ACETONE

1. Introduction

Acetone [67-64-1] (2-propanone, dimethyl ketone, CH_3COCH_3), molecular weight 58.08 (C_3H_6O), is the simplest and most important of the ketones. It is a color-less, mobile, flammable liquid with a mildly pungent, somewhat aromatic odor, and is miscible in all proportions with water and most organic solvents. Acetone is an excellent solvent for a wide range of gums, waxes, resins, fats, greases, oils, dyestuffs, and cellulosics. It is used as a carrier for acetylene, in the manufacture of a variety of coatings and plastics, and as a raw material for the chemical

synthesis of a wide range of products such as ketene, methyl methacrylate, bisphenol A, diacetone alcohol, methyl isobutyl ketone, hexylene glycol (2-methyl-2,4-pentanediol), and isophorone. World production of acetone in 1999 was about 4.27 million metric tons per year, of which about 1.4 million was made in the United States. Most of the world's manufactured acetone is obtained as a coproduct in the process for phenol from cumene and most of the remainder from the dehydrogenation of isopropyl alcohol. Numerous natural sources of acetone make it a normal constituent of the environment. It is readily biodegradable.

2. Physical and Thermodynamic Properties

Selected physical properties are given in Table 1 and some thermodynamic properties in Table 2. Vapor pressure (P) and enthalpy of vaporization (H) over the temperature range 178.45–508.2 K can be calculated with an error of <3%

Table 1. **Physical Properties**[a]

Property	Value		
melting point, °C	−94.6		
boiling point at 101.3 kPa[b], °C	56.29		
refractive index, n_D			
at 20°C	1.3588		
at 25°C	1.35596		
electrical conductivity at 298.15 K, S/cm	5.5×10^{-8}		
critical temperature, °C	235.05		
critical pressure, kPa[b]	4701		
critical volume, L/mol	0.209		
critical compressibility	0.233		
triple point temperature, °C	−94.7		
triple point pressure, Pa[b]	2.59375		
acentric factor	0.306416		
solubility parameter at 298.15 K, $(J/m^3)^{1/2}$ [c]	19773.5		
dipole moment, C·m[d]	9.61×10^{-30}		
molar volume at 298.15 K, L/mol	0.0739		
molar density, mol/L			
solid at −99°C	16.677		
liquid at 298.15 K	13.506		
Selected physical properties as a function of temperature			
temperature, °C	0	20	40
surface tension, mN/m (= dyn/cm)	26.2	23.7	21.2
vapor pressure, kPa[b]	9.3	24.7	54.6
specific gravity at 20°C	0.807	0.783	0.759
viscosity, mPa·s (= cP)	0.40	0.32	0.27

[a] Extensive tables and equations are given in (1) for viscosity, surface tension, thermal conductivity, molar density, vapor pressure, and second virial coefficient as functions of temperature.
[b] To convert kPa to mmHg, multiply by 7.501.
[c] To convert $(J/m^3)^{1/2}$ to $(cal/m^3)^{1/2}$, divide by 2.045.
[d] To convert C·m to debyes, divide by 3.336×10^{-30}.

Table 2. **Thermodynamic Properties**[a–c]

Property	Value
specific heat of liquid at 20°C, J/g	2.6
specific heat of vapor at 102°C, J/(mol·K)	92.1
heat of vaporization at 56.1°C, kJ/mol	29.1
enthalpy of vaporization, kJ/mol	30.836
enthalpy of fusion at melting point, J/mol	5691.22
heat of combustion of liquid, kJ/mol	1787
enthalpy of combustion, kJ/mol	−1659.17
entropy of liquid, J/(mol·K)	200.1
entropy of ideal gas, J/(mol·K)	295.349
Gibbs energy of formation, kJ/mol	−152.716
enthalpy of formation, kJ/mol	
ideal gas	−217.15
gas	−216.5
liquid	−248

[a] Extensive tables and equations are given in (1) for enthalpy of vaporization and heat capacity at constant pressure.
[b] At 298.15 K unless otherwise noted.
[c] To convert J to cal, divide by 4.184.

from the following equations wherein the units are P, kPa; H, mJ/mol; T, K; and T_r = reduced temperature, T/T_c (1):

$$\log (P) = 70.72 - 5685/T - 7.351 \ln (T) + 0.0000063 T^2$$

$$\log (H) = \log (49,170,000) + \left(1.036 - 1.294 T_r + 0.672 T_r^2\right) \log (1 - T_r)$$

Spectral characterization data are given in Table 3 (2).

3. Chemical Properties

The closed cup flash point of acetone is −18°C and open cup −9°C. The autoignition temperature is 538°C, and the flammability limits are 2.6–12.8 vol% in air at 25°C (3).

