BAYHIBIT® AM

BAYHIBIT® AM is a highly effective scale and corrosion inhibitor, which active ingredient PBTC was developed by the Bayer AG. Main field of application are the treatment of cooling and process water as well as the area of cleaning formulations.

Chemical name

BAYHIBIT® AM is a 50 % solution of 2-Phosphonobutane-1,2,4-tricarboxylic acid (abbreviation: PBTC) in water

CAS Reg. No.

37971-36-1

Structural formula

Empirical formula

C_{7}H_{11}O_{9}P

Molecular weight

270.13 g/mol

Physical form

clear, colorless to yellowish, low-viscous, almost odorless liquid

Health and safety information

Safety data and precautions which must be observed under all circumstances are to be found in EU Safety Data Sheet No. 000969.
Specified Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Nominal Value</th>
<th>Unit</th>
<th>Test Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Active agent content</td>
<td>50 ± 1</td>
<td>% by mass</td>
<td>2022-2303301-00D</td>
</tr>
<tr>
<td>Orthophosphate content (as ( \text{PO}_4^{3-} ))</td>
<td>≤ 0.2</td>
<td>% by mass</td>
<td>2022-2303601-00D</td>
</tr>
<tr>
<td>Density at 20 °C</td>
<td>1.285 ± 0.015</td>
<td>g / cm³</td>
<td>DIN 51 757</td>
</tr>
<tr>
<td>Turbidity</td>
<td>≤ 10</td>
<td>NTU (= TE/F)</td>
<td>DIN 38 404, part 2</td>
</tr>
<tr>
<td>Gardner color</td>
<td>≤ 2</td>
<td>-</td>
<td>DIN 53 995</td>
</tr>
<tr>
<td>Hazen color (at dispatch)</td>
<td>≤ 100</td>
<td>(APHA)</td>
<td>ISO 6271</td>
</tr>
</tbody>
</table>

Additional Information

<table>
<thead>
<tr>
<th>Property</th>
<th>Typical Value</th>
<th>Unit</th>
<th>Test Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBTC share *)</td>
<td>ca. 84</td>
<td>mol-%</td>
<td>2012-0567802-00D</td>
</tr>
<tr>
<td>Viscosity at 20 °C</td>
<td>17.5 ± 7.5</td>
<td>mPa · s</td>
<td>DIN 53 015</td>
</tr>
<tr>
<td>Refractive index at 20 °C ( (\text{n}^{20}_D) )</td>
<td>1.417</td>
<td>-</td>
<td>DIN 53 491</td>
</tr>
<tr>
<td>pH value of the aqueous solution with 2 % BAYHIBIT® AM</td>
<td>1.6 ± 0.1</td>
<td>-</td>
<td>DIN 38 404, part 5</td>
</tr>
<tr>
<td>Iron (as Fe)</td>
<td>ca. 5</td>
<td>mg / l</td>
<td>AC-F/V/246/03/88</td>
</tr>
<tr>
<td>Total chlorine (as Cl)</td>
<td>ca. 4</td>
<td>mg / l</td>
<td>2011-0380801-93D</td>
</tr>
<tr>
<td>Hazen color (ex works)</td>
<td>10</td>
<td>(APHA)</td>
<td>ISO 6271</td>
</tr>
</tbody>
</table>

*) referred to phosphorus compounds

These material properties are typical properties and, unless specifically indicated otherwise, are not to be considered as delivery specification.
Packaging
Road tanker
ISO tank container
1250 kg IBC container
250 kg polyethylene drum

Storage
The product can be stored in tightly sealed original packaging without a deterioration of quality for a period of at least two years in case of appropriate storage. Material which has solidified on account of cold (solidifying point approx. – 15 °C) can be defrosted without a reduction of quality.

Materials
The following materials have proved suitable for the metering tanks, pumps and lines for BAYHIBIT® AM:
glass, stainless steel (e.g. DIN W1.4571 = US AISI 316 TI), plastics such as polyethylene, polytetrafluoro ethylene (PTFE) and polyvinyl chloride (PVC). Seals should be made from PTFE or graphite.

