

Safety data sheet
according to 1907/2006/EC, Article 31

Printing date 31.07.2016

Revision: 31.07.2016

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

· **1.1 Product identifier**

· **Trade name:** 1,5-cyclooctadiene{(4S)-(-)-2-[(5R)-6-(diphenylphosphino)spiro[4.4]nona-1.6-dien-1-yl]-4,5-dihydro-4-phenyloxazole}iridium(I) tetrakis[3,5-bis(trifluoromethyl)phenyl]borate, 97% (R,S)-(COD)Ir[Ph-SpinPHOX]

· **Item number:** 77-5047

· **CAS Number:**

1195511-59-1

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

No further relevant information available.

· **1.3 Details of the supplier of the safety data sheet**

· **Manufacturer/Supplier:**

Strem Chemicals, Inc.

7 Mulliken Way

NEWBURYPORT, MA 01950

USA

info@strem.com

· **Further information obtainable from:** Technical Department

· **1.4 Emergency telephone number:**

EMERGENCY: CHEMTREC: + 1 (800) 424-9300

During normal opening times: +1 (978) 499-1600

SECTION 2: Hazards identification

· **2.1 Classification of the substance or mixture**

· **Classification according to Regulation (EC) No 1272/2008**



GHS07

Skin Irrit. 2 H315 Causes skin irritation.

Eye Irrit. 2 H319 Causes serious eye irritation.

STOT SE 3 H335 May cause respiratory irritation.

· **2.2 Label elements**

· **Labelling according to Regulation (EC) No 1272/2008**

The substance is classified and labelled according to the CLP regulation.

· **Hazard pictograms**



GHS07

· **Signal word** Warning

· **Hazard-determining components of labelling:**

1,5-cyclooctadiene{(4S)-(-)-2-[(5R)-6-(diphenylphosphino)spiro[4.4]nona-1.6-dien-1-yl]-4,5-dihydro-4-phenyloxazole}iridium(I) tetrakis[3,5-bis(trifluoromethyl)phenyl]borate, 97%

· **Hazard statements**

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

(Contd. on page 2)

Safety data sheet
according to 1907/2006/EC, Article 31

Printing date 31.07.2016

Revision: 31.07.2016

Trade name: 1,5-cyclooctadiene{(4S)-(-)-2-[(5R)-6-(diphenylphosphino)spiro[4.4]nona-1.6-dien-1-yl]-4,5-dihydro-4-phenyloxazole}iridium(I) tetrakis[3,5-bis(trifluoromethyl)phenyl]borate, 97% (R,S)-(COD)Ir[Ph-SpinPHOX]

(Contd. of page 1)

· **Precautionary statements**

- P101 *If medical advice is needed, have product container or label at hand.*
- P102 *Keep out of reach of children.*
- P103 *Read label before use.*
- P231 *Handle under inert gas.*
- P222 *Do not allow contact with air.*
- P305+P351+P338 *IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.*
- P403+P233 *Store in a well-ventilated place. Keep container tightly closed.*
- P422 *Store contents under inert gas.*
- P501 *Dispose of contents/container in accordance with local/regional/national/international regulations.*

· **2.3 Other hazards**

· **Results of PBT and vPvB assessment**

- **PBT:** Not applicable.
- **vPvB:** Not applicable.

SECTION 3: Composition/information on ingredients

· **3.1 Chemical characterisation: Substances**

· **CAS No. Description**

1195511-59-1 1,5-cyclooctadiene{(4S)-(-)-2-[(5R)-6-(diphenylphosphino)spiro[4.4]nona-1.6-dien-1-yl]-4,5-dihydro-4-phenyloxazole}iridium(I) tetrakis[3,5-bis(trifluoromethyl)phenyl]borate, 97%

SECTION 4: First aid measures

· **4.1 Description of first aid measures**

- **After inhalation:** In case of unconsciousness place patient stably in side position for transportation.
- **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
- **After eye contact:**
Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.
- **After swallowing:** If symptoms persist consult doctor.
- **4.2 Most important symptoms and effects, both acute and delayed** No further relevant information available.
- **4.3 Indication of any immediate medical attention and special treatment needed**
No further relevant information available.

SECTION 5: Firefighting measures

· **5.1 Extinguishing media**

· **Suitable extinguishing agents:**

CO₂, powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

· **5.2 Special hazards arising from the substance or mixture** No further relevant information available.

· **5.3 Advice for firefighters**

- **Protective equipment:** No special measures required.

