CAROAT® – Potassium Monopersulfate Compound

CAROAT® is the preferred reagent for a wide range of applications wherever a strong oxidizing or bleaching agent is required. There are other molecules which can be used for these applications but CAROAT® has the particular advantage of containing no halogens. Oxidative processes may be performed without the risk of forming hazardous halogenated by-products. CAROAT® is supplied as a free-flowing and stable powder with a high quality consistency and a long storage life under cool and dry conditions.

CAROAT® is a triple salt of potassium monopersulfate, potassium hydrogen sulfate and potassium sulfate. The active constituent is the potassium salt of Caro’s acid, peroxomono-nosulfate (KMPS). With an annual production of several thousand tons, United Initiators has a leading position in the worldwide production of KMPS.

Applications

Denture Cleaners
A major application of CAROAT® is denture cleansing. It acts by bleaching food residues and organic discolorations. Other organic deposits are effectively oxidized, facilitating their removal.

In formulas adjusted to an acidic to neutral condition, CAROAT® plays the role of bleaching agent. In weakly alkaline formulas, an effervescent effect can be obtained with CAROAT® in the presence of sodium perborate monohydrate in a weight ratio of approx. 3:1, which disintegrates the tablets and features a mechanical cleaning effect on the dentures.

CAROAT® oxidizes the hydrogen peroxide liberated from the perborate, forming gaseous oxygen. In weakly acidic to neutral formulas, formation of gas supporting the removal of deposits is achieved through the reaction of acidic components with sodium hydrogen carbonate.

Metal Treatment and Metal Extraction
CAROAT® is the premium etching agent for the surface treatment of metals and alloys in the metal fabricating industry. When dissolved in water or in diluted sulfuric acid, CAROAT® forms micro-etching solutions for the preparation of non-ferrous metal finishes. Such solutions are suitable for the pre-cleaning of metal surfaces and the removal of passivating oxidized surface layers. Due to its high oxidizing power in aqueous solution, CAROAT® can also be used for the extraction of metals and for the separation from ores.

CAROAT® oxidizes the hydrogen peroxide liberated from the perborate, forming gaseous oxygen. In weakly acidic to neutral formulas, formation of gas supporting the removal of deposits is achieved through the reaction of acidic components with sodium hydrogen carbonate.

Etching of Printed Circuit Boards (PCBs)
CAROAT® is the product of choice for the microetching of copper conductors in the production of printed circuit boards, yielding clean, uniformly etched, and oxide-free surfaces that match the highest demands in quality. This is indispensable for downstream processes, such as the plating-through holes of two-sided boards or the lamination of multilayer boards.

CAROAT® matches all of the key requirements for this application, such as highest purity and high powder flowability.

Repulping of Paper
CAROAT® is used as active ingredient for chlorine-free formulations for the repulping of wet strength paper. In this process, polymers applied for paper production such as polyamide (PA) and polyamine-epichlorhydrin (PAE) are effectively oxidized by thermal activation alone.

Running the pulper at 60 °C is already sufficient for a successful repulping process in an average of less than 30 minutes.

Other types of resins, like urea-formaldehyde or melamine-formaldehyde-resins can be repulped with CAROAT®, if alkalization or acidification has to be avoided for reduction of cellulose loss. In contrary to chlorine-based systems such as sodium hypochlorite, (NaOCl), CAROAT® does not form problematic chlorinated compounds, such as Adsorbable Organic Halides (AOX).

Also, CAROAT® based solutions bear a lower corrosivity than those based on hypochlorite, which is often an issue in case of chlorine-based systems.

CAROAT® based systems are easy to prepare, handle and are remarkably efficient. As CAROAT® also decomposes organic-based chromophores, it also features a pronounced bleaching effect.

Pretreatment of Wool
In the textile industry, CAROAT® is a key agent to render wool shrink-resistant and non-felting. This oxidation process smoothens the surface of the wool fibers. Examples of the advantages of CAROAT® over other processes (e.g., such involving active chlorine) are avoiding yellowing, additional brightness, and the softer feel of the wool fibers.

