Material Safety Data Sheet
Benzoic-d5 acid, 99+ atom % D

ACC# 68509

Section 1 - Chemical Product and Company Identification

MSDS Name: Benzoic-d5 acid, 99+ atom % D
Catalog Numbers: AC202770010
Synonyms: Benzenemethanoic acid; Benzenecarboxylic acid; Phenylcarboxylic acid; Phenylformic acid; Carboxybenzene; Benzeneformic acid; Dracylic acid.
Company Identification:

Acros Organics N.V.
One Reagent Lane
Fair Lawn, NJ 07410

For information in North America, call: 800-ACROS-01
For emergencies in the US, call CHEMTREC: 800-424-9300

Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name	Percent	EINECS/ELINCS
1079-02-3	Benzoic-d5 acid	>99	214-089-0

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Appearance: white crystalline powder.
Warning! Causes eye, skin, and respiratory tract irritation. May cause allergic respiratory and skin reaction. May be harmful if swallowed, inhaled, or absorbed through the skin.
Target Organs: Respiratory system, eyes, skin.

Potential Health Effects
Eye: Causes severe eye irritation and possible injury.
Skin: Causes moderate skin irritation. May cause allergic contact dermatitis. May be absorbed through the skin in harmful amounts. Absorption through the skin has produced labored breathing in humans. Benzoic acid can cause redness and swelling with itching (non-immunological contact urticaria or hives) in most people at the site of application. Inidviduals can react without having been previously exposed to benzoic acid.
Ingestion: May cause gastrointestinal irritation with nausea, vomiting and diarrhea. May be harmful if swallowed.
Inhalation: Inhalation of dust may cause irritation of the nose and throat. Intermittent breathing of dust over a 4-week period produced interstitial fibrosis in the lungs of rats. Benzoic acid begins to sublime at 100°C.
Chronic: Prolonged or repeated skin contact may cause dermatitis.

Section 4 - First Aid Measures

Eyes: In case of contact, immediately flush eyes with plenty of water for a t least 15 minutes. Get medical aid immediately.
Skin: In case of contact, flush skin with plenty of water. Remove contaminated clothing and shoes. Get medical aid if irritation develops and persists. Wash clothing before reuse.
Ingestion: If swallowed, do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Get medical aid.
Inhalation: If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid.
Notes to Physician: Persons with asthma, chronic respiratory disease, skin disorders, eye problems or allergies may be at increased risk from exposure to this substance.

Section 5 - Fire Fighting Measures

General Information: As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Water runoff can cause environmental damage. Dike and collect water used to fight fire. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion. This material in sufficient quantity and reduced particle size is capable of creating a dust explosion. Reacts with most metals in the presence of moisture, liberating extremely flammable hydrogen gas.
Extinguishing Media: Use water spray, dry chemical, carbon dioxide, or chemical foam.
Flash Point: 121 deg C (249.80 deg F)
Autoignition Temperature: 570 deg C (1,058.00 deg F)
Explosion Limits, Lower: Not available.
Upper: Not available.
NFPA Rating: (estimated) Health: 2; Flammability: 1; Instability: 0

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.
Spills/Leaks: Avoid runoff into storm sewers and ditches which lead to waterways. Clean up spills immediately, observing precautions in the Protective Equipment section. Avoid generating dusty conditions. Provide ventilation. Cover with soda ash or sodium bicarbonate and place in a closed container for disposal.

Section 7 - Handling and Storage

Handling: Wash thoroughly after handling. Use with adequate ventilation. Minimize dust generation and accumulation. Avoid contact with eyes, skin, and clothing. Wash clothing before reuse. Avoid breathing dust.
Storage: Store in a cool, dry, well-ventilated area away from incompatible substances.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls: Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Use adequate ventilation to keep airborne concentrations low.
Exposure Limits

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
Benzoic-d5 acid	none listed	none listed	none listed
Benzoic acid	none listed	none listed	none listed

OSHA Vacated PELs: Benzoic-d5 acid: No OSHA Vacated PELs are listed for this chemical. Benzoic acid: No OSHA Vacated PELs are listed for this chemical.
Personal Protective Equipment
Eyes: Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin: Wear appropriate protective gloves to prevent skin exposure.
Clothing: Wear appropriate protective clothing to prevent skin exposure.
Respirators: A respiratory protection program that meets OSHA's 29 CFR 1910.134 and ANSI Z88.2 requirements or European Standard EN 149 must be followed whenever workplace conditions warrant respirator use.

Section 9 - Physical and Chemical Properties

Physical State: Crystalline powder
Appearance: white
Odor: pleasant odor
pH: 2.8 (satd soln)
Vapor Pressure: 0.0012 mm Hg @ 25 deg C
Vapor Density: 4.21 (air=1)
Evaporation Rate: Negligible.
Viscosity: Not available.
Boiling Point: 249.2 deg C @ 760 mm Hg
Freezing/Melting Point:120-122 deg C
Decomposition Temperature: Not available.
Solubility: 3.4 g/l @ 25°C
Specific Gravity/Density: Not available.
Molecular Formula:C7D5HO2
Molecular Weight:127.15

Section 10 - Stability and Reactivity

Chemical Stability: Stable under normal temperatures and pressures. Volatile in steam.
Conditions to Avoid: Dust generation, excess heat.
Incompatibilities with Other Materials: Strong oxidizing agents, strong bases, amines, ammonia, isocyanates, Solutions attack some metals..
Hazardous Decomposition Products: Carbon monoxide, carbon dioxide, phenol, benzene.
Hazardous Polymerization: Has not been reported

Section 11 - Toxicological Information

RTECS#:
CAS# 1079-02-3 unlisted.
CAS# 65-85-0: DG0875000
LD50/LC50:
Not available.

