

# SAFETY DATA SHEET

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

## 1.1 Product identifiers

Product Number:	D0502
Product name:	Ohira-Bestmann Reagent solution(~10% in acetonitrile)
CAS Registry Nr:	90965-06-3

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

Laboratory chemicals, Manufacture of substances.

## 1.3 Details of the supplier of the safety data sheet

Company:	Chemodex AG	
	CH - 9000 St. Gallen	
	Switzerland, Europe	
	Tel: +41 71 244 48 25	
	Fax: +41 71 244 48 26	
	Email: info@chemodex.com	
	Website: www.chemodex.com	

## 1.4 Emergency telephone number

Tox Info Suisse: +41 44 251 51 51
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## **SECTION 2: Hazards identification**

2.1 Classification of the substance or mixture

#### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 2)	H225	
Acute toxicity, Oral (Category 4)	H302	
Acute toxicity, Inhalation (Category 4)	H332	
Eye irritation (Category 2A)	H319	
For the full text of the H-Statements mentioned in this Section, see Section 16.		

# 2.2 GHS Label elements, including precautionary statements

Pictogram	
Signal word	Danger

## Hazard statement(s)

H225	Highly flammable liquid and vapour.	
H302 + H332	Harmful if swallowed 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.		
P240	Ground/bond container and receiving equipment.		
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.		
P242	Use only non-sparking tools.		
P243	Take precautionary measures against static discharge.		
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.		
P264	Wash skin thoroughly after handling.		
P270	Do not eat, drink or smoke when using this product.		
P271	Use only outdoors or in a well-ventilated area.		
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.		
P301 + P312	IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell.		
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.		
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.		
P312	Call a POISON CENTER or doctor/ physician if you feel unwell.		
P330	Rinse mouth.		
P337 + P313	If eye irritation persists: Get medical advice/ attention.		
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.		
P403 + P235	Store in a well-ventilated place. Keep cool.		
P501	Dispose of contents/ container to an approved waste disposal plant.		

# 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

# SECTION 3: Composition/information on ingredients

3.2 Mixtures

Formula:	C5H9N2O4P
Molecular weight:	192.11 g/mol

## Hazardous components

Component		Classification	Concentration		
Acetonitrile					
CAS-No.	75-05-8	Flam. Liq. 2; Acute	90 - 100 %		
EC-No.	200-835-2	Tox. 4; Eye Irrit. 2A;			
Index-No.	608-001-00-3	H225, H302 + H312 +			
Registration number	01-2119471307-38-XXXX	H332, H319			

For the full text of the H-Statements mentioned in this Section, see Section 16.

## **SECTION 4: First aid measures**

4.1 Description of first aid measures

#### **General advice**

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

## If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

# In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

## If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

#### 4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

#### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

## **SECTION 5: Firefighting measures**

## 5.1 Extinguishing media

Suitable extinguishing media Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

#### 5.2 Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NOx), Oxides of phosphorus

#### 5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

## **SECTION 6: Accidental release measures**

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas. For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

## 6.3 Methods and material for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections

For disposal see section 13.

## **SECTION 7: Handling and storage**

## 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Use explosion-proof equipment.Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

#### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Recommended storage temperature 2 - 8 °C

#### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

## **SECTION 8: Exposure controls/personal protection**

## 8.1 Control parameters

## Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Acetonitrile	75-05-8	TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Lower Respiratory Tract irritation Not classifiable as a human carcinogen Danger of cutaneous absorption		
		TWA	20 ppm 34 mg/m3	USA. NIOSH Recommended Exposure Limits
		Forms cyanide in the body.		
		TWA	40 ppm 70 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	40 ppm 70 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	60 ppm 105 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000

#### 8.2 Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

#### Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

#### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

#### **Body Protection**

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### **Respiratory protection**

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multipurpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air

respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

## Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

## **SECTION 9: Physical and chemical properties**

9.1 Information on basic physical and chemical properties

a)	Appearance:	Form: Liquid
b)	Odour:	pungent
C)	Odour Threshold:	No data available
d)	pH:	No data available
e)	Melting point/freezing point:	No data available
f)	Initial boiling point and boiling range	No data available
g)	Flash point:	No data available
h)	Evaporation rate:	No data available
i)	Flammability (solid, gas):	No data available
j)	Upper/lower flammability or	
	explosive limits:	No data available
k)	Vapour pressure:	No data available
I)	Vapour density:	No data available
m)	Relative density:	No data available
n)	Water solubility:	No data available
o)	Partition coefficient (n-	
	octanol/water):	No data available
p)	Auto-ignition temperature:	No data available
q)	Decomposition temperature:	No data available
r)	Viscosity:	No data available
s)	Explosive properties:	No data available
t)	Oxidizing properties:	No data available

## 9.2 Other safety information

No data available

## **SECTION 10: Stability and reactivity**

## 10.1 Reactivity

No data available

## 10.2 Chemical stability

Stable under recommended storage conditions.

#### 10.3 Possibility of hazardous reactions

Vapours may form explosive mixture with air.

