SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier
NMR-SAMPLE 40% p-Dioxan in Benzol-d6 (13C SENSITIVITY ASTM-Test)

Further trade names
Z10724, Z10035, Z10163, Z10164
Z100929, Z10242, Z10255, Z10165, Z10166

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture
For R&D use only.

Uses advised against
Not for drug, household or other uses.

1.3. Details of the supplier of the safety data sheet

Company name: Bruker BioSpin AG
Street: Industriestrasse 26
Place: CH-8117 Fällanden
Telephone: +41 44 825 9111 / 9622
Telefax: +41 44 825 96 96
Internet: www.bruker.com
Responsible Department: Responsible for the safety data sheet: sds@gbk-ingelheim.de
Emergency telephone : +49 (0) 6132 / 84463 (GBK GmbH, Ingelheim)
(001) 352 323 3500 - Transport, EMTEL ID: 94135
+41 44 251 51 51 - Swiss Toxicological Information Center (24 h)

1.4. Emergency telephone number:

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture according to 1272/2008/EC

Hazard categories:
Flammable liquid: Flam. Liq. 2
Skin corrosion/irritation: Skin Irrit. 2
Serious eye damage/eye irritation: Eye Irrit. 2
Germ cell mutagenicity: Muta. 1B
Carcinogenicity: Carc. 1A
Carcinogenicity: Carc. 2
Specific target organ toxicity - single exposure: STOT SE 3
Specific target organ toxicity - repeated exposure: STOT RE 1

Hazard Statements:
Highly flammable liquid and vapour.
Causes skin irritation.
Causes serious eye irritation.
May cause respiratory irritation.
May cause genetic defects.
May cause cancer.
Suspected of causing cancer.
Causes damage to organs through prolonged or repeated exposure.

2.2. Label elements

Hazard components for labelling
benzene
1,4-dioxane

Signal word: Danger

Pictograms:
Hazard statements

H225 Highly flammable liquid and vapour.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.
H340 May cause genetic defects.
H350 May cause cancer.
H351 Suspected of causing cancer.
H372 Causes damage to organs through prolonged or repeated exposure.

Precautionary statements

P201 Obtain special instructions before use.
P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P235 Keep cool.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P308+P313 IF exposed or concerned: Get medical advice/attention.
P370+P378 In case of fire: Use water to extinguish.

SECTION 3: Composition/information on ingredients

3.2. Mixtures

Chemical characterization
CPID 259577-83

Hazardous components

<table>
<thead>
<tr>
<th>CAS No</th>
<th>Chemical name</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>71-43-2</td>
<td>benzene</td>
<td>60 %</td>
</tr>
<tr>
<td>123-91-1</td>
<td>1,4-dioxane</td>
<td>40 %</td>
</tr>
</tbody>
</table>

Full text of H and EUH statements: see section 16.

SECTION 4: First aid measures

4.1. Description of first aid measures

General information
Self-protection for first-aid personnel required! Highly flammable Toxic: danger of serious damage to health by prolonged exposure in contact with skin and if swallowed. Ensure adequate ventilation. If patient is not breathing, apply artificial respiration. Do not breathe vapour. May cause cancer. May cause heritable genetic damage. May cause liver injury and blood disorders.

After inhalation
Take affected person into fresh air. If patient is not breathing, apply artificial respiration. Seek medical treatment immediately.

After contact with skin
Wash off immediately with plenty of water for at least 15 minutes. Remove contaminated clothing immediately and dispose of safely. Seek medical treatment immediately.

After contact with eyes
Rinse immediately with plenty of water, also under the eyelids. If eye irritation persists consult a physician.

After ingestion
Do not induce vomiting. Attention, beware danger of aspiration. Rinse out mouth and give plenty of water to drink. Seek medical treatment immediately.
medical treatment immediately.

4.2. Most important symptoms and effects, both acute and delayed
Toxic: danger of serious damage to health by prolonged exposure in contact with skin and if swallowed. Irritating to eyes, respiratory system and skin.

4.3. Indication of any immediate medical attention and special treatment needed
Treat symptoms.

SECTION 5: Firefighting measures

5.1. Extinguishing media
Suitable extinguishing media
Foam, carbon dioxide (CO2), dry chemical

Unsuitable extinguishing media
No data available.

5.2. Special hazards arising from the substance or mixture
Sensitive to Static Discharge.
Burning may release the following flue gases such as: carbon monoxide (CO), carbon dioxide (CO2), Biphenyl.

