Acetone

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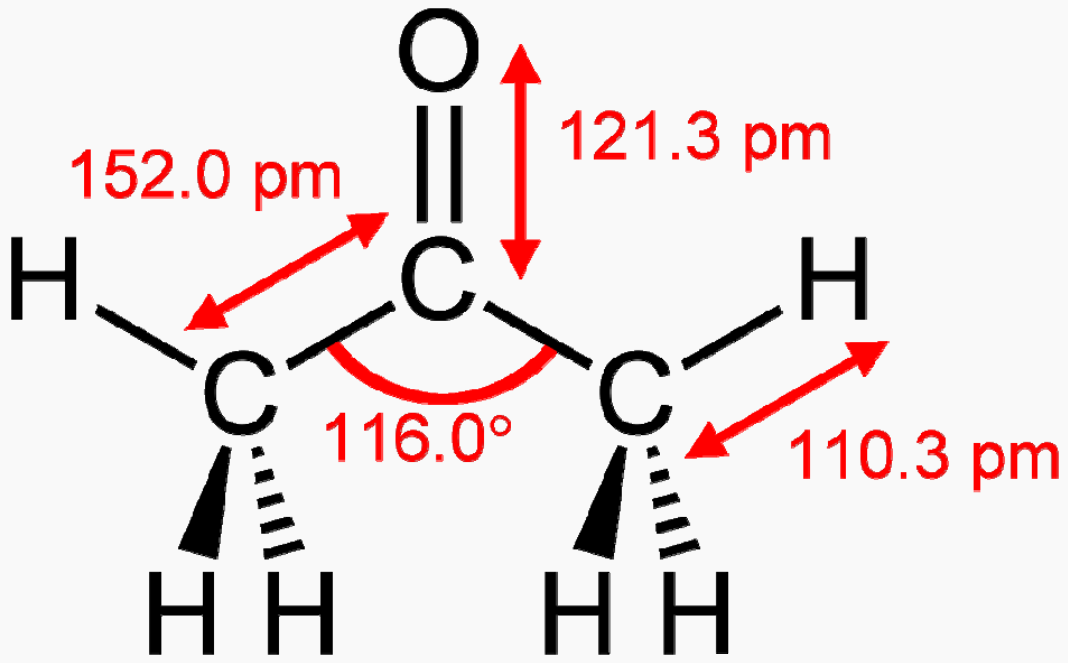	
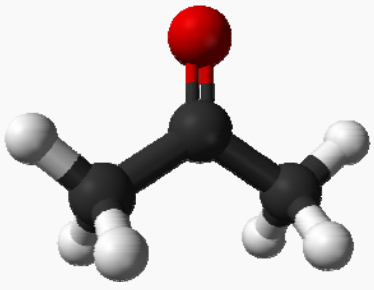	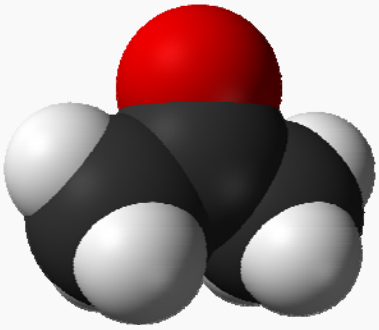
[IUPAC name](#)	propanone

Other names	β-ketopropane, dimethyl ketone, dimethylformaldehyde, DMK, propanone, 2-propanone, propan-2-one, β-ketopropane
Identifiers	
CAS number	**[67-64-1]**
RTECS number	AL31500000
SMILES	`CC(=O)C`
InChI	1/C3H6O/c1-3(2)4/h1-2H3
ChemSpider ID	175
Properties	
Molecular formula	C_3H_6O
Molar mass	58.08 g mol^{-1}
Appearance	Colorless liquid
Density	0.79 g/cm^3
Melting point	–94.9 °C, 178 K, -139 °F
Boiling point	56.53 °C, 330 K, 134 °F
Solubility in water	miscible
Acidity (pK_a)	24.2
Refractive index (n_D)	1.359 (20 °C)
Viscosity	0.32 cP (20 °C)
Structure	

Molecular shape	trigonal planar at C=O
Dipole moment	2.91 D
Hazards	
MSDS	External MSDS
R-phrases	R11, R36, R66, R67
S-phrases	(S2), S9, S16, S26
Flash point	-17 °C
Autoignition temperature	465 °C
Explosive limits	4.0–57.0
LD_{50}	>2000 mg/kg, oral (rat)
Related compounds	
Related solvents	Water Ethanol Isopropanol Toluene
Supplementary data page	
Structure and properties	*n*, ε_r, etc.
Thermodynamic data	Phase behaviour Solid, liquid, gas
Spectral data	UV, IR, NMR, MS
Except where noted otherwise, data are given for materials in their standard state (at 25 °C, 100 kPa)	

Acetone is the organic compound with the formula $OC(CH_3)_2$. This colorless, mobile, flammable liquid is the simplest example of the ketones. Owing to the fact that acetone is miscible with water, and virtually all organic solvents, it serves as an important solvent in its own right, typically the solvent of choice for cleaning purposes in the laboratory. More than 3 billion kilograms are produced annually, mainly as a precursor to polymers.[2] Familiar household uses of acetone are as the active ingredient in nail polish remover and as paint thinner and sanitary cleaner/ nail polish remover base. It is a common building block in organic chemistry. In addition to being manufactured, acetone also occurs naturally, even being biosynthesized in small amounts in the human body.