Formation of halogenated organic compounds (AOX) in the wastewater is also prevented in this process.
Swimming Pool Water Treatment
CAROAT® is the ideal alternative for the shock treatment by superchlorination for the disinfection of pools & spas.
Advantages of CAROAT® are:
• No chloramines or chlorine odors
  CAROAT® is oxygen-based, containing no chlorine and thus cannot form chloramines or chlorine odor. CAROAT® accelerates the degradation of chloramine produced by the chlorine sanitizer.
• No unhealthy THMs (trihalomethanes)
  The high oxidation potential of CAROAT® is based on oxygen, not on chlorine. Thus, hazardous THMs such as chloroform cannot be formed from CAROAT®.
• Increases efficiency of the sanitizer
  By using CAROAT® to oxidize the constantly introduced contaminants, the chlorine is able to remain in its free and most efficient form thus readily available for doing its job of exterminating bacteria and viruses. No more need to raise the chlorine level!
• Sparkling clear water
  CAROAT® significantly improves water clarity, yielding sparkling clean and crystal clear water.
• Protects pool and spa surfaces
  Even though CAROAT® is aggressive in eliminating swimmer waste and other contaminants, it does not damage the vinyl liners of pools and does not bleach the surfaces – no more fading!
• Same day shock & swim
  Swimming can resume after a short waiting period. No significant down time, which can be especially troublesome in commercial pools!
• Can be used day & night
  In contrary to chlorine, CAROAT® is unaffected by UV degradation and therefore is particularly suited for day or night application.
• Harmless, non-toxic
  CAROAT® is approved and widely used for conditioning of drinking water in many countries worldwide.

Waste Treatment and Detoxification of Cyanide Solutions
CAROAT® solutions readily oxidize pollutants in waste streams, such as sulfides and sulfites, amines, mercaptans and various oxidizable organic compounds. Effectiveness of the waste treatment with CAROAT® should always be monitored analytically.
Waste-waters with a high content of heavy-metal cyanides can be detoxified using CAROAT®. While hydrogen peroxide (H₂O₂) oxidizes only free cyanides, CAROAT® can also break down complex cyanides (except those of iron and gold) rapidly and completely, due to its higher oxidation potential.
Also, oxidation of cyanides with CAROAT® can prevent the formation of hazardous AOX (adsorbable organic halides).

Chemical Synthesis
CAROAT® is a very strong and selective oxidizing agent for different applications substituting chlorine chemistry.
In organic chemistry, such as for pharmaceutical and agrochemical intermediates, CAROAT® works as a highly selective reagent for stereoselective dioxirane chemistry (epoxidation of olefins), Baeyer-Villiger reactions and the selective oxidizations of reduced nitrogen and sulfur groups.

Disinfection
CAROAT® is the active ingredient in formulations used for disinfection in animal husbandry such as for poultry farming and stabilizing disinfection for the suppression and prevention of diseases such as foot and mouth disease, bird flu and swine flu.
CAROAT® is also used for the disinfection of hard surfaces in hospitals or in other areas requiring increased hygiene standards.
CAROAT® is notified and pre-registered according to the EU Biocide Directive.

Treatment of Yeast
CAROAT® can be used for selective elimination of undesired bacteria in yeast suspensions. The yeast itself is not damaged by this treatment when CAROAT® is dosed appropriately.
Chemical and Physical Properties

Redox Potential
The standard electrode potential $E_0$ for the half-cell reaction
$\text{HSO}_5^– + 2 \text{H}^+ + 2 \text{e}^- \leftrightarrow \text{SO}_4^{2–} + \text{H}_2\text{O}$
is $+1.82 \text{ V}$ (25 °C, activity 1).
The lower the pH, the stronger is the oxidizing power that CAROAT® can develop.
With this high oxidation potential, CAROAT® can oxidize, for example chloride ions to chlorine, iron(II) to iron(III) and hydrogen peroxide to oxygen.

Stability in Solid Form
Under cool, dry conditions, CAROAT® has a long storage life in closed containers.
The active oxygen loss per month is less than 0.5% relative to its original activity.

