Date of Issue:
06 December 2019

SAFETY DATA SHEET

1. Substance and Source Identification

Product Identifier

SRM Number: 2269
SRM Name: Perdeuterated PAH-I Solution in Hexane/Toluene
Other Means of Identification: Not applicable.

Recommended Use of This Material and Restrictions of Use

This Standard Reference Material (SRM) is intended primarily for use as an internal standard, or surrogate internal standard, solution that is used to spike both the unknown sample and the calibration or external standard solution of non-labeled PAHs. A unit of SRM 2269 consists of five 2 mL ampoules, each containing approximately 1.2 mL of a solution of five perdeuterated polycyclic aromatic hydrocarbons (PAHs) in hexane/toluene (96:4 volume fraction).

Company Information

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2. Hazards Identification

Classification

Physical Hazard:	Flammable liquid	Category 2
Health Hazard:	Skin Corrosion/Irritation	Category 2
	Serious Eye damage/Eye Irritation	Category 2B
	Reproductive Toxicity	Category 2
	STOT, Single Exposure	Category 3
	STOT, Repeated Exposure	Category 2
	Aspiration Hazard	Category 1

Label Elements

Symbol

Signal Word

DANGER

Hazard Statement(s)

H225	Highly flammable liquid and vapor.
H305	May be fatal if swallowed and enters airways.
H315+H320	Causes skin and eye irritation.
H336	May cause drowsiness or dizziness.
H361	Suspected of damaging fertility or the unborn child.
H373	May cause damage to organs (eyes, skin, respiratory system, central nervous system, liver, kidneys) through prolong or repeated exposure (inhalation, ingestion, skin contact).

Precautionary Statement(s)

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat, sparks, open flames or hot surfaces. No smoking.
P241	Use explosion-proof electrical ventilating and lighting equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P260	Do not breathe fumes, mist, vapors or spray.
P264	Wash hands thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P280	Wear protective gloves, protective clothing, and eye protection.
P301+P310	If swallowed: Immediately call a doctor.
P303+P361+P353	If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P304+P340	If inhaled: Remove victim to fresh air and keep at rest in a position 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.
P308+P313	IF exposed or concerned: Get medical attention.
P331	Do NOT induce vomiting.
P362+P364	Take off contaminated clothing and wash it before reuse.
P403+P233	Store in a well-ventilated place. Keep container tightly closed.
P405	Store locked up.
P501	Dispose of contents and container according to local regulations.

Hazards Not Otherwise Classified: Not applicable.

Ingredients(s) with Unknown Acute Toxicity: Not applicable.

3. Composition and Information on Hazardous Ingredients

Substance: Hexane/Toluene with trace amounts of perdeuterated PAHs.

Other Designations:

Hexane (hexyl hydride; normal hexane; n-hexane)
Toluene (methylbenzene; toluol; 1-methylbenzene; methylbenzol; phenylmethane; methyl benzene)

NOTE: This material contains trace amounts of perdeuterated PAHs, which have been reported to have toxic, mutagenic, and/or carcinogenic properties, and should be handled with care. The components listed below are in compliance with OSHA's 29 CFR 1910.1200; for the actual values of components, see the Certificate of Analysis.

Hazardous Component(s)	CAS Number	EC Number (EINECS)	Nominal Concentration (%)
Hexane	110-54-3	203-777-6	96
Toluene	108-88-3	203-625-9	4

4. First Aid Measures

Description of First Aid Measures:

Inhalation: If adverse effects occur, remove to uncontaminated area. If not breathing, give artificial respiration or oxygen by qualified personnel. Seek immediate medical attention.

Skin Contact: Wash skin with soap and water for at least 15 minutes while removing contaminated clothing and shoes. Get immediate medical attention. Thoroughly clean and dry contaminated clothing before reuse. Destroy contaminated shoes.

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

Ingestion: Aspiration hazard! ***Do not*** induce vomiting. If vomiting occurs, keep head lower than hips to help prevent aspiration. Get immediate medical attention. Give artificial respiration if not breathing.

Most Important Symptoms/Effects, Acute and Delayed: Respiratory tract, skin, and eye irritation; aspiration hazard, nervous system depression, and nerve damage.

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. The vapor is heavier than air. Vapors or gases may ignite at distant ignition sources and flash back. Vapor/air mixtures are explosive. Electrostatic discharges may be generated by flow or agitation resulting in ignition or explosion. See Section 9, "Physical and Chemical Properties" for flammability properties.

