A

Acetic Acid Glacial **Monograph Number:** 56 **CAS Registry Number:** 64-19-7 **Trademarks:** Aci-Jel (Ortho) **Molecular Formula:** $C_2H_4O_2$ **Molecular Weight:** 60.05. **Percent Composition:** C 40.00%, H 6.71%, O 53.29% **Line Formula:** CH_3COOH **Literature References:** Obtained in the destructive distillation of wood; from acetylene and water, via acetaldehyde by oxidation with air. Manuf processes: Bhattacharyya, Sourirajan, *J. Appl. Chem. (London)* **6,** 442 (1956); *eidem, ibid.* **9,** 126 (1959); Elce *et al.,* **US 2800504** (1957 to Distillers Co.); Wirth, **US 2818428** (1957 to British Petroleum); McKusick and Hoover, **US 2940913** and **US 2940914** (both 1960 to Du Pont); *Faith, Keyes & Clark's Industrial Chemicals,* F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 8-15. Toxicity data: H. F. Smyth *et al., Arch. Ind. Hyg. Occup. Med.* **4,** 119 (1951). *Review:* F. S. Wagner in *Kirk-Othmer Encyclopedia of Chemical Technology* **vol. 1** (Wiley-Interscience, New York, 3rd ed., 1978) pp 124-147. **Properties:** Liquid; pungent odor. *Produces burns of the skin!* $d^{16.67}$ (liq) 1.053; $d^{16.60}$ (solid) 1.266. d_{25}^{25} 1.049. bp 118°. mp 16.7°. n_D^{20} 1.3718. Flash pt, closed cup: 103°F (39°C). *Caution: Flammable!* Contracts slightly on freezing. It is an excellent solvent for many organic compounds; also dissolves phosphorus, sulfur and halogen acids. Miscible with water, alcohol, glycerol, ether, carbon tetrachloride. Practically insol in carbon disulfide. Weakly ionized in aq solns: pKa 4.74. pH of aq solns 1.0*M* = 2.4; 0.1*M* = 2.9; 0.01*M* = 3.4. LD_{50} in rats (g/kg): 3.53 orally (Smyth). **Melting point:** mp 16.7° **Boiling point:** bp 118° **Flash point:** Flash pt, closed cup: 103°F (39°C) **pKa:** pKa 4.74 **Index of refraction:** n_D^{20} 1.3718 **Density:** $d^{16.67}$ (liq) 1.053; $d^{16.60}$ (solid) 1.266; d_{25}^{25} 1.049 **Toxicity data:** LD_{50} in rats (g/kg): 3.53 orally (Smyth) **NOTE:** *Incompat.* Carbonates, hydroxides, many oxides, and phosphates, etc. **CAUTION:** Ingestion may cause severe corrosion of mouth and G.I. tract, with vomiting, hematemesis, diarrhea, circulatory collapse, uremia, death. Chronic exposure may cause erosion of dental enamel, bronchitis, eye irritation, *cf. Patty's Industrial Hygiene and Toxicology* **vol. 2C,** G. D. Clayton, F. E. Clayton, Eds. (Wiley-Interscience, New York, 3rd ed., 1982) p 4909-4911. **Use:** Manuf various acetates, acetyl compounds, cellulose acetate, acetate rayon, plastics and rubber in tanning; as laundry sour; printing calico and dyeing silk; as acidulant and preservative in foods; solvent for gums, resins, volatile oils and many other substances. Widely used in commercial organic syntheses. Pharmaceutic aid (acidifier). **Therap-Cat-Vet:** Vesicant, caustic, destruction of warts.

B

Benzamide **Monograph Number:** 1059 **CAS Registry Number:** 55-21-0 **Additional Names:** Benzoylamide **Molecular Formula:** C_7H_7NO **Molecular Weight:** 121.14. **Percent Composition:** C 69.40%, H 5.82%, N 11.56%, O 13.21% **Line Formula:** $C_6H_5CONH_2$ **Literature References:** Prepd from benzoyl chloride and ammonium carbonate. Lab prepn: Gattermann-Wieland, *Praxis des organischen Chemikers* (de Gruyter, Berlin, 40th ed., 1961) p 119. Alternate procedure using concd ammonia soln: A. I. Vogel, *Practical Organic Chemistry* (Longmans, London, 3rd ed., 1959) p 797. **Properties:** Crystals. d^4 1.341. mp 130°. bp 288°. One gram dissolves in 74 ml water, more sol in boiling water, in 6 ml alc, 3.3 ml pyridine. Sol in hot benzene, slightly in ether; sol in ammonia with formation of a small quantity of benzonitrile. **Melting point:** mp 130° **Boiling point:** bp 288° **Density:** d^4 1.341 **Derivative Type:** *N*-Chloro deriv. **Properties:** mp 116°. Sol in water; insol in alcohol or benzene. **Melting point:** mp 116°