Table 3. **Spectral Parameters for Acetone**[a]

Method	Property
Absorption peaks, cm^{-1}	
infrared: SADG 77	3000, 1715, 1420, 1360, 1220, 1090, 900, 790, 530
Raman: SAD 162	3010, 2930, 2850, 2700, 1740, 1710, 1430, 1360, 1220, 1060, 900, 790, 520, 490, 390
Absorption peaks, nm	
ultraviolet: SAD 89	270 (in methanol)
Chemical shift, ppm	
^{1}H nmr: SAD 9228	2.1 (CDCl$_3$)
^{13}C nmr: JJ 28 FT	30.6, 206.0 (CDCl$_3$)
m/e (relative abundance)	
mass spec: Wiley 30	43(100), 58(42), 15(14), 42(6), 27(4), 39(3), 26(3), 29(2) molecular ion = 58.04

[a] Ref. 2.

Acetone shows the typical reactions of saturated aliphatic ketones. It forms crystalline compounds such as acetone sodium bisulfite [540-92-1], $(CH_3)_2C(OH)SO_3Na$, with alkali bisulfites. The highly reactive compound ketene [463-51-4], $CH_2=C=O$, results from the pyrolysis of acetone. Reducing agents convert acetone to pinacol [76-09-5], isopropyl alcohol [67-63-0], or propane [74-98-6]. Reductive ammonolysis produces isopropyl amines. Acetone is stable to many of the usual oxidants such as Fehling's solution, silver nitrate, cold nitric acid, and neutral potassium permanganate, but it can be oxidized with some of the stronger oxidants such as alkaline permanganate, chromic acid, and hot nitric acid. Metal hypohalite, or halogen in the presence of a base, oxidizes acetone to the metal acetate and a haloform, eg, iodoform. Halogens alone substitute for the H atoms, yielding haloacetones. Acetone is a metabolic product in humans and some other mammals and is a normal constituent of their blood and urine. In diabetics, it is present in relatively large amounts.

Compounds with active hydrogen add to the carbonyl group of acetone, often followed by the condensation of another molecule of the addend or loss of water. Hydrogen sulfide forms hexamethyl-1,3,5-trithiane probably through the transitory intermediate thioacetone that readily trimerizes. Hydrogen cyanide forms acetone cyanohydrin [75-86-5] $(CH_3)_2C(OH)CN$, which is further processed to methacrylates. Ammonia and hydrogen cyanide give $(CH_3)_2C(NH_2)CN$ [19355-69-2] from which the widely used polymerization initiator, azobisisobutyronitrile [78-67-1] is made (4).
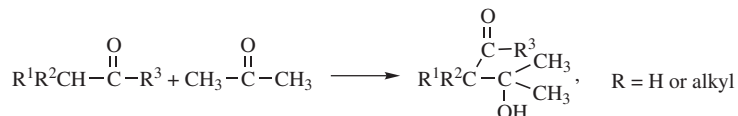
Primary amines form Schiff bases, $(CH_3)_2C=NR$. Ammonia induces an aldol condensation followed by 1,4-addition of ammonia to produce diacetone amine (from mesityl oxide), 4-amino-4-methyl-2-pentanone [625-04-7], $(CH_3)_2C(NH_2)CH_2COCH_3$, and triacetone amine (from phorone), 2,2,6,6-tetramethyl-4-piperidinone [826-36-8]. Hydroxylamine forms the oxime and hydrazine compounds $(RNHNH_2)$ form hydrazones $(RNHN=C(CH_3)_2)$. Acetone and nitrous acid give the isonitroso compound that is the monoxime of pyruvaldehyde [306-44-5], $CH_3COCH=NOH$. Mercaptans form hemimercaptols by addition and mercaptols, $(CH_3)_2C(SR)_2$, by substitution following the addition.

With aldehydes, primary alcohols readily form acetals, $RCH(OR')_2$. Acetone also forms acetals (often called ketals), $(CH_3)_2C(OR)_2$, in an exothermic reaction, but the equilibrium concentration is small at ambient temperature. However, the methyl acetal of acetone, 2,2-dimethoxypropane [77-76-9], was once made commercially by reaction with methanol at low temperature for use as a gasoline additive (5). Isopropenyl methyl ether [116-11-0], useful as a hydroxyl blocking agent in urethane and epoxy polymer chemistry (6), is obtained in good yield by thermal pyrolysis of 2,2-dimethoxypropane. With other primary, secondary, and tertiary alcohols, the equilibrium is progressively less favorable to the formation of ketals, in that order. However, acetals of acetone with other primary and secondary alcohols, and of other ketones, can be made from 2,2-dimethoxypropane by transacetalation procedures (7,8). Because they hydrolyze extensively, ketals of primary and especially secondary alcohols are effective water scavengers.

Acetone has long been used as an agent to block the reactivity of hydroxyl groups in 1,2- and 1,3-diols, especially in carbohydrate chemistry. The equilibrium for the formation of acetals with hydroxyls in these compounds is more favorable because the products are five- and six-membered ring compounds,

1,3-dioxolanes and dioxanes, respectively. With glycerol the equilibrium constant for formation of the dioxolane is ∼0.50 at 23°C and 0.29 at 48°C in a mixture resulting from acidification of equal volumes of acetone and glycerol at ambient temperature. The equilibrium can be displaced toward acetal formation by the use of a water scavenger, eg, an anhydrous metal salt such as copper sulfate.

