Eco-friendly oxidizing reagent

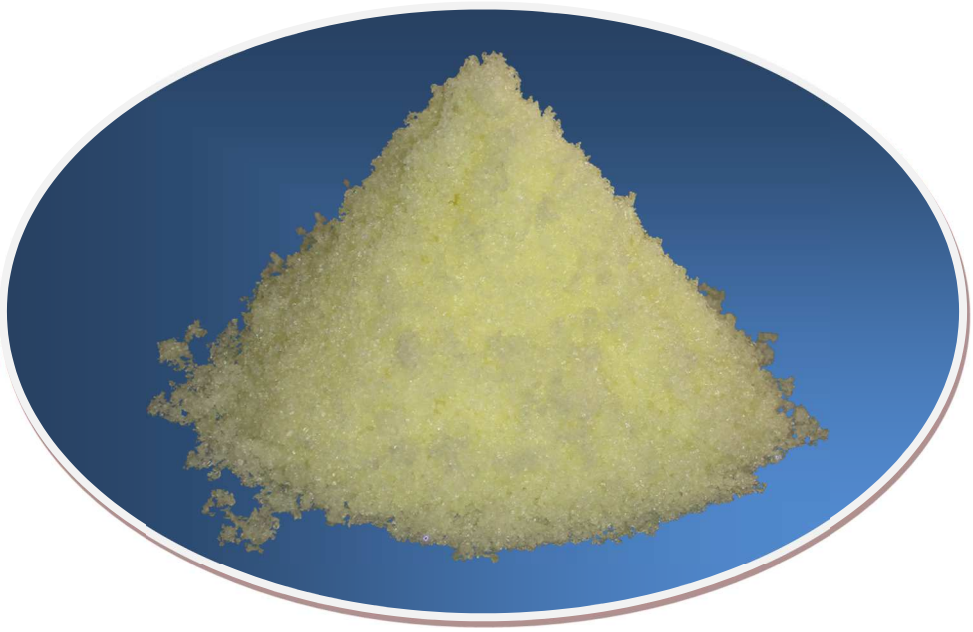
The world's first industrial production !

SHC5®

Sodium HypoChlorite Pentahydrate (5)

$NaClO \cdot 5H_2O$

Technical Data



日本軽金属株式会社
Nippon Light Metal Co., Ltd.

Notable features of SHC5®

(1) High concentration

- High volumetric efficiency leads to better productivity and waste water reduction.

(2) High purity

- The oxidizing reagent containing minimal amounts of NaCl and NaOH.

(3) High stability

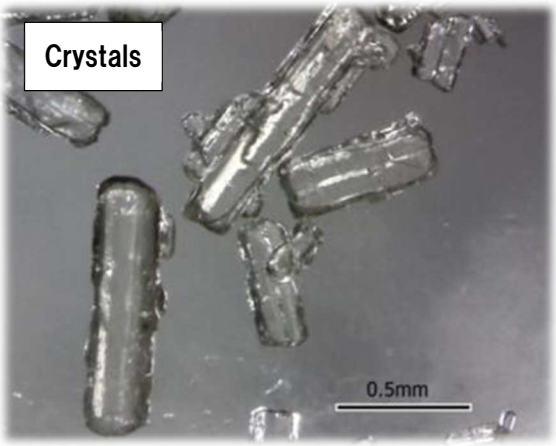
- Stable for 1 year below 7℃ in a sealing and lightproof container.

(4) Adjustable to highly concentrated aqueous solution

- Easy to prepare any concentration of aqueous solution at room temperature (approx. ≦30%).

(5) Applicable to organic synthesis

- Alcohol and sulfide can be oxidized selectively.
- Various oxidation reactions are possible for both homogeneous and heterogeneous systems.



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～What is sodium hypochlorite pentahydrate (SHC5®) ?～