Benzoic Acid **Monograph Number:** 1092 **CAS Registry Number:** 65-85-0 **Additional Names:** Benzenecarboxylic acid; phenylformic acid; dracylic acid **Molecular Formula:** $C_7H_6O_2$ **Molecular Weight:** 122.12. **Percent Composition:** C 68.85%, H 4.95%, O 26.20% **Literature References:** Occurs in nature in free and combined forms. Gum benzoin may contain as much as 20%. Most berries contain appreciable amounts (around 0.05%). Excreted mainly as hippuric acid by almost all vertebrates, except fowl. Mfg processes include the air oxidation of toluene, the hydrolysis of benzotrichloride, and the decarboxylation of phthalic anhydride: *Faith, Keyes & Clark's Industrial Chemicals,* F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 138-144. Lab prepn from benzyl chloride: A. I. Vogel, *Practical Organic Chemistry* (Longmans, London, 3rd ed, 1959) p 755; from benzaldehyde: Gattermann-Wieland, *Praxis des organischen Chemikers* (de Gruyter, Berlin, 40th ed, 1961) p 193. Prepn of ultra-pure benzoic acid for use as titrimetric and calorimetric standard: Schwab, Wicher, *J. Res. Nat. Bur. Standards* **25,** 747 (1940). *Review:* A. E. Williams in *Kirk-Othmer Encyclopedia of Chemical Technology* **vol. 3** (Wiley-Interscience, New York, 3rd ed., 1978) pp 778-792. **Properties:** Monoclinic tablets, plates, leaflets. d 1.321 (also reported as 1.266). mp 122.4°. Begins to sublime at ~100°. bp_{760} 249.2°; bp_{400} 227°; bp_{200} 205.8°; bp_{100} 186.2°; bp_{60} 172.8°; bp_{40} 162.6°; bp_{20} 146.7°; bp_{10} 132.1°. Volatile with steam. Flash pt 121°C. pK (25°) 4.19. pH of satd soln at 25°: 2.8. Soly in water (g/l) at 0° = 1.7; at 10° = 2.1; at 20° = 2.9; at 25° = 3.4; at 30° = 4.2; at 40° = 6.0; at 50° = 9.5; at 60° = 12.0; at 70° = 17.7; at 80° = 27.5; at 90° = 45.5; at 95° = 68.0. Mixtures of excess benzoic acid and water form two liquid phases beginning at 89.7°. The two liquid phases unite at the critical soln temp of 117.2°. Composition of critical mixture: 32.34% benzoic acid, 67.66% water: *see* Ward, Cooper, *J. Phys. Chem.* **34,** 1484 (1930). One gram dissolves in 2.3 ml cold alc, 1.5 ml boiling alc, 4.5 ml chloroform, 3 ml ether, 3 ml acetone, 30 ml carbon tetrachloride, 10 ml benzene, 30 ml carbon disulfide, 23 ml oil of turpentine; also sol in volatile and fixed oils, slightly in petr ether. The soly in water is increased by alkaline substances, such as borax or trisodium phosphate, *see also* Sodium Benzoate. **Melting point:** mp 122.4° **Boiling point:** bp_{760} 249.2°; bp_{400} 227°; bp_{200} 205.8°; bp_{100} 186.2°; bp_{60} 172.8°; bp_{40} 162.6°; bp_{20} 146.7°; bp_{10} 132.1° **Flash point:** Flash pt 121°C **pKa:** pK (25°) 4.19 **Density:** d 1.321 (also reported as 1.266) **Derivative Type:** Barium salt dihydrate **Additional Names:** Barium benzoate **Molecular Formula:** $C_{14}H_{10}BaO_4.2H_2O$ **Molecular Weight:** 415.59. **Percent Composition:** C 40.46%, H 3.40%, Ba 33.04%, O 23.10% **Properties:** Nacreous leaflets. *Poisonous!* Soluble in about 20 parts water; slightly sol in alc. **Derivative Type:** Calcium salt trihydrate **Additional Names:** Calcium benzoate **Molecular Formula:** $C_{14}H_{10}CaO_4.3H_2O$ **Molecular Weight:** 336.35. **Percent Composition:** C 49.99%, H 4.80%, Ca 11.92%, O 33.30% **Properties:** Orthorhombic crystals or powder. d 1.44. Soluble in 25 parts water; very sol in boiling water. **Density:** d 1.44 **Derivative Type:** Cerium salt trihydrate **Additional Names:** Cerous benzoate **Molecular Formula:** $C_{21}H_{15}CeO_6.3H_2O$ **Molecular Weight:** 557.51. **Percent Composition:** C 45.24%, H 3.80%, Ce 25.13%, O 25.83% **Properties:** White to reddish-white powder. Sol in hot water or hot alc. **Derivative Type:** Copper salt dihydrate **Additional Names:** Cupric benzoate **Molecular Formula:** $C_{14}H_{10}CuO_4.2H_2O$ **Molecular Weight:** 341.81. **Percent Composition:** C 49.20%, H 4.13%, Cu 18.59%, O 28.08% **Properties:** Light blue, cryst powder. Slightly soluble in cold water, more in hot water; sol in alc or in dil acids with separation of benzoic acid. **Derivative Type:** Lead salt dihydrate **Additional Names:** Lead benzoate **Molecular Formula:** $C_{14}H_{10}O_4Pb.2H_2O$ **Molecular Weight:** 485.20. **Percent Composition:** C 34.62%, H 2.89%, O 19.79%, Pb 42.70% **Properties:** Cryst powder. *Poisonous!* Slightly sol in water. **Derivative Type:** Manganese salt tetrahydrate **Additional Names:** Manganese benzoate **Molecular Formula:** $C_{14}H_{10}MnO_4.4H_2O$ **Molecular Weight:** 369.23. **Percent Composition:** C 45.54%, H 4.91%, Mn 14.88%, O 34.67% **Properties:** Pale-red powder. Sol in water, alc. Also occurs with $3H_2O$. **Derivative Type:** Nickel salt trihydrate **Additional Names:** Nickel benzoate **Molecular Formula:** $C_{14}H_{10}NiO_4.3H_2O$ **Molecular Weight:** 354.97. **Percent Composition:** C 47.37%, H 4.54%, Ni 16.53%, O 31.55% **Properties:** Light-green odorless powder. Slightly sol in water; sol in ammonia; dec by acids. **Derivative Type:** Potassium salt trihydrate **Additional Names:** Potassium benzoate **Molecular Formula:** $C_7H_5KO_2.3H_2O$ **Molecular Weight:** 214.26. **Percent Composition:** C 39.24%, H 5.17%, K 18.25%, O 37.34% **Properties:** Crystalline powder. Sol in water, alc. **Derivative Type:** Silver salt **Additional Names:** Silver benzoate **Molecular Formula:** $C_7H_5AgO_2$ **Molecular Weight:** 228.98. **Percent Composition:** C 36.72%, H 2.20%, Ag 47.11%, O 13.97% **Properties:** Light-sensitive powder. Sol in 385 parts cold water, more sol in hot water; very slightly sol in alc. **Derivative Type:** Uranium salt **Additional Names:** Uranium benzoate; uranyl benzoate **Molecular Formula:** $C_{14}H_{10}O_6U$ **Molecular Weight:** 512.25. **Percent Composition:** C 32.83%, H 1.97%, O 18.74%, U 46.47% **Properties:** Yellow powder. Slightly sol in water, alc. **CAUTION:** Mild irritant to skin, eyes, mucous membranes. **Use:** Preserving foods, fats, fruit juices, alkaloidal solns, etc; manuf benzoates and benzoyl compds, dyes; as a mordant in calico printing; for curing tobacco. As standard in volumetric and calorimetric analysis. Pharmaceutic aid (antifungal). **Therap-Cat-Vet:** Has been used with salicylic acid as a topical antifungal.