Production

Acetone is produced directly or indirectly from propene. Most commonly, in the cumene process, benzene is alkylated with propene and the resulting cumene (isopropylbenzene) is oxidized to give phenol and acetone:

$$C_6H_5CH(CH_3)_2 + O_2 \rightarrow C_6H_5OH + OC(CH_3)_2$$

This conversion entails the intermediacy of cumene hydroperoxide, $C_6H_5C(OOH)(CH_3)_2$.

Acetone is also produced by the direct oxidation of propene with a Pd(II)/Cu(II) catalysts, akin to the Wacker process.

Older production methods

Previously, acetone was produced by the dry distillation of acetates, for example calcium acetate. During World War I acetone was produced via bacterial fermentation, as developed by Chaim Weizmann (later the first president of Israel) in order to help the British war effort.[2] This Acetone Butanol Ethanol process was abandoned due to the small yields.[2]

Biosynthesis

See also: ketosis

Small amounts of acetone are produced in the body by the decarboxylation of ketone bodies.

Uses

About half of the world's production of acetone is consumed as a precursor to methyl methacrylate. This application begins with the initial conversion of acetone to its cyanohydrin:

$$(CH_3)_2CO + HCN \rightarrow (CH_3)_2C(OH)CN$$

In a subsequent step, the nitrile is hydrolyzed to the unsaturated amide, which is esterified:

$$(CH_3)_2C(OH)CN + CH_3OH \rightarrow CH_2{=}(CH_3)CCO_2CH_3 + NH_3$$

The second major use of acetone entails its condensation with phenol to give bisphenol A:

$$(CH_3)_2CO + 2\ C_6H_5OH \rightarrow (CH_3)_2C(C_6H_4OH)_2 + H_2O$$

Bisphenol-A is a component of many polymers such as polycarbonates, polyurethanes, and epoxy resins.

Combustion

$(CH_3)_2CO + 4O_2 \rightarrow 3CO_2 + 3H_2O$

As a solvent

Acetone is a good solvent for most plastics and synthetic fibres including those used in Nalgene bottles made of polystyrene, polycarbonate and some types of polypropylene.[3]. It is ideal for thinning fiberglass resin, cleaning fiberglass tools and dissolving two-part epoxies and superglue before hardening. It is used as a volatile component of some paints and varnishes. As a heavy-duty degreaser, it is useful in the preparation of metal prior to painting; it also thins polyester resins, vinyl and adhesives.

Many millions of kilograms of acetone are consumed in the production of the solvents methyl isobutyl alcohol and methyl isobutyl ketone. These products arise via an initial aldol condensation to give diacetone alcohol.[2]

$$2\ (CH_3)_2CO \rightarrow (CH_3)_2C(OH)CH_2C(O)CH_3$$

Acetone is used as a solvent by the pharmaceutical industry and as a denaturation agent in denatured alcohol.[4] Acetone is also present as an excipient in some pharmaceutical products.[5]

Storage of acetylene

Although flammable itself, acetone is also used extensively as a solvent for the safe transporting and storing of acetylene, which cannot be safely pressurized as a pure compound. Vessels containing a porous material are first filled with acetone followed by acetylene, which dissolves into the acetone. One liter of acetone can dissolve around 250 liters of acetylene.[6][7]

Laboratory uses

In the laboratory, acetone is used as a polar aprotic solvent in a variety of organic reactions, such as S_N2 reactions. The use of acetone solvent is also critical for the Jones oxidation. It is a common solvent for rinsing laboratory glassware because of its low cost, volatility, and ability to dissolve water. For similar reasons, acetone is also used as a drying agent. Acetone can be cooled with dry ice to -78 °C without freezing; acetone/dry ice baths are commonly used to conduct reactions at low temperatures. Acetone is fluorescent under ultraviolet light, and acetone vapor may be used as a fluorescent tracer in fluid flow experiments.[8]

Domestic and other niche uses

Acetone is often the primary component in cleaning agents such as nail polish remover. Ethyl acetate, another organic solvent, is sometimes used as well. Acetone is a component of superglue remover and it easily removes residues from glass and porcelain.

It can be used as an artistic agent; when rubbed on the back of a laser print or photocopy placed face-down on another surface and burnished firmly, the toner of the image is allowed to transfer to the destination surface.