Physical Properties of CAROAT® and Typical Analytical Data

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Comment¹</th>
<th>¹ S = technically specified; T = typical value ² ² Self-accelerating decomposition temperature; relates to a container size of one bag (25 kg, 55 lbs) only. Data applies for material from our Pullach site.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical Formula</td>
<td>2KHSO₅, KHSO₄, K₂SO₄</td>
<td>approx.</td>
<td></td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>g/mol</td>
<td>614.8</td>
<td></td>
</tr>
<tr>
<td>Composition</td>
<td>%</td>
<td>45 KHSO₅, 25 KHSO₄, 30 K₂SO₄</td>
<td>approx.</td>
</tr>
<tr>
<td>Active Oxygen Content</td>
<td>%</td>
<td>&gt; 4.5 / 4.7</td>
<td>S/T</td>
</tr>
<tr>
<td>Moisture</td>
<td>%</td>
<td>&lt; 0.3</td>
<td>S</td>
</tr>
<tr>
<td>Bulk Density</td>
<td>g/cm³</td>
<td>1.10</td>
<td>T</td>
</tr>
<tr>
<td>Particle Distribution</td>
<td></td>
<td>&gt; 0.8 mm: 0–2%</td>
<td>&gt; 0.1 mm: 0.8 mm: 90–100%</td>
</tr>
<tr>
<td>Solubility in water (20 °C)</td>
<td>g/l</td>
<td>260</td>
<td>approx.</td>
</tr>
<tr>
<td>Insolubles</td>
<td>ppm</td>
<td>&lt; 10</td>
<td>T</td>
</tr>
<tr>
<td>pH (1% in water)</td>
<td></td>
<td>2.0</td>
<td>T</td>
</tr>
<tr>
<td>pH (10% in water)</td>
<td></td>
<td>1.6</td>
<td>T</td>
</tr>
<tr>
<td>Sodium (Na)</td>
<td>ppm</td>
<td>&lt; 900</td>
<td>T</td>
</tr>
<tr>
<td>Copper (Cu)</td>
<td>ppm</td>
<td>&lt; 0.1</td>
<td>T</td>
</tr>
<tr>
<td>Chromium (Cr)</td>
<td>ppm</td>
<td>&lt; 0.3</td>
<td>T</td>
</tr>
<tr>
<td>Iron (Fe)</td>
<td>ppm</td>
<td>&lt; 3</td>
<td>T</td>
</tr>
<tr>
<td>Manganese (Mn)</td>
<td>ppm</td>
<td>&lt; 0.2</td>
<td>T</td>
</tr>
<tr>
<td>Zink (Zn)</td>
<td>ppm</td>
<td>&lt; 2.0</td>
<td>T</td>
</tr>
<tr>
<td>Color</td>
<td></td>
<td>white</td>
<td></td>
</tr>
<tr>
<td>Odor</td>
<td></td>
<td>none</td>
<td></td>
</tr>
<tr>
<td>SADT² (dry state)</td>
<td>°C/°F</td>
<td>&gt;80/176</td>
<td>T</td>
</tr>
<tr>
<td>SADT² (3.6% humidity)</td>
<td>°C/°F</td>
<td>65/140</td>
<td>T</td>
</tr>
</tbody>
</table>

Stability in Aqueous Solution
Stability of aqueous solutions depends on the pH, the temperature, and the impurities present. Aqueous CAROAT® solutions are acidic. If the pH is raised beyond 7, the stability drops to a minimum at pH 9, while decomposition is delayed between pH 13 and pH 14 (see Figure above).
The content of the hydrogen sulfate is then increased $2\text{HSO}_5^– \rightarrow 2\text{SO}_4^{2–} + \text{O}_2$ and thus the pH decreases. In the case of alkaline formulas, this shift in pH must be taken into account meaning that an excess of alkali needs to be applied in order to reach the desired pH.
A 3% CAROAT® solution at room temperature and the intrinsic pH, held for seven weeks in completely softened water, still contains approx. 95% of the starting content. At higher temperatures, decomposition takes place significantly faster (see figure on lower left). Nevertheless, United Initiators recommends to always apply fresh and un- or low-polluted solutions of CAROAT®, where applicable.
A 20% CAROAT® solution at 25 °C and the intrinsic pH, held for seven weeks in completely softened water, still contains more than 90% of the starting content (see figure on lower right). Heavy metals cause decomposition of CAROAT® solutions, but not to the extent observed for most other active oxygen compounds.

Shelf Life of CAROAT® Solutions at Different Storage Temperatures

Half Life of a 3% CAROAT® Solution as Function of pH
(3% solution, temperature = 23 °C)
Working with CAROAT®

United Initiators is committed to provide technical support for the properties and correct and safe use of CAROAT®. Upon request, detailed analytical specifications can be provided.

Analytical Determination of Active Oxygen

The iodide-thiosulfate method is well suited to the determination of peroxomonosulfate in CAROAT®. In the case of formulas containing CAROAT® along with other active-oxygen compounds, the other compounds are determined at the same time. If an additional titration is performed with cerium(IV) sulfate, in which only hydrogen peroxide-releasing compounds react, the CAROAT® content can be calculated by taking the difference between the values from the two titrations.