Benzonitrile **Monograph Number:** 1098 **CAS Registry Number:** 100-47-0 **Additional Names:** Phenyl cyanide; cyanobenzene **Molecular Formula:** C_7H_5N **Molecular Weight:** 103.12. **Percent Composition:** C 81.53%, H 4.89%, N 13.58% **Line Formula:** C_6H_5CN **Literature References:** Prepd by heating Na benzenesulfonate with NaCN or by adding benzenediazonium chloride soln to a hot aq NaCN soln contg $CuSO_4$ and distilling. Lab prepn: A. I. Vogel, *Practical Organic Chemistry* (Longmans, London, 3rd ed, 1959) p 608. **Properties:** Liquid, odor of volatile oil of almond. bp_{760} 190.7°, bp_{100} 123.5°, bp_{10} 69.2°, bp_1 28.2°. mp -12.75°. d_{15}^{15} 1.010. n_D^{20} 1.5289. Fire pt 167°F. Slightly sol in cold water; sol to the extent of 1% in water at 100°; miscible with common organic solvents. **Melting point:** mp -12.75° **Boiling point:** bp_{760} 190.7°; bp_{100} 123.5°; bp_{10} 69.2°; bp_1 28.2° **Index of refraction:** n_D^{20} 1.5289 **Density:** d_{15}^{15} 1.010 **Use:** Solvent.