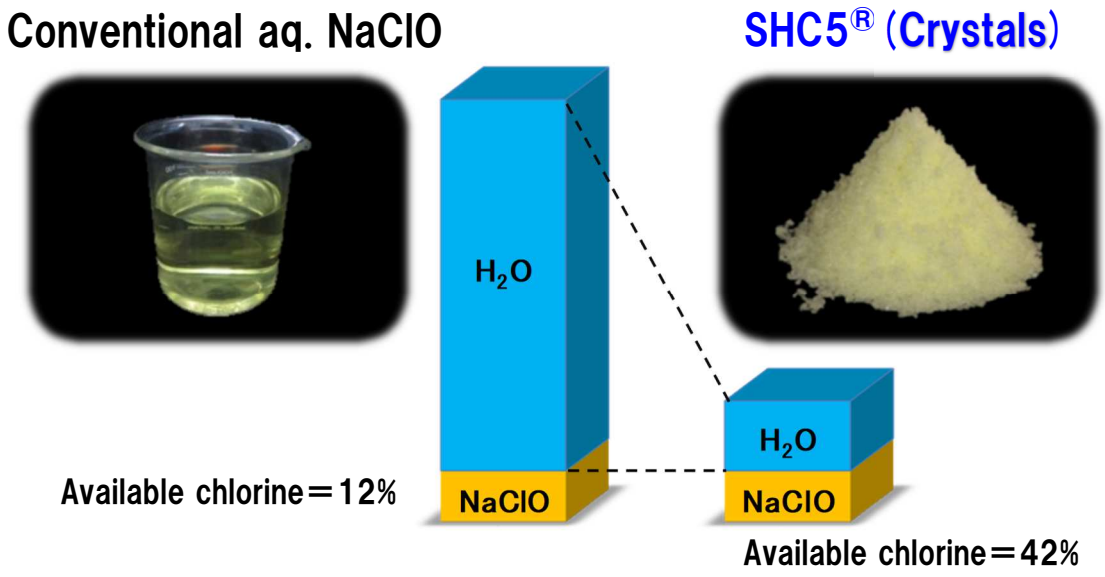
Although the existence of "sodium hypochlorite pentahydrate" has been known for a long time, only aqueous solution of about 12% has been industrially available. Nippon Light Metal Company has succeeded in producing sodium hypochlorite pentahydrate in industrial scale for the first time in the world and launched a new product in 2013, under the name of "SHC5®" which is abbreviated name of **S**odium **H**ypo**C**hlorite Penta (**5**) hydrate. SHC5® has higher volumetric efficiency compared with conventional aqueous solution and it has been revealed that SHC5® shows a unique reactivity in organic reactions.

1. Notable features of SHC5®

(1) High concentration

- The available chlorine concentration of SHC5® is 42% (44% as NaClO), while that of conventional aqueous sodium hypochlorite solution is 12%.
- SHC5® is about 3.5 times higher in concentration ratio.
- Significant waste reduction is achievable.

< Comparison of conventional aq. NaClO solution with SHC5® under the same molar condition >



✔Volume decreased to approx.1/3

✔Waste decreased to approx.1/5

(2) High purity

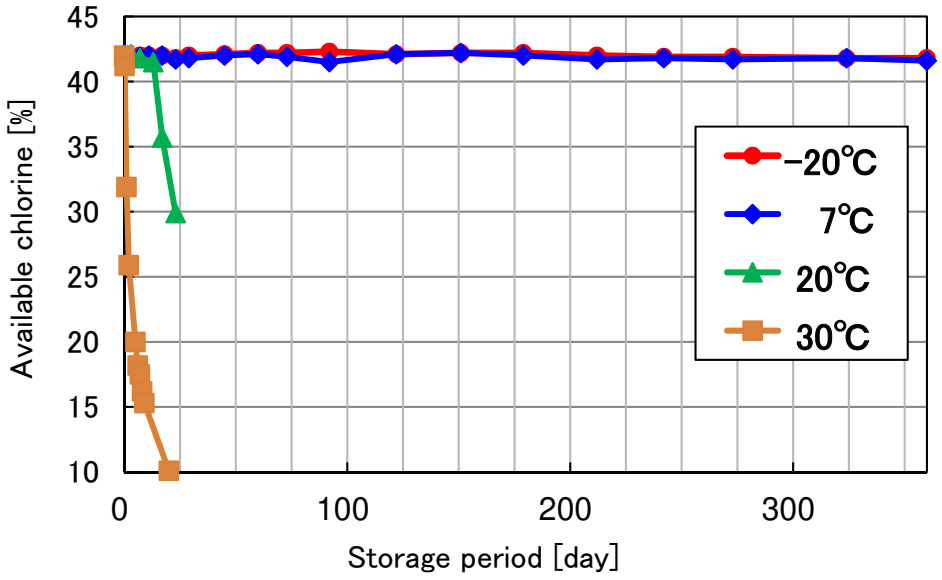
- SHC5® prepared by our patented manufacturing process is a high-purity product with reduced NaOH, NaCl, $NaClO_3$, $NaBrO_3$ and metal impurities such as iron and chromium.

※ Conventional aqueous NaClO solution is prepared by introducing chlorine gas (Cl_2) into aqueous sodium hydroxide (NaOH) solution. It essentially contains sodium chloride (NaCl) produced during manufacturing process and various impurities derived from raw materials.