Acetone undergoes aldol additions,

$$R^1R^2CH{-}\overset{\overset{\displaystyle O}{\|}}{C}{-}R^3 + CH_3{-}\overset{\overset{\displaystyle O}{\|}}{C}{-}CH_3 \longrightarrow R^1R^2C{-}\underset{\underset{\displaystyle OH}{|}}{C}\overset{\nearrow}{\underset{\searrow}{}}\begin{matrix} \overset{\overset{\displaystyle O}{\|}}{C}{-}R^3 \\ CH_3 \\ CH_3 \end{matrix}, \qquad R = H\ or\ alkyl$$

and further reacts with the products, forming aldol chemicals, diacetone alcohol (4-hydroxy-4-methyl-2-pentanone [123-42-2]), mesityl oxide (4-methyl-3-penten-2-one [141-79-7]), isophorone (3,5,5-trimethyl-2-cyclohexenone [78-59-1]), phorone (2,6-dimethyl-2,5-heptadien-4-one [504-20-1]), and mesitylene (1,3,5-trimethyl-benzene [108-67-8]). From these are produced the industrial solvents methyl iso-butyl ketone (MIBK, 4-methyl-2-pentanone [108-10-1]), methylisobutylcarbinol (MIBC, 4-methyl-2-pentanol [108-11-2]), hexylene glycol (2-methyl-2,4-pentane-diol [107-41-5]), and others. Acetone enters the typical nucleophilic addition and condensation reactions of ketones both at its carbonyl group and at its methyl groups, with aldehydes, other ketones, and esters. The Claisen reaction with ethyl acetate gives acetylacetone (2,4-pentanedione [123-54-6]); Mannich reaction with secondary amines gives R_2NCH_2 substituted acetones; and the Reformatzky reaction gives β-hydroxy esters. Glycidic esters (esters with a 2-epoxy group) can be made by condensation of acetone and chloroacetic esters with a metal alkoxide.

The para and ortho positions of phenols condense at the carbonyl group of acetone to make bisphenols, eg, bisphenol A, 4,4′-(1-methylethylidene)bisphenol [80-05-07]). If the H atom is activated, ClCH− compounds add to the carbonyl group in the presence of strong base; chloroform gives chloretone (1,1,1-tri-chloro-2-methyl-2-propanol [57-15-8]).

4. Manufacture

Acetone was originally observed ∼1595 as a product of the distillation of sugar of lead (lead acetate). In the nineteenth century, it was obtained by the destructive distillation of metal acetates, wood, and carbohydrates with lime, and pyrolysis of citric acid. Its composition was determined by Liebig and Dumas in 1832.

Until World War I, acetone was manufactured commercially by the dry distillation of calcium acetate from lime and pyroligneous acid (wood distillate) (9). During the war processes for acetic acid from acetylene and by fermentation supplanted the pyroligneous acid (10). In turn, these methods were displaced by the process developed for the bacterial fermentation of carbohydrates (cornstarch and molasses) to acetone and alcohols (11). At one time, Publicker Industries, Commercial Solvents and National Distillers had combined biofermentation capacity of 22,700 metric tons of acetone per year. Biofermentation became

noncompetitive $\sim$1960 because of the economics of scale of the isopropyl alcohol dehydrogenation and cumene hydroperoxide processes.

Production of acetone by dehydrogenation of isopropyl alcohol began in the early 1920s and remained the dominant production method through the 1960s. In the mid-1960s, virtually all United States acetone was produced from propylene. A process for direct oxidation of propylene to acetone was developed by Wacker Chemie (12), but is not believed to have been used in the United States. However, by the mid-1970s 60% of United States acetone capacity was based on cumene hydroperoxide [80-15-9], which accounted for $\sim$65% of the acetone produced.

Acetone was a coproduct of the Shell process for glycerol [56-8-5]. Propylene was hydrated to isopropyl alcohol. Some of the alcohol was catalytically oxidized to acrolein and some was oxidized to give hydrogen peroxide and acetone. Some more of the isopropyl alcohol and the acrolein reacted to give allyl alcohol and acetone. The allyl alcohol was then treated with the peroxide to give glycerol. About 1.26 kg of acetone resulted per kilogram of glycerol.

Direct oxidation of hydrocarbons and catalytic oxidation of isopropyl alcohol have also been used for commercial production of acetone.

Most of the world's acetone is now obtained as a coproduct of phenol by the cumene process. More then 90% of U.S. acetone is produced by this process. Cumene is oxidized to the hydroperoxide and cleaved to acetone and phenol. The yield of acetone is believed to average about 94%, and $\sim$0.60–0.62 unit weight of acetone is obtained per unit of phenol (13).
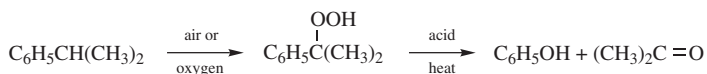
Dehydrogenation of isopropyl alcohol accounts for most of the acetone production not obtained from cumene. The vapor is passed over a brass, copper, or other catalyst at 400–500°C, and a yield of $\sim$95% is achieved (1.09 unit weight of alcohol per unit of acetone) (13).