n-Butyl Acetate **Monograph Number:** 1534 **CAS Registry Number:** 123-86-4 **CAS Name:** Acetic acid butyl ester **Molecular Formula:** $C_6H_{12}O_2$ **Molecular Weight:** 116.16. **Percent Composition:** C 62.04%, H 10.41%, O 27.55% **Line Formula:** $CH_3COO(CH_2)_3CH_3$ **Literature References:** Prepd from acetic acid and butyl alcohol: Leyes, Othmer, *Ind. Eng. Chem.* **37,** 968 (1945); Vogel, *J. Chem. Soc.* **1948,** 624; Zettlemoyer *et al.,* **US 2644839** (1953 to FMC); *Faith, Keyes & Clark's Industrial Chemicals,* F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 171-177. Toxicity data: H. F. Smyth *et al., Arch. Ind. Hyg. Occup. Med.* **10,** 61 (1954). **Properties:** Liquid. d^{20}_{20} 0.8826. bp 125-126°. mp -77°. n^{20}_D 1.3951. Flash pt, closed cup: 72°F (22°C). Sol in about 120 parts water at 25°; misc with alcohol, ether; sol in most hydrocarbons. LD_{50} orally in rats: 14.13 g/kg (Smyth). **Melting point:** mp -77° **Boiling point:** bp 125-126° **Flash point:** Flash pt, closed cup: 72°F (22°C) **Index of refraction:** n^{20}_D 1.3951 **Density:** d^{20}_{20} 0.8826 **Toxicity data:** LD_{50} orally in rats: 14.13 g/kg (Smyth) **CAUTION:** Potential symptoms of overexposure are headache, drowsiness, narcosis; irritation of eyes, upper respiratory system and skin. *See NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 97-140, 1997) p 36. **Use:** Manuf lacquer, artificial leather, photographic films, plastics, safety glass.