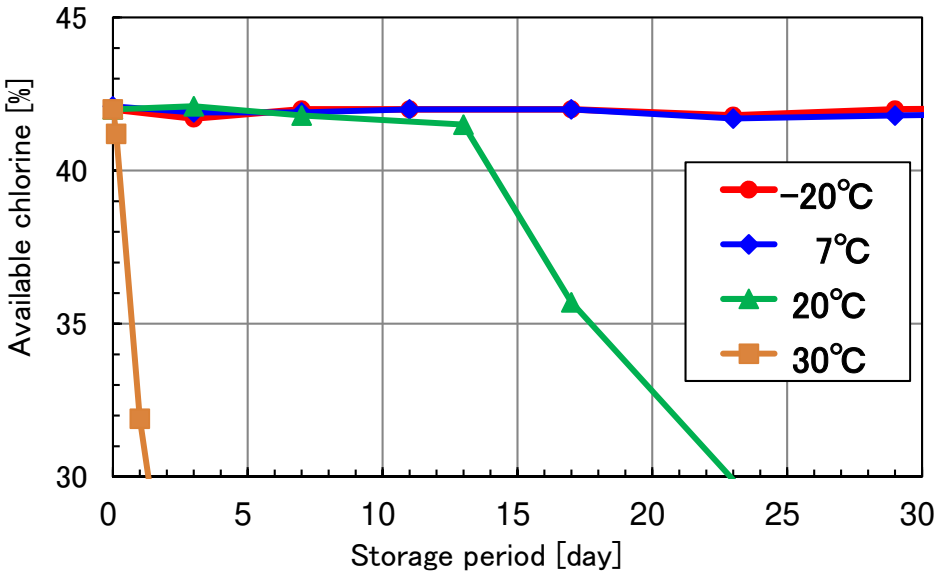
(3) High stability

- SHC5® is stable for 1 year below 7℃ in a tightly sealed plastic container stored in the dark.
- High available chlorine concentration is maintained for about 1 week at 20℃, but decomposition accelerates and produces sodium chloride and sodium chlorate ($NaClO_3$) ※ during prolonged storage. It decomposes markedly in the molten state (30℃).

※ Decomposition of SHC5® produces sodium chlorate ($NaClO_3$) which violently reacts in contact with organic materials, sulfur and metal powder. SHC5® should be kept away from them. Make sure to seal tightly and store below 7℃ in the dark.



Stability of SHC5®



Stability of SHC5® (Enlarged figure of 30 days)

2. Chemical and physical properties

Chemical property

	Chemical components	SHC5®	Conventional aq. NaClO soln.
Specification	Available chlorine※ [%] (Typical value)	≧39.0 (42.0)	≧12.0 (12.8)
	Aqueous solution	Pale yellow transparent	-
Composition	NaOH [%]	0.05	0.8
	NaCl [%]	0.12	12.4
	$NaClO_3$ [%]	0.05	0.9
	$NaBrO_3$ [%]	0.005	0.01

※ The concentration of available chlorine can be calculated by converting the weight percent of sodium hypochlorite into its equivalent as chlorine molecule shown in the following equation. One molecule of sodium hypochlorite corresponds to one molecule of chlorine.

$$\text{Available chlorine concentration} = \frac{\text{Molecular weight of chlorine (70.9)}}{\text{Molecular weight of sodium hypochlorite (74.4)}} \times \text{weight percent of NaClO}$$

$$= 0.95 \times \text{weight percent of NaClO}$$

Physical property

	SHC5®	Conventional aq. NaClO soln.
Molecular formula	$NaClO \cdot 5H_2O$	NaClO
Molecular weight	164.52	74.44
Appearance	Pale yellow crystals	Pale yellow liquid
Density [g/cm³]	-	1.1-1.2
Untapped bulk density [g/cm³]	0.8	-
Solubility	Insoluble in organic solvent※	-
Heat of dissolution [J/g]	293 (Endothermic)	-
Melting point [℃]	25-27	-

※ Alcohol is not suitable for solvent as it reacts with SHC5®.