Minor amounts of acetone are made by other processes. Until mid-1980 Shell Chemical Company obtained acetone and hydrogen peroxide as coproducts of noncatalytic oxidation of isopropyl alcohol with oxygen in the liquid phase. Yield to acetone was $\sim$90%. In a process analogous to the cumene process, Eastman Chemical Products, Inc., and The Goodyear Tire & Rubber Company produce hydroquinone and acetone from diisopropylbenzene [25321-09-9] in the United States. Similarly, Mitsui Petrochemical Industries, Ltd., in Japan produces coproduct acetone with cresol from cymene [25755-15-1]. BP Chemicals, Ltd., in the United Kingdom recovers by-product acetone from the manufacture of acetic acid by the oxidation of light petroleum distillate.

Producers of acetone in the United States and their capacities and feedstocks are given in Table 4 (14).

4.1. Cumene Hydroperoxide Process for Phenol and Acetone. Benzene is alkylated to cumene, and then is in oxidized to cumene hydroperoxide, which in turn is cleaved to phenol and acetone.

$$C_6H_5CH(CH_3)_2 \xrightarrow[\text{oxygen}]{\text{air or}} C_6H_5\overset{\overset{\text{OOH}}{|}}{C}(CH_3)_2 \xrightarrow[\text{heat}]{\text{acid}} C_6H_5OH + (CH_3)_2C = O$$

One kilogram of phenol production results in $\sim$0.6 kg of acetone or about $\sim$0.40–0.45 kg of acetone per kilogram of cumene used.

Table 4. **U.S. Producers of Acetone and Their Capacities**

Company	Location	Annual[a] capacity, 10^3 t
Cumene feedstock		
Aristech Chemical Corporation	Haverhill, Ohio	203
JLM Chemicals	Blue Island, Ill.	30
Dow Chemical U.S.A.	Oyster Creek, Tex.	181
General Electric Company	Mount Vernon, Ind.	197
Georgia Gulf Corporation	Plaquemine, La.	45
Shell Oil Company	Deer Park, Tex.	185
Texaco Corporation	El Dorado, Kans.	38.6
Isopropyl alcohol feedstock		
Shell Oil Company	Deer Park, Tex.	190
Union Carbide Corporation	Institute, W.Va.	77
Diisopropylbenzene feedstock		
Eastman Kodak Company	Kingsport, Tenn.	11.3[b]
The Goodyear Tire and Rubber Company, Chemical Division	Bayport, Tex.	6.8[b]

[a] As of April 5, 1999 (14).
[b] Small amounts, in manufacture of hydroquinone.

There are many variations of the basic process and the patent literature is extensive. Several key patents describe the technology (15). The process steps are oxidation of cumene to a concentrated hydroperoxide, cleavage of the hydroperoxide, neutralization of the cleaved products, and distillation to recover acetone.

In the first step, cumene is oxidized to cumene hydroperoxide with atmospheric air or air enriched with oxygen in one or a series of oxidizers. The temperature is generally between 80 and 130°C and pressure and promoters, such as sodium hydroxide, may be used (16). A typical process involves the use of three or four oxidation reactors in series. Feed to the first reactor is fresh cumene and cumene recycled from the concentrator and other reactors. Each reactor is partitioned. At the bottom there may be a layer of fresh 2–3% sodium hydroxide if a promoter (stabilizer) is used. Cumene enters the side of the reactor, overflows the partition to the other side, and then goes on to the next reactor. The air (oxygen) is bubbled in at the bottom and leaves at the top of each reactor.

The temperatures decline from a high of 115°C in the first reactor to 90°C in the last. The oxygen ratio as a function of consumable oxygen is also higher in the later reactors. In this way, the rate of reaction is maintained as high as possible, while minimizing the temperature-promoted decomposition of the hydroperoxide.

This procedure may result in a concentration of cumene hydroperoxide of 9–12% in the first reactor, 15–20% in the second, 24–29% in the third, and 32–39% in the fourth. Yields of cumene hydroperoxide may be in the range of 90–95% (17). The total residence time in each reactor is likely to be in the range of 3–6 h. The product is then concentrated by evaporation to 75–85% cumene hydroperoxide. The hydroperoxide is cleaved under acid conditions with agitation in a vessel at 60–100°C. A large number of nonoxidizing inorganic acids are useful for this reaction, eg, sulfur dioxide (18).

After cleavage, the reaction mass is a mixture of phenol, acetone and a variety of other products such as cumylphenols, acetophenone, dimethyl-phenylcarbinol, α-methylstyrene, and hydroxyacetone. It may be neutralized with a sodium phenoxide solution (19) or other suitable base or ion-exchange resins. Process water may be added to facilitate removal of any inorganic salts. The product may then go through a separation and a wash stage, or go directly to a distillation tower.

A crude acetone product is recovered by distillation from the reaction mass. One or two additional distillation columns may be required to obtain the desired purity. If two columns are used, the first tower removes impurities such as acetaldehyde and propionaldehyde. The second tower removes undesired heavies, the major component being water.

