ACULYN™ 46 Rheology Modifier/Stabilizer
An Efficient Shear Thinning Thickener Compatible with Cationics

Description

ACULYN 46 rheology modifier is a nonionic Hydrophobically-modified Ethoxylated URethane (HEUR) thickener designed for personal care applications. As with other ACULYN rheology modifiers, the polymer is a liquid product for easier handling and manufacturing efficiency. ACULYN 46 is offered at 18 to 20% solids, is stable from pH 2 to 12 and compatible with peroxide and other oxidizing agents. The polymer has a well-established toxicological profile and is safe in normal use.

CTFA/INCI Name: PEG-150/Stearyl Alcohol/SMDI Copolymer

Features

- Highly associative
- Peroxide stable
- Yields clear gels
- Particulate stabilizer
- Pseudoplastic rheology
- Cold-processable
- Nonionic
- Liquid
- Stable in anionic, cationic, nonionic and Zwitterionic surfactant systems
- Formulation compatible
- Stable pH/viscosity response
- Microbe resistant
- Acid compatibility
- Lack of odor
- Salt tolerant

Applications

- Aqueous antiperspirants
- Cationic silicone emulsions
- Creams
  - Medicated creams
  - Make-ups
  - Mascara
  - Alpha-Hydroxy acid creams
- Hair Products
  - Permanent waves
  - Conditioners
- Peroxide-containing formulations
  - Hair bleaches/dyes
  - Anti-acne (benzoyl peroxide) lotions
  - Hydrogen peroxide skin disinfectants
- Sunscreen formulations

Benefits

- Easy to handle
- Can be used with electrolytes
- No neutralization necessary
- Ability to stabilize suspensions
- No preparation necessary
- Compatible with nonionic, anionic, Zwitterionic and cationic surfactants
- Non-hygroscopic
- Increased manufacturing efficiency
- Stable in pH 2 to 12 formulations
- Allows for use of continuous production processes with use of in-line static mixers
- Effective in thickening acid media such as solutions of organic acids
- Can be processed with membrane pumps and, when diluted, with turbine mixers and high speed propellers
- Thickens and stabilizes oxidizing media
- Does not promote or support contaminations, unlike natural thickeners
- Able to formulate clear products
- Supported by comprehensive environmental, health and safety data
- Mild, soft, non-greasy, non-sticky
- Reproducible viscosity
- Stabilization of hydrophobic (low solubility) components
ACULYN 46 Chemistry

ACULYN 46 is a Hydrophobically-modified Ethoxylated URethane (HEUR) and is synthesized from stearyl alcohol, a diisocyanate and a polyethylene glycol. The general structure for Aculyn 46 is shown below.

Mechanism of Action

Aculyn HEUR rheology modifiers thicken via an associative mechanism. The hydrophobic parts of HEUR polymers build up associations with other hydrophobes present in the formulation. However, because the polymer is nonionic in nature, no neutralization is needed and the polymer will function equivalently in a pH range from 2 through 12.

The pendant hydrophobic groups in Aculyn HEUR polymers are free to build associations with one another and with other hydrophobes available in the formulation, such as surfactants, particulates, emulsion droplets and dyes. This phenomenon creates a network structure that results in a significant viscosity build.
These associative structures can also act to stabilize and disperse particulates in a formulation.

The chart below shows features indicative of the behavior of HEUR rheology modifiers under different conditions. Please note that these behaviors may vary to some extent according to specific formulations.

All ACULYN rheology modifiers are easy to formulate, have good to excellent salt tolerance, compatibility with anionics and nonionics and low odor. Additionally, HEUR polymers have excellent compatibility with low pH and cationic systems and excellent stability in one-part peroxide systems.

