

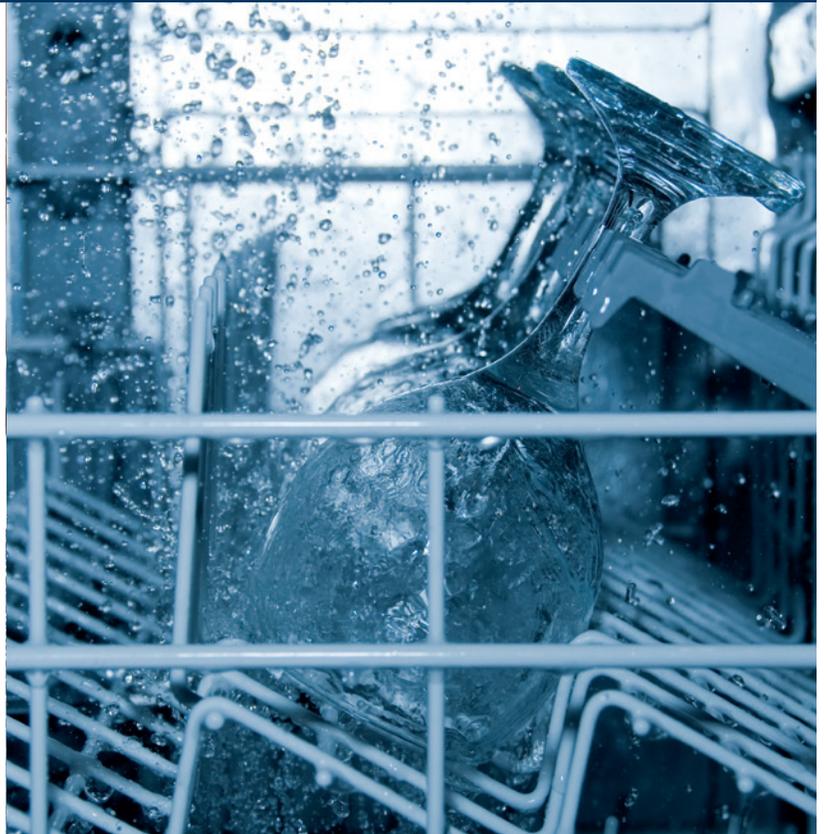


SASOL

NOVEL G12 ETHOXYLATES

New Guerbet Surfactants

Sasol Performance Chemicals



About Us

Sasol Performance Chemicals develops and markets a broad portfolio of organic and inorganic commodity and specialty chemicals and comprises three key business divisions: Organics, Advanced Materials and Wax. Our offices in 18 countries serve customers around the world with a multifaceted portfolio of state-of-the-art chemical products and solutions for a wide range of applications and industries.

Surfactants, surfactant intermediates, fatty alcohols, linear alkyl benzene (LAB), short-chain linear alpha olefins, mineral oil-based and synthetic paraffin waxes, high-purity and ultra-high-purity alumina as well as high-quality carbon solutions form the basis of our key product range.

As individual as the industrial applications they serve, the tailor-made solutions offered by our products create real business value for customers. Ongoing research activities result in a continuous stream of innovative product concepts that help our customers position themselves successfully in future markets.

Our products are used in countless applications in our daily lives to add value, security and comfort. Typical examples include detergents, cleaning agents, personal care, construction, paints, inks and coatings, metalworking and lubricants, hot-melt adhesives, bitumen modification and catalyst support for automotive catalysts and refineries as well as other specialty applications including oil and gas recovery, agriculture, plastic stabilization, and polymer production. Every day, our researchers explore ways to improve our products and develop innovations that improve the quality of people's lives.



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1. Introduction

The **NOVEL G12** product series are nonionic surfactants based on defined mid-chain branched Guerbet 12 alcohols. The individual grades of the **NOVEL G12** product series differ in the number of moles of ethylene oxide added to the starting alcohol. The **NOVEL G12** ethoxylates are new distinctive surfactants produced with unique catalyst and hydrophobe feedstock that result in interesting properties, useful in a wide range of applications.



