Methyl acetate Usage And Synthesis

Description	Methyl acetate, also known as MeOAc , acetic acid methyl ester or methyl ethanoate, is a carboxylate ester with the formula CH3COOCH3. It is a flammable liquid with a characteristically pleasant smell reminiscent of some glues and nail polish removers. Methyl acetate is occasionally used as a solvent, being weakly polar and lipophilic, but its close relative ethyl acetate is a more common solvent being less toxic and less soluble in water. Methyl acetate has a solubility of 25% in water at room temperature. At elevated temperature its solubility in water is much higher. Methyl acetate is not stable in the presence of strong aqueous bases or aqueous acids. Methyl acetate is VOC exempt.
Chemical Properties	Methyl acetate has a pleasant, fruity odor and slightly bitter flavor. May be prepared by boiling acetic acid and methanol in the presence of acid catalysts; or by heating methanol with an excess carbon monoxide under pressure in the presence of a catalyst (phosphoric acid, cobalt salts). Methyl acetate occurs naturally in low concentrations in mint, fungus,grapes, banana, coffee (Furia and Bellanca, 1975) and is a volatile constituent of nectarines (Takeoka et al., 1988). It is also present in some distilled alcoholic beverages (Shimoda et al., 1993). It is produced industrially via the carbonylation of methanol as a byproduct of acetic acid production or by esterification of acetic acid with methanol in the presence of strong acid such as sulfuric acid.
Chemical Properties	Methyl acetate has a pleasant, fruity odor and slightly bitter flavor.
Physical properties	Colorless liquid with a pleasant odor. An odor threshold concentration of 48 ppb_v was reported by Nagata and Takeuchi (1990). Cometto-Mu?iz and Cain (1991) reported an average nasal pungency threshold concentration of 112,500 ppm_v.
Occurrence	Reported found in apple, banana, sweet and sour cherry, tangerine juice, black currants, guava, grapes, melon, peach, pear, pineapple, strawberry, cabbage, tomato, clove bud, peppermint oil, vinegar, bread, cheeses, butter, yogurt, beef, beer, cognac, rum, whiskies, cider, sherry, grape wines, cocoa, coffee, filbert, peanut, honey, soybean, olive, passion fruit, fruit brandies, fig, gin, kiwifruit, clary sage, arrack and nectarine.
Uses	Methyl acetate is used as a solvent forlacquers, resins, oils, and nitrocellulose; inpaint removers; as a flavoring agent; and inthe manufacture of artificial leather.
Uses	Solvent for lacquers, oils, and resins
Uses	Solvent for nitrocellulose, acetylcellulose, and many resins and oils; manufacture of artificial leather.

Preparation	Methyl acetate is produced industrially via the carbonylation of methanol as a byproduct of the production of acetic acid.Methyl acetate also arises by esterification of acetic acid with methanol in the presence of strong acids such as sulfuric acid, this production process is famous because of Eastman Kodak's intensified process using a reactive distillation. **2–1-Reactions** In the presence of strong bases such as sodium hydroxide or strong acids such as hydrochloric acid or sulfuric acid it is hydrolyzed back into methanol and acetic acid, especially at elevated temperature. The conversion of methyl acetate back into its components, by an acid , is a first-order reaction with respect to the ester. The reaction of methyl acetate and a base, for example sodium hydroxide, is a second-order reaction with respect to both reactants. **3-Applications** A major use of methyl acetate is as a volatile low toxicity solvent in glues, paints, and nail polish removers. Acetic anhydride is produced by carbonylation of methyl acetate in a process that was inspired by the Monsanto acetic acid synthesis.
Aroma threshold values	Detection: 1.5 to 47 ppm
Taste threshold values	Taste characteristics at 60 ppm: green, ethereal, fruity, fresh, rum and whiskey-like.
General Description	A clear colorless liquid with a fragrant odor. Moderately toxic. Flash point 14°F. Vapors heavier than air.
Air & Water Reactions	Highly flammable. Water soluble.
Reactivity Profile	Methyl acetate presents a fire or explosion hazard when exposed to strong oxidizing agents. Emits irritating fumes and acrid smoke when heated to decomposition, [Lewis, 3rd ed., 1993, p. 826]. Methyl acetate reactivity is consistent with other compounds of the ester group.
Hazard	Flammable, dangerous fire and explosion risk, explosive limits in air 3–16%. Irritant to respiratory tract. Headache, dizziness, nausea, eye damage (degeneration of ganglion cells in the retina).
Health Hazard	(Very similar to those of methyl alcohol, which constitutes 20% of commercial grade.) Inhalation causes headache, fatigue, and drowsiness; high concentrations can produce central nervous system depression and optic nerve damage. Liquid irritates eyes and may cause defatting and cracking of skin. Ingestion causes headache, dizziness, drowsiness, fatigue; may cause severe eye damage.
Health Hazard	The toxic effects from exposure to methylacetate include inflammation of the eyesvisual and nervous disturbances, tightnessof the chest, drowsiness, and narcosis. Ithydrolyzes in body to methanol, which