GB

(Contd. on page 3)

Safety data sheet
according to 1907/2006/EC, Article 31

Printing date 31.07.2016

Revision: 31.07.2016

Trade name: 1,5-cyclooctadiene{(4S)-(-)-2-[(5R)-6-(diphenylphosphino)spiro[4.4]nona-1.6-dien-1-yl]-4,5-dihydro-4-phenyloxazole}iridium(I) tetrakis[3,5-bis(trifluoromethyl)phenyl]borate, 97% (R,S)-(COD)Ir[Ph-SpinPHOX]

(Contd. of page 2)

SECTION 6: Accidental release measures

- **6.1 Personal precautions, protective equipment and emergency procedures** Not required.
- **6.2 Environmental precautions:** No special measures required.
- **6.3 Methods and material for containment and cleaning up:**
Dispose contaminated material as waste according to item 13.
Ensure adequate ventilation.
- **6.4 Reference to other sections**
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

SECTION 7: Handling and storage

- **7.1 Precautions for safe handling** Open and handle receptacle with care.
- **Handling:** Handle under inert gas.
- **Information about fire - and explosion protection:** No special measures required.
- **7.2 Conditions for safe storage, including any incompatibilities**
- **Storage:** Store contents under inert gas.
- **Requirements to be met by storerooms and receptacles:** No special requirements.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:** Keep container tightly sealed.
- **7.3 Specific end use(s)** No further relevant information available.

SECTION 8: Exposure controls/personal protection

- **Additional information about design of technical facilities:** No further data; see item 7.
- **8.1 Control parameters**
- **Ingredients with limit values that require monitoring at the workplace:** Not required.
- **Additional information:** The lists valid during the making were used as basis.
- **8.2 Exposure controls**
- **Personal protective equipment:**
- **General protective and hygienic measures:**
Keep away from foodstuffs, beverages and feed.
Immediately remove all soiled and contaminated clothing
Wash hands before breaks and at the end of work.
Avoid contact with the eyes and skin.
- **Respiratory protection:**
In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use self-contained respiratory protective device.
- **Protection of hands:**



Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

(Contd. on page 4)

Safety data sheet
according to 1907/2006/EC, Article 31

Printing date 31.07.2016

Revision: 31.07.2016

Trade name: 1,5-cyclooctadiene{(4S)-(-)-2-[(5R)-6-(diphenylphosphino)spiro[4.4]nona-1.6-dien-1-yl]-4,5-dihydro-4-phenyloxazole}iridium(I) tetrakis[3,5-bis(trifluoromethyl)phenyl]borate, 97% (R,S)-(COD)Ir[Ph-SpinPHOX]

(Contd. of page 3)

Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

· **Material of gloves**

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

· **Penetration time of glove material**

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

· **Eye protection:**



Tightly sealed goggles

· **9.1 Information on basic physical and chemical properties**

· **General Information**

· **Appearance:**

Form:	Powder
Colour:	Red
Odour:	Odourless
Odour threshold:	Not determined.

· **pH-value:** Not applicable.

· **Change in condition**

Melting point/Melting range:	172-174 °C
Boiling point/Boiling range:	Undetermined.

· **Flash point:** Not applicable.

· **Flammability (solid, gaseous):** Not determined.

· **Ignition temperature:**

Decomposition temperature: Not determined.

· **Self-igniting:** Not determined.

· **Danger of explosion:** Product does not present an explosion hazard.

· **Explosion limits:**

Lower:	Not determined.
Upper:	Not determined.

· **Vapour pressure:** Not applicable.

· **Density:** Not determined.

· **Relative density:** Not determined.

· **Vapour density:** Not applicable.

· **Evaporation rate:** Not applicable.

· **Solubility in / Miscibility with water:** Insoluble.

· **Partition coefficient (n-octanol/water):** Not determined.

· **Viscosity:**

Dynamic: Not applicable.

(Contd. on page 5)

Safety data sheet
according to 1907/2006/EC, Article 31

Printing date 31.07.2016

Revision: 31.07.2016

Trade name: 1,5-cyclooctadiene{(4S)-(-)-2-[(5R)-6-(diphenylphosphino)spiro[4.4]nona-1.6-dien-1-yl]-4,5-dihydro-4-phenyloxazole}iridium(I) tetrakis[3,5-bis(trifluoromethyl)phenyl]borate, 97% (R,S)-(COD)Ir[Ph-SpinPHOX]

(Contd. of page 4)

Kinematic:	Not applicable.
· Solvent content:	
Organic solvents:	0.0 %
VOC (EC)	0.00 %
· 9.2 Other information	No further relevant information available.

SECTION 10: Stability and reactivity

- **10.1 Reactivity** No further relevant information available.
- **10.2 Chemical stability**
- **Thermal decomposition / conditions to be avoided:** No decomposition if used according to specifications.
- **10.3 Possibility of hazardous reactions** No dangerous reactions known.
- **10.4 Conditions to avoid** No further relevant information available.
- **10.5 Incompatible materials:** No further relevant information available.
- **10.6 Hazardous decomposition products:** No dangerous decomposition products known.

