficiency syndrome (AIDS) (see Antiviral agents).

The effect of acid structure on skin penetration and skin irritation has been studied (57).

1.6.3. Agricultural Applications

One of the largest uses for neopentanoic acid is in the preparation of agricultural chemicals. Neopentanoic acid or its derivatives are used in the preparation of a number of commercial herbicides, such as tebuthiuron [39014-18-1], metamitron [41394-05-2], metribuzin [21087-64-9], clomazone [81777-89-1], and oxadiazon [19666-30-9], and others (58–63). As with pharmaceuticals, the pivalate ester of a herbicide has been prepared to increase the resistance to hydrolysis, allowing the preparation of aqueous dispersions (64). A combination of a pivalic acid amide and metribuzin results in a synergism that broadens the range of applicability of the herbicide (65). The amides themselves also show nematocidal and fungicidal activity. The preparation of organotin compounds for use as miticides also involves the use of neopentanoic acid (66).

1.6.4. Cosmetics

Esters of neopentanoic acid are used as perfumes or perfume precursors (8, 67), as liquid binders (68), and in emollient and moisturizing compositions (69).

1.6.5. Fuels, Lubricants, and Transmission Fluids

Polyol esters of neopentanoic acid have been used as high vacuum pumping liquids that are stable in chemically aggressive environments (70). Esters such as 6-(*p*-anilinophenoxy)hexyl pivalate are used as antioxidants for synthetic ester lubricants (71). Pivalic anhydride [1538-75-6] has been claimed as an antiknock additive for gasoline (72).

1.6.6. Miscellaneous Applications

The fruity odor of a series of esters, including a number of esters of neopentanoic acid, has been related to the structure of the ester, with an emphasis on pearlike odor (73). Methyl pivaloylacetate [55107-14-7], $(CH_3)_3CCOOCH_2COOCH_3$, prepared by condensation of methyl pivalate and methyl acetate, is used as an intermediate in the preparation of photographic chemicals (74). Degradable organic material such as aviation turbo-kerosene can be preserved by using basic zinc carboxylates, such as zinc pivalate [15827-10-8], for their biocidal activity (75) (see Aviation and other gas turbine fuels).

2. C_{10} Trialkylacetic Acids

2.1. Physical Properties

The C_{10} trialkylacetic acids, referred to as neodecanoic acid [26896-20-8] or as Versatic 10 [52627-73-3], are liquids at room temperature. Typical physical properties for commercially available material are given in Table 2. These materials are typically mixtures of isomers, hence no structures are given throughout this section.

2.2. Chemical Properties

Like neopentanoic acid, neodecanoic acid, $C_{10}H_{20}O_2$, undergoes reactions typical of carboxylic acids. For example, neodecanoic acid is used to prepare acid chlorides, amides (76), and esters (7, 11, 77, 78), and, like

Table 2. Physical Properties of Commercially Available Neodecanoic Acid[a]

Property	Value
mp, °C	<-40
bp, °C	250–257
acid value, mg KOH/g	325
color	100 (Pt/Co)
specific gravity at 20/20°C	0.915
viscosity, mm^2/s (=cSt)	
at 20°C	35.7
at 60°C	7
flash point, °C (Tag closed cup)	105
water, wt%	0.05
vapor pressure, kPa[b] at 60°C	0.012
solubility in water, g/100 mL H_2O at 25°C	0.017
heat of vaporization, kJ/kg[c], at the boiling point and 101.3 kPa[b]	249.5
ionization constant, $K_a \times 10^{-6}$ at 25°C	4.2

[a] Ref. 1.

[b] To convert kPa to mm Hg, multiply by 7.5.

[c] To convert kJ to kcal, divide by 4.184.

neopentanoic acid, is reduced to give alcohols and alkanes (21, 24). One area of reaction chemistry that is different from the C_5 acids is the preparation of metal salts. Both neopentanoic acid and neodecanoic acid, like all carboxylic acids, can form metal salts. However, in commercial applications, metal salt formation is much more important for neodecanoic acid than it is for neopentanoic acid.

2.2.1. Metal Salt Formation

At least three methods are commonly used to prepare metals salts. The first of these is known as the double decomposition method.

$$\mathrm{CoCl_2\ (aq) + 2Na\,(neodec)\ (org) \longrightarrow Co\,(neodec)_2\ (org) + 2\ NaCl\ (aq)}$$

where neodec = the anion of neodecanoic acid

Typically, a slight excess of acid is used, resulting in salts that are neutral or slightly acidic. This method has been applied to the preparation of zirconium salts (79).

A second method for preparing acid salts is termed fusion, represented by

$$\mathrm{Co\,(OH)_2 + 2\ neodecanoic\ acid \longrightarrow Co\,(neodec)_2 + 2\ H_2O}$$

In this method, a metal oxide or hydroxide is slurried in an organic solvent, neodecanoic acid is slowly added, and the mixture is refluxed to remove the water. Salts that are basic can be prepared by using less than stoichiometric amounts of acid. This method has been used in the preparation of metal salts of silver (80) and vanadium (81). The third method of preparation is similar to the fusion process, the difference is the use of finely divided metal as the starting material instead of the metal oxide or hydroxide. This method has been applied to the preparation of cobalt neodecanoate (82). Salts of tin (83) and antimony (84) have been prepared by the fusion method, starting with lower carboxylic acids, then replacing these acids with neodecanoic acid.