The **NOVEL G12** product group is characterized by the following properties:

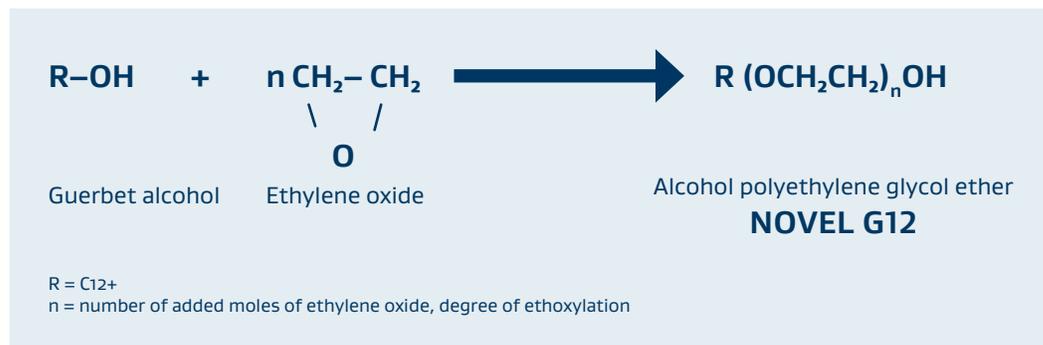
- High wetting efficiency
- Customized foaming properties
- Broad HLB series
- Strong emulsifying power
- Outstanding detergency and cleaning performance
- Chemical stability over a wide pH range
- Easy handling and storage due to low viscosity and solidification points
- Readily biodegradable: OECD Test Guideline 301B (28 d) > 60%

These favorable properties have opened up numerous fields of application for the **NOVEL G12** surfactants such as detergents, cleaning, personal care, textile auxiliaries, metalworking, emulsifying technology and other chemical-industrial applications.

These products are subject to EPA review of a submitted consolidated PMN. The results of this review will be made publically available via the Federal Register. For further information, please contact manager of Product Safety and Regulatory Affairs, Nita Moniaga at nita.moniga@us.sasol.com

2. NOVEL G12

2.1 Process Description



NOVEL G12 ethoxylates are manufactured by the ethoxylation processes using Sasol's proprietary NOVEL catalyst technology. These alcohol polyethylene glycol ethers are produced by a chemical reaction of the alcohol with varying amounts of ethylene oxide via Sasol proprietary technology. The individual grades of **NOVEL G12** ethoxylates differ in the number n of added moles of ethylene oxide and thus in the length of the polyethylene glycol ether chain. The letter n denotes the average degree of ethoxylation.

2.2 NOVEL G12 Properties

The **NOVEL G12** products are special ethoxylates based on unique branched alcohols with a very narrow distribution of homologues.

Figure 1 shows a typical ethoxymer distribution of an alcohol ethoxylate with 9 EO. The navy blue line shows the ethoxylate catalyzed with potassium hydroxide and the light blue line illustrates the ethoxylate catalyzed with Sasol's proprietary NOVEL catalyst technology. The narrow distribution of NOVEL technology presents several interesting characteristics such as lower free alcohol content and lower levels of higher molecular weight ethoxylates. The peaking ethoxymer distribution lowers the pour point, allowing easy handling, and improves the efficiency by increasing the amount of desired ethoxymers in the product. Furthermore, the narrow-range ethoxylates (NRE) typically show lower interfacial tension between oil and water compared to the broad-range ethoxylates (BRE).

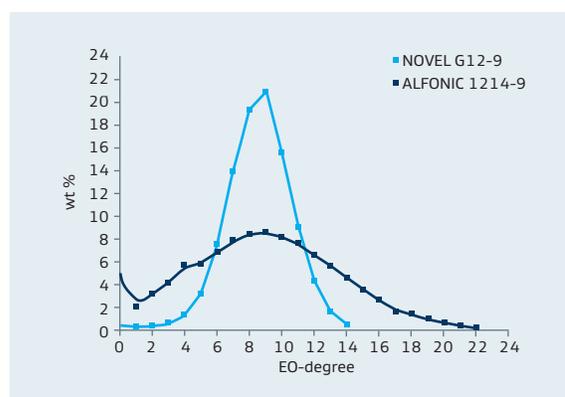


Figure 1: Comparison between NOVEL (NRE) and ALFONIC 1214-9 (BRE) ethoxymer distribution of **NOVEL G12-9**.