The yield of acetone from the cumene–phenol process is believed to average 94%. By-products include significant amounts of α-methylstyrene [98-83-9] and acetophenone [98-86-2] as well as small amounts of hydroxyacetone [116-09-6], and mesityl oxide [141-79-7]. By-product yields vary with the producer. The α-methylstyrene may be hydrogenated to cumene for recycle or recovered for monomer use. Yields of phenol and acetone decline by 3.5–5.5% when the α-methylstyrene is not recycled (20).

4.2. Purification. A process for the purification of acetone containing cumene as an impurity using solvent extraction with triethylene glycol has been patented (21).

4.3. Dehydrogenation of Isopropyl Alcohol. Isopropyl alcohol is dehydrogenated in an endothermic reaction.

$$CH_3CHOHCH_3 + 66.5 \text{ kJ/mol (at } 327°C) \longrightarrow CH_3COCH_3 + H_2$$
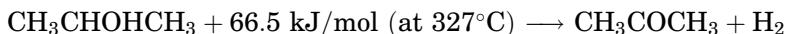
The equilibrium is more favorable to acetone at higher temperatures. At 325°C, 97% conversion is theoretically possible. The kinetics of the reaction has been studied (22). A large number of catalysts have been investigated, including copper, silver, platinum, and palladium metals, as well as sulfides of transition metals of groups 4(IVB), 5(VB), and (VIB)6 of the periodic table. These catalysts are made with inert supports and are used at 400–600°C (23). Lower temperature reactions (315–482°C) have been successfully conducted using zinc oxide-zirconium oxide combinations (24), and combinations of copper–chromium oxide and of copper and silicon dioxide (25).

It is usual practice to raise the temperature of the reactor as time progresses to compensate for the loss of catalyst activity. When brass spelter is used as a catalyst, the catalyst must be removed at intervals of 500–1000 h and treated with a mineral acid to regenerate a catalytically active surface (26). When 6–12% zirconium oxide is added to a zinc oxide catalyst and the reaction temperatures are not excessive, the catalyst life is said to be a minimum of 3 months (24). The dehydrogenation is carried out in a tubular reactor. Conversions are in the range of 75–95 mol %. A process described by Shell International Research (23) is a useful two-stage reaction to attain high conversion, with lower energy cost and lower capital cost. The first stage uses a tubular reactor at 420–550°C to convert up to 70% of the alcohol to acetone. The second stage

employs an unheated fixed-bed reactor with the same catalyst used in the tube reaction to complete the conversion at ~85%.

Although the selectivity of isopropyl alcohol to acetone via vapor-phase dehydrogenation is high, there are a number of by-products that must be removed from the acetone. The hot reactor effluent contains acetone, unconverted isopropyl alcohol, and hydrogen, and may also contain propylene, polypropylene, mesityl oxide, diisopropyl ether, acetaldehyde, propionaldehyde, and many other hydrocarbons and carbon oxides (24,27).

The mixture is cooled and noncondensable gases are scrubbed with water. Some of the resultant gas stream, mainly hydrogen, may be recycled to control catalyst fouling. The liquids are fractionally distilled, taking acetone overhead and a mixture of isopropyl alcohol and water as bottoms. A caustic treatment may be used to remove minor aldehyde contaminants prior to this distillation (28). In another fractionating column, the aqueous isopropyl alcohol is concentrated to ~88% for recycle to the reactor.

A yield of ~95% of theoretical is achieved using this process (1.09 units of isopropyl alcohol per unit of acetone produced). Depending on the process technology and catalyst system, such coproducts as methyl isobutyl ketone and diisobutyl ketone can be produced with acetone (29).

5. Production and Shipment

Acetone is produced in large quantities and is usually shipped by producers to consumers and distributors in drums and larger containers. Distributors repackage the acetone into containers ranging in size from small bottles to drums or even tank trucks. Specialty processors make available various grades and forms of acetone such as high purity, specially analyzed, analytical reagent grade, chromatography and spectrophotometric grades, and isotopically labeled forms, and ship them in ampoules, vials, bottles, or other containers convenient for the buyers.

The Department of Transportation (DOT) hazard classification for acetone is Flammable Liquid, identification number UN1090. DOT regulations concerning the containers, packaging, marking, and transportation for overland shipment of acetone are published in the *Federal Register* (30). Regulations and information for transportation by water in the United States are published in the *Federal Register* (31) and by the U.S. Coast Guard (32). Rules and regulations for ocean shipping have been published by the International Maritime Organization (IMO), a United Nations convention of nations with shipping interests, in the IMOBCH Code (33). The IMO identification number is 3.1. Because additions and changes to the regulations appear occasionally, the latest issue of the regulations should be consulted.