2.3. Manufacture

The C_{10} trialkylacetic acids are prepared using the same process and catalysts as are used for the preparation of neopentanoic acid. For the C_{10} acids, a branched C_9 olefin stream is typically used. Because the reaction proceeds by means of a carbenium ion mechanism, rearrangement of the olefin occurs, resulting in a C_{10} acid composed of a large number of isomers. In addition to the carbonylation reaction, olefin dimerization and oligomerization, along with olefin disproportionation also occur, resulting in trialkylacetic acids with carbon numbers less than and greater than 10.

2.4. Economic Aspects and Shipment

The C_{10} trialkylacetic acids are produced in volumes totaling tens of thousands of metric tons per year. The C_{10} acids are shipped in bulk sea vessels, tank cars, tank trucks, and drums.

2.5. Health and Safety Factors

The C_{10} trialkylacetic acids have toxicities similar to those for other neo acids: oral LD_{50} in rats is 2.0 g/kg, and dermal LD_{50} in rabbits is 3.16 g/kg.

The primary hazard associated with C_{10} trialkylacetic acids is eye irritation. In contact with the eyes, the material is irritating and may injure eye tissue if not removed promptly. Any contact with the eyes should be immediately flushed with large amounts of water. Medical attention should also be obtained. For skin contact, flush with large quantities of water, using soap if available. To extinguish fires, use foam, dry chemical, or water spray.

2.6. Uses

2.6.1. Polymers, Resins, and Coatings

Peroxyesters of neodecanoic acid, such as *tert*-butyl peroxyneodecanoate [26748-41-4] and α-cumyl peroxyneodecanoate [26748-47-0], constitute one of the most important uses for neodecanoic acid. These materials are used as free-radical initiators in the polymerization of vinyl chloride (85), acrylates (86), ethylene (87), styrene [100-42-5] (87), and in the copolymerization of vinyl chloride with other monomers, such as propylene [115-07-1] (88), or acrylates (89). The peroxyesters are also used as curing agents for resins (90).

Metal salts of neodecanoic acid have also been used as catalysts in the preparation of polymers. For example, bismuth, calcium, barium, and zirconium neodecanoates have been used as catalysts in the formation of polyurethane elastomers (91, 92). Magnesium neodecanoate [57453-97-1] is one component of a catalyst system for the preparation of polyolefins (93); vanadium, cobalt, copper, or iron neodecanoates have been used as curing catalysts for conjugated-diene butyl elastomers (94).

The metal salts of neodecanoic acid have found wide usage as driers for paints and inks (95, 96). Metal neodecanoates that are used include silver (80), cobalt (82), and zirconium (79), along with lead, copper, manganese, and zinc (see Driers and metallic soaps).

Neodecanoic acid is also used as the carrier for metals in poly(vinyl chloride) heat stabilizers (qv). Metals used in this application include barium, cadmium, and zinc. Tin as the neodecanoate salt has also been claimed as a heat stabilizer for maleic anhydride (97).

2.6.2. Adhesion Promoters

One of the growing uses for neodecanoic acid has been in the preparation of adhesion promoters for radial tires. In this application, cobalt or nickel neodecanoate, along with other components, is used during tire manufacture to promote the adhesion or bonding of the rubber to the steel cord. The result is high adhesive strength, good thermal aging resistance and improved resistance to moisture aging (98–100).

2.6.3. Metal-Working and Hydraulic Fluids

In the preparation of fluids for metal-working and hydraulics, the trend has been to replace organic-based materials with aqueous-based materials. Neodecanoic acid has found application in these newer fluids as a corrosion inhibitor and a viscosity improver. For example, neodecanoic acid is used in an aqueous hydraulic fluid concentrate for corrosion inhibition and improved antiwear properties (101), in the preparation of a thickened aqueous hydraulic fluid to reduce viscosity loss (102), and in a water-soluble metal working oil to reduce corrosion (103). In a similar vein, neodecanoic acid has been used in antifreeze concentrates for corrosion inhibition (104).

2.6.4. Metal Extraction

As with other carboxylic acids, neodecanoic acid can be used in the solvent extraction of metal ions from aqueous solutions. Recent applications include the extraction of zinc from river water for determination by atomic absorption spectrophotometry (105), the coextraction of metals such as nickel, cobalt, and copper with iron (106), and the recovery of copper from ammoniacal leaching solutions (107).

2.6.5. Fuels and Lubricants

Rare-earth neodecanoates have been claimed as additives for diesel fuels that reduce the precipitation of particles and gum (108). Neodecanoic acid has also been used in the preparation of ashless detergent additives for fuels and lubricants that reduce engine deposits in internal combustion engines (109).