C

Cyclohexane **Monograph Number:** 2752 **CAS Registry Number:** 110-82-7 **Additional Names:** Hexahydrobenzene; hexamethylene; hexanaphthene **Molecular Formula:** C_6H_{12} **Molecular Weight:** 84.16. **Percent Composition:** C 85.63%, H 14.37% **Literature References:** Occurs in petr (0.5-1.0%). Obtained in the distillation of petr or by hydrogenation of benzene. In the distillation of petr the C_4-400°F boiling range naphthas are fractionated to obtain a C_5-200°F naphtha contg 10-14% cyclohexane which on superfractionation yields an 85% concentrate (which is sold as such); further purification necessitates isomerization of pentanes to cyclohexane, heat cracking for removing open chain hydrocarbons and sulfuric acid treatment to remove aromatic compds. The hydrogenation of benzene is done in the liq phase at 150° using Raney nickel catalyst and at least 10 atm H_2 pressure: Sabatier, *Ind. Eng. Chem.* **18,** 1005 (1926). Review and bibliography: Sachanen, *Chemical Constituents of Petroleum* (New York, 1945). Prepn of high purity cyclohexane: Seyer *et al., Ind. Eng. Chem.* **31,** 759 (1939). Cyclohexane can exist in two interconvertible conformations, the boat and the chair. In the chair form its 12 extracyclic bonds fall into two classes: six lie parallel to the main axis of symmetry and are designated "axial", while six extend radially outward at ±109.5° angles to the axis and are designated as "equatorial", Barton *et al., Nature* **172,** 1096 (1954); *Science* **119,** 49 (1954). Solubility: F. P. Schwarz, *Anal. Chem.* **52,** 10 (1980). Toxicity: Lazarew, *Arch. Exp. Pathol. Pharmacol.* **143,** 223 (1929). Physical properties and methods of purification: L. Scheflan, M. B. Jacobs, *The Handbook of Organic Solvents* (Van Nostrand, 1953) p 233; *Techniques of Chemistry,* A. Weissberger, Ed., **vol. II,** 3rd ed., entitled *"Organic Solvents"* by J. D. Riddick, W. B. Bunger (Wiley-Interscience, New York, 1970) p 592. *Review:* M. L. Campbell in *Kirk-Othmer Encyclopedia of Chemical Technology,* **vol. 12** (Wiley-Interscience, New York, 3rd ed., 1980) pp 931-937. **Properties:** Flammable liq. Solvent odor. Pungent when impure. d_4^{20} 0.7781; d_4^{80} 0.7206. mp +6.47°. bp_{760} 80.7°; bp_{400} 60.8°; bp_{200} 42.0°; bp_{100} 25.5°; bp_{60} 14.7°; bp_{40} 6.7°. n_D^{20} 1.4264. Flash pt, closed cup: 1°F (-18°C). Flammability limits in air 1.3-8.4% v/v. Soly in water at 23.5°C (w/w): 0.0052%. 100 ml of methanol dissolves 57 grams at 20°C; miscible with ethanol, ethyl ether, acetone, benzene, carbon tetrachloride. LC in mice: ~60-70 mg/l air (Lazarew). **Melting point:** mp +6.47° **Boiling point:** bp_{760} 80.7°; bp_{400} 60.8°; bp_{200} 42.0°; bp_{100} 25.5°; bp_{60} 14.7°; bp_{40} 6.7° **Flash point:** Flash pt, closed cup: 1°F (-18°C) **Index of refraction:** n_D^{20} 1.4264 **Density:** d_4^{20} 0.7781; d_4^{80} 0.7206 **Toxicity data:** LC in mice: ~60-70 mg/l air (Lazarew) **CAUTION:** Potential symptoms of overexposure are irritation of eyes, skin and respiratory system; drowsiness; dermatitis; narcosis, coma. *See NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 97-140, 1997) p 82. **Use:** Solvent for lacquers and resins. Paint and varnish remover. In the extraction of essential oils. In analytical chemistry for mol wt determinations (cryoscopic constant 20.3). In the manuf of adipic acid, benzene, cyclohexyl chloride, nitrocyclohexane, cyclohexanol and cyclohexanone. In the manuf of solid fuel for camp stoves. In fungicidal formulations (possesses slight fungicidal action). In the industrial recrystn of steroids.

E

Ethyl Acetate **Monograph Number:** 3792 **CAS Registry Number:** 141-78-6 **CAS Name:** Acetic acid ethyl ester **Additional Names:** acetic ether; vinegar naphtha **Molecular Formula:** $C_4H_8O_2$ **Molecular Weight:** 88.10. **Percent Composition:** C 54.53%, H 9.15%, O 36.32% **Line Formula:** $CH_3COOC_2H_5$ **Literature References:** Obtained by the slow distillation of a mixture of acetic acid, ethyl alc, and sulfuric acid: Alheritiere, Mercier, **US 2787636** (1957 to Usines de Melle); *Faith, Keyes, & Clark's Industrial Chemicals,* F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 350-354. Toxicity: H. F. Smyth *et al., Am. Ind. Hyg. Assoc. J.* **23,** 95 (1962). **Properties:** Clear, volatile, flammable liq; characteristic fruity odor; pleasant taste when diluted. Slowly dec by moisture, then acquires an acid reaction. Absorbs water (up to 3.3% w/w). d_4^{20} 0.902; d_{25}^{25} 0.898. bp 77°. mp -83°. Ignition temp 800°F. Explosive limits (% vol in air): 2.2 to 11.5. n_D^{20} 1.3719. Vapor density 3.04 (air = 1). One ml dissolves in 10 ml water at 25°; more sol at lower and less sol at higher temps. Misc with alc, acetone, chloroform, ether. Azeotropic mixture with water (6.1% w/w) bp 70.4°. Azeotropic mixture with water (7.8% w/w) and alc (9.0% w/w) bp 70.3°. *Keep tightly closed in a cool place and away from fire.* LD_{50} orally in rats: 11.3 ml/kg (Smyth). **Melting point:** mp -83° **Boiling point:** bp 77°; bp 70.4°; bp 70.3° **Index of refraction:** n_D^{20} 1.3719 **Density:** d_4^{20} 0.902; d_{25}^{25} 0.898 **Toxicity data:** LD_{50} orally in rats: 11.3 ml/kg (Smyth) **CAUTION:** Potential symptoms of overexposure are irritation of eyes, skin, nose and throat; narcosis; dermatitis. *See NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 97-140, 1997) p 130. **Use:** Pharmaceutic aid (flavor); artificial fruit essences; solvent for nitrocellulose, varnishes, lacquers, and aeroplane dopes; manuf smokeless powder, artificial leather, photographic films and plates, artificial silk, perfumes; cleaning textiles, etc.

