BYK

TECHNICAL INFORMATION

FULCAT HETEROGENEOUS CLAY CATALYSTS

Contents

Introduction to FULCAT

From pharma to commodity chemicals, BYK's FULCAT product range provides only the best heterogeneous clay catalysts, with and without acid modification. The FULCAT catalyst product range, prepared from sustainably sourced natural clays, is designed to be reused and recycled, providing an efficient and green solution for a range of chemistries. Covering Brønsted and Lewis acidity, FULCAT catalysts have been optimized to provide excellent activity in such reactions as Friedel-Crafts alkylation, siloxane polymerization, dimerization, isomerization, dehydration, and more.

BYK's experience in selecting clay minerals and acid processing ensures high-quality FULCAT products with low chloride content and high surface area that consistently add value to chemical production. To support customers in all kinds of applications, BYK has invested in a dedicated catalyst testing laboratory with capability for catalyst characterization and evaluation of FULCAT in a broad range of reactions. BYK's catalyst testing capabilities enable reaction-specific optimization of the FULCAT product range, as well as a high level of quality assurance.

Note

To ensure the best appearance and full functionality, please open in Adobe Acrobat.

BYK's catalyst testing lab

Chromatography analysis suite

High-pressure high-temperature reactor

FULCAT product range

FULCAT-22 B
- BYK's market leading Friedel-Crafts alkylation catalyst
- Potent Lewis acid active sites provide exceptional alkylation reactivity
- Optimized particle size distribution for extra-fast filtration

FULCAT-22 F
- BYK's "all-rounder"
- High reactivity in a large range of reactions, including:
  - Friedel-Crafts alkylation
  - (trans)esterification
  - alcohol dehydration
  - alkene isomerization

FULCAT-22 S
- High surface area, ultra-low sulfur catalyst developed for the siloxane polymerization market
- Strong Brønsted acid sites provide fast siloxane polymerization kinetics
- Also recommended for fatty acid isomerization reactions

FULCAT-435
- High surface area, low acid value activated catalyst
- For applications where low levels of free acid and high adsorption rates are desirable, for example fatty acid chemistry

FULCAT-22 D
- Low-sulfur natural clay catalyst
- Active Lewis acid sites within the phyllosilicate structure provides high reactivity in the dimerization of
  - tall oil fatty acids
  - rapeseed oil fatty acids
  - soybean oil fatty acids

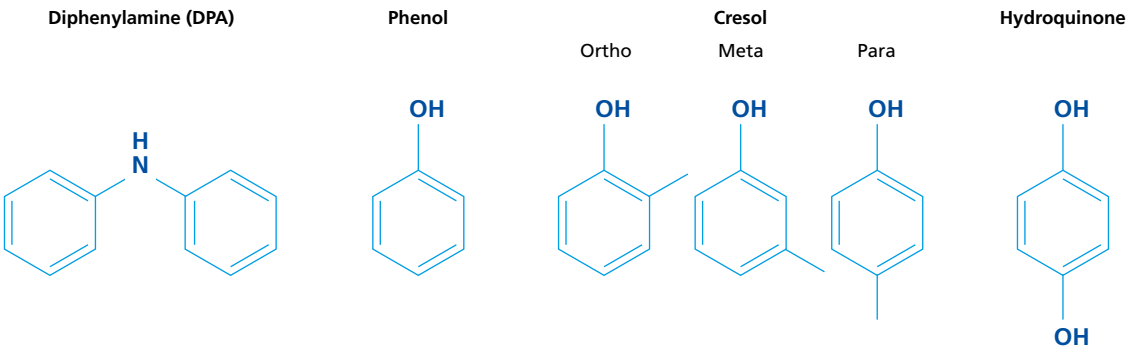
Antioxidants

Antioxidants are an important class of materials that are used in almost all consumer markets. The FULCAT product range is of particular importance to the production of automotive antioxidants. From rubber in the tires to oils in the engine, antioxidants are crucial to ensure smooth running and longevity.