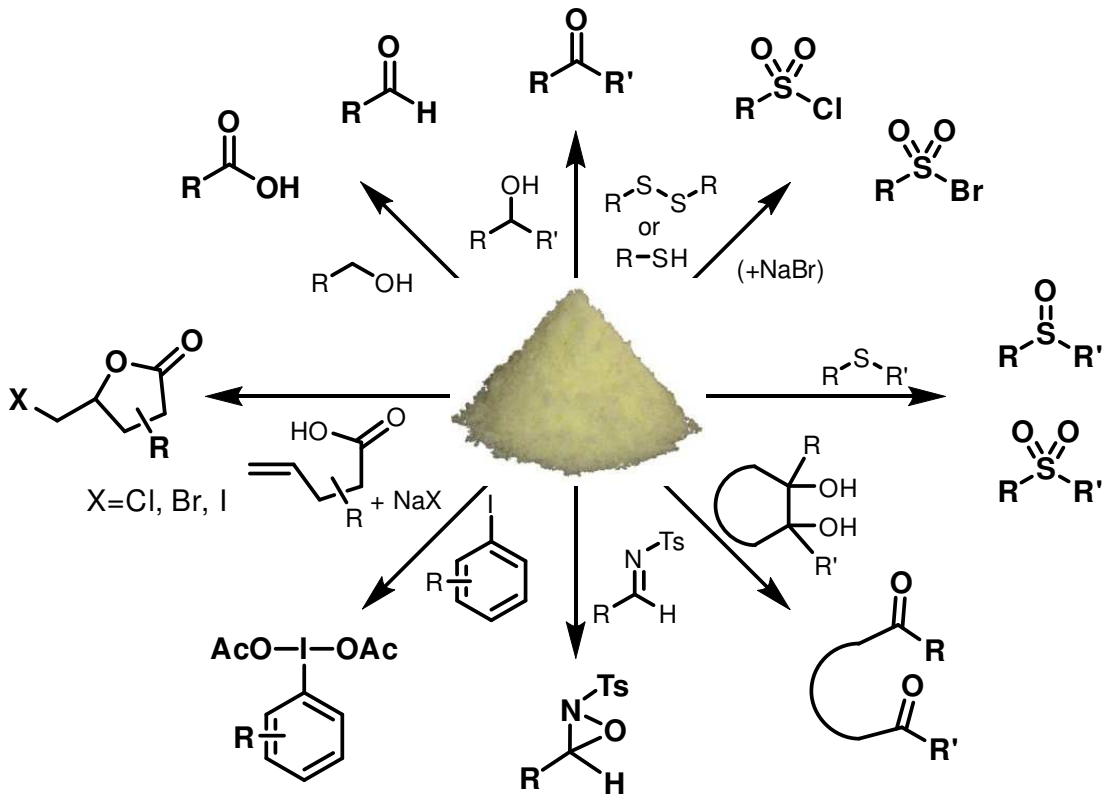
3. Solubility

- Insoluble in most organic solvents. (Alcoholic solvents may react with SHC5® and corresponding oxidized compounds are formed.)
- Any concentration of the solution (approx. ≦30%) can be prepared simply by dissolving SHC5® with water.
- 20% NaClO solution prepared from SHC5® is stable even after 24 hours at 20℃.

Target concentration (Available Chlorine) [%]	SHC5® [g]	Water [g]	Density (solution) [g/cm^3]
0.1	2.4	996.7	1.00
1.0	24.0	983.0	1.01
5.0	124.0	918.0	1.04
10.0	258.8	828.2	1.09
13.0	345.1	769.9	1.12
15.0	405.0	729.0	1.13
20.0	562.4	618.6	1.18
25.0	732.1	497.9	1.23
30.0	914.3	365.7	1.28

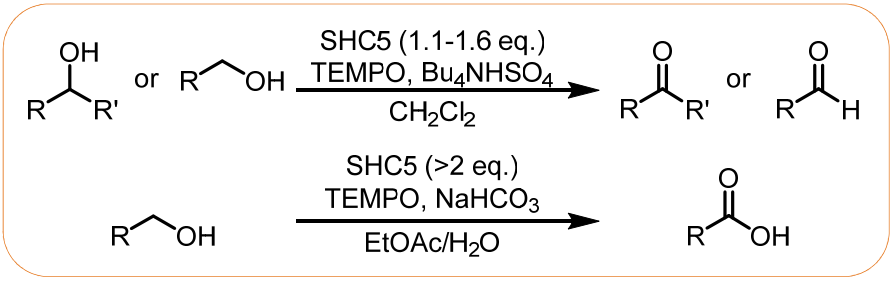
4. Oxidizability of SHC5®

- Most of other oxidizing reagents have toxic and explosive issues. However, SHC5® does not have these kinds of risks and it is an eco-friendly oxidizing reagent, producing only sodium chloride and water as by-products.
- Owing to high available chlorine concentration (42%) of SHC5®, it allows higher volumetric efficiency.
- SHC5® can be applied to various reactions as shown below.

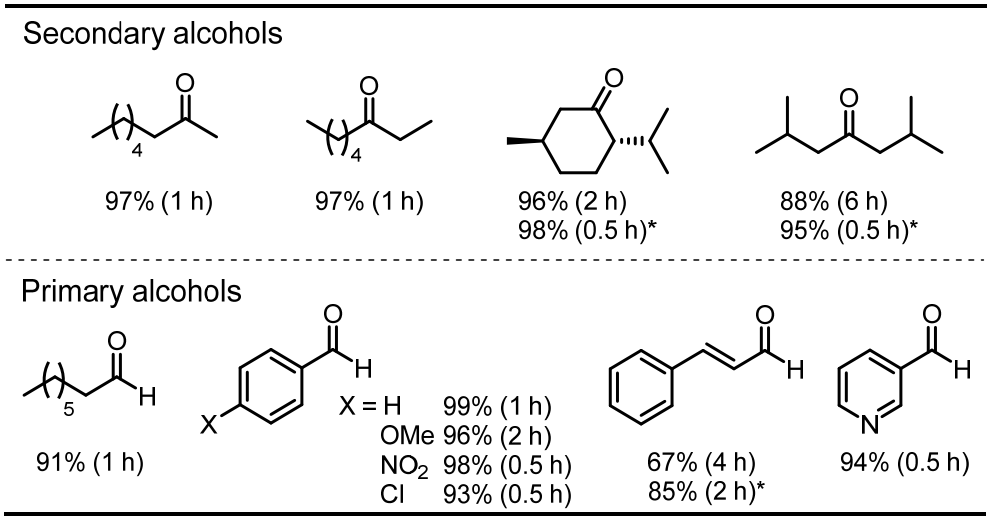


(1) Oxidation reactions of alcohols

- The oxidation reactions of various alcohols proceed smoothly without pH adjustment and corresponding ketones or aldehydes are obtained selectively. (Patent number : JP 6176177)
- Oxidations of primary alcohols to carboxylic acids are also possible with a simple modification of the reaction conditions.