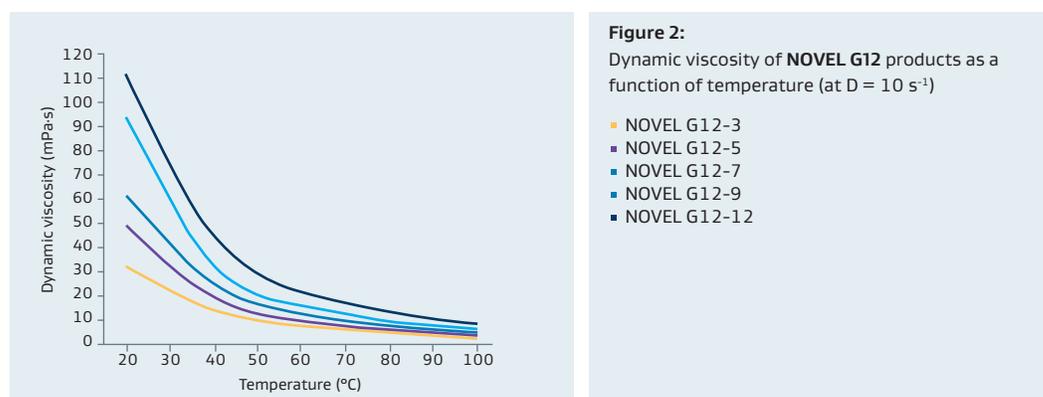
3. Technical Product Data

3.1 Viscosity

The **NOVEL G12** ethoxylate products are easily handled and stored as the EO chains (here from 3 to 12 moles) are liquid and have low viscosity at room temperature. Within this product series, the viscosity increases as the temperature decreases and as the degree of ethoxylation increases.

This favorable behavior results not only in easy handling and transportation, but also in high activity and performance when used or processed at lower temperatures. In contrast to **NOVEL G12** products, which are liquid at room temperature, commonly used ethoxylates based on linear C12-14 alcohols and even branched isotridecanol with 9–10 mole EO show a pasty to solid appearance.

Figure 2 shows the temperature-dependent viscosity profile of the **NOVEL G12** ethoxylates determined at a constant shear rate of 10 s^{-1} .



3.2 Gel Formation with Water

The pour point is measured using ASTM D97. The surfactant is added to a measurement device and cooled down. The lowest temperature where flowability can still be observed represents the pour point. Low pour points are very important properties for product storage and handling and for low-temperature applications. In general, the pour point increases with increasing ethoxylation degree. Due to the branched structure, **NOVEL G12** products show very low pour points compared to many other products found in the market.

Table 1:
Physical states of aqueous **NOVEL G12** solutions at 20°C, homogeneity and gel phases.

	Water Content in%									
	0	10	20	30	40	50	60	70	80	90
NOVEL G12-3	●	●	●	●	●	●	●	●	●	●
NOVEL G12-5	●	●	●	▲	▲	▲	▲	●	●	●
NOVEL G12-7	●	●	●	▲	▲	▲	●	●	●	■
NOVEL G12-9	●	■	■	▲	▲	■	■	■	■	■
NOVEL G12-12	●	■	■	▲	▲	■	■	■	■	■

- Clear liquid
- ▲ Gel or paste
- Cloudy liquid, homogeneous
- Cloudy, nonhomogeneous

3.3 Hydroxyl Numbers and Cloud Points

The two most relevant parameters to characterize nonionic surfactants, especially alcohol ethoxylates, are the hydroxyl number (OH number) and the cloud point (CP). While the determination of the OH number is an analytical titration of the product with potassium hydroxide solution. The CP is measured by heating up a solution of the given product in DI water or butyldiglycol solution until the solution becomes cloudy. For applications, the CP will give an indication of the solubility of the ethoxylates. It is important to evaluate different products, as the performance of nonionic surfactants can change with process conditions.

Table 2:
Typical hydroxyl numbers
(OH number) and cloud points of
NOVEL G12 products.

