

DOPED ALUMINAS

Silica-Aluminas
Mixed Metal Oxides
Hydrotalcites

Sasol Performance Chemicals



SASOL



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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.



1. Alumina Production Process

Sasol Inorganics produces high- and ultra-high-purity alumina primarily through synthetic aluminum alkoxide processing routes. The alumina is produced either as co-product with synthetic linear alcohols (Ziegler method) or directly from aluminum metal (on-purpose route).

Several production steps must be completed to produce the different alumina-based products. In the first step, an aqueous intermediate (alumina slurry) is produced, which is further tailored in the subsequent processing steps to obtain the various products sold on the market. These can be alumina hydrates, calcined aluminas and doped versions thereof.