**Features of HEUR Rheology Modifiers**

<table>
<thead>
<tr>
<th>Feature</th>
<th>Rating</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ease of formulation</td>
<td>Good</td>
</tr>
<tr>
<td>Associative</td>
<td>Yes</td>
</tr>
<tr>
<td>Salt tolerance</td>
<td></td>
</tr>
<tr>
<td>NaCl</td>
<td>Excellent</td>
</tr>
<tr>
<td>D/trivalent ions</td>
<td>Excellent</td>
</tr>
<tr>
<td>Shear thinning behavior</td>
<td>Good</td>
</tr>
<tr>
<td>Residual monomer levels</td>
<td>Very Low</td>
</tr>
<tr>
<td>Solvent compatibility</td>
<td>Good</td>
</tr>
<tr>
<td>Low pH compatibility</td>
<td>Excellent</td>
</tr>
<tr>
<td>Anionic surfactant compatibility</td>
<td>Good</td>
</tr>
<tr>
<td>Nonionic surfactant compatibility</td>
<td>Excellent</td>
</tr>
<tr>
<td>Cationic surfactant compatibility</td>
<td>Excellent</td>
</tr>
<tr>
<td>Zwitterionic surfactant compatibility</td>
<td>Excellent</td>
</tr>
<tr>
<td>Peroxide stability</td>
<td></td>
</tr>
<tr>
<td>1 part system</td>
<td>Excellent</td>
</tr>
<tr>
<td>2 part system</td>
<td>Excellent</td>
</tr>
<tr>
<td>Lack of odor</td>
<td>Excellent</td>
</tr>
</tbody>
</table>
ACULYN 46 Behavior Profile

ACULYN 46 rheology modifier possesses many properties that make this polymer highly desirable for use in personal care applications, as shown in the data presented below.

Rheology

ACULYN 46 has a positive effect on the feel of formulations. When a formulation is shear thinning, such as in the interaction of ACULYN 46 with dicetyl dimethyl ammonium dichloride (DCDMAC), which is shown in Figure 1 below, it tends to feel ‘heavy’ or less oily on the skin.

**FIGURE 1. Interaction of 1% Aculyn 46 with 2.7% DCDMAC**

![Graph showing viscosity vs. RPM for 1% Aculyn 46 with 2.7% DCDMAC](image)

2.75% dicetyl dimethyl ammonium chloride solids

Surfactant Interactions

ACULYN 46 does not interact strongly with hydrophilic surfactants such as sodium lauryl sulfate (SLS) because the hydrophobe on the surfactant (C_{12}) does not counterbalance the high hydrophilicity of the sulfate group. However, when a more hydrophobic surfactant such as the C_{14-15} pareth-7 surfactant is employed, the longer chains (C_{13}, C_{14}, C_{15}) and the lower hydrophilicity of the ethylene oxide groups causes the surfactant to interact/associate with the ACULYN 46. This association effectively builds a network and structure in the solution, causing an increase in viscosity. Dicetyl dimethyl ammonium chloride (DCDMAC) is even more hydrophobic, and consequently interacts more strongly with ACULYN 46. The viscosity at higher surfactant levels (1.5% and 2% surfactant) is greater with DCDMAC than with the C_{14-15} pareth-7, indicating a stronger interaction and a stronger network in solution. See Figure 2.
ACULYN 46 rheology modifier is compatible with cationic surfactants, acids and peroxides as well as other ingredients commonly found in cosmetic and toiletry products.

This product is shipped as a low viscosity water-based liquid that thickens on addition to a formulation due to interactions with a surfactant or dispersed phase. A proprietary solvent-free viscosity suppressant is used to provide ease of handling of the ACULYN 46 HEUR polymer as it is shipped. When the ACULYN 46 HEUR rheology modifier is added to the formulation, the viscosity suppressant is released from the ACULYN 46 polymer, allowing the thickener to interact with the ingredients in the formulation.

This technology accounts for the behavior of ACULYN 46 when it is added to a formulation containing a surfactant. Depending on the surfactant type, a small amount of surfactant will increase the viscosity dramatically until a maximum is reached. After reaching this maximum, the ACULYN 46 polymer will behave like a traditional associative thickener or rheology modifier.

ACULYN 46 rheology modifier should be added slowly and steadily near the periphery of the mixing tank. The rate of addition should be adjusted to allow uniform incorporation of the thickener. Rapid addition may cause excessive thickening or flocculation due to highly localized thickener concentrations.