CAS# 65-85-0:
Draize test, rabbit, eye: 100 mg Severe;
Draize test, rabbit, skin: 500 mg/24H Mild;
Inhalation, rat: LC50 = >26 mg/m3/1H;
Oral, mouse: LD50 = 1940 mg/kg;
Oral, rat: LD50 = 1700 mg/kg;

Skin, rabbit: LD50 = >10 gm/kg;

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Human TDLo skin of 6 mg/kg produced dyspnea (difficult or labored breathing) and allergic dermatitis.

Carcinogenicity:

CAS# 1079-02-3: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

CAS# 65-85-0: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

Epidemiology: No information available.

Teratogenicity: No information available.

Reproductive Effects: No information available.

Mutagenicity: Benzoic acid and sodium benzoate have been tested for mutagenicity or genotoxicity in prokaryotes, eukaryotes, and several mammalian test systems. No positive results have been reported.RTECS data for benzoic acid: Mutations in microorganisms: Escherichia coli = 10 mmol/L. DNA inhibition: Human lymphocyte = 5 mmol/L. EPA GENETOX PROGRAM 1988, Negative: Histidine reversion-Ames test; S cerevisiae-homozygosis.

Neurotoxicity: No information available.

Other Studies:

Section 12 - Ecological Information

Ecotoxicity: Fish: Mosquito Fish: LC50 = 180 mg/L; 96 Hr; UnspecifiedBacteria: Phytobacterium phosphoreum: EC50 = 16.9 mg/L; 96 Hr; Microtox test @ 15°C If released on land, benzoic acid should leach into the ground due to its low soil adsorption and biodegrade (half-life <1 wk). If released in water, benzoic acid should also readily biodegrade (half-life 0.2-3.6 days). Adsorption to sediment and volatilization should not be significant.

Environmental: No information available.

Physical: No information available.

Other: Antifungal agent.

Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.

RCRA P-Series: None listed.

RCRA U-Series: None listed.

Section 14 - Transport Information

	US DOT	Canada TDG
Shipping Name:	Not regulated as a hazardous material	No information available.
Hazard Class:		
UN Number:		
Packing Group:		

Section 15 - Regulatory Information

US FEDERAL

TSCA

CAS# 1079-02-3 is not listed on the TSCA inventory. It is for research and development use only.

CAS# 65-85-0 is listed on the TSCA inventory.

Health & Safety Reporting List

None of the chemicals are on the Health & Safety Reporting List.

Chemical Test Rules

None of the chemicals in this product are under a Chemical Test Rule.

Section 12b

None of the chemicals are listed under TSCA Section 12b.

TSCA Significant New Use Rule

None of the chemicals in this material have a SNUR under TSCA.

CERCLA Hazardous Substances and corresponding RQs

CAS# 65-85-0: 5000 lb final RQ; 2270 kg final RQ

SARA Section 302 Extremely Hazardous Substances

None of the chemicals in this product have a TPQ.

SARA Codes

CAS # 65-85-0: immediate.

Section 313 No chemicals are reportable under Section 313.

Clean Air Act:

This material does not contain any hazardous air pollutants.

This material does not contain any Class 1 Ozone depletors.

This material does not contain any Class 2 Ozone depletors.

Clean Water Act:

CAS# 65-85-0 is listed as a Hazardous Substance under the CWA.

None of the chemicals in this product are listed as Priority Pollutants under the CWA.

None of the chemicals in this product are listed as Toxic Pollutants under the CWA.

OSHA:

None of the chemicals in this product are considered highly hazardous by OSHA.

STATE

CAS# 1079-02-3 is not present on state lists from CA, PA, MN, MA, FL, or NJ.
CAS# 65-85-0 can be found on the following state right to know lists: California, New Jersey, Pennsylvania, Massachusetts.

California Prop 65

California No Significant Risk Level: None of the chemicals in this product are listed.

European/International Regulations

European Labeling in Accordance with EC Directives

Hazard Symbols:

XN

Risk Phrases:

R 22 Harmful if swallowed.
R 36/37/38 Irritating to eyes, respiratory system and skin.
R 42/43 May cause sensitization by inhalation and skin contact.

Safety Phrases:

S 22 Do not breathe dust.
S 24 Avoid contact with skin.
S 26 In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
S 37/39 Wear suitable gloves and eye/face protection.
S 45 In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

WGK (Water Danger/Protection)

CAS# 1079-02-3: No information available.
CAS# 65-85-0: 1

Canada - DSL/NDSL

CAS# 65-85-0 is listed on Canada's DSL List.

Canada - WHMIS

This product has a WHMIS classification of D2B.

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

Canadian Ingredient Disclosure List

CAS# 65-85-0 is listed on the Canadian Ingredient Disclosure List.

Section 16 - Additional Information

MSDS Creation Date: 9/02/1997
Revision #9 Date: 8/31/2005