i) Application of oxidation to aldehyde/ketone

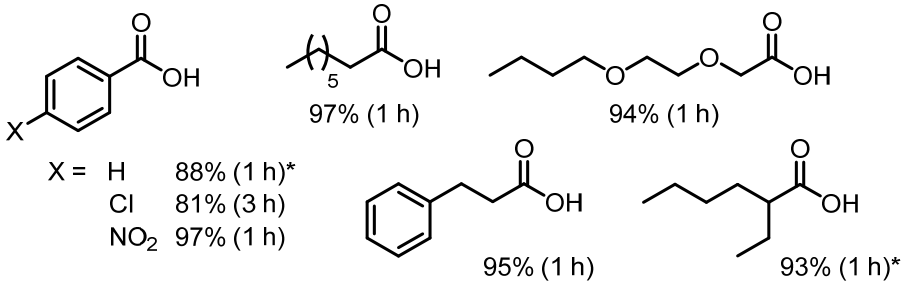


* 1-Me-AZADO was used instead of TEMPO.

Synlett **2014**, *25*, 596-598.

Tetrahedron **2016**, *72*, 2818-2827.

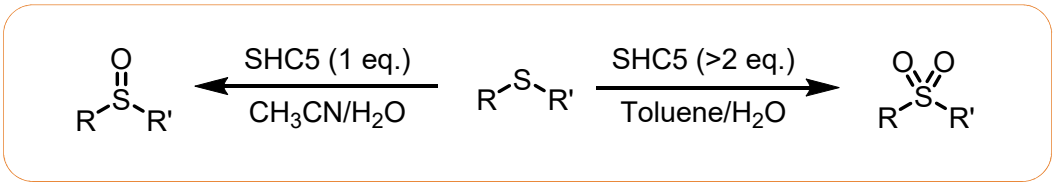
ii) Application of oxidation to carboxylic acid



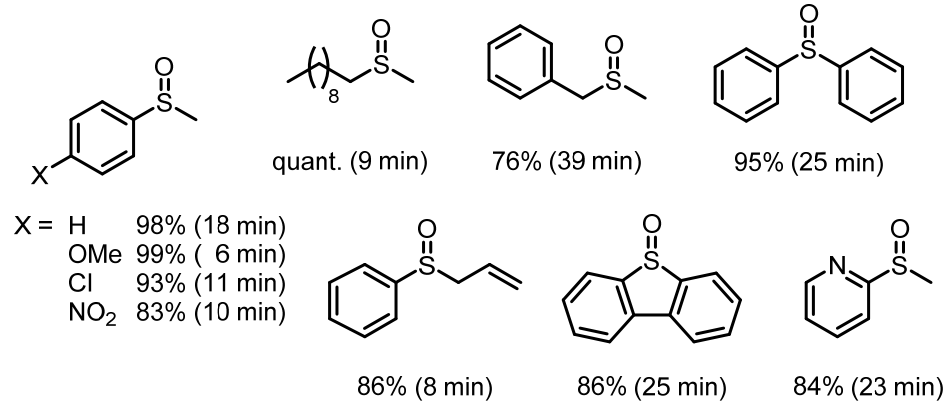
* AZADOL® was used instead of TEMPO.
AZADOL® is a registered trademark of Nissan Chemical Industries, Ltd.

(2) Oxidation reactions of sulfur compounds

- **Selective oxidations of sulfides to sulfoxides or sulfones are realized by simple selection of the solvent. (Patent publication number : JP 2017-52730)**

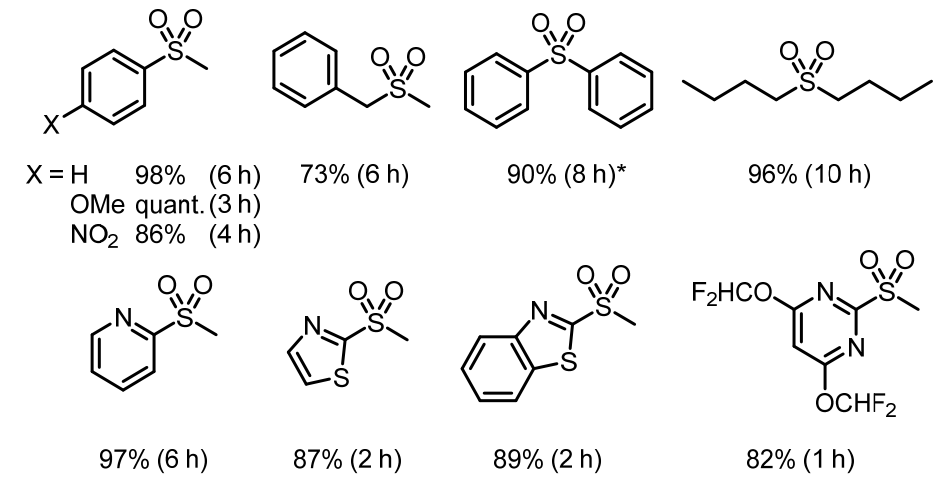


i) Application of oxidation to sulfoxide



Synlett **2015**, *26*, 2547-2552.