Peculiarity
No labeling is required for BAYHIBIT® AM under Germany’s regulations on hazardous substances and the equivalent EU Directives.

BAYHIBIT® AM - effects

Scale inhibition
BAYHIBIT® has proved highly effective as a threshold inhibitor. Very low additions (ppm range), i.e. in far less than sub-stoichiometric concentrations (calculated on the hardness of the water), prevent the formation of scale and incrustations, respectively. Even water which is highly over-saturated with hardness constituents such as calcium carbonate remain without scale when BAYHIBIT® is added.
The outstanding effectiveness of BAYHIBIT is proved by a multitude of practically orientated trials, which can be discussed and are available.

Dispersion
The adsorption of the PBTC anion on inorganic particles suspended in water results in a negative charge on their surfaces and thus in an improvement in dispersibility. This is why neutralized BAYHIBIT® is used as a dispersion agent / deflocculation agent for inorganic slurries and slips.

Corrosion inhibition
Under the conditions found in cooling water, BAYHIBIT® is a good corrosion inhibitor for carbon steel. In the case of relatively soft water, it is common to combine BAYHIBIT® with synergistic substances (phosphates, zinc salts). In water of higher hardness or with sufficiently high alkalinity (approx. 300 mg/l or more, calculated as calcium carbonate), formulations containing BAYHIBIT® and no inorganic components – known as all-organic formulations – are highly effective. In alkaline cleaning agents, the corrosion-inhibiting effects of BAYHIBIT® on aluminium can be a benefit.
BAYHIBIT® AM - properties

Solubility
BAYHIBIT® AM can be mixed in any ratio with water. It is soluble in lyes, e.g. sodium hydroxide solution, and in acids, e.g. sulfuric acid. Because of its outstanding solubility, even formulations which already contain high concentrations of other active substances can be optimized by the addition of BAYHIBIT® AM.

Neutralization
BAYHIBIT® AM is a strong acid. When it is mixed with alkali, a heat of neutralization of around 210 kJ (approx. 50 kcal) is released per mole PBTC. This is why the final temperature of a solution produced without cooling by neutralizing BAYHIBIT® AM (commercial product) with 20 % sodium hydroxide solution is around 50 °C higher than the temperature of the starting solutions. If higher concentrations of sodium hydroxide are used, it must be expected that the solution will begin to boil if it is not cooled.

The safety precautions which normally apply for acid-base neutralization must therefore be observed when mixing BAYHIBIT® AM commercial product with concentrated sodium hydroxide solution.

Stability to hydrolysis
BAYHIBIT® can be used in aqueous solutions, lyes and acids up to temperatures considerably above 100 °C. Investigations of the stability have shown that, for example, the half-life (50 % degradation to orthophosphate) in process water with a pH of 9 and a temperature of 200 °C is around 20 hours.

Inhibitor loss / turbidity region
When combined with polyvalent cations, threshold inhibitors can form poorly soluble salts which, when they exceed the solubility limits, often result in turbidity. Field experience and special trials have shown that the tendency of the inhibitor to precipitate caused by, for example, Ca²⁺ and Fe(III) is much lower in BAYHIBIT® than in other phosphonates. For this reason, inhibitor losses are low when BAYHIBIT® is used. (cp. fig.1)

Fig. 1: Tendency of the phosphonates to form undissolved calcium salts

<table>
<thead>
<tr>
<th>Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca²⁺ concentration = 200 mg/l</td>
</tr>
<tr>
<td>pH 8.5</td>
</tr>
<tr>
<td>temperature 60°C</td>
</tr>
<tr>
<td>storage time 24 h</td>
</tr>
</tbody>
</table>

![Graph showing tendencies of phosphonates](image)
Stability to chlorine, bleaching lye and other oxidizing agents

Because of its outstanding stability to chlorine and bleaching lye, BAYHIBIT® is often used together with bleaching lye in disinfectant alkaline cleaning agents.

