

SAFETY DATA SHEET

1. SUBSTANCE AND SOURCE IDENTIFICATION

Product Identifier

SRM Number: 869b
SRM Name: Column Selectivity Test Mixture for Liquid Chromatography
(Polycyclic Aromatic Hydrocarbons)
Other Means of Identification: Not applicable.

Recommended Use of This Material and Restrictions of Use

This Standard Reference Material (SRM) is a mixture of three polycyclic aromatic hydrocarbons (PAHs) in acetonitrile: benzo[*a*]pyrene (BaP), 1,2:3,4:5,6:7,8-tetrabenzonaphthalene (TBN, alternate name, dibenzo[*g,p*]chrysene), and phenanthro[3,4-*c*]phenanthrene (PhPh). SRM 869b is useful for characterizing liquid chromatographic (LC) column selectivity for separation of PAHs. A unit of SRM 869b consists of 5 ampoules, each containing 1.1 mL of the PAH mixture.

Company Information

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2. HAZARDS IDENTIFICATION

NOTE: The health and safety information provided in this SDS is for acetonitrile.

Classification

Physical Hazard:	Flammable Liquid	Category 2
Health Hazard:	Acute Toxicity, Oral	Category 4
	Acute Toxicity, Dermal	Category 4
	Acute Toxicity, Inhalation	Category 4
	Eye Damage/Irritation	Category 2A

Label Elements

Symbol



Signal Word

DANGER

Hazard Statement(s)

H225 Highly flammable liquid and vapor.
H302+H312+H332 Harmful if swallowed, in contact with skin, or if inhaled.
H319 Causes serious eye irritation.

Precautionary Statement(s)

P210 Keep away from heat, sparks, open flames, hot surfaces. — No smoking.
P233 Keep container tightly closed.
P241+P242 Use explosion-proof electrical and ventilating equipment. Use only non-sparking tools.
P243 Take precautionary measures against static discharge.
P261 Avoid breathing fumes, mist, vapors, or spray.
P264 Wash hands thoroughly after handling.

P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated room.
P280	Wear protective gloves, eye protection, and protective clothing.
P301+P330	If swallowed: Rinse mouth.
P303+P361+P353	If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P304+P340	If inhaled: Remove person to fresh air and keep comfortable for breathing.
P305+P351+P338	If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P312	Call a doctor if you feel unwell.
P337+P313	If eye irritation persists: Get medical attention.
P362+P363	Take off contaminated clothing and wash it before reuse.
P403+P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents and container according to local regulations.

Hazards Not Otherwise Classified: None.

Ingredients(s) with Unknown Acute Toxicity: None.

3. COMPOSITION AND INFORMATION ON HAZARDOUS INGREDIENTS

Substance: PAHs in acetonitrile

Other Designations: Acetonitrile (cyanomethane; ethanenitrile; ethyl nitrile; methanecarbonitrile; methyl cyanide)

This material contains trace amounts of PAHs. Though many PAHs have been reported to have mutagenic and/or carcinogenic properties, the trace amounts found in this SRM do not require individual SDS information, see OSHA 29 CFR 1910.1200. For the actual concentrations, see the NIST Certificate of Analysis.

Hazardous Component(s)	CAS Number	EC Number (EINECS)	Nominal Mass Concentration (%)
Acetonitrile	75-05-8	200-835-2	>99

4. FIRST AID MEASURES

Description of First Aid Measures

Inhalation: If adverse effects occur, remove to well-ventilated (uncontaminated) area. If breathing is difficult, qualified personnel may administer oxygen. If not breathing, qualified personnel should give artificial respiration. Seek immediate medical attention.

Skin Contact: Rinse affected skin with water for at least 15 minutes, then wash thoroughly with soap or mild detergent and water. Seek medical attention if need; bring the container.

Eye Contact: Immediately flush eyes, including under the eyelids, with copious amounts of water for at least 15 minutes. Seek immediate medical attention.

Ingestion: If ingested, immediately call a doctor. If vomiting occurs, keep head lower than the hips to help prevent aspiration.

Most Important Symptoms/Effects, Acute and Delayed: Difficulty breathing, chest pain, vomiting, dizziness, confusion, convulsions, unconsciousness and coma. Note: health effects may be delayed.