Small containers up to 4–5 L (~1 gal) are usually glass. Acetone is also shipped by suppliers of small quantities in steel pails of 18 L. Depending on the size of the container, small amounts are shipped by parcel delivery services or truck freight. Quantities that can be accepted by some carriers are limited by law and special "over-pack" outer packaging may be required. Usual materials for larger containers are carbon steel for 55-gal (0.21 m^3) drums, stainless

steel or aluminum for tank trucks, and carbon steel, lined steel, or aluminum for rail tank cars. The types of tank cars and trucks that can be used are specified by law, and shippers may have particular preferences. Barges and ships are usually steel, but may have special inner or deck-mounted tanks. Increasing in use, especially for international shipments, are intermodal (IM) portable containers, tanks suspended in frameworks suitable for interchanging among truck, rail, and ship modes of transportation.

Containers less than bulk must bear the red diamond-shaped FLAMMABLE LIQUID label. Bulk containers must display the red FLAMMABLE placard in association with the UN1090 identification. Fire is the main hazard in emergencies resulting from spills. Some manufacturers provide transportation emergency response information. A listing of properties and hazard response information for acetone is published by the U.S. Coast Guard in its CHRIS manual (34). Two books on transportation emergencies are available (35). Immediate information can be obtained from CHEMTREC (36). Interested parties may contact their suppliers for more detailed information on transportation and transportation emergencies.

Tank cars contain up to 10, 20, or 30 thousand gal $(10,000 \text{ gal} = 38 \text{ m}^3)$ of material, tank trucks 6000 gal (22.7 m^3), and barges 438,000 gal $(\sim 1270 \text{ tons})$. International shipments by sea are typically ~ 2000 tons.

6. Economic Aspects

The economics of acetone production and its consequent market position are unusual. Traditional laws of supply and demand cannot be applied because supply depends on the production of phenol and demand is controlled by the uses of acetone. Therefore, coproduct acetone from the cumene to phenol process will continue to dominate market supply. Deliberate production of acetone from isopropyl alcohol accommodates demand in excess of that supplied by the phenol process. More than 75% of world and 90% of U.S. production comes from the cumene to phenol process.

Current U.S. and World production data are shown in Tables 5 and 6 (37). Consumption of acetone is expected to grow at a rate of $\sim 3\%$ through 2003 annually, but phenol demand and consequent coproduct acetone production are expected to grow at a rate of 4%, thus resulting in excess supplies. The fastest growing outlet for acetone is for bisphenol A, mainly for growth in polycarbonate. Although bisphenol A production consumes 1 mol of acetone, it yields a net amount of 1 mol of acetone production because 2 mol of acetone accompany the production of the required phenol. Production of "on-purpose" acetone will probably decline as supplies of by-product acetone increase.

In 1998, demand for acetone was 1.26×10^9 kg $(2.78 \times 10^9 \text{ lb})$. Estimated demand for 2003 is 1.46×10^9 kg $(3.22 \times 10^9 \text{ lb})$ (14).

Prices as of 1999, were for the United States, 9.5–10.5 cents/lb (4.3–4.7 cents/kg) fob Gulf Coast; 11 cents/lb (4.9 cents/kg) fob first quarter contract. In Europe, $209–231/metric ton,: $264.50/metric ton; contract. In Asia/Pacific, $270–310/metric ton spot (37).

Table 5. **United States Production of Acetone, 10^3 t**[a]

Company	Production, 10^3 t
Sun	
Frankford, Pa	310
Mount Vernon Phenol[b]	
Mount Vernon, Ind.	197
Aristech	
Haverhill, Ohio	197
Shell Chemical	
Deer Park, Texas	185
Dow Chemical	
Freeport, Texas	176
Georgia Gulf	
Plaquemine, La.	140
Pasadena, Texas	44
Union Carbide	
Institute, W. Va.	77
Texaco[c]	
El Dorado, Kan.	30
JLM Industries	
Blue Island, Ill.	26

[a] As of Feb. 1999, from Ref. 37.
[b] Joint Venture of G.E. Plastics. JLM Marketing and Citgo Group.
[c] Refinery: Output marketed by Plaza Group, Houston.

Table 6. **World Production of Acetone, 10^3 t**[a]

Country	Production, 10^3t
North America	
Canada	16
Mexico	
Fenoquimia	
Cosoleacaque, Veracruz	83
South America	
Argentina	18
Brazil	
Rhodia	
Paulinia	78
Western Europe	
Belgium	
Phenolchemie	
Antwerp	252
Finland	
Borealis Polymers	
Porvoo	78
France	
Rhône-Poulenc	
Roussillon	96
Shell Chimie	
Berre	75
Germany	
Phenolchemie	
Gladbeck	318

Table 6   (*Continued*)

Country	Production, 10^3t
DOMO Group	
Leuna	57
Italy	
EniChem	
Mantova	174
Porto Torres	108
Netherlands	
Shell Nederland	
Rotterdam	80
DSM Chemicals	
Botlek	66
Spain	
Ertisa	
Huelva	96
U.K	
BP Amoco	
Hull	62
Shell Chemicals	
Ellesmere Port	40
Eastern Europe	
Russia	
Salavat	
Salvat	96
Orgesteklo	
Dzerzhinsk	82
Others	322
Middle East	18
South Africa	17
Asia/Pacific	
China	126
India	36
Japan	
Mitsui Toatsu	120
Mitsui Sekka	120
Mitsubishi Kaggaku	108
Korea	
Kumho	132
Taiwan	
Formosa Chemical	221
Taiwan Prosperity Chemical	60