To ensure optimum performance of the ACULYN 46 rheology modifier, the following procedure is recommended:

1. Introduce most of the formulation water into the reactor.
2. Add ACULYN 46 polymer and stir vigorously for a minimum of 5 minutes.
3. Add the most hydrophilic (high HLB) surfactants and ingredients and stir for a minimum of 5 minutes.
4. Add the remaining components, saving the most hydrophobic component for last.
Environmental, Health and Safety Record

Toxicology

**Acute Toxicology Profile**
*Toxicity data for a compositionally similar product are below.*

<table>
<thead>
<tr>
<th>Test/Species</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oral LD&lt;sub&gt;50&lt;/sub&gt; — rat</td>
<td>&gt; 5 g/kg non-toxic</td>
</tr>
<tr>
<td>Dermal LD&lt;sub&gt;50&lt;/sub&gt; — rabbit</td>
<td>&gt; 5 g/kg non-toxic</td>
</tr>
<tr>
<td>Eye irritation — rabbit</td>
<td>Non-irritating (US and EEC)</td>
</tr>
<tr>
<td>Skin irritation — rabbit</td>
<td>Slightly irritating (US), Non-irritating (EEC)</td>
</tr>
</tbody>
</table>

*US = United States classification*
*EEC = European Economic Community classification*

**Sensitization Toxicity Profile**
*Toxicity data for a compositionally similar product are below.*

<table>
<thead>
<tr>
<th>Test/Species</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitization, Guinea pig</td>
<td>Non-sensitizer</td>
</tr>
</tbody>
</table>

**Genetic Toxicity Profile**

<table>
<thead>
<tr>
<th>Test/Species</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ames Test</td>
<td>Non-mutagenic with and without metabolic activation</td>
</tr>
<tr>
<td>In vitro Chromosomal Aberration Test</td>
<td>Non-mutagenic with and without metabolic activation</td>
</tr>
<tr>
<td>In vivo Cytogenetics</td>
<td>Non-mutagenic with and without metabolic activation</td>
</tr>
<tr>
<td>In vivo Mouse Micronucleus</td>
<td>Non-mutagenic</td>
</tr>
</tbody>
</table>

**Human Toxicity Profile**

<table>
<thead>
<tr>
<th>Test/Species</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>HRIPT</td>
<td>Non-sensitizing and Non-irritating</td>
</tr>
</tbody>
</table>

**Ecotoxicity Profile**
*Toxicity data for a compositionally similar product are below.*

<table>
<thead>
<tr>
<th>Test/Species</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Algae EC&lt;sub&gt;50&lt;/sub&gt; — 72 hr</td>
<td>229 mg/L — non-toxic</td>
</tr>
<tr>
<td>Daphnia magna EC&lt;sub&gt;50&lt;/sub&gt; — 48 hr</td>
<td>229 mg/L — non-toxic</td>
</tr>
<tr>
<td>Rainbow Trout LC&lt;sub&gt;50&lt;/sub&gt; — 96 hr</td>
<td>750 mg/L — non-toxic</td>
</tr>
</tbody>
</table>

**Overall Evaluation**

ACULYN 46 is considered non-toxic by single oral and dermal exposure, produces minimal to no irritation to the eyes and skin, a non-sensitizer, non-mutagenic in genetic toxicity assays and non-toxic to aquatic organisms as well as non-irritating or sensitizing in Human Patch testing. This material is safe and appropriate for use in a broad range of rinse-off and leave-on personal care applications.

ACULYN 46 is cleared under the major chemical inventories such as CTFA, MITI, EINECS, TSCA, AICS and Canada.
Storage and Handling

Storage

ACULYN 46 is supplied at 19% solids with a maximum viscosity of 3000 mPa.s at room temperature (25°C). The polymer is supplied as clear to slightly opaque liquid that thickens to a clear liquid.

The recommended storage temperature is 4°C to 49°C. Keep from freezing. Product, which has been subjected to freezing, will not perform satisfactorily.

Material Safety Data Sheets

Rohm and Haas Material Safety Data Sheets (MSDS) contain pertinent information that you may need to protect your employees and customers against any known health or safety hazards associated with our products. Under the OSHA Hazard Communication Standard, workers must have access to and understand MSDS on all hazardous substances to which they are exposed. Thus, it is important that you provide appropriate training and information to your employees and make sure they have available to them MSDS on any hazardous products in the workplace.

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