Ethyl Alcohol **Monograph Number:** 3795 **CAS Registry Number:** 64-17-5 **CAS Name:** Ethanol **Additional Names:** absolute alcohol; anhydrous alcohol; dehydrated alcohol; ethyl hydrate; ethyl hydroxide **Molecular Formula:** C_2H_6O **Molecular Weight:** 46.07. **Percent Composition:** C 52.14%, H 13.13%, O 34.73% **Line Formula:** C_2H_5OH **Literature References:** Manuf: by fermentation of starch, sugar, and other carbohydrates; from ethylene, acetylene, sulfite waste liquors, and synthesis gas (CO + H); by hydrolysis of ethyl sulfate, and oxidation of methane. Toxicity: G. S. Wiberg *et al., Toxicol. Appl. Pharmacol.* **16,** 718 (1970). Embryotoxicity in mammals: N. A. Brown *et al., Science* **206,** 573 (1979). Possible mechanism for actions of ethanol on the brain: G. Aston-Jones *et al., Nature* **296,** 857 (1982). Ethanol-induced chromosomal abnormalities in mice: M. H. Kaufman, *ibid.* **302,** 258 (1983). Disruption of reproductive function in female primates following alcohol self-administration: N. K. Mello *et al., Science* **221,** 677 (1983). Review of metabolism and toxicity: C. S. Lieber in *Reviews in Biochemical Toxicology* **vol. 5,** E. Hodgson *et al.,* Eds. (Elsevier, New York, 1983) pp 267-312; of pharmacology: L. Pohorecky, J. Brick, *Pharmacol. Ther.* **36,** 335-427 (1988); of hepatotoxicity: C. S. Lieber, L. M. DeCarli, *J. Hepatol.* **12,** 394-401 (1991). General reviews: P. Baud, "Ethyl Alcohol Industry" in Grignard, *Traité de Chimie Organique* **vol. 5** (Masson, 1937) pp 841-975; Zabel, *Chem. Inds.* (now *Chem. Week*) **64,** 212 (1949); *Faith, Keyes & Clark's Industrial Chemicals,* F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 355-364; P. D. Sherman, P. R. Kavasmaneck, "Ethanol" in *Kirk-Othmer Encyclopedia of Chemical Technology* **vol. 9** (Interscience, New York, 3rd ed., 1980) pp 338-380. **Properties:** Clear, colorless, very mobile, flammable liquid; pleasant odor; burning taste. Absorbs water rapidly from air. d_4^{20} 0.789. bp