[a] Ref. 37

7. Specifications, Standards, and Quality Control

The ASTM "Standard Specification for ACETONE," D329, requires 99.5% grade acetone to conform to the following: apparent specific gravity 20/20°C, 0.7905–0.7930; 25/25°C, 0.7860–0.7885 (ASTM D891); color, not more than No. 5 on the platinum–cobalt scale (ASTM D1209); distillation range, 1.0°C, which shall include 56.1°C (ASTM D1078); nonvolatile matter, not >5 mg/100 mL (D1353); odor, characteristic, nonresidual (ASTM D1296); water, not >0.5 wt %

(ASTM D1364); acidity (as free acetic acid), <0.002 wt %, equivalent to 0.019 mg of KOH per gram of sample (ASTM D1613); water miscibility, no turbidity or cloudiness at 1:10 dilution with water (ASTM D1722); alkalinity (as ammonia), not >0.001 wt % (ASTM D1614); and permanganate time, color of added $KMnO_4$ must be retained at least 30 min at 25°C in the dark (ASTM D1363).

Higher or lower quality at more or less cost will meet the needs of some consumers. Acetone is often produced under contract to meet customer specifications that are different from those of ASTM D329. Some specialty grades are analyzed reagent, isotopically labeled, clean room, liquid chromatography, spectroscopic, ACS reagent (38), semiconductor (low metals), and Federal Specification O-A-51G.

Specification tests are performed on plant streams once or twice per worker shift, or even more often if necessary, to assure the continuing quality of the product. The tests are also performed on a sample from an outgoing shipment, and a sample of the shipment is usually retained for checking on possible subsequent contamination. Tests on specialty types of acetone may require sophisticated instruments, eg, mass spectrometry for isotopically labeled acetone.

8. Analytical and Test Methods, Storage

In current industrial practice, gas chromatographic analysis (gc) is used for quality control. The impurities, mainly a small amount of water (by Karl–Fischer) and some organic trace constituents (by gc), are determined quantitatively, and the balance to 100% is taken as the acetone content. Compliance to specified ranges of individual impurities can also be assured by this analysis. The gas chromatographic method is accurately correlated to any other tests specified for the assay of acetone in the product. Contract specification tests are performed on the product to be shipped. Typical wet methods for the determination of acetone are acidimetry (39), titration of the liberated hydrochloric acid after treating the acetone with hydroxylamine hydrochloride; and iodimetry (40), titrating the excess of iodine after treating the acetone with iodine and base (iodoform reaction).

Carbon steel tanks of welded construction, as specified in the American Petroleum Institute Standard 650 (41), are recommended for acetone storage. Gaskets should be ethylene–propylene rubber or Viton rubber. An inert gas pad should be used. Provisions should be made to prevent static charge buildup during filling. Design considerations of the National Fire Prevention Association Code 30 and local fire codes should be followed. Tank venting systems should comply with local vapor emission standards and conform with National Fire Prevention Association recommendations. Where the purity of the acetone is to be optimized, an inorganic zinc lining is recommended (42). One such lining is Carbozinc 11, metallic zinc in an ethyl silicate binder, available from Carboline Co., St. Louis, Missouri.

9. Health and Safety Factors

Acetone is among the solvents of comparatively low acute and chronic toxicity. High vapor concentrations produce anesthesia, and such levels may be irritating to the eyes, nose, and throat, and the odor may be disagreeable. Acetone does not

have sufficient warning properties to prevent repeated exposures to concentrations that may cause adverse effects. In industry, no injurious effects have been reported other than skin irritation resulting from its defatting action, or headache from prolonged inhalation (43). Direct contact with the eyes may produce irritation and transient corneal injury.

Material Safety Data Sheets (MSDS) issued by suppliers of acetone are required to be revised within 90 days to include new permissible exposure limits (PEL). Current OSHA PEL is 1000 ppm TWA (44) and ACGIH threshold limit values (TLV) (44) are 500 ppm TWA and 750 ppm STEL. A report on human experience (44) concluded that exposure to 1000 ppm for an 8-h day produced no effects other than slight, transient irritation of the eyes, nose, and throat.

There are many natural sources of acetone including forest fires, volcanoes, and the normal metabolism of vegetation, insects, and higher animals (45). Acetone is a normal constituent of human blood, and it occurs in much higher concentrations in diabetics. Its toxicity appears to be low to most organisms. Acetone is ubiquitous in the environment, but is not environmentally persistent because it is readily biodegraded. In general, acetone is an environmentally benign compound, widely detected but in concentrations that are orders of magnitude below toxicity thresholds.

Acetone can be handled safely if common sense precautions are taken. It should be used in a well-ventilated area, and because of its low flash point, ignition sources should be absent. Flame will travel from an ignition source along vapor flows on floors or bench tops to the point of use. Sinks should be rinsed with water while acetone is being used to clean glassware, to prevent the accumulation of vapors. If prolonged or repeated skin contact with acetone could occur, impermeable protective equipment such as gloves and aprons should be worn.