Determination with Potassium Iodide/Sodium Thiosulfate

This method is based on the oxidative liberation of iodine from potassium iodide in acidic solution:

\[
\text{KHSO}_5 + 3 \text{KI} + \text{H}_2\text{SO}_4 \rightarrow \text{KHSO}_4 + \text{KI}_3 + \text{H}_2\text{O} + \text{K}_2\text{SO}_4
\]

After a reaction time of 20 minutes, the iodine eliminated is titrated with sodium thiosulfate:

\[
\text{KI}_3 + 2 \text{Na}_2\text{S}_2\text{O}_3 \rightarrow \text{KI} + \text{Na}_2\text{S}_4\text{O}_6 + 2 \text{NaI}
\]

Titration with Cerium(IV) Sulfate

In acidic solution, hydrogen peroxide reduces cerium(IV) to cerium(III) with the evolution of oxygen:

\[
2\text{Ce (SO}_4)_2 + \text{H}_2\text{O}_2 \rightarrow \text{Ce(SO}_4)_3 + \text{H}_2\text{SO}_4 + \text{O}_2
\]

The end point of the titration is easily identified potentiometrically. Organic substances, however, are partly determined along with the desired product.

**PACKAGING**

<table>
<thead>
<tr>
<th>Type</th>
<th>Material</th>
<th>Container wt</th>
<th># of containers per pallet</th>
<th>Total product wt per pallet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bag</td>
<td>PE</td>
<td>25 kg / 55 lbs</td>
<td>40</td>
<td>1000 kg / 2200 lbs</td>
</tr>
<tr>
<td>Supersack / Big Bag</td>
<td>PP sack w/ PE inliner</td>
<td>1000 kg / 2200 lbs</td>
<td>1</td>
<td>1000 kg / 2200 lbs</td>
</tr>
</tbody>
</table>

For information on alternative packaging options, please contact your sales representative at UI.
Safety at work with CAROAT®

When handled and stored properly, CAROAT® and its aqueous solutions do not pose a threat to human health. Before working with a persulfate, please carefully study the appropriate SDS. CAROAT® and its solutions can be handled safely in containers of glass, stainless steel, ceramics or plastic. For CAROAT® mixtures containing sodium chloride, we recommend the addition of a corrosion inhibitor such as sodium nitrate. The possible formation of active chlorine may otherwise lead to corrosion.

Personal Protection
As CAROAT® is a very strong oxidizer, certain precautions are necessary when working with this substance. This starts with wearing suitable protective equipment such as protective goggles and appropriate protective gloves, but it is also advisable to wear protective full-length clothing.

Safe Handling
• Keep material away from sources of heat and direct sunlight
• Keep material away from combustible materials
• Protect from moisture, as SADT (self accelerated decomposition temperature) of persulfates will be significantly reduced.
• Contaminants such as rust, dust and ash may also trigger decomposition and/or reduce SADT
• Product residues should be processed quickly and never be returned back into the storage container.
• Use tools of plastic, stainless steel when removing persulfates from containers. Always maintain a clean working environment.
• Do not breathe product, vapor or dust

Dealing with Spillage
• Sweep up solid product and collect separately
• Collected residues need to be treated as special waste
• Avoid formation of dust
• Flush minor residues with ample amounts of water

First Aid
• Eye contact
  Rinse immediately and thoroughly with water, minimum 15 minutes.
  Protect non-injured eye. Immediately consult a physician.
• Skin contact
  Immediately flush contaminated skin areas with plenty of soap and water.
  Remove contaminated clothing immediately. If skin irritation persists, seek medical advice.
• Ingestion
  Rinse mouth and drink plenty of water (approx. two glasses). Do not induce vomiting.
  Consult a physician immediately.
• Inhalation
  Remove injured individual to fresh air. Consult a physician immediately.
• When consulting a physician
  Same treatment as for acid burns should be administered. Treatment for inhalation is the same as for irritating gases. Development of a late pulmonary edema may be possible.

Storage
• Store separately from other dangerous and incompatible substances (e.g. aqueous liquids, redox-active chemicals)
• Store dry at temperatures preferably < 30 °C / 86 °F and in original sealed containers.
• Try to maintain a minimum distance of 20 – 30 cm / 1 ft. between pallets and/or bulk bags
• Do not stack pallets

Shipping Regulations
CAROAT® is subject to the shipping regulations for Class 8, “Corrosive Substances”.

Technical Name
Land: Contains potassium peroxomonosulfate
Sea/air: Corrosive solid, n.o.s. (cont. potassium peroxomonosulfate)

The information and statements contained herein are provided free of charge. They are believed to be accurate at the time of publication, but United Initiators makes no warranty with respect thereto, including but not limited to any results to be obtained or infringement of any proprietary rights. Use or application of such information or statements is at user’s sole discretion, without any liability on the part of United Initiators. Nothing herein shall be construed as a license or recommendation for use which infringes upon any proprietary rights. All sales are subject to United Initiators’ General Conditions of Sale and Delivery.