Indication of any immediate medical attention and special treatment needed, if necessary: If any of the above symptoms are present, seek immediate medical attention.

5. FIRE FIGHTING MEASURES

Fire and Explosion Hazards: Severe fire hazard. Vapor/air mixtures are explosive above the flash point. Vapors or gases may ignite at distant ignition sources and flash back. See Section 9, "Physical and Chemical Properties" for flammability properties.

Extinguishing Media

Suitable: Regular dry chemical, carbon dioxide, water, or alcohol-resistant foam.

Unsuitable: None listed.

Specific Hazards Arising from the Chemical: Not applicable.

Special Protective Equipment and Precautions for Fire-Fighters: Move container from fire area if it can be done without personal risk. Avoid inhalation of material or combustion by-products. Wear full protective clothing and NIOSH-approved self-contained breathing apparatus (SCBA).

NFPA Ratings (0 = Minimal; 1 = Slight; 2 = Moderate; 3 = Serious; 4 = Severe)

Health = 2 Fire = 3 Reactivity = 0

6. ACCIDENTAL RELEASE MEASURES

Personal Precautions, Protective Equipment and Emergency Procedures: Use suitable protective equipment; see Section 8, “Exposure Controls and Personal Protection”. Keep out of waters supplies and sewers.

Methods and Materials for Containment and Clean up: Avoid heat, flames, sparks and other sources of ignition. Stop leak if possible without personal risk, with water spray to reduce vapors. Absorb spilled material with sand or non-combustible material and collect in appropriate container for disposal.

7. HANDLING AND STORAGE

Safe Handling Precautions: See Section 8, “Exposure Controls and Personal Protection”.

Storage and Incompatible Materials: Store in a well-ventilated area. Keep separated from incompatible substances (see Section 10, “Stability and Reactivity”).

8. EXPOSURE CONTROLS AND PERSONAL PROTECTION

Exposure Limits

OSHA (PEL):	40 ppm (70 mg/m ³) TWA Prevent or reduce skin absorption (related to cyanide compounds).
ACGIH (TLV):	20 ppm TWA Skin – potential significant contribution to overall exposure by the cutaneous route.
NIOSH (REL):	20 ppm (34 mg/m ³) TWA 500 ppm IDLH

Engineering Controls: Provide local exhaust or process enclosure ventilation system. Ensure compliance with applicable exposure limits.

Personal Protection Measures: In accordance with OSHA 29 CFR 1910.132, subpart I, wear appropriate Personal Protective Equipment (PPE) to minimize exposure to this material.

Respiratory Protection: If workplace conditions warrant a respirator, a respiratory protection program that meets OSHA 29CFR 1910.134 must be followed. Refer to NIOSH 42 CFR 84 for applicable certified respirators.

Eye Protection: Splash resistant safety goggles and emergency eyewash are recommended.

Skin and Body Protection: Chemical resistant clothing and gloves are recommended.

9. PHYSICAL AND CHEMICAL PROPERTIES

Descriptive Properties	Acetonitrile
	>99 %
Molar Mass (g/mol)	41.05
Molecular Formula	CH ₃ CN
Appearance (physical state, color, etc.)	clear, colorless liquid
Odor	sweet odor
Odor threshold	40 ppm
pH	not available
Evaporation rate (butyl acetate = 1)	5.79
Melting point/freezing point	-46 °C (-50.8 °F)
Relative Density as Specific Gravity (water = 1)	0.7857
Density	not available
Vapor Pressure	73 mmHg at 20 °C
Vapor Density (air = 1)	1.42
Viscosity	0.35 cP at 20 °C

Descriptive Properties

Acetonitrile

>99 %

Solubilities

soluble in water
solvent: alcohol, ether, ethyl acetate, methyl acetate, benzene, acetone, chloroform, carbon tetrachloride, ethylene chloride, acetamide solutions, unsaturated hydrocarbons
not available

Partition coefficient (n-octanol/water)

Thermal Stability Properties

Autoignition Temperature

524 °C (975.2 °F)

Thermal Decomposition

not available

Initial boiling point and boiling range

82 °C (179.6 °F)

Explosive Limits, LEL (Volume %)

3 %

Explosive Limits, UEL (Volume %)

16 %

Flash Point (Open Cup)

6 °C (42.8 °F)

Flammability (solid, gas)

not applicable

10. STABILITY AND REACTIVITY

Reactivity: Stable at normal temperatures and pressure.