78.5°. mp -114.1°. n_D^{20} 1.361. Flash pt, closed cup: 13°C. Miscible with water and with many organic liquids. *Keep tightly closed, cool, and away from flame!* LD_{50} in young, old rats (g/kg): 10.6, 7.06 orally (Wiberg). The terms ***95% alcohol*** and ***alcohol*** (when used alone) refer to a binary azeotrope having a distillate composition of 95.57% ethyl alcohol (by wt) and bp 78.15°. ***Alcohol, USP*** is specified as containing not less than 92.3% and not more than 93.8% by weight, corresponding to not less than 94.9% and not more than 96.0% by vol of C_2H_5OH at 15.56°. d_{25}^{25} 0.810; d 0.816 at 15.56° (60°F). ***Diluted alcohol***, prepd from equal vols 95% alcohol and water, contains about 41.5% by wt or about 48.9% by vol of C_2H_5OH. d_{25}^{25} 0.931; d 0.936 at 15.56° (60°F). *See U.S.P.* **XXI,** 22, 1530 (1985). **Melting point:** mp -114.1° **Boiling point:** bp 78.5°; bp 78.15° **Flash point:** Flash pt, closed cup: 13°C **Index of refraction:** n_D^{20} 1.361 **Density:** d_4^{20} 0.789; d_{25}^{25} 0.810; d 0.816 at 15.56° (60°F); d_{25}^{25} 0.931; d 0.936 at 15.56° (60°F) **Toxicity data:** LD_{50} in young, old rats (g/kg): 10.6, 7.06 orally (Wiberg) **CAUTION:** Potential symptoms of overexposure are irritation of eyes, skin, nose; headache, nausea, vomiting, drowsiness, fatigue, narcosis; cough; flushing, rapid pulse, sweating; mental excitement or depression, impaired perception, incoordination, stupor, coma; liver damage; anemia; reproductive and teratogenic effects. *See NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 97-140, 1997) p 132; *Clinical Toxicology of Commercial Products,* R. E. Gosselin *et al.,* Eds. (Williams & Wilkins, Baltimore, 5th ed., 1984) Section III, pp 166-171. **Use:** Most ethyl alcohol is used in alcoholic beverages in suitable dilutions. Other uses are as solvent in laboratory and industry, in the manufacture of denatured alcohol, pharmaceuticals (rubbing compds, lotions, tonics, colognes), in perfumery, in organic synthesis. Octane booster in gasoline. Pharmaceutic aid (solvent). **Therap-Cat:** Antiseptic. **Therap-Cat-Vet:** Antiseptic. To destroy nerve tissue. Solvent and dehydrating agent.

Ethyl Benzoate **Monograph Number:** 3802 **CAS Registry Number:** 93-89-0 **CAS Name:** Benzoic acid ethyl ester **Molecular Formula:** $C_9H_{10}O_2$ **Molecular Weight:** 150.17. **Percent Composition:** C 71.98%, H 6.71%, O 21.31% **Line Formula:** $C_6H_5COOC_2H_5$ **Properties:** Colorless, clear, refractive liq; aromatic odor; vapors cause cough. d_4^{25} 1.050. bp 211-213°. mp -34°. n_D^{20} 1.506. Almost insol in water; miscible with alcohol, chloroform, ether, petr ether. LD_{50} orally in rats: 6.48 g/kg, Smyth *et al., Arch. Ind. Hyg. Occup. Med.* **10,** 61 (1954). **Melting point:** mp -34° **Boiling point:** bp 211-213° **Index of refraction:** n_D^{20} 1.506 **Density:** d_4^{25} 1.050 **Toxicity data:** LD_{50} orally in rats: 6.48 g/kg, Smyth *et al., Arch. Ind. Hyg. Occup. Med.* **10,** 61 (1954) **Use:** In perfumery under the name ***Essence de Niobe***; in manuf of ***Peau d'Espagne***; artificial fruit essence.

I

Isoamyl Acetate **Monograph Number:** 5127 **CAS Registry Number:** 123-92-2 **Additional Names:** Amylacetic ester **Molecular Formula:** $C_7H_{14}O_2$ **Molecular Weight:** 130.18. **Percent Composition:** C 64.58%, H 10.84%, O 24.58% **Line Formula:** $CH_3COOCH_2CH_2CH(CH_3)_2$ **Literature References:** The technical product is also known as ***pear oil*** or ***banana oil***. **Properties:** Colorless, neutral liq; pear-like odor and taste. d_4^{15} 0.876. Pure isoamyl acetate bp 142°. n_D^{21} 1.400; the ordinary grade of commerce boils between 120-145°. Flash pt, closed cup: 92°F (33°C); open cup: 100°F (38°C). Sol in 400 parts water; miscible with alcohol, ether, ethyl acetate, amyl alcohol. Soly of water in isoamyl acetate (25°) 1.6% by volume. **Boiling point:** bp 142° **Flash point:** Flash pt, closed cup: 92°F (33°C); open cup: 100°F (38°C) **Index of refraction:** n_D^{21} 1.400 **Density:** d_4^{15} 0.876 **CAUTION:** Potential symptoms of overexposure are irritation of eyes, skin, nose and throat; dermatitis. *See NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 97-140, 1997) p 174. **Use:** In alcohol solution as a pear flavor in mineral waters and syrups; as solvent for old oil colors, for tannins, nitrocellulose, lacquers, celluloid, and camphor; swelling bath sponges; covering unpleasant odors, perfuming shoe polish; manuf artificial silk, leather or pearls, photographic films, celluloid cements, waterproof varnishes, bronzing liquids, and metallic paints; dyeing and finishing textiles. A special grade of the amyl acetate has been used for burning in the Hefner lamp serving as a photometric standard.