Extinguishing Media:

Suitable: Regular dry chemical, carbon dioxide, water, regular foam.
Unsuitable: None listed.

Specific Hazards Arising from the Chemical: Thermal decomposition products: oxides of carbon, hydrocarbons.

Special Protective Equipment and Precautions for Fire-Fighters: Avoid inhalation of material or combustion byproducts. 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: Avoid heat, flames, sparks and other sources of ignition. Stop leak if possible without personal risk. Immediately contact emergency personnel, Isolate hazard area, and deny entry. Reduce vapors with water spray. Use suitable protective equipment; see Section 8, "Exposure Controls and Personal Protection".

Methods and Materials for Containment and Clean up: Do not touch spilled material. Notify safety personnel of spills. Absorb with sand or other non-combustible material. Collect spilled material in appropriate container for disposal. Avoid and remove sources of ignition. Keep out of water supplies and sewers.

7. HANDLING AND STORAGE

Safe Handling Precautions: Open glass ampoules carefully to prevent contamination and injury. See Section 8, "Exposure Controls and Personal Protection".

Storage: Sealed ampoules, as received, should be stored in the dark at temperatures lower than 30 °C. Store and handle in accordance with all current regulations and standards. Keep separated from incompatible substances (See Section 10, "Stability and Reactivity").

8. EXPOSURE CONTROLS AND PERSONAL PROTECTION

Exposure Limits:

Hexane:

NIOSH (REL): 180 mg/m^3; 50 ppm (TWA)
3960 mg/m^3; 1100 ppm (IDLH, 10 % LEL)
ACGIH (TLV): 180 mg/m^3; 50 ppm (TWA)
Skin - potential significant contribution to overall exposure by the cutaneous route.
OSHA (PEL): 1800 mg/m^3; 500 ppm (TWA)

Toluene:

NIOSH (REL): 375 mg/m^3; 100 ppm (TWA)
560 mg/m^3; 150 ppm (STEL)
1885 mg/m^3; 500 ppm (IDLH)
ACGIH (TLV): 75 mg/m^3; 20 ppm (TWA)
OSHA (PEL): 750 mg/m^3; 200 ppm (TWA)
1130 mg/m^3; 300 ppm (Ceiling)

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

Personal Protection: 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/Face Protection: Wear splash resistant safety goggles with a face shield. An eyewash station should be readily available near areas of use.

Skin and Body Protection: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product. Chemical-resistant gloves should be worn at all times when handling chemicals.

9. PHYSICAL AND CHEMICAL PROPERTIES

Descriptive Properties:

Appearance (physical state, color, etc.):	colorless liquid
Molecular Formula:	not applicable
Molar Mass (g/mol):	not applicable
Odor:	gasoline-like odor
Odor threshold:	64 ppm to 244 ppm (hexane)
pH:	not available
Evaporation rate (butyl acetate = 1):	15.8 (hexane)
Melting point/freezing point (ºC):	–95 (–139 ºF) (hexane)
Sublimation Point (ºC):	not applicable
Decomposition (ºC):	not applicable
Relative Density as specific gravity (water = 1):	0.6606 g/cm^3 at 25 ºC (hexane)
Vapor Pressure:	124 mmHg at 20 ºC (hexane)
Vapor Density (air = 1):	3.0 (hexane)
Viscosity (cP):	0.32 cP at 25 °C (hexane)
Solubility(ies):	water solubility: 0.014 % at 20 °C; soluble in ethanol, ether, chloroform, acetone, organic solvents (hexane)
Partition coefficient (n-octanol/water):	log Kow = 3.90 (hexane)

Thermal Stability Properties:

Autoignition Temperature (ºC):	225 (437 ºF) (hexane)
Thermal Decomposition (ºC):	not applicable
Initial boiling point and boiling range (ºC):	69 (156 ºF) (hexane)
Explosive Limits, LEL (Volume %):	1.1 (hexane)
Explosive Limits, UEL (Volume %):	7.5 (hexane)
Flash Point (ºC):	–22 (–7.6 ºF) CC (hexane)
Flammability (solid, gas):	not applicable

10. STABILITY AND REACTIVITY

Reactivity: Stable at normal temperatures and pressure.

Stability: X Stable _____ Unstable

Possible Hazardous Reactions: No data available.

Conditions to Avoid: Avoid heat, flames, sparks and other sources of ignition. Ampoules may rupture or explode if exposed to heat. Keep out of water supplies and sewers.