5.3. Advice for firefighters
In case of fire, wear suitable respiratory equipment with positive air supply. Use personal protective clothing.

Additional information
Highly flammable Vapours are heavier than air. Formation of explosive mixtures with air. Flashbacks can occur. Closed NMR sample tubes may rupture when heated and may cause severe injury of eyes and skin. Collect contaminated firefighting water separately, must not be discharged into the drains.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures
The appropriate action is to be taken immediately if the product is spilled or leaks. Take affected person away from danger area. Ensure adequate ventilation. Avoid contact with the skin and the eyes. Do not breathe vapour. Wear self-contained breathing apparatus and protective suit.

6.2. Environmental precautions
Do not discharge into the drains/surface waters/ground water. Inform competent authority about release into the sewage, ground or into waters.

6.3. Methods and material for containment and cleaning up
Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder). Shovel into suitable container for disposal. Ensure adequate ventilation.

6.4. Reference to other sections
Information for disposal see section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling
Advice on safe handling
Handling should only be allowed by trained personnel.

Indication of danger: Highly flammable Toxic: danger of serious damage to health by prolonged exposure in contact with skin and if swallowed. Suspected of causing cancer. Mutagen. Irritant

Advice on protection against fire and explosion
Sensitive to Static Discharge.

Further information on handling
Do not open the glass tube. Avoid contact with skin, eyes and clothing. Use only in a chemical fume hood. Do not breathe vapour. Heating will cause pressure rise with risk of bursting. See also chapter: 10

7.2. Conditions for safe storage, including any incompatibilities
Requirements for storage rooms and vessels
To be kept tightly closed, in a cool and dry place. Keep away from sources of ignition - No smoking.

Advice on storage compatibility
Store separately from other hazardous and incompatible substances. See also chapter: 10
7.3. Specific end use(s)

NMR Sample

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

<table>
<thead>
<tr>
<th>CAS No</th>
<th>Substance</th>
<th>ppm</th>
<th>mg/m³</th>
<th>fibres/ml</th>
<th>Category</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>123-91-1</td>
<td>1,4-Dioxane</td>
<td>20</td>
<td>73</td>
<td></td>
<td>TWA (8 h)</td>
<td>WEL</td>
</tr>
<tr>
<td></td>
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<td></td>
<td></td>
<td></td>
<td>STEL (15 min)</td>
<td>WEL</td>
</tr>
<tr>
<td>71-43-2</td>
<td>Benzene</td>
<td>1</td>
<td>3.25</td>
<td></td>
<td>TWA (8 h)</td>
<td>WEL</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>STEL (15 min)</td>
<td>WEL</td>
</tr>
</tbody>
</table>

8.2. Exposure controls

Appropriate engineering controls

Ensure adequate ventilation, especially in confined areas. Use only in a chemical fume hood.

Protective and hygiene measures

Take the usual precautions when handling with chemicals.

Wash hands before breaks and at the end of workday. When using do not eat, drink or smoke. Avoid contact with skin, eyes and clothing. Do not breathe vapour. If you feel unwell, seek medical advice.

Workers should be trained on good working practices and informed on applicable local regulations.

Eye/face protection

In case of eye contact wear safety goggles or face protection (EN 166).

Eye wash bottle with pure water (EN 15154).

Hand protection

Chemical-resistant gloves (EN 374). Fluorocarbon rubber - Viton (0,4 mm), Nitrile rubber (recommended: minimum protection index 2, corresponding to a permeation rate > 30 minutes according to EN 374).

Follow the recommendations of the glove manufacturer for breakthrough properties especially for workplace conditions involving mechanical stress and contact duration.

Skin protection

Protective clothing.

Respiratory protection

In case of vapour / mist formation use respirator.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state: Liquid

Colour: Colourless, clear

Odour: characteristic

Changes in the physical state

Melting point: 6.8 °C *)

Initial boiling point and boiling range: 79.1 °C *)

Flash point: -11 °C *)

Explosive properties

In use, may form flammable/explosive vapour-air mixture. *)

Lower explosion limits: 1.4 vol. %

Upper explosion limits: 8 vol. %

Ignition temperature: 555 °C *)

Print date: 20.11.2015
The product is not self-igniting *)
Vapour pressure: 99.46 hPa *)
Density: 0.95 g/cm³ *)
Solubility in other solvents Organic solvent: Soluble *)

9.2. Other information
Vapor density: 2.77 g/l
*) All data refer to the solution

SECTION 10: Stability and reactivity

10.1. Reactivity
No data available.

10.2. Chemical stability
Stable under normal conditions.

10.3. Possibility of hazardous reactions
Formations of peroxides possible. Reactions with light.

10.4. Conditions to avoid
To avoid thermal decomposition, do not overheat.

10.5. Incompatible materials
Peroxides, oxidizing agents, oxygen, perchlorates, hydrides, metal salts, strong acids and strong bases.