Some automotive enthusiasts add acetone at around 1 part in 500 to their fuel, following claims of dramatic improvement in fuel economy and engine life.[9] This practice is controversial as the body of systematic testing shows that acetone has no measurable effect or may in fact reduce engine life by adversely affecting fuel system parts.[10][11] Debates on this subject and the perennial claims of a "Big Oil" cover-up intensified when the practice was addressed on the popular American TV show MythBusters in 2006, and shown to have negative effect in the televised fuel economy test.[12]

Safety

Flammability

The most common hazard associated with acetone is its extreme flammability. It auto-ignites at a temperature of 465 °C (869 °F). At temperatures greater than acetone's flash point of −20 °C (−4 °F), air mixtures of between 2.5% and 12.8% acetone, by volume, may explode or cause a flash fire. Vapors can flow along surfaces to distant ignition sources and flash back. Static discharge may also ignite acetone vapors.[13]

Acetone peroxide

Main article: acetone peroxide

When oxidized, acetone forms acetone peroxide as a byproduct, which is a highly unstable compound. It may be formed accidentally, e.g. when waste hydrogen peroxide is poured into waste solvent containing acetone. Acetone peroxide is more than ten times as friction and shock sensitive as nitroglycerin. Due to its instability, it is rarely used, despite its easy chemical synthesis.

Toxicology

Acetone is believed to exhibit only slight toxicity in normal use, and there is no strong evidence of chronic health effects if basic precautions are followed.[14]

At very high vapor concentrations, acetone is irritating and, like many other solvents, may depress the central nervous system. It is also a severe irritant on contact with eyes, and a potential pulmonary aspiration risk. In one documented case, ingestion of a substantial amount of acetone led to systemic toxicity, although the patient eventually

fully recovered.[15] Some sources estimate LD_{50} for human ingestion at 1.159 g/kg; LD_{50} inhalation by mice is given as 44 g per cubic meter, over 4 hours.[16]

Interestingly, acetone has been shown to have anticonvulsant effects in animal models of epilepsy, in the absence of toxicity, when administered in millimolar concentrations.[17] It has been hypothesized that the high-fat low-carbohydrate ketogenic diet used clinically to control drug-resistant epilepsy in children works by elevating acetone in the brain.[17]

Environmental effects

Acetone evaporates rapidly, even from water and soil. Once in the atmosphere, it is degraded by UV light with a 22-day half-life. Acetone dissipates slowly in soil, animals, or waterways since it is sometimes consumed by microorganisms;[18] however, it is a significant issue with respect to groundwater contamination due to its high solubility in water. The LD_{50} of acetone for fish is 8.3 g/l of water (or about 0.8%) over 96 hours, and its environmental half-life is about 1 to 10 days. Acetone may pose a significant risk of oxygen depletion in aquatic systems due to the microbial activity consuming it.[19]

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External links

- International Chemical Safety Card 0087
- National Pollutant Inventory: Acetone
- NIOSH Pocket Guide to Chemical Hazards
- Calculation of vapor pressure, liquid density, dynamic liquid viscosity, surface tension of acetone
- Hazardous substances databank entry at the national library of medicine

v · d · e

Cholesterol and steroid metabolic intermediates

Mevalonate pathway	**to HMG-CoA**	Acetyl-CoA · Acetoacetyl-CoA · HMG-CoA
	Ketone bodies	**Acetone** · Acetoacetic acid · beta-Hydroxybutyric acid
	to DMAPP	Mevalonic acid · Phosphomevalonic acid · 5-Diphosphomevalonic acid · Isopentenyl pyrophosphate · Dimethylallyl pyrophosphate
	Geranyl-	Geranyl pyrophosphate · Geranylgeranyl pyrophosphate
	Carotenoid	Prephytoene diphosphate · Phytoene
Non-mevalonate pathway		DOXP · MEP · CDP-ME · CDP-MEP · MEcPP · HMB-PP · IPP · DMAPP
To Cholesterol		Farnesyl pyrophosphate · Squalene · 2,3-Oxidosqualene · Lanosterol
		Lanosterol · Lathosterol · 7-Dehydrocholesterol · Cholesterol
		Lanosterol · Zymosterol · 7-Dehydrodesmosterol · Desmosterol · Cholesterol
Steroid	**Corticosteroids (C21 pregnane)**	**Mineralocorticoids** Pregnenolone ·

			Progesterone · 11-Deoxycorticosterone · Corticosterone · Aldosterone
		Glucocorticoids	Pregnenolone · 17-Hydroxypregnenolone · 17-Hydroxyprogesterone · 11-Deoxycortisol · Cortisol
			Cortisol · Cortisone
	Sex steroids	**Androgens** (C19 andrane)	DHEA · Androstenedione/5-Androstenediol · Testosterone · Dihydrotestosterone
			DHEA sulfate · Epitestosterone
		Estrogens (C18 estrane)	Estrone · Estradiol · Estriol
Nonhuman	**Phytosterols**		Stigmasterol · Brassicasterol
	Ergosterols		Ergosterol · Ergocalciferol

see also enzymes, disorders

Major families of biochemicals

Saccharides/Carbohydrates/Glycosides · Amino acids/Peptides/Proteins/Glycoproteins · Lipids/Terpenes/Steroids/Carotenoids · Alkaloids/Nucleobases/Nucleic acids · Cofactors/Flavonoids/Polyketides/Tetrapyrroles