Incompatible Materials: Oxidizing materials, halogens, combustible materials, acids, metal salts.

Fire/Explosion Information: See Section 5, "Fire Fighting Measures".

Hazardous Decomposition: Thermal decomposition will produce oxides of carbon, hydrocarbons.

Hazardous Polymerization: _____ Will Occur X Will Not Occur

11. TOXICOLOGICAL INFORMATION

Route of Exposure: X Inhalation X Skin X Ingestion

Symptoms Related to the Physical, Chemical and Toxicological Characteristics: Respiratory tract, skin, and eye irritation; aspiration hazard, nervous system depression, and nerve damage.

Potential Health Effects (Acute, Chronic and Delayed):

Inhalation: Inhalation of hexane can cause eye, nose, throat and respiratory irritation. Acute exposure to considerable concentrations may cause cough, wheezing, headache, dizziness, nausea, gastrointestinal symptoms, central nervous system depression and asphyxia. Prolonged exposure may result in motor sensory and central nervous system abnormalities.

Skin Contact: Contact with liquid may cause irritation and dermatitis due to defatting.

Eye Contact: Irritation with redness and pain and conjunctivitis.

Ingestion: Aspiration hazard; ingestion of hexane can cause lung damage and death.

Numerical Measures of Toxicity:

Acute Toxicity: Not classified.

Hexane:	Rat, Oral LD50: 15 840 mg/kg Rat, Dermal LD50: 3000 mg/kg Rat, Inhalation LC50: 48 000 ppm (4 h)
Toluene:	Rat, Oral LD50: 636 mg/kg Rat, Dermal LD50: 8390 mg/kg Rat, Inhalation LC50: 49 g/m^3 (4 h)

Skin Corrosion/Irritation: Category 2

Hexane:	Hexane is irritating to skin, and can cause redness, pain and blister formation.
Toluene:	Rabbit, Dermal: 435 mg (mild); 500 mg (moderate); 20 mg (moderate, 24 h)

Serious Eye Damage/Eye Irritation: Category 2B

Hexane: Rabbit, Eye: 10 mg (mild);

Inhalation of hexane has been report to cause eye irritation, but is rapidly reversible when exposure is discontinued. Vapors at 880 ppm for 15 minutes caused irritation.

Toluene: Rabbit, Eye: 870 µg (mild); 100 mg/30 s rinse (mild); 2 mg (severe, 24 h)

Respiratory Sensitization: No data available.

Skin Sensitization: No data available.

Germ Cell Mutagenicity: Not classified.

Hexane:	Saccharomyces cerevisiae, sex chromosome loss and nondisjunction: 132 mmol/L
Toluene:	Human, Inhalation: 252 µg/L (19 years)

Carcinogenicity: Not classified.

Listed as a Carcinogen/Potential Carcinogen ____ Yes X No

Hexane is not listed by NTP, IARC or OSHA as a carcinogen.

Toluene is not listed by NTP or OSHA as a carcinogen; IARC lists toluene as Group 3, *not classifiable*.

Reproductive Toxicity: Category 2B

Hexane: Endpoints listed for reproductive effects on embryo or fetus: fetotoxicity (except death, e.g., stunted fetus).

Rat, Inhalation, TCLo: 238 g/kg (pregnant 6 d to 15 d)
Rat, Inhalation, TCLo: 1000 ppm (6 h, pregnant 8 d to 16 d)
Rat, Inhalation, TCLo: 5000 ppm (20 h, pregnant 6 d to 19 d)

Toluene: Endpoints listed for reproductive effects on embryo or fetus

Rat, Oral, TDLo: 7280 mg/kg (pregnant 6 d to 19 d), fetotoxicity (except death, e.g., stunted fetus)
Mouse, Oral, TDLo: 9 g/kg (pregnant 6 d to 15 d), fetal death

Specific Target Organ Toxicity, Single Exposure: Category 3 (narcotic effects)

Acute exposure by inhaling considerable concentrations of hexane may cause nervous system depression including headache, nausea, dizziness, giddiness, coughing, numbness in the extremities, difficulty walking, defects of memory, excitement followed by depression, and unconsciousness.

Specific Target Organ Toxicity, Repeated Exposure: Category 2

Prolonged or repeated exposure to hexane may cause damage to organs (eyes, skin, respiratory system, central nervous system, liver, kidneys).

Aspiration Hazard: Category 1

This SRM contains ≥10 % hexane and it is classified as Category 1.