Phenolic/aminic antioxidants
Phenylamine and phenolic-based antioxidants are widely used in rubber and/or lubricant formulations. The base aromatics are functionalized with a variety of organic chemistries to provide antioxidant performance tailored to their end-use environment.

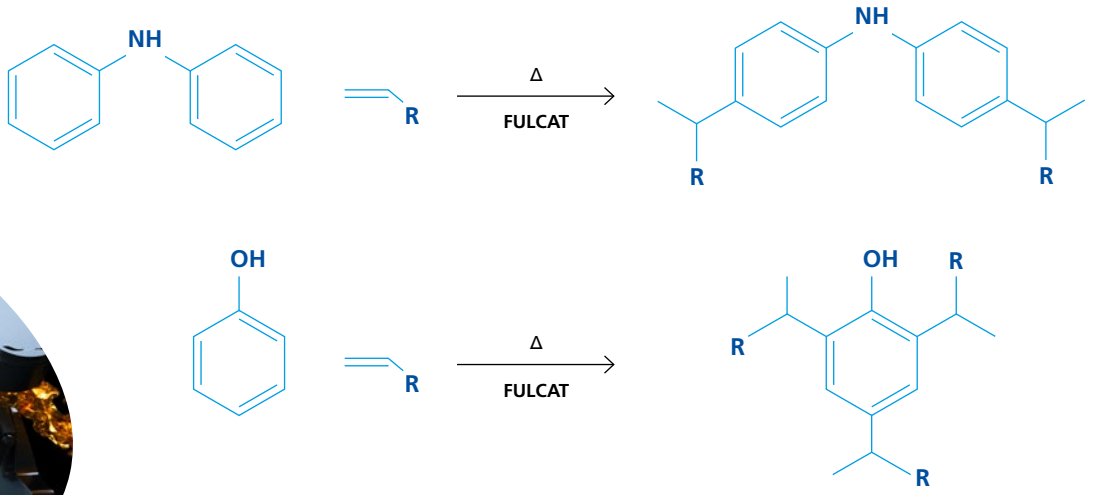
The FULCAT product range is especially suitable for the production of antioxidants by alkylation of phenylamines and phenolics (G. 02). These Friedel-Crafts type alkylation reactions are catalyzed by Lewis acids. BYK recommends FULCAT-22 B for this application. FULCAT-22 B has been developed to have market-leading Lewis acidity combined with low catalyst deactivation and excellent filtration properties. Furthermore, FULCAT-22 B is considerably less toxic than the traditional aluminum chloride Lewis acid catalyst and is easily removed from the reaction mixture to give a pure end product.

Example phenolic and aromatic amine antioxidant reagents



G. 01

Friedel-Crafts alkylation reactions



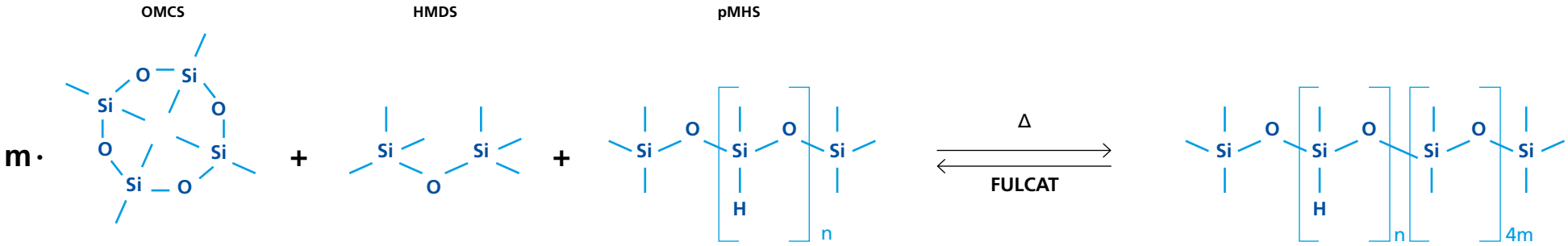
G. 02

Silicone fluids

Silicone fluids (polydimethylsiloxanes), typically prepared from cyclic dimethylsiloxane monomers, are widely used as lubricants due to their low surface tension, heat resistance, chemical resistance, shear resistance, water resistance, and viscosity stability. FULCAT-22 F and FULCAT-22 S demonstrate excellent catalytic activity in the polymerization of cyclic dimethylsiloxanes.