	OH Number in mg KOH/g	Cloud Point in°C		
		10% actives in 25% butyldiglycol solution	1% in DI water	10% NaCl solution
NOVEL G12-3	174	40	–	–
NOVEL G12-5	137	58	–	–
NOVEL G12-7	113	70	29	–
NOVEL G12-9	96	77	57	28.5
NOVEL G12-12	78	–	86	54

3.4 Foam Profile

The foaming properties of alcohol ethoxylates depend on the length, branching of the alcohol and on the ethoxylation degree.

Compared to commonly used linear mid-cut ethoxylates, **NOVEL G12** ethoxylates demonstrate more moderate foam formation and low foam stability (see Figure 3). The reason for this foam profile is the branched structure of the alcohol feedstock. **NOVEL G12-3** is hardly soluble in water and shows nearly no foam formation. With higher EO-degrees the solubility in water increases and the foaming properties will also increase.

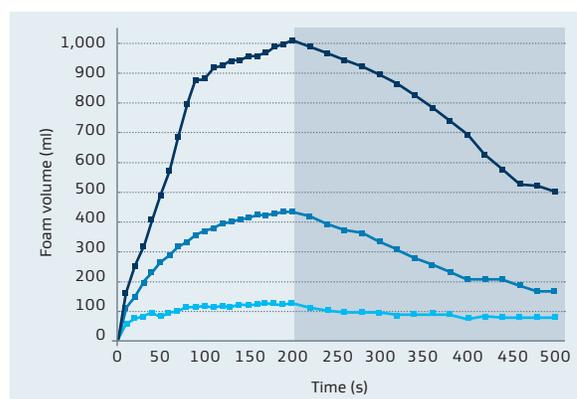


Figure 3:
Foam formation of **NOVEL G12**
ethoxylates. Measured with SITA Foam
Tester R-2000, 1 g/l, 250 ml test
solution, 25°C, 15 x 20 s stirring time
with 1,000 rpm (left). Foam decay
measurement after foam formation
(right).

- NOVEL G12-5
- NOVEL G12-7
- NOVEL G12-9

Moderate foam formation and low foam stabilities are advantages, especially in the industrial and institutional applications with high mechanical action such as high-pressure spraying, or shear mixing. **NOVEL G12** types with low EO-content such as **NOVEL G12-3** can even be used as a defoamer.

3.5 Wetting on Cotton

Excellent wetting behavior of surfactants is one of the most important properties on various fabrics. Some of the most common textile applications are the pretreatment of raw materials, e.g. wool, silk or cotton, removal of stains such as natural fats and waxes in fabrics, synthesis of rayon fabrics, dye-processes, hydrophobisation, antistatic auxiliaries and many more.

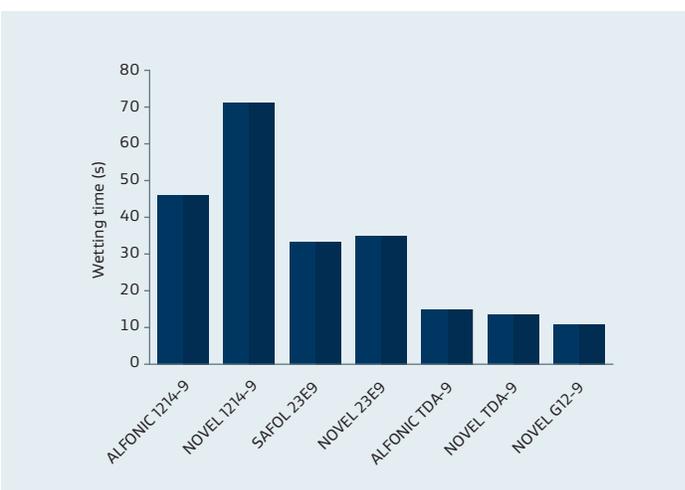
The wetting efficiency on fabrics like cotton is measured using the Cotton Disc Method (DIN EN 1772). For this test method, cotton fabric with a diameter of 30 mm is immersed in a surfactant solution using a clip (see Figure 4). The wetting time is the time it takes for the cotton fabrics' buoyancy to become neutral and to sink down to the bottom. When the surfactant molecules diffuse in the fabric of the disc and remove the entrapped air in the fabric, the air bubbles will rise to the surface. Excellent wetting times of fast-acting surfactants are typically below 15 s.