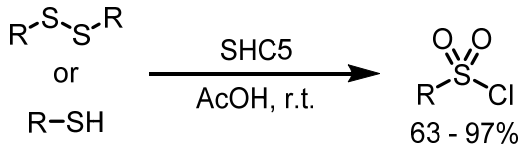
ii) Application of oxidation to sulfone



* $R_3MeN^+Cl^-$ (R = C_8 ~ C_{10}) was added.

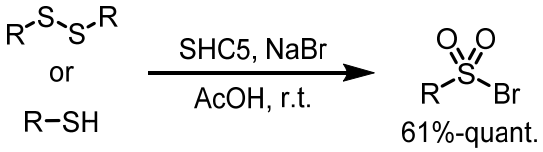
42nd Symposium on Progress in Organic Reactions and Syntheses 2016, 2P-53. (Japanese)

- The reaction of disulfide or thiol with SHC5® in acetic acid gives corresponding sulfonyl chloride in a short time and in high yield. (Patent number : JP 6149667)



Chem. Lett. **2015**, *44*, 185-187.

- In the presence of sodium bromide (NaBr), the reaction gives high yield of the corresponding sulfonyl bromide. (Patent publication number : JP 2017-52728)

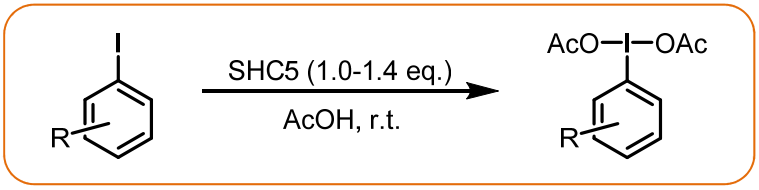


41st Symposium on Progress in Organic Reactions and Syntheses **2015**, 2P-33. (Japanese)

(3) Other oxidation reactions

<Synthesis of (Diacetoxyiodo) arenes>

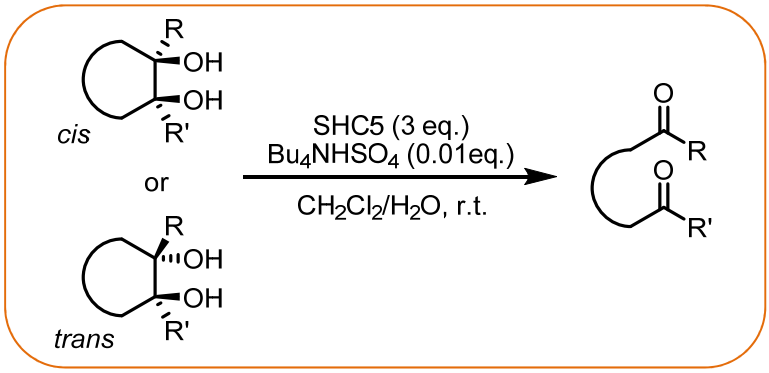
- (Diacetoxyiodo) arenes are easily and safely synthesized by SHC5®.



J. Org. Chem. **2018**, *83*, 14262-14268.

<Cleavage of glycols>

- *Trans*-isomer which is usually resisted to this type of reaction can also be applied for the oxidative cleavage by SHC5®.

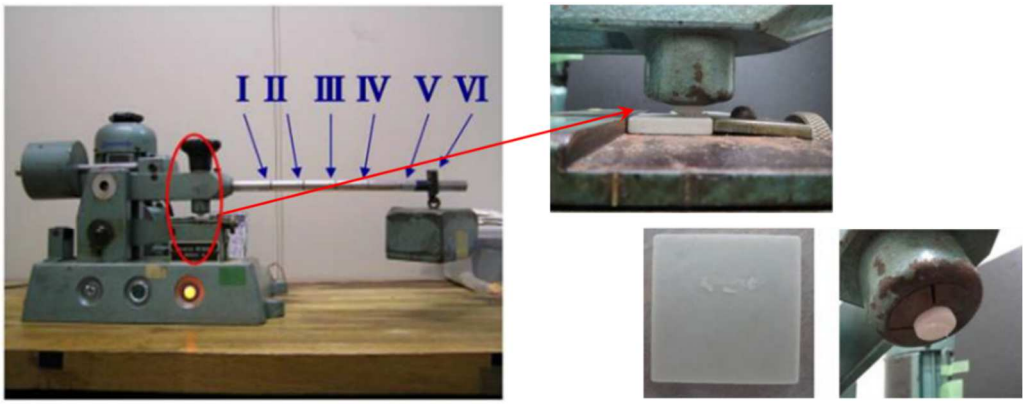


J. Org. Chem. **2019**, *84*, 8330-8336.

5. Safety assessment

According to the testing methods of explosives based on the Japanese Industrial Standards (JIS K 4810), the BAM friction test and the drop hammer test have been applied to SHC5®. The results of both tests were negative. This means that SHC5® is not an explosive compound under normal conditions.