Functional silicone fluids
Replacing some of the methyl groups with reactive organic functionalities like hydride (G. 03) or vinyl results in functional silicone fluids. Functional silicone fluids can be used as building blocks in the manufacture of more complex silicone-based molecules. Due to the very low surface tension of the polydimethylsiloxane back bone, functional silicone fluids are excellent components of surface additives. Such silicone-based surface additives are used in a broad range of applications, from personal care to decorative coatings. Modification of the functional fluids, for example grafting polyethers on to hydride functionality via hydrosilylation reactions, is often catalyzed by precious metal catalysts. Such catalysts can easily be fouled by sulfur species. FULCAT-22 S has been developed to combine exceptional catalytic performance alongside ultra-low sulfur content specifically to produce functional silicone fluids.

Siloxane polymerization

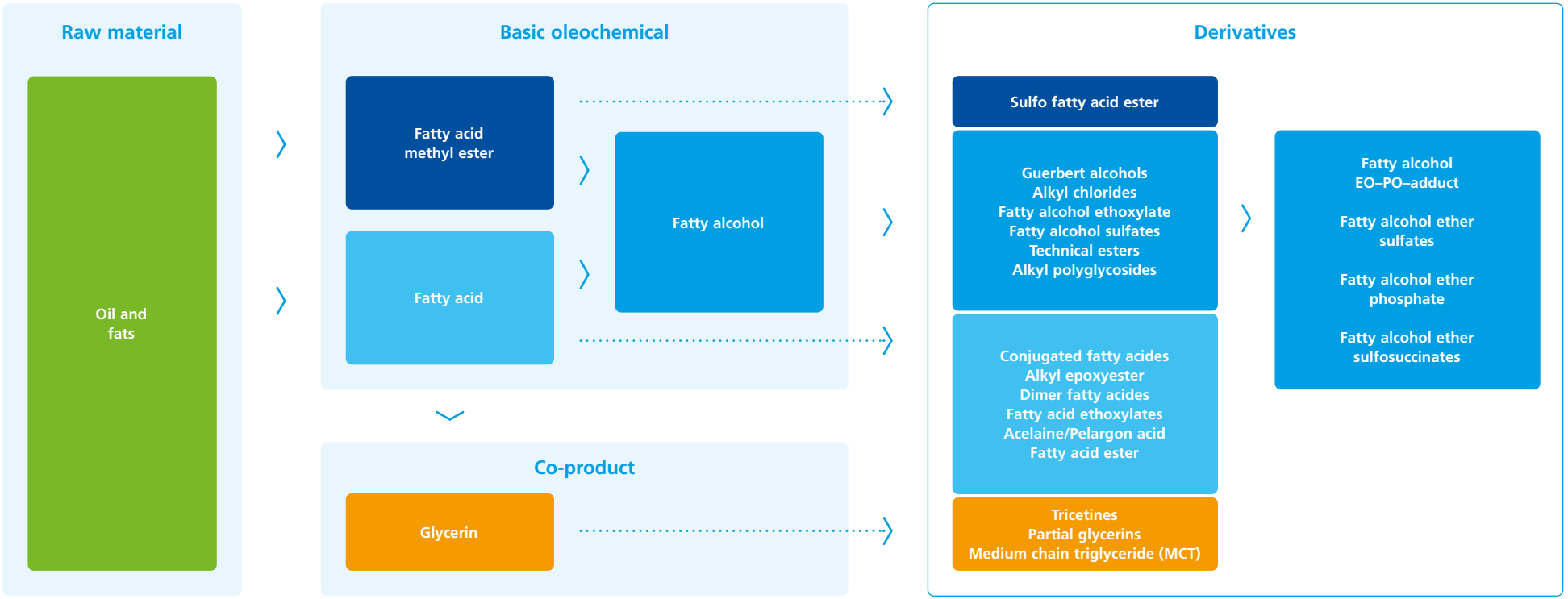


OMCS = octamethylcyclotetrasiloxane HMDS = hexamethyldisiloxane pMHS = polymethylhydrosiloxane. G. 03

Oleochemicals

Oleochemicals are compounds derived from natural oils and fats. Typically talked about are glycerin, fatty acids, and their derivatives. Derivatives of fatty acids include fatty acid dimers, fatty acid esters, fatty alcohols, fatty amines, and more. Fatty acids and their derivatives are used in a broad range of applications, including detergents and surfactants, paints, lubricants, and food stuffs. Intelligent and responsible use of sustainably sourced oleochemicals is, and will continue to be, an important part of a sustainable global chemical future. FULCAT clay catalysts add value to the derivatization of fatty acids.