Figure 5 shows the wetting test results of different 9 EO mid-cut alcohol ethoxylates with different branching structures and ethoxylation catalysts (ALFONIC, the broad-range ethoxylates and NOVEL, the narrow-range ethoxylates). The wetting time decreases with higher degree of branching. **NOVEL G12-9** is an outstanding wetting agent in aqueous solutions and is even more efficient than ITDA with 9 EO.

Figure 4 (left):
Cotton disc test.



Figure 5 (right):
Wetting times of different 9 EO ethoxylates, based on different branching structures and broad-range catalyst (KOH) and narrow-range catalyst (NOVEL). Cotton disc test at 1,000 ppm surfactant concentration at 25°C.



3.6 Surface Tension and Critical Micelle Concentration

When adding surfactants to water, the surface tension decreases. The surface tension of pure water is 72 mN/m. With **NOVEL G12** ethoxylates, the surface tension can be decreased below 30 mN/m. Surfactants tend to form micelles above a certain concentration. This concentration is called critical micelle (formation) concentration (CMC). In most applications, the usage concentration of surfactants must be above CMC to achieve the lowest-possible surface tension and detergency. Table 3 shows the surface tension and CMCs of the **NOVEL G12** products.

Table 3:
Surface tension and critical micelle concentration of **NOVEL G12** ethoxylates. The products were measured using a KRÜSS K100 Force Tensiometer (plate method) at 0.5 g/l

Product	Surface Tension @ 0.5 g/l (mN/m)	Critical Micelle Concentration (mg/l)
NOVEL G12-3	Not water-soluble	Not water-soluble
NOVEL G12-5	Not water-soluble	Not water-soluble
NOVEL G12-7	27.5	109
NOVEL G12-9	27.6	210
NOVEL G12-12	29.9	330

Because **NOVEL G12-3** and **NOVEL G12-5** are not water-soluble, their surface tension and CMC cannot be measured with these standardized methods.

Interfacial tension can also be measured between an aqueous solution and a defined soil using the pendant drop method. Figure 6 shows this for soybean oil and a 1,000 ppm concentrated solution. Lower interfacial tension requires less energy to emulsify the oil. In other words, surfactants with a low interfacial tension can significantly increase the cleaning performance depending on the given soil.

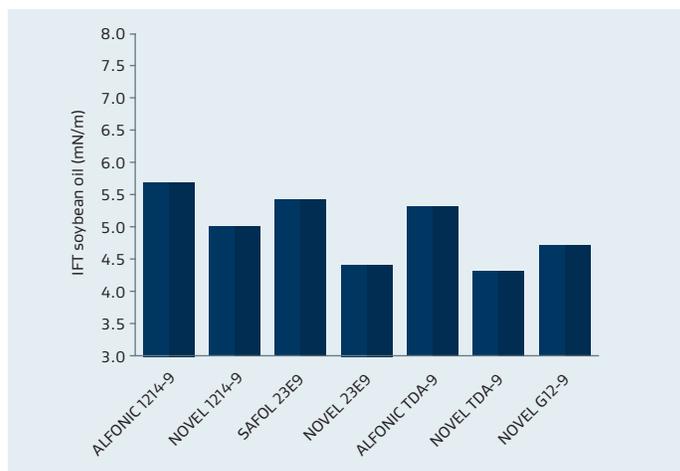


Figure 6:
Interfacial tension (IFT) between soybean oil and surfactant solution (1,000 ppm) at 23°C using the pendant drop method.

3.7 Wetting on Hard Surfaces

The contact angles of aqueous surfactant solutions indicate their ability to wet on a given surface. Commonly used surfaces are glass, steel and plastics. For this product group, the wetting properties improve as the contact angle decreases. Due to their branched structure, **NOVEL G12** ethoxylates show an overall excellent wetting property on most surfaces as shown in Table 4.

Table 4:
Contact angles measured at equilibrium on different surfaces at 1 g/l in deionized water and 25°C using a KRÜSS Drop Shape Analyzer (sessile drop method).