10.6. Hazardous decomposition products
Biphenyl, carbon monoxide (CO), carbon dioxide (CO2).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity
Based on available data, the classification criteria are not met.
benzene-d₆, CAS-No.: 1076-43-3
LD₅₀/oral/rat: 930 mg/kg
LD₅₀/dermal/rabbit: > 8260 mg/kg
LC₅₀/inhalation/rat: 44 mg/l/4h

Irritation and corrosivity
Causes skin irritation.
Causes serious eye irritation.
1,4-dioxane, CAS-No.: 123-91-1
Skin irritation (rabbit): Slightly irritating.
Eyes irritation (rabbit): Severe irritant
benzene-d₆, CAS-No.: 1076-43-3
Skin irritation (rabbit): Irritant
Eyes irritation (rabbit): Severe irritant

Sensitising effects
Based on available data, the classification criteria are not met.
benzene-d₆, CAS-No.: 1076-43-3: No data available.
1,4-dioxane, CAS-No.: 123-91-1: No sensitizing effect known.

STOT-single exposure
May cause respiratory irritation. (1,4-dioxane)

Severe effects after repeated or prolonged exposure
Causes damage to organs through prolonged or repeated exposure. (benzene)

Carcinogenic/mutagenic/toxic effects for reproduction
May cause genetic defects. (benzene)
May cause cancer. (benzene)
Suspected of causing cancer. (1,4-dioxane)
benzene-d₆, CAS-No.: 1076-43-3: May cause cancer. Mutagen.
1,4-dioxane, CAS-No.: 123-91-1: May cause cancer. Repeated exposure may cause skin dryness or cracking.
Aspiration hazard
Based on available data, the classification criteria are not met.

SECTION 12: Ecological information

12.1. Toxicity
The product has not been tested. The information is derived from the properties of the individual components.
1,4-dioxane, CAS-No.: 123-91-1:
EC50: 8450 mg/l (24 h, Daphnia magna)
EC50: 2700 mg/l (16 h, Pseudomonas putida)
EC5: 5340 mg/l (72 h, Echinodontium sulphatatum)
benzene-d6, CAS-No.: 1076-43-3:
EC50: 200 mg/l (48 h, Daphnia magna)
LC50/fish: 34 mg/l (96 h, Carassius auratus)
LC50/fish: 5.3 mg/l (96 h, Oncorhynchus mykiss)
EC10: 168 mg/l (Pseudomonas putida)
IC50: 530 mg/l (Chlorella vulgaris)

12.2. Persistence and degradability
1,4-dioxane, CAS-No.: 123-91-1: < 5% / 28 d (Modif.OECD Screen.T.); Slightly biodegradable
benzene-d6, CAS-No.: 1076-43-3:
BOD: > 60 %
BODS to COD: > 50 %
DOC: > 70 %

12.3. Bioaccumulative potential
There is no indication of bioaccumulation potential.

12.4. Mobility in soil
benzene-d6, CAS-No.: 1076-43-3: Log Pow: 2.65

12.5. Results of PBT and vPvB assessment
Not determined.

12.6. Other adverse effects
No data available.

Further information
Do not flush into surface water or sanitary sewer system.

SECTION 13: Disposal considerations

13.1. Waste treatment methods
Advice on disposal
Do not flush into surface water or sanitary sewer system. This product is to be brought to a properly certified waste site approved to handle energy wastes.

Waste disposal number of waste from residues/unused products
160506 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; gases in pressure containers and discarded chemicals; laboratory chemicals, consisting of or containing hazardous substances, including mixtures of laboratory chemicals
Classified as hazardous waste.

Waste disposal number of contaminated packaging
150107 WASTE PACKAGING; ABSORBENTS, WIPE CLOTHS, FILTER MATERIALS AND PROTECTIVE CLOTHING NOT OTHERWISE SPECIFIED; packaging (including separately collected municipal packaging waste); glass packaging

Contaminated packaging
Disposal in accordance with local regulations.