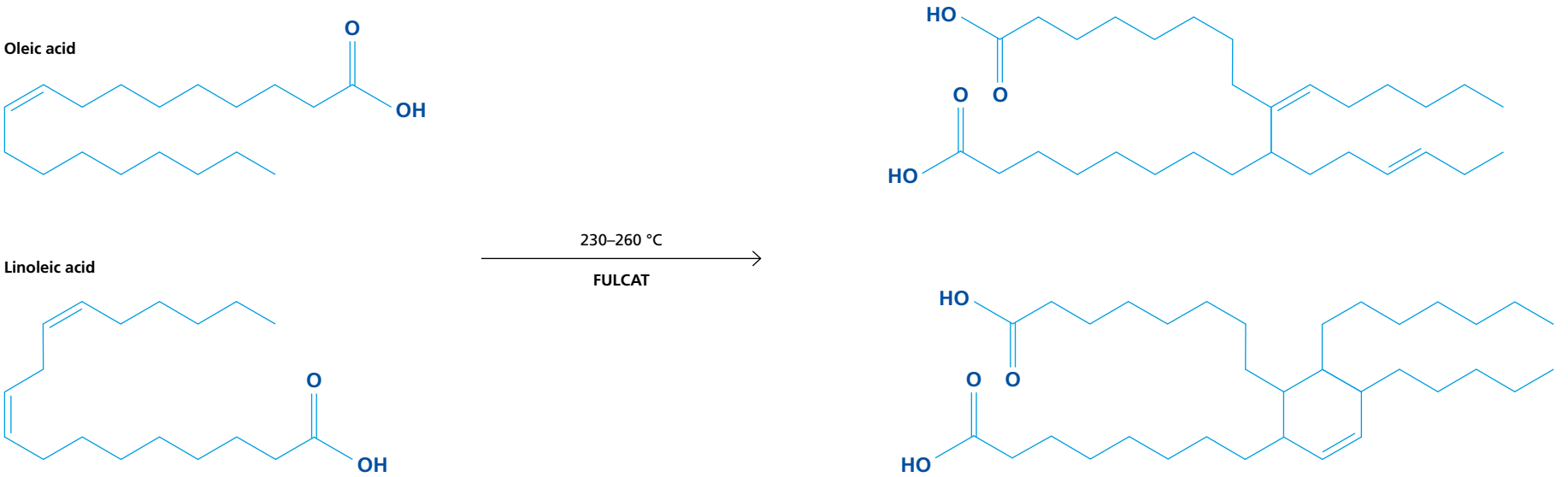
Oleochemical value chain



Fatty acid dimers

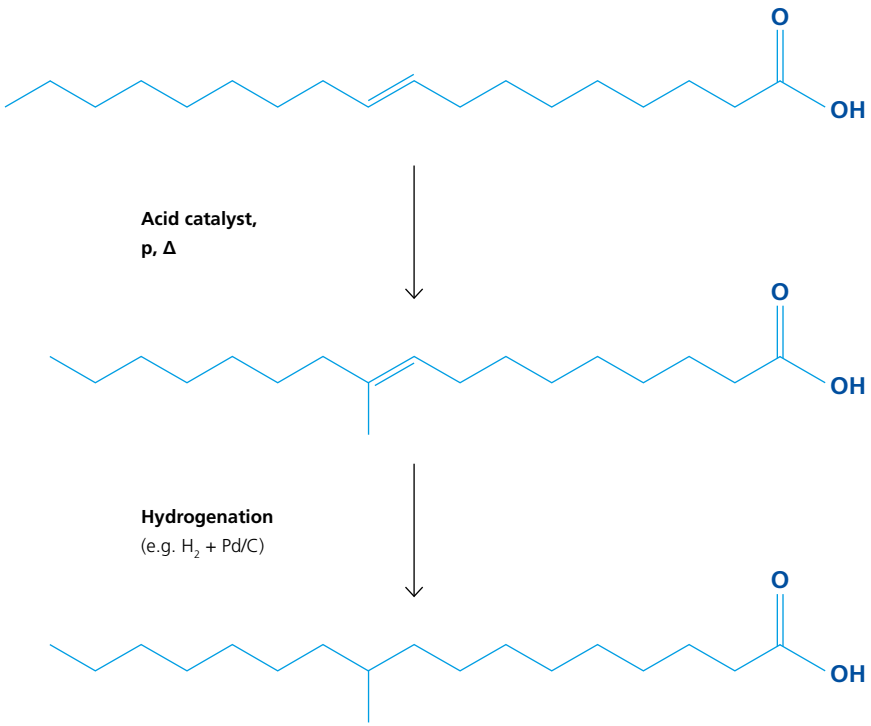
Dimer acids are produced from mixed monounsaturated/ polyunsaturated starting materials such as tall oil fatty acids, rapeseed oil fatty acids, and soybean oil fatty acids. Dimer acids are important raw materials for such chemical processes as the production of: polyesters, polyamides, polyurethanes, inks, adhesives, lubricants, corrosion inhibitors, and epoxy resin curing agents. The dimerization reaction proceeds via a combination of dehydrogenation, isomerization, and Diels-Alder cycloaddition mechanisms. FULCAT-22 D is a mineral acid-free natural clay catalyst with excellent catalytic activity in the dimerization reaction.

Example dimerization for linoleic acid and oleic acid (major constituents of tall oil fatty acid) to produce cyclic and acyclic dimer acids



Isomerization/hydrogenation
Fatty acid hydrogenation is widely used to manufacture saturated fatty acids and fatty alcohols. Of particular interest for FULCAT is the conversion of oleic acid to isostearic acid via an isomerization/hydrogenation mechanism (see G. 06). Isostearic acid is a low-viscosity, high-stability base oil that is used extensively in the cosmetics industry. Due to their high surface area, strong Brønsted acid sites and low sulfur content, FULCAT-22 S and FULCAT-435 make excellent isomerization acid catalysts for the initial conversion of oleic acid to isostearic acid.

Conversion of oleic acid to isostearic acid via acid-catalysed isomerization and hydrogenation



G. 06

Adsorbants

Due to their high surface area and high surface affinity for organics, acid-activated clays have a long history of being used as adsorbants in the purification of hydrocarbons. Examples of such purification processes include:

- Oxide scavengers in the processing of fatty acids
- Purifying white mineral oils (or paraffin oils)
- Removal of isoprene and azo-compounds from benzene streams

The high surface area and low free acid content of FULCAT-435 and FULCAT-22 S make them an ideal choice as high-performance adsorbants for a wide range of purification processes.