Stability: Stable Unstable

Possible Hazardous Reactions: Not applicable.

Conditions to Avoid: Avoid heat, flames, sparks, and other sources of ignition. Minimize contact with material. Avoid inhalation of material or combustion by-products. Keep out of water supplies and sewers.

Incompatible Materials: Acids, bases, combustible materials, metals, oxidizing materials, and reducing agents.

Hazardous Decomposition: Oxides of carbon, nitrogen, and cyanides.

Hazardous Polymerization: Will Occur Will Not Occur

11. TOXICOLOGICAL INFORMATION

Route of Exposure: Inhalation Skin Ingestion

Symptoms Related to the Physical, Chemical and Toxicological Characteristics: Nausea, vomiting, respiratory failure, hypotension, convulsions.

Potential Health Effects (Acute, Chronic, and Delayed)

Inhalation: Acute and chronic exposure to high concentrations of acetonitrile may cause irritation of the nose and throat, cough with bloody sputum, nausea, vomiting of blood or bile-like substance, chest or abdominal pain, dizziness, headache, dyspnea or tachypnea, low blood pressure, shock, unconsciousness, coma and death due to nervous system depression. Chronic exposure may also cause anorexia, profuse sweating, hypersalivation, rigidity of the neck, urinary frequency, and albuminuria.

Skin Contact: Acute exposure to acetonitrile may result in irritation, absorption may occur resulting in systemic toxicity.

Eye Contact: Acute exposure to acetonitrile may cause irritation and tearing. Chronic exposure may cause conjunctivitis.

Ingestion: Ingestion of sufficient amounts may cause systemic toxicity as detailed for inhalation.

Numerical Measures of Toxicity

Acute Toxicity: Category 4 for Oral, Dermal, and Inhalation.

Rabbit, Dermal, LD50: >2000 mg/kg

Rat, Oral, LD50: 2460 mg/kg

Rat, Inhalation, LC50: 17 100 ppm (4 h); 7551 ppm (8 h)

Skin Corrosion/Irritation: Not classified.

Rabbit, Skin: 500 mg open skin, mild

Serious Eye Damage/Eye Irritation: Category 2A.

Rabbit, Eyes: 100 µL (24 h) moderate

Respiratory Sensitization: No data available.

Skin Sensitization: No data available.

Germ Cell Mutagenicity: No data available.

Carcinogenicity: Not classified.

Listed as a Carcinogen/Potential Carcinogen _____ **Yes** _____ **X** **No**

Acetonitrile is not listed by IARC, NTP, or OSHA as a carcinogen/potential carcinogen.

Tumorigenic: Rat, Inhalation, TCLo: 400 ppm (6 h)

Mutagenic: Hamster: 5 g/L; *Drosophila melanogaster*: 131 ppm; *Saccharomyces cerevisiae*: 47 600 ppm

Reproductive Toxicity: Not classified.

Hamster, Inhalation, TCLo: 8000 ppm (1 h, pregnant 8 d)

Hamster, Oral, TDLo: 300 mg/kg (pregnant 8 d)

Rat, Inhalation, TCLo: 1800 ppm (6 h, pregnant 6 d to 20 d)

Specific Target Organ Toxicity, Single Exposure: Not classified.

Specific Target Organ Toxicity, Repeated Exposure: Not classified.

Aspiration hazard: Not classified.

12. ECOLOGICAL INFORMATION

Ecotoxicity Data: Fish, Bluegill (*Lepomis macrochirus*), LC50: 1850 mg/L (96 h) static

Persistence and Degradability: No data available.

Bioaccumulative Potential: No data available.

Mobility in Soil: No data available.

Other Adverse effects: No data available.

13. DISPOSAL CONSIDERATIONS

Waste Disposal: Dispose in accordance with all applicable federal, state, and local regulations. Subject to US EPA 40 CFR 262; hazardous waste number U003.