M

Methylene Chloride **Monograph Number:** 6088 **CAS Registry Number:** 75-09-2 **CAS Name:** Dichloromethane **Additional Names:** methylene dichloride; methylene bichloride **Molecular Formula:** CH_2Cl_2 **Molecular Weight:** 84.93. **Percent Composition:** C 14.14%, H 2.37%, Cl 83.49% **Literature References:** Prepn by chlorination of methane: Lukes *et al.,* **US 2792435** (1957 to Diamond Alkali); Pitt, Bender, **US 2979541** (1961 to Stauffer); Burks, Obrecht, **US 3126419** (1964 to Stauffer). Review of mfg processes: *Faith, Keyes & Clark's Industrial Chemicals,* F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 530-538. Toxicity data: E. T. Kimura *et al., Toxicol. Appl. Pharmacol.* **19,** 699 (1971). **Properties:** Colorless liquid; vapor is not flammable and when mixed with air is not explosive. Soluble in ~50 parts water; miscible with alc, ether, DMF. bp_{760} 39.75°. mp -95°. d_4^0 1.36174; d_4^{15} 1.33479; d_4^{20} 1.3255; d_4^{30} 1.30777. n_D^{20} 1.4244. LD_{50} orally in young adult rats: 1.6 ml/kg (Kimura). **Melting point:** mp -95° **Boiling point:** bp_{760} 39.75° **Index of refraction:** n_D^{20} 1.4244 **Density:** d_4^0 1.36174; d_4^{15} 1.33479; d_4^{20} 1.3255; d_4^{30} 1.30777 **Toxicity data:** LD_{50} orally in young adult rats: 1.6 ml/kg (Kimura) **CAUTION:** Potential symptoms of overexposure are fatigue, weakness, sleepiness, lightheadedness; numbness or tingle of limbs; nausea; irritation of eyes and skin. *See NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 97-140, 1997) p 208. This substance is reasonably anticipated to be a human carcinogen: *Ninth Report on Carcinogens* (PB2000-107509, 2000) p III-107. **Use:** Solvent in paint removers, for cellulose acetate; degreasing and cleaning fluids; as solvent in food processing. Pharmaceutic aid (solvent). Aerosol propellant; insecticide.

P

1-Pentanol **Monograph Number:** 7195 **CAS Registry Number:** 71-41-0 **Additional Names:** Pentyl alcohol; *n*-amyl alcohol; *n*-butyl carbinol **Molecular Formula:** $C_5H_{12}O$ **Molecular Weight:** 88.15. **Percent Composition:** C 68.13%, H 13.72%, O 18.15% **Line Formula:** $CH_3(CH_2)_4OH$ **Literature References:** Prepn from 1-pentene: Brown, Rao, *J. Am. Chem. Soc.* **81,** 6434 (1959); Brown, **US 2925437** (1960). Toxicity study: P. M. Jenner *et al., Food Cosmet. Toxicol.* **2,** 327 (1964). Review of manuf by fractionation of fusel oil and via chlorination of pentanes, and properties: *Industrial Chemicals,* W. L. Faith *et al.,* Eds. (John Wiley, New York, 2nd ed., 1957) pp 107-114. **Properties:** Liquid, mild characteristic odor. bp 137.5°. mp -79°. d_4^{20} 0.8146; d_4^{25} 0.8110. n_D^{20} 1.4103: Mumford, Phillips, *J. Chem. Soc.* **1950,** 75. Flash pt, closed cup: 100°F (38°C). Slightly sol in water (2.7 g/100 ml at 22°); misc with alc, ether. LD_{50} orally in rats: 3030 mg/kg (Jenner). **Melting point:** mp -79° **Boiling point:** bp 137.5° **Flash point:** Flash pt, closed cup: 100°F (38°C) **Index of refraction:** n_D^{20} 1.4103: Mumford, Phillips, *J. Chem. Soc.* **1950,** 75 **Density:** d_4^{20} 0.8146; d_4^{25} 0.8110 **Toxicity data:** LD_{50} orally in rats: 3030 mg/kg (Jenner) **CAUTION:** Irritating to eyes, respiratory passages. Narcotic: E. Browning, *Toxicity and Metabolism of Industrial Solvents* (Elsevier, New York, 1965) pp 356-367. **Use:** In organic syntheses; as solvent.