SECTION 11: Toxicological information

- **11.1 Information on toxicological effects**
- **Acute toxicity** Based on available data, the classification criteria are not met.
- **Primary irritant effect:**
- **Skin corrosion/irritation**
Causes skin irritation.
- **Serious eye damage/irritation**
Causes serious eye irritation.
- **Respiratory or skin sensitisation** Based on available data, the classification criteria are not met.
- **CMR effects (carcinogenicity, mutagenicity and toxicity for reproduction)**
- **Germ cell mutagenicity** Based on available data, the classification criteria are not met.
- **Carcinogenicity** Based on available data, the classification criteria are not met.
- **Reproductive toxicity** Based on available data, the classification criteria are not met.
- **STOT-single exposure**
May cause respiratory irritation.
- **STOT-repeated exposure** Based on available data, the classification criteria are not met.
- **Aspiration hazard** Based on available data, the classification criteria are not met.

SECTION 12: Ecological information

- **12.1 Toxicity**
- **Aquatic toxicity:** No further relevant information available.
- **12.2 Persistence and degradability** No further relevant information available.
- **12.3 Bioaccumulative potential** No further relevant information available.
- **12.4 Mobility in soil** No further relevant information available.
- **Additional ecological information:**
- **General notes:** Not known to be hazardous to water.
- **12.5 Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.

(Contd. on page 6)

Safety data sheet
according to 1907/2006/EC, Article 31

Printing date 31.07.2016

Revision: 31.07.2016

Trade name: 1,5-cyclooctadiene{(4S)-(-)-2-[(5R)-6-(diphenylphosphino)spiro[4.4]nona-1.6-dien-1-yl]-4,5-dihydro-4-phenyloxazole}iridium(I) tetrakis[3,5-bis(trifluoromethyl)phenyl]borate, 97% (R,S)-(COD)Ir[Ph-SpinPHOX]

(Contd. of page 5)

· **12.6 Other adverse effects** No further relevant information available.

SECTION 13: Disposal considerations

- **13.1 Waste treatment methods**
- **Recommendation**
Must not be disposed together with household garbage. Do not allow product to reach sewage system.
- **Uncleaned packaging:**
- **Recommendation:** Disposal must be made according to official regulations.

SECTION 14: Transport information

- | | |
|--|-----------------|
| · 14.1 UN-Number | |
| · ADR, ADN, IMDG, IATA | not regulated |
| · 14.2 UN proper shipping name | |
| · ADR, ADN, IMDG, IATA | not regulated |
| · 14.3 Transport hazard class(es) | |
| · ADR, ADN, IMDG, IATA | |
| · Class | not regulated |
| · 14.4 Packing group | |
| · ADR, IMDG, IATA | not regulated |
| · 14.5 Environmental hazards: | |
| · Marine pollutant: | No |
| · 14.6 Special precautions for user | Not applicable. |
| · 14.7 Transport in bulk according to Annex II of Marpol and the IBC Code | Not applicable. |
| · UN "Model Regulation": | not regulated |

SECTION 15: Regulatory information

- **15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**
- **Directive 2012/18/EU**
- **Named dangerous substances - ANNEX I** Substance is not listed.
- **15.2 Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

SECTION 16: Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

- **Department issuing MSDS:** Technical Department.
- **Contact:** Technical Director

(Contd. on page 7)

Safety data sheet
according to 1907/2006/EC, Article 31

Printing date 31.07.2016

Revision: 31.07.2016

Trade name: 1,5-cyclooctadiene{(4S)-(-)-2-[(5R)-6-(diphenylphosphino)spiro[4.4]nona-1.6-dien-1-yl]-4,5-dihydro-4-phenyloxazole}iridium(I) tetrakis[3,5-bis(trifluoromethyl)phenyl]borate, 97% (R,S)-(COD)Ir[Ph-SpinPHOX]

(Contd. of page 6)

· Abbreviations and acronyms:

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

GHS: Globally Harmonised System of Classification and Labelling of Chemicals

CAS: Chemical Abstracts Service (division of the American Chemical Society)

VOC: Volatile Organic Compounds (USA, EU)

PBT: Persistent, Bioaccumulative and Toxic

vPvB: very Persistent and very Bioaccumulative

Skin Irrit. 2: Skin corrosion/irritation, Hazard Category 2

Eye Irrit. 2: Serious eye damage/eye irritation, Hazard Category 2

STOT SE 3: Specific target organ toxicity - Single exposure, Hazard Category 3

GB