Brønsted acid catalysis

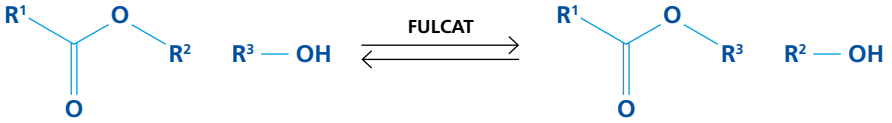
Clay catalysts, especially after acid activation, display very high levels of surface acidity. A combined effect of residual protons and ionization of bound water means that FULCAT clay catalysts can achieve surface pKa's as low as -8. This high surface acidity ensures FULCAT acid clay catalysts display good reactivity in a range of Brønsted acid-catalyzed reactions. BYK's first recommendation for Brønsted acid catalysis is FULCAT-22 F.

Carbonyl chemistry
The broad range of carbonyl chemistry makes it one of the cornerstones of chemical production. Carbonyl chemistry includes functionalities such as: esters, carboxylic acids, amides, ketones, and aldehydes. Carbonyl chemistry is driven by Brønsted acid activation of the carbonyl carbon-oxygen bond. The carbon-oxygen bond is activated by the uptake of a proton by a lone electron pair on the oxygen.

FULCAT-22 F is a an excellent source of Brønsted acidity and as a result displays strong catalytic activity in such reactions as esterification, transesterification, and reductive amination.

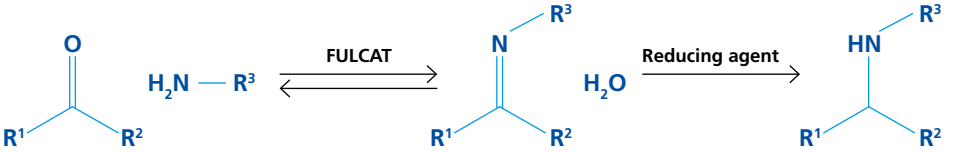
(Trans)esterification reactions are used in the production of fine chemicals, agricultural chemicals, and pharmaceutical chemicals. Example reactions include the production of fatty acid esters from fatty acids or fatty acid methyl esters, and the manufacture of polyesters. In the reductive amination of an amine and a ketone, FULCAT catalyzes the formation of the imine intermediate. An important commercial example of this reaction is the reductive amination of methyl isobutyl ketone with 4-aminodiphenylamine to produce 6PPD (N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine) – an antioxidant for rubber compositions.

(Trans)esterification



G.07

Reductive amination



G.08

Alcohol dehydration

FULCAT-22 F provides excellent catalytic performance in the acid-catalyzed dehydration of alcohols. This has a range of applications from forming alkenes and/or reactive carbocation intermediates from secondary and tertiary alcohols to forming ethers from primary alcohols.

Isomerization

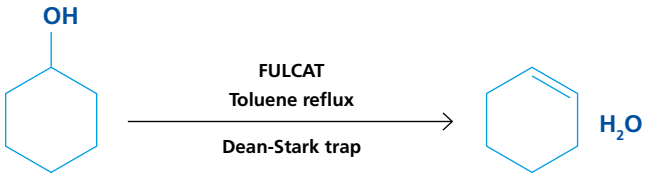
Alkene isomerization is catalyzed by Brønsted acids. Alkene isomerization can be used to rearrange molecules to their most thermodynamically stable stereoisomer, for example: the cis-trans rearrangement and alkene migration, or to redistribute double bonds statistically. BYK's recommendation for this application is FULCAT-22 F if low sulfur is not required and FULCAT-22 S if low sulfur is required (for example in the preparation of isostearic acid).

Hydrolysis

As the reverse of dehydration reactions such as alcohol dehydration and esterification, hydrolysis is also catalyzed by Brønsted acids. This means that FULCAT-22 F, as well as being the recommended catalyst for dehydration reactions, is also recommended as a catalyst for the hydrolysis of ethers, esters, and amides.