Product	Contact Angle an Equilibrium State (at 25°C) in °		
	Teflon	Glass	Steel
NOVEL G12-3	52.41	14.54	34.93
NOVEL G12-5	36.38	25.59	Complete wetting
NOVEL G12-7	34.85	23.89	24.58
NOVEL G12-9	28.41	18.84	23.98
NOVEL G12-12	32.55	23.46	30.65

The best wetting product for a formulation is selected based on the type of the hard surface. Due to the overall excellent wetting performance, further properties like foam formation, which is dependent on the ethoxylation degree, can be considered when selecting a product. **NOVEL G12-9** exhibits excellent wetting properties on plastics such as Teflon, glass and steel, together with moderate foam formation. In contrast, **NOVEL G12-5** shows similar properties but low foaming ability.

Due to its outstanding wetting ability on metal surfaces, **NOVEL G12-5** could be suitable as a degreasing component for water-based applications. The low foaming properties allow easy handling for several applications even for high-pressure surface treatments.

3.8 Solidification Points

The solidification temperatures of alcohol ethoxylates increase with increasing EO-degrees. **NOVEL G12** ethoxylates with 3 to 12 EO are liquid products, so they can be easily handled. In addition, the **NOVEL G12** ethoxylates have significantly lower solidification points compared to the linear C12-14 alcohol ethoxylates such as ALFONIC 1214 ethoxylates (see Figure 7).

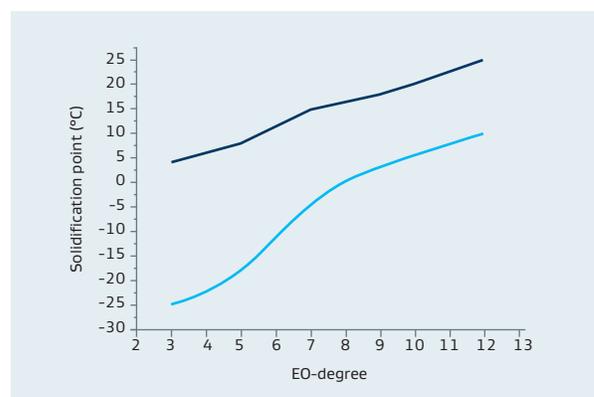


Figure 7:
Comparison of the solidification points of **NOVEL G12** ethoxylates with those of ALFONIC 1214 ethoxylates.
■ C12-14 ETO
■ NOVEL G12

3.9 Pour Points

The determination of the pour point is measured using ASTM D97. The surfactant is filled into the measurement device and cooled down. The lowest temperature where flowability can still be observed represents the pour point. Low pour points are very important properties for product storage and handling and for low-temperature applications. In general, the pour point increases with increasing ethoxylation degree. Due to the branched structure, **NOVEL G12** products show very low pour points compared to many other products found in the market.

Product	Pour Point (°C)
NOVEL G12-3	< -20
NOVEL G12-5	-13
NOVEL G12-7	-3
NOVEL G12-9	9
NOVEL G12-12	15

Table 5:
Typical pour points of **NOVEL G12** products.

3.10 Typical Product Properties

Table 6: Typical product data of **NOVEL G12**

Product Name			NOVEL G12-3	NOVEL G12-5	NOVEL G12-7	NOVEL G12-9	NOVEL G12-12
Chemical composition		C12 alcohol with n EO	n = 3	n = 5	n = 7	n = 9	n = 9
CAS no.			CAS 60636-37-5				
Technical Data							
Appearance	at 20°C		Hazy liquid	Hazy liquid	Hazy liquid	Hazy liquid	Hazy liquid
Cloud point	10% actives in 25% BDG solution	°C	40	58	70	77	–
	1% actives in DI water	°C	–	–	30	57	86
	10% NaCl sol.	°C	–	–	–	29	54
pH value	2% in DI water	–	6–8	6–8	6–8	6–8	6–8
Density	at 20°C	g/ml	0.930	0.964	0.988	1.008	1.028
	at 60°C	g/ml	0.900	0.934	0.957	0.977	0.997
Solidification point		°C	< –20	–20	–3	4	10
Pour point		°C	< –20	–13	–3	9	15
Viscosity (Brookfield)	at 20°C	mPa·s	47	51	65	113	141
	at 60°C	mPa·s	16	20	26	28	33
Water		% by weight	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5
Polyethylene glycol		% by weight	< 2	< 2	< 2	< 2	< 2
HLB value (calculated)	calculated	–	8.2	10.7	12.4	13.5	14.7
OH number		mg KOH/g	174	137	113	96	78

Source reference

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