12. ECOLOGICAL INFORMATION

Ecotoxicity Data:

Hexane:

Fish Toxicity: fathead minnow (*Pimephales promelas*) LC50 (flow-through): 2.1 mg/L to 2.98 mg/L (96 h)
Invertebrate: water flea (*Daphnia magna*) EC50: >1000 mg/L (24 h)

Toluene:

Fish Toxicity: rainbow trout (*Oncorhynchus mykiss*) LC50 (flow-through): 5.9 mg/L to 7.8 mg/L (96 h)
Invertebrate: freshwater water flea (*Daphnia magna*) EC50 (static): 5.5 mg/L to 9.8 mg/L (48 h)

Persistence and Degradability: Degradation of hexane by microorganisms.

Bioaccumulative Potential: Potentially high for hexane based on estimated BCF of 170 in fish.

Mobility in Soil: High mobility for hexane based on estimated Koc of 130.

Other Adverse effects: No data available.

13. DISPOSAL CONSIDERATIONS

Waste Disposal: Dispose of waste in accordance with all applicable federal, state, and local regulations. Subject to disposal regulations: U.S. EPA 40 CFR 262, Hazardous Waste Number: D001 (Hexane), U220 (Toluene).

14. TRANSPORTATION INFORMATION

U.S. DOT and IATA: UN1208, Hexanes, Hazard Class 3, Packing Group II, Excepted Quantities E2.

15. REGULATORY INFORMATION

U.S. Regulations:

CERCLA Sections 102a/103 (40 CFR 302.4): 5000 lbs (2270 kg) final RQ for hexane and toluene.

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 concentration for hexane and toluene.

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:	Yes.
FIRE:	Yes.
REACTIVE:	No.
PRESSURE:	No.

State Regulations:

California Proposition 65: WARNING! This product contains a chemical (toluene) known to the state of California to cause reproductive/developmental effects.

U.S. TSCA Inventory: Hexane and toluene are listed.

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

Canadian Regulations:

WHMIS Information: Not provided for this material.

16. OTHER INFORMATION

Issue Date: 06 December 2019

Sources: ChemAdvisor, Inc., SDS *n-Hexane*, 09 December 2015.

PubChem Database, U.S. National Library of Medicine, *Hexane CAS 110-54-3*, available at https://pubchem.ncbi.nlm.nih.gov/ (accessed Dec 2019).

NIOSH Pocket Guide to Chemical Hazards, *Hexane CAS 110-54-3*, available at https://www.cdc.gov/niosh/npg/npgd0322.html (accessed Dec 2019); also see *RTECS #: MN9275000*; available at https://www.cdc.gov/niosh-rtecs/MN8D8678.html (accessed Dec 2019).

ChemAdvisor, Inc., SDS *Toluene*, 09 December 2015.

PubChem Database, U.S. National Library of Medicine, *Toluene CAS 108-88-3*, available at https://pubchem.ncbi.nlm.nih.gov/ (accessed Dec 2019).

NIOSH Pocket Guide to Chemical Hazards, *Toluene CAS 108-88-3*; available at https://www.cdc.gov/niosh/npg/npgd0619.html (accessed Dec 2019); also see *RTECS #: XS5250000*; available at http://www.cdc.gov/niosh-rtecs/XS501BD0.html (accessed Dec 2019).

Key of Acronyms:

ACGIH	American Conference of Governmental Industrial Hygienists	NRC	Nuclear Regulatory Commission
ALI	Annual Limit on Intake	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
EC50	Effective Concentration, 50%	RM	Reference Material
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 Transport Association	SCBA	Self-Contained Breathing Apparatus
IDLH	Immediately Dangerous to Life and Health	SRM	Standard Reference Material
LC50	Lethal Concentration, 50 %	STEL	Short Term Exposure Limit
LD50	Lethal Dose, 50 %	TLV	Threshold Limit Value
LEL	Lower Explosive Limit	TPQ	Threshold Planning Quantity
MSDS	Material Safety Data Sheet	TSCA	Toxic Substances Control Act
NFPA	National Fire Protection Association	TWA	Time Weighted Average
NIOSH	National Institute for Occupational Safety and Health	UEL	Upper Explosive Limit
NIST	National Institute of Standards and Technology	WHMIS	Workplace Hazardous Materials Information System
n.o.s.	Not Otherwise Specified		

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 certified 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 https://www.nist.gov/srm.