(1) BAM friction test (JIS K 4810:2003 Testing methods of explosives)

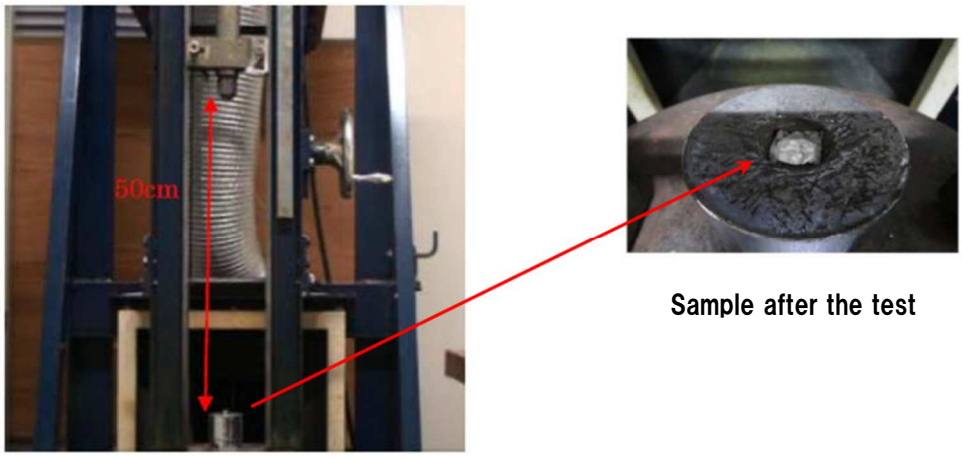


Friction panel after the test

Result of BAM friction test

Condition (position)	Result	JIS grade
Limiting Load:353 N (VI)	Negative (0/6)	Grade 7

(2) Drop hammer test (JIS K 4810:2003 Testing methods of explosives)



Sample after the test

Result of Drop hammer test

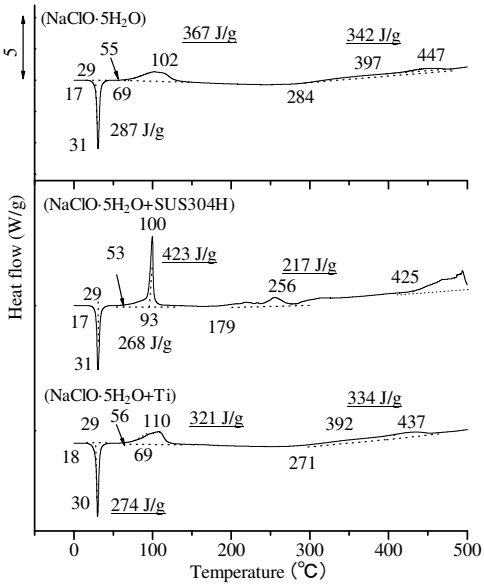
Condition	Result	JIS grade
Limiting impact energy: 24.5 J	Negative (0/6)	Grade 8

National Institute of Advanced Industrial Science and Technology, measured in 2016

6. Thermal behavior (DSC measurement)

(1) Stability with metals

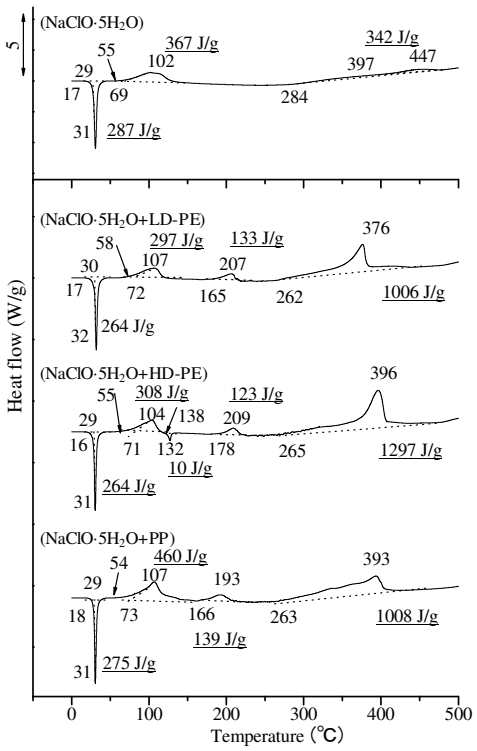
- The sharp peak was observed at 100℃ in DSC measurement with SUS304H. This result shows that stainless steel reacts with SHC5®, thus stainless vessels cannot be used as reactors. On the other hand, titanium did not react with SHC5®, thus the reaction of SHC5® can be performed in titanium vessels as well as glass wares.



DSC chart with SUS304H and Ti

(2) Stability with resins

- No changes are observed in the results of the measurement with high- and low-density polyethylene (PE) and polypropylene (PP) around room temperature. On the other hand, decomposition of resins was observed in the high temperature range. These show that above resins are able to be used as containers only below 25℃.