2.6.6. Electrical and Electronic Applications

Silver neodecanoate [62804-19-7] has been used in the preparation of a capacitor-end termination composition (110), lead and stannous neodecanoate have been used in circuit-board fabrication (111), and stannous neodecanoate has been used to form patterned semiconductive tin oxide films (112). The silver salt has also been used in the preparation of ceramic superconductors (113). Neodecanoate salts of barium, copper, yttrium, and europium have been used to prepare superconducting films and patterned thin-film superconductors. To prepare these materials, the metal salts are deposited on a substrate, then decomposed by heat to give the thin film (114–116) or by a focused beam (electron, ion, or laser) to give the patterned thin film (117, 118). The resulting films exhibit superconductivity above liquid nitrogen temperatures.

2.6.7. Miscellaneous Applications

Polyamides, prepared from polyamines and neodecanoic acid, are used as wash-cycle antistatic agents (qv) (76). Salts of neodecanoic acid have been used in the preparation of supported catalysts, such as silver neodecanoate for the preparation of ethylene oxide catalysts (119), and the nickel soap in the preparation of a hydrogenation catalyst (120). Metal neodecanoates, such as magnesium, lead, calcium, and zinc, are used to improve the adherence of plasticized poly(vinyl butyral) sheet to safety glass in car windshields (121). Platinum complexes using neodecanoic acid have been studied for antitumor activity (122). Neodecanoic acid and its esters are used in cosmetics as emollients, emulsifiers, and solubilizers (77, 123, 124). Zinc or copper salts of neoacids are used as preservatives for wood (125).

2.7. Glycidyl and Vinyl Esters

Glycidyl neodecanoate [26761-45-5], sold commercially as GLYDEXX N-10 (Exxon) or as Cardura E10 (Shell), is prepared by the reaction of neodecanoic acid and epichlorohydrin under alkaline conditions, followed by purification. Physical properties of the commercially available material are given in Table 3. The material is a mobile liquid monomer with a mild odor and is used primarily in coatings. For example, it is used as an

Table 3. Physical Properties of Commercially Available Glycidyl Neodecanoates

Property	Cardura E10[a]	GLYDEXX N-10[b]
color (Pt/Co scale)	<60	45
density at 20°C, g/mL	0.958–0.968	
water content	<0.1% mass/mass	0.05 wt %
epoxy equivalent weight,[c] g	244–256	250
flash point, °C	126[d]	128[e]
residual epichlorohydrin	<10 mg/kg	<5 ppm
viscosity, mPa·s(=cP)		
25°C	7.13	
100°C	1.31	
150°C	0.72	
vapor pressure at 37.8°C, kPa[f]	0.9	
boiling range at 101.3 kPa,[f] °C	251–278	
freezing point, °C	<−60	
solubility in water at 20°C	0.01 % mass/mass	

[a] Ref. 126.
[b] Ref. 127.
[c] Grams of resin containing 1 g-equivalent of epoxide.
[d] PMCC = Pensky−Martin closed cup.
[e] Tagliabue closed cup.
[f] To convert kPa to mm Hg, multiply by 7.5.

Table 4. Physical Properties of VeoVa 10[a]

Property	Value
color (Pt/Co)	<15
density at 20°C, g/mL	0.875–0.885
water content, % mass/mass	<0.1
acid value, mg KOH/g	<1.0
vinyl unsaturation, mol/kg	4.85–5.10
kinematic viscosity at 20°C, mm^{2}s(=cSt)	2.2
vapor pressure, kPa[b]	
at 30°C	<0.1
at 110°C	4.3
at 210°C	101
boiling range, °C at 13.3 kPa[b]	133–136
flash point,[c] °C	75
freezing point, °C	<−20
solubility in water at 20°C, % mass/mass	<0.1

[a] Ref. 128.
[b] To convert kPa to mm Hg, multiply by 7.5.
[c] PMCC = Pensky−Martin closed cup closed cup.

intermediate for the production of a range of alkyd resins (qv) and acrylics, and as a reactive diluent for epoxy resins (qv).

Total world production of glycidyl neodecanoate is ca 7–10 thousand metric tons per year, with production by Exxon in the United States and by Shell in The Netherlands. The product is shipped in bulk or in drums and must be protected from contact with atmospheric water during storage.

Vinyl neodecanoate [26544-09-2] is prepared by the reaction of neodecanoic acid and acetylene in the presence of a catalyst such as zinc neodecanoate. Physical properties of the commercially available material, VeoVa 10 from Shell, are given in Table 4. The material is a mobile liquid with a typical mild ester odor used in a number of areas, primarily in coatings, but also in construction, adhesives, cosmetics, and a number of miscellaneous areas. Copolymerization of vinyl neodecanoate with vinyl acetate gives coating materials with excellent performance on alkaline substrates and in exterior weathering conditions.

The only producer of vinyl neodecanoate is Shell in The Netherlands, who markets the material as VeoVa 10. Production is several tens of thousands of metric tons per year. The vinyl ester is shipped in bulk or in lined drums, stabilized with 5 ppm of the monomethyl ether of hydroquinone [95-71-6] MEHQ.

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M. J. KEENAN
M. A. KREVALIS
Exxon Chemical Co.

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