10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials

acids, Bases, Oxidizing agents, Reducing agents, Alkali metals

10.6 Hazardous decomposition products

Other decomposition products - No data available In the event of fire: see section 5

## **SECTION 11: Toxicological information**

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male - 1,320 - 6,690 mg/kg (Acetonitrile)
LC50 Inhalation - Mouse - 4 h - 3587 ppm (Acetonitrile)
(OECD Test Guideline 403)
LC50 Inhalation - Rat - 4 h - 26.8 mg/l (Acetonitrile)
LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg (Acetonitrile)
(OECD Test Guideline 402)
No data available (Acetonitrile)
Skin corrosion/irritation
Skin - Rabbit (Acetonitrile)
Result: No skin irritation
(OECD Test Guideline 404)
Serious eye damage/eye irritation
Eyes - Rabbit (Acetonitrile)
Result: Irritating to eyes. (OECD Test Guideline 405)
Respiratory or skin sensitisation
Buehler Test - Guinea pig (Acetonitrile)
Did not cause sensitisation on laboratory animals.
(OECD Test Guideline 406)
Germ cell mutagenicity
Hamster (Acetonitrile)
ovary
Result: negative
Mutation in mammalian somatic cells.
Ames test (Acetonitrile)
S. typhimurium
Result: Not mutagenic in Ames Test.

Hamster (Acetonitrile) ovary Result: Equivocal evidence. Sister chromatid exchange Mutagenicity (micronucleus test) (Acetonitrile) Mouse Result: Positive results were obtained in some in vivo tests. Carcinogenicity No evidence of carcinogenicity in animal studies. (Acetonitrile) IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC. NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP. OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA. **Reproductive toxicity** No data available (Acetonitrile) Animal testing did not show any effects on fertility. (Acetonitrile) Specific target organ toxicity - single exposure The substance or mixture is not classified as specific target organ toxicant, single exposure. (Acetonitrile) Specific target organ toxicity - repeated exposure The substance or mixture is not classified as specific target organ toxicant, repeated exposure. Aspiration hazard No aspiration toxicity classification (Acetonitrile) Additional Information **RTECS: Not available** Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhoea, Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness, impaired judgment, Lack of coordination, stupor, death (Acetonitrile) Lungs - Lung oedema - Based on Human Evidence

## **SECTION 12: Ecological information**

12.1 Toxicity

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 1,640.00 mg/l - 96 h (Acetonitrile) NOEC - Oryzias latipes - 102 mg/l - 21 d (Acetonitrile)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 3,600 mg/l - 48 h (Acetonitrile) (OECD Test Guideline 202) NOEC - Daphnia magna (Water flea) - 160 mg/l - 21 d (Acetonitrile)

#### 12.2 Persistence and degradability

Biodegradability	Result: 84 % - Readily biodegradable.
	(OECD Test Guideline 301C)

#### 12.3 Bioaccumulative potential

No bioaccumulation is to be expected (log Pow  $\leq 4$ ).

## 12.4 Mobility in soil

Not expected to adsorb on soil. (Acetonitrile)

## 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

## 12.6 Other adverse effects

Avoid release to the environment.		
Stability in water	(Acetonitrile)	
	Remarks: Hydrolyses slowly.	

## **SECTION 13: Disposal considerations**

## 13.1 Waste treatment methods

## Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. **Contaminated packaging** 

Dispose of as unused product.

## **SECTION 14: Transport information**

## DOT (US)

UN number: 1648	Class: 3 Packing group: II	
Proper shipping name:	Acetonitrile, solution	
Reportable Quantity (RQ):	5556 lbs	
Marine pollutant:	No	
Poison Inhalation Hazard:	No	

## IMDG

UN number: 1648	Class: 3	Packing group: EMS-No:	ll F-E, S-D
Proper shipping name:	ACETONITRILE, SOLUT	ΓΙΟΝ	
Marine pollutant:	No		

## ΙΑΤΑ

UN number: 1648	Class: 3	Packing group: II
Proper shipping name:	Acetonitrile, solution	

## **SECTION 15: Regulatory information**

## SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

## SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313: Acetonitrile CAS-No. 75-05-8 Revision Date 2007-07-01

## SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

## **Massachusetts Right To Know Components**

Acetonitrile CAS-No. 75-05-8 Revision Date 2007-07-01

## Pennsylvania Right To Know Components

Acetonitrile CAS-No. 75-05-8 Dimethyl (1-diazo-2-oxopropyl)phosphonate CAS-No. 90965-06-3 Revision Date 2007-07-01

## New Jersey Right To Know Components

Acetonitrile CAS-No. 75-05-8 Dimethyl (1-diazo-2-oxopropyl)phosphonate CAS-No. 90965-06-3 Revision Date 2007-07-01

## California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

## **SECTION 16: Other information**

## Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H302	Harmful if swallowed.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled
H319	Causes serious eye irritation.
H332	Harmful if inhaled.

## **HMIS Rating**

Health hazard: 2 Chronic Health Hazard: \* Flammability: 3 Physical Hazard 0

## **NFPA Rating**

Health hazard: 2 Fire Hazard: 3 Reactivity Hazard: 0

## **Further information**

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