	prob ably produces the atrophy of the optic nerve.A 4-hour exposur e to 32,000 ppm was lethalto rats. Oral and dermal toxicities of this compound are low. An oral LD50 value inrats is on the order of 50 00 mg/kg.
Fire Hazard	Behavior in Fire: Vapor is heavier than air and may travel a consid erable distance to a source of ignition and flash back.
Chemical Reactivity	Reactivity with Water Reacts slowly to form acetic acid and methyl alcohol; the reaction is not violent; Reactivity with Common Material s: No reaction; Stability During Transport: Stable; Neutralizing Agent s for Acids and Caustics: Not pertinent; Polymerization: Not pertinen t; Inhibitor of Polymerization: Not pertinent.
Safety Profile	Moderately toxic by several routes. A human systemic irritant by inh alation. A moderate skin and eye irritant. Mutation data reported. Da ngerous fire hazard when exposed to heat, flame, or oxidizers. Mod erate explosion hazard when exposed to heat or flame. When heate d to decomposition it emits acrid smoke and fumes. See also ESTE RS.
Chemical Synthesis	By boiling acetic acid and methanol in the presence of acid catalyst s, or by heating methanol with an excess of carbon monoxide unde r pressure in the presence of a catalyst (phosphoric acid, cobalt salt s).
Potential Exposure	Methyl acetate is used as a solvent in lacquers and paint removers; and as an intermediate in pharmaceutical manufacture.
Environmental fate	*Photolytic.* A rate constant of 2.00 x 10^{-13} cm^3/molecule?sec was rep orted for the reaction of methyl acetate and OH radicals in aqueous solution (Wallington et al., 1988b). *Chemical/Physical.* Slowly hydrolyzes in water yielding methyl alcohol and acetic acid (NIOSH, 1997). The estimated hydrolysis half-life in water at 25 °C and pH 7 is 2.5 yr (Mabey and Mill, 1978). At an influent concentration of 1,030 mg/L, treatment with GAC resu lted in an effluent concentration of 760 mg/L. The adsorbability of th e carbon used was 54 mg/g carbon (Guisti et al., 1974).
Shipping	UN1231 Methyl acetate, Hazard Class: 3; Labels: 3-Flammable liqui d.
Purification Methods	Methanol in methyl acetate can be detected by measuring its solubil ity in water. At 20o, the solubility of methyl acetate in water is ca 3 5g per 100mL, but 1% MeOH confers complete miscibility. Methanol can be removed by conversion to methyl acetate, by refluxing for 6hours with acetic anhydride (85mL/L), followed by fractional distillati on. Acidic impurities can be removed by shaking with anhydrous K2 CO3 and distilling. An alternative treatment is with acetyl chloride, fo llowed by washing with concentrated NaCl and drying with CaO or

	MgSO4. (Solid CaCl2 cannot be used because it forms a crystalline addition compound.) Distillation from copper stearate destroys peroxides. Free alcohol or acid can be eliminated from methyl acetate by shaking with strong aqueous Na2CO3 or K2CO3 (three times), then with aqueous 50% CaCl2 (three times), saturated aqueous NaCl (twice), drying with K2CO3 and distilling it from P2O5. [Beilstein 2 IV 122.]
Incompatibilities	Vapor may form explosive mixture with air. A Strong reducing agent. Incompatible water, acids, nitrates, strong oxidizers; alkalis. Attacks some plastics. Attacks many metals in presence of water. Reacts slowly with water, forming acetic acid and methanol. Decomposes in heat; on contact with air, bases, strong oxidizers; UV-light; possible fire and explosion hazard
Waste Disposal	Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. All federal, state, and local environmental regulations must be observed.

Methyl acetate Preparation Products And Raw materials

Raw materials	Methanol-->Acetic acid-->Dehydrolyzing agent
Preparation Products	METHYL 3-(2,2-DICHLOROVINYL)-2,2-DIMETHYL-(1-CYCLOPROPANE) CARBOXYLATE-->ethyl 3-(2,2-dichlorovinyl)-2,2-dimethyl-1-cyclopropanecarboxylate-->methyl(±)cis，trans-2，2-dimethyl-3-(2-methyl-1-propenyl cyclopropane carboxylate)-->Ethyl chrysanthemumate-->Sulindac-->Misoprostol-->Lornoxicam-->Benalaxyl-->Clopidogrel-->METHYL 3-(THIEN-2-YL)ACRYLATE-->dimethyl trans，trans-chrysanthemumdicarboxylate-->Methyl nicotinoylacetate