When manufacturing formulations which contain BAYHIBIT® AM, alkali and bleaching lye, BAYHIBIT® AM must always be neutralized before addition of the latter. Like all acids, acidic BAYHIBIT® AM generates toxic chlorine gas when mixed with bleaching lye.

Under cooling water conditions (neutral to slightly alkaline environment), the high stability of PBTC to chlorine and hypochlorite is also not matched by most other phosphonates. The product also has outstanding stability to bromine and hypobromite which are generated by adding chlorine to bromide. Bromine does not affect PBTC even after many hours but destroys HEDP, for example very quickly (cp. fig. 2).

Unlike aminomethylene phosphonates such as ATMP or DTPMP, PBTC is also stable under operating conditions to chlorine dioxide, which is used to prevent reinfection in bottle-washing plants.

**Fig. 2: Stability of phosphonates to chlorine and bromine**

| Conditions for test a): |
| total hardness SE = 3.0 mmol/l (300 mg/l as CaCO₃); total alkalinity K₀.₄₃ = 3.2 mmol/l (160 mg/l as CaCO₃); start pH = 8.5; storage temperature 60°C |
| phosphonate concentration: 10 mg/l; chlorine concentration (as bleaching lye): 10 mg/l |

| Conditions for parallel test b): |
| as in a) plus 1 mg/l bromide |

The residual phosphonate concentration was calculated from the analytical determined orthophosphate concentration.
BAYHIBIT® AM - ecology and toxicology

Biodegradation
Bacteria which degrade BAYHIBIT® were isolated from natural sources (activated sludge, river water and river sediment). Degradation is rapid if a second carbon source is available to the bacteria and inorganic phosphate is present in concentrations of just a few mg/l.

In pond water, biodegradation was found to take place under natural conditions without isolation and adaptation of the bacterial population. The half-life was 28 days. Only 0.3 % of radioactively marked PBTC could still be found in the water after 208 days.

In contrast, in biodegradability tests using standard methods (e.g. OECD 301 D, 302 B), PBTC was found to be not easily degradable.

Degradation by light
In water, PBTC is degraded by light. The rate of degradation depends on the intensity of the light and on the other constituents in the natural water. In the presence of traces of iron or nitrate, the half-life of PBTC is just a few hours.

Adsorption on activated sludge and sediment
Trials have shown that more than 95% of PBTC is adsorbed by activated sludge. If the water treatment plant has a third treatment stage (phosphate precipitation with aluminium or iron (III) salts) PBTC residues are also precipitated with the consequence that the discharge from the waste water treatment plant contains virtually no PBTC.

PBTC is eliminated from standing water over resting sediment through adsorption on the sediment with a half-life of five days. If the sediment is kept in suspension, the adsorption process is much quicker (half-life of just a few hours).

Complex formation
PBTC is a much weaker complexing agent than EDTA. There is no reason to expect a remobilization of heavy metals from sediment by PBTC. This has been confirmed by laboratory trials.

Ecotoxicity
Trials have shown that BAYHIBIT® has no harmful effect on aquatic organisms (fish, daphnia, algae, bacteria) or on terrestrial organisms (Earthworms) and sediment organisms (midge larvae).

Toxicity to mammals
a) Acute toxicity (rat, oral);
   \( \text{LD}_{50} > 6.500 \text{ mg BAYHIBIT® AM/kg} \)

b) Subchronic toxicity (rat, three-month feeding test with PBTC-Na₄ salt; max. test conc. 5000 mg kg⁻¹)
   All concentrations tested were tolerated without symptoms.

Conclusion
Tests to date (local irritation, inhalation toxicity, mutagenicity) did not result in harmful effects which means that BAYHIBIT® can be considered as not harmful to health. This conclusion is confirmed by the OECD in its Initial Assessment (March 1996): PBTC represents no risk to the environment or to humans.
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