Hydrolysis reactions are critical depolymerization pathways for polyesters, polyamides, and polyethers. As the global chemical industry looks to move to sustainable chemical feedstocks, the ability to break down polymers and biomass will become increasingly important; FULCAT clay catalysts offer the potential for a clean and green solution.

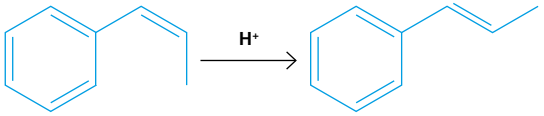
Alcohol dehydration



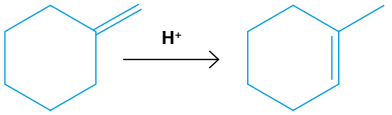
G. 09

Alkene isomerization

Example cis-trans rearrangement



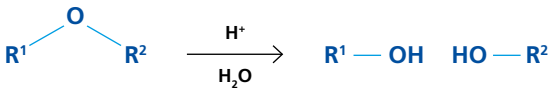
Example thermodynamic bond migration



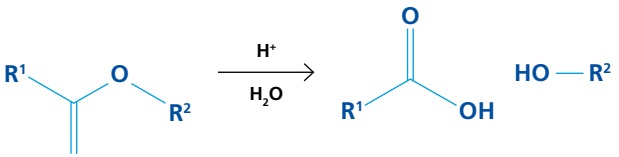
G. 10

Hydrolysis

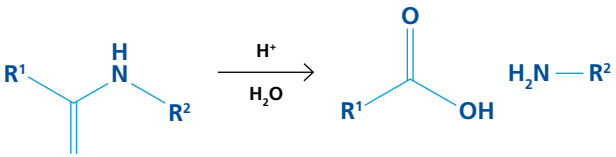
Ether hydrolysis



Ester hydrolysis



Amide hydrolysis



G. 11

FULCAT selection chart

Product	Application					Desired properties				
	Antioxidants	Silicone fluids	Oleochemicals - Dimerization	Oleochemicals - Isomerization/ Hydrogenation	Absorbants	Brønsted catalysts	Lewis catalyst	High surface area	Low sulfur	Low moisture
FULCAT-22 B	●			○		○	●	○		
FULCAT-22 D			●				●		○	
FULCAT-22 F	○	○		●		●	○	○		
FULCAT-22 S		●		○	○	○	○	●	●	●
FULCAT-435					●			●	○	○

● First recommendation ○ Second recommendation

T. 01

FULCAT benefits

FULCAT-22 B
- Acid-activated clay catalyst
- Market-leading Lewis acidity and filtration performance
- Recommended for Friedel-Crafts alkylation reactions, particularly in the production of aminic and phenolic antioxidants

FULCAT-22 F
- Acid-activated clay catalyst
- Active Lewis and Brønsted acid provide high reactivity in a large range of reactions, including:
  - Friedel-Crafts alkylation
  - (trans)esterification
  - alcohol dehydration
  - alkene isomerization

FULCAT-22 S
- Acid-activated clay catalyst
- Combines high surface area and ultra-low sulfur with strong Brønsted and Lewis acid sites
- Recommended for use when sulfur would cause problems to concurrent or downstream processes
- Particularly developed for fatty acid isomerization and functional silicone fluid production

FULCAT-22 D
- Low-sulfur natural clay catalyst
- Active Lewis acid sites within the phyllosilicate structure provides high reactivity in the dimerization of;
  - tall oil fatty acids
  - rapeseed oil fatty acids
  - soybean oil fatty acids

FULCAT-435
- Acid-activated clay catalyst
- High surface area, low acid value
- For applications where low levels of free acid and high adsorption rates are desirable, for example fatty acid chemistry or purification processes

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