SECTION 14: Transport information

Land transport (ADR/RID)

14.1. UN number:
UN 1993

14.2. UN proper shipping name:
FLAMMABLE LIQUID, N.O.S. (benzene-d6, 1,4-dioxane, mixture)
14.3. Transport hazard class(es): II
14.4. Packing group: 3
Hazard label: F1

Special Provisions: 274 601 640C
Limited quantity: 1 L
Excepted quantity: E2
Transport category: 2
Hazard No: 33
Tunnel restriction code: D/E

Inland waterways transport (ADN)
14.1. UN number: UN 1993
14.2. UN proper shipping name: FLAMMABLE LIQUID, N.O.S. (benzene-d6, 1,4-dioxane, mixture)
14.3. Transport hazard class(es): II
14.4. Packing group: 3
Hazard label: F1

Special Provisions: 274 601 640C
Limited quantity: 1 L
Excepted quantity: E2

Marine transport (IMDG)
14.1. UN number: UN 1993
14.2. UN proper shipping name: FLAMMABLE LIQUID, N.O.S. (benzene-d6, 1,4-dioxane, mixture)
14.3. Transport hazard class(es): II
14.4. Packing group: 3
Hazard label: A3

Special Provisions: 274
Limited quantity: 1 L
Excepted quantity: E2
EmS: F-E, S-E

Air transport (ICAO)
14.1. UN number: UN 1993
14.2. UN proper shipping name: FLAMMABLE LIQUID, N.O.S. (benzene-d6, 1,4-dioxane, mixture)
14.3. Transport hazard class(es): II
14.4. Packing group: 3
Hazard label: A3

Special Provisions: A3
Limited quantity Passenger: 1 L
NMR-SAMPLE 40% p-Dioxan in Benzol-d6 (13C SENSITIVITY ASTM-Test)

Passenger LQ: Y341
Excepted quantity: E2
IATA-packing instructions - Passenger: 353
IATA-max. quantity - Passenger: 5 L
IATA-packing instructions - Cargo: 364
IATA-max. quantity - Cargo: 60 L

14.5. Environmental hazards
ENVIRONMENTALLY HAZARDOUS: no

14.6. Special precautions for user
Handle in accordance with good industrial hygiene and safety practice.

14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code
The transport takes place only in approved and appropriate packaging.

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulatory information
Additional information
The product is labeled in accordance with Regulation (EC) no. 1272/2008 (GHS).

National regulatory information

15.2. Chemical safety assessment
For this substance a chemical safety assessment has not been carried out.

SECTION 16: Other information

Changes
Section 8, 13, 14, 15.

Abbreviations and acronyms
ADR = Accord européen relatif au transport international des marchandises Dangereuses par Route
RID = Règlement concernant le transport international ferroviaire de marchandises dangereuses
ADN = Accord européen relatif au transport international des marchandises dangereuses par voie de navigation intérieure
IMDG = International Maritime Code for Dangerous Goods
IATA/ICAO = International Air Transport Association / International Civil Aviation Organization
MARPOL = International Convention for the Prevention of Pollution from Ships
IBC-Code = International Code for the Construction and Equipment of Ships Carrying Dangerous Chemicals in Bulk
GHS = Globally Harmonized System of Classification and Labelling of Chemicals
REACH = Registration, Evaluation, Authorization and Restriction of Chemicals
CAS = Chemical Abstract Service
EN = European norm
ISO = International Organization for Standardization
DIN = Deutsche Industrie Norm
PBT = Persistent Bioaccumulative and Toxic
vPvB = Very Persistent and very Bio-accumulative
LD = Lethal dose
LC = Lethal concentration
EC = Effect concentration
IC = Median immobilisation concentration or median inhibitory concentration

Relevant H and EUH statements (number and full text)
H225 Highly flammable liquid and vapour.
H304 May be fatal if swallowed and enters airways.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.
H340 May cause genetic defects.
H350 May cause cancer.
Further Information

Data of items 4 to 8, as well as 10 to 12, do partly not refer to the use and the regular employing of the product (in this sense consult information on use and on product), but to liberation of major amounts in case of accidents and irregularities.

The information describes exclusively the safety requirements for the product(s) and is based on the present level of our knowledge.

The delivery specifications are contained in the corresponding product sheet.

This data does not constitute a guarantee for the characteristics of the product(s) as defined by the legal warranty regulations.

(n.a. = not applicable; n.d. = not determined)

(Information about the composition are based on information from the sub-contractor)

(The data for the hazardous ingredients were taken respectively from the last version of the sub-contractor's safety data sheet.)