Compatibility of acetone with other materials should be carefully considered, especially in disposal of wastes. It reacts with chlorinating substances to form toxic chloroketones, and potentially explosively with some peroxy compounds and a number of oxidizing mixtures. Mixed with chloroform, acetone will react violently in the presence of bases. Other incompatibilities are listed in the Sax handbook (43).

Vapor flammability range in air (2.6–12.8 vol %) and low flash point (−18°C, 0°F) make fire the major hazard of acetone. Quantities larger than laboratory hand bottles should be stored in closed metal containers. Gallon glass bottles should be protected against impacts. Areas where acetone is in contact with the ambient air should be free of ignition sources (flames, sparks, static charges, and hot surfaces above the autoignition temperature, ~500–600°C depending on the reference consulted). Fires may be controlled with carbon dioxide or dry chemical extinguishers. Recommended methods of handling, loading, unloading, and storage can be obtained from Material Safety Data Sheets and inquiries directed to suppliers of acetone.

10. Uses

Acetone is used as a solvent and as a reaction intermediate for the production of other compounds that are mainly used as solvents and/or intermediates for

consumer products. Forty five percent is used as acetone cyanohydrin for methyl methacrylate, 20% for bisphenol A, solvent uses, 17% MIBK and MIBC 8%, and miscellaneous 10% (14).

10.1. Direct Solvent Use.   A large volume, direct solvent use of acetone is in formulations for surface coatings and related washes and thinners, mainly for acrylic and nitrocellulose lacquers and paints. It is used as a solvent in the manufacture of pharmaceuticals and cosmetics (∼7000 metric tons in nail polish removers), in spinning cellulose acetate fibers, in gas cylinders to store acetylene safely, in adhesives and contact cements, in various extraction processes, and in the manufacture of smokeless powder. It is a wash solvent in fiberglass boat manufacturing, a cleaning solvent in the electronics industry, and a solvent for degreasing wool and degumming silk.

10.2. Acrylics.   Acetone is converted via the intermediate acetone cyano-hydrin to the monomer methyl methacrylate (MMA) [80-62-6]. The MMA is poly-merized to poly(methyl methacrylate) (PMMA) to make the familiar clear acrylic sheet. PMMA is also used in molding and extrusion powders. Hydrolysis of acet-one cyanohydrin gives methacrylic acid (MAA), a monomer that goes directly into acrylic latexes, carboxylated styrene–butadiene polymers, or ethylene–MAA ionomers. As part of the methacrylic structure, acetone is found in the following major end-use products: acrylic sheet molding resins, impact modifiers and pro-cessing aids, acrylic film, ABS and polyester resin modifiers, surface coatings, acrylic lacquers, emulsion polymers, petroleum chemicals, and various copoly-mers (see METHACRYLIC ACID AND DERIVATIVES; METHACRYLIC POLYMERS).

10.3. Bisphenol A.   One mole of acetone condenses with 2 mol of phenol to form bisphenol A [80-05-07], which is used mainly in the production of poly-carbonate and epoxy resins. Polycarbonates (qv) are high strength plastics used widely in automotive applications and appliances, multilayer containers, and housing applications. Epoxy resins (qv) are used in fiber-reinforced lami-nates, for encapsulating electronic components, and in advanced composites for aircraft–aerospace and automotive applications. Bisphenol A is also used for the production of corrosion- and chemical-resistant polyester resins, polysulfone resins, polyetherimide resins, and polyarylate resins.

10.4. Aldol Chemicals.   The aldol condensation of acetone molecules leads to the group of aldol chemicals that are themselves used mainly as sol-vents. The initial condensation product is diacetone alcohol (DAA), which is dehydrated to mesityl oxide. Because of its toxicity effects, mesityl oxide is no longer produced for sale, but is used captively to make methyl isobutyl ketone (MIBK) and methylisobutylcarbinol (MIBC) by hydrogenation. DAA is hydro-genated to hexylene glycol. Three molecules of acetone give isophorone and phorone, which is hydrogenated todiisobutyl ketone (DIBK) [108-83-8] and diiso-butylcarbinol (DIBC) [108-82-7].

MIBK is a coatings solvent for nitrocellulose lacquers and vinyl and acrylic polymer coatings, an intermediate for rubber antioxidants and specialty surfac-tants, and a solvent for the extraction of antibiotics. MIBC is used mainly for the production of zinc dialkyl dithiophosphates, which are used as lubricating oil additives. It is a flotation agent for minerals and a solvent for coatings. Besides its use as a chemical intermediate, DAA is used as a solvent for nitrocellulose, cellulose acetate, oils, resins, and waxes, and in metal cleaning compounds.

Hexylene glycol is a component in brake fluids and printing inks. Isophorone is a solvent for industrial coatings and enamels. DIBK is used in coatings and leather finishes.

10.5. Other Uses. More than 70 thousand metric tons of acetone is used in small volume applications some of which are to make functional compounds such as antioxidants, herbicides, higher ketones, condensates with formaldehyde or diphenylamine, and vitamin intermediates.

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