DSC chart with resins

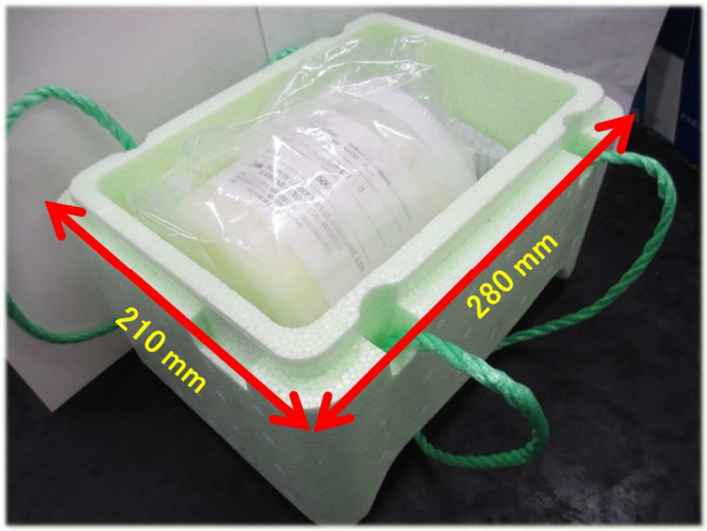
7. Precautions for handling, storage, disposal and transportation

(1) Package

- 500 g : High-density polyethylene container
  10 kg : 0.1 mm thickness polyethylene bag, heat-sealed, delivered in double packing
- Refrigerated transport by reefer truck or frozen delivery are required.

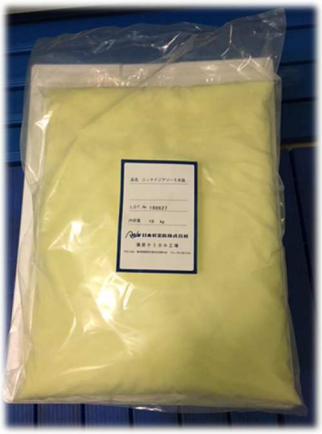
<500 g sample - Package appearance>

Inner package
Φ125×H130 mm



Outer package
W280×D210×H190 mm (Incl. upper lid)

<10 kg - Package appearance>



- Bag size (PE)
  450×670 mm

(2) Precautions for handling

- Contact with metal, cloth and paper causes heating and decomposition. Avoid contacting SHC5® with weighing paper and metal spoon. Use glass or plastic equipment.
- Avoid exposure to heat and light. SHC5® melts above 25℃. Decomposition is accelerated with heat, light or carbon dioxide in the air. Weighing should be quickly as possible.
- The used equipment should be washed with a large amount of water, and waste water needs to be treated with reducing reagent such as sodium sulfite for disposal.
- Avoid skin/eye contact and breathing in vapor, mists or aerosols. Wear protective equipment and eye protection when using. Wash with plenty of water and seek medical attention immediately in case of contact on skin or in eye.
- Avoid contacting SHC5® with acid. Harmful chlorine gas will be generated.
- For other hazards, please refer to the instructions for conventional aqueous NaClO solution.

(3) Precautions for storage and disposal

- Store below 7℃ in sealed container and keep away from light. Use up as soon as possible after opening.
- SHC5® is deliquescent material. The decomposition is accelerated by light and carbon dioxide in the air. Keep tightly sealed to preclude contact with light, moisture and air.
- For disposal, dissolving with a large amount of water and treatment with reducing reagents such as sodium sulfite are required prior to discharge.

(4) Transport information

- There is no regulation for domestic land transportation in Japan. All transports need to be conducted according to above "precautions for handling" and "precautions for storage and disposal".
- For the transport by air or by sea, this product is classified as hazardous materials which require a specific shipping arrangement based on UN number 3212. It is highly recommended to consult with freight forwarders about details in advance and follow their instructions.

8. Japanese regulatory information

- METI registration number : (1) -237
- Industrial Safety and Health Act : Existing chemical substances
  Enforcement Order of Industrial Safety and Health Act
  Annex 1 Dangerous goods oxidizing substance
- Fire Service Act : Not applicable
- Toxic Substances Control Law : Not applicable
- HS code : 2828.90-000
- UN Number : UN3212 Class 5.1 (Oxidizing substance)
  Product name: Inorganic hypochlorite
- Ship Safety Law : Notification of regulations for the carriage and
  storage of hazardous materials in ship
  Annex Article 1 Oxidizing substance
- Aviation Law : Enforcement regulation Article 194
  Oxidizing substance
- Act on Port Regulations : Enforcement regulation Article 12
  Dangerous goods (Oxidizing substance)
- Water Pollution Prevention Act : Specified substance
  (Article 2-4, Enforcement order Article 3-3)
- Marine Pollution Prevention Law : Not applicable
- Law for Promotion of Chemical Management (PRTR Law)
  : Not applicable

Refrigeration or cold storage is required for this product. Avoid contact to skin or clothing. Make sure properties, handling methods and others in Safety Data Sheet (SDS) before use. The data shown in this catalog are typical values, not the guaranteed values. Suitability should be ascertained when using this product for application not described in this catalog.

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