14. TRANSPORTATION INFORMATION

U.S. DOT and IATA: UN1648; Acetonitrile solution; Hazard Class 3; Packing Group II; Excepted Quantity: E2.

15. REGULATORY INFORMATION

U.S. Regulations

CERCLA Sections 102a/103 (40 CFR 302.4): 5000 lb (2270 kg) final RQ

SARA Title III Section 302 (40 CFR 355.30): Not regulated.

SARA Title III Section 304 (40 CFR 355.40): Not regulated.

SARA Title III Section 313 (40 CFR 372.65): 1.0 % de minimis concentrations.

OSHA Process Safety (29 CFR 1910.119): Not regulated.

SARA Title III Sections 311/312 Hazardous Categories (40 CFR 370.21):

ACUTE HEALTH: Yes

CHRONIC HEALTH: No

FIRE: Yes

REACTIVE: No

PRESSURE: No

State Regulations: California Proposition 65: Not listed.

U.S. TSCA Inventory: Acetonitrile is listed.

TSCA 12(b), Export Notification: Not listed.

Canadian Regulations: WHMIS Information is not provided for this material.

16. OTHER INFORMATION

Issue Date: 08 January 2015

Sources: ChemADVISOR, Inc., SDS *Acetonitrile*, 09 September 2014.

CDC, NIOSH, *Acetonitrile*, RTECS# AL7700000, CAS No. 75-05-8; available at <http://www.cdc.gov/niosh-rtecs/AL757E20.html> (accessed Jan 2015).

International Programme on Chemical Safety, Environmental Health Criteria 154, *Acetonitrile*, World Health Organization, Geneva, 1993; available at <http://www.inchem.org/documents/ehc/ehc/ehc154.htm> (accessed Jan 2015).

European Chemicals Agency (ECHA), Information on Chemicals, Registered Substances, *Acetonitrile* CAS No. 75-05-8, Harmonised classification; available at <http://echa.europa.eu/> (accessed Jan 2015).

Key of Acronyms:

ACGIH	American Conference of Governmental Industrial Hygienists	NTP	National Toxicology Program
CAS	Chemical Abstracts Service	OSHA	Occupational Safety and Health Administration
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act	PEL	Permissible Exposure Limit
CFR	Code of Federal Regulations	RCRA	Resource Conservation and Recovery Act
DOT	Department of Transportation	REL	Recommended Exposure Limit
EINECS	European Inventory of Existing Commercial Chemical Substances	RQ	Reportable Quantity
EPCRA	Emergency Planning and Community Right-to-Know Act	RTECS	Registry of Toxic Effects of Chemical Substances
IARC	International Agency for Research on Cancer	SARA	Superfund Amendments and Reauthorization Act
IATA	International Air Transportation Agency	SCBA	Self-Contained Breathing Apparatus
IDLH	Immediately Dangerous to Life and Health	SRM	Standard Reference Material
LC50	Lethal Concentration	STOT	Specific Target Organ Toxicity
LD50	Median Lethal Dose or Lethal Dose, 50 %	STEL	Short Term Exposure Limit
LEL	Lower Explosive Limit	TLV	Threshold Limit Value
MSDS	Material Safety Data Sheet	TPQ	Threshold Planning Quantity
NFPA	National Fire Protection Association	TSCA	Toxic Substances Control Act
NIOSH	National Institute for Occupational Safety and Health	TWA	Time Weighted Average
NIST	National Institute of Standards and Technology	UEL	Upper Explosive Limit
n.o.s.	Not Otherwise Specified	WHMIS	Workplace Hazardous Materials Information System

Disclaimer: Physical and chemical data contained in this SDS are provided only for use in assessing the hazardous nature of the material. The SDS was prepared carefully, using current references; however, NIST does not certify the data in the SDS. The values for this material are given in the NIST Certificate of Analysis.

Users of this SRM should ensure that the SDS in their possession is current. This can be accomplished by contacting the SRM Program: telephone (301) 975-2200; fax (301) 948-3730; e-mail srmmsds@nist.gov; or via the Internet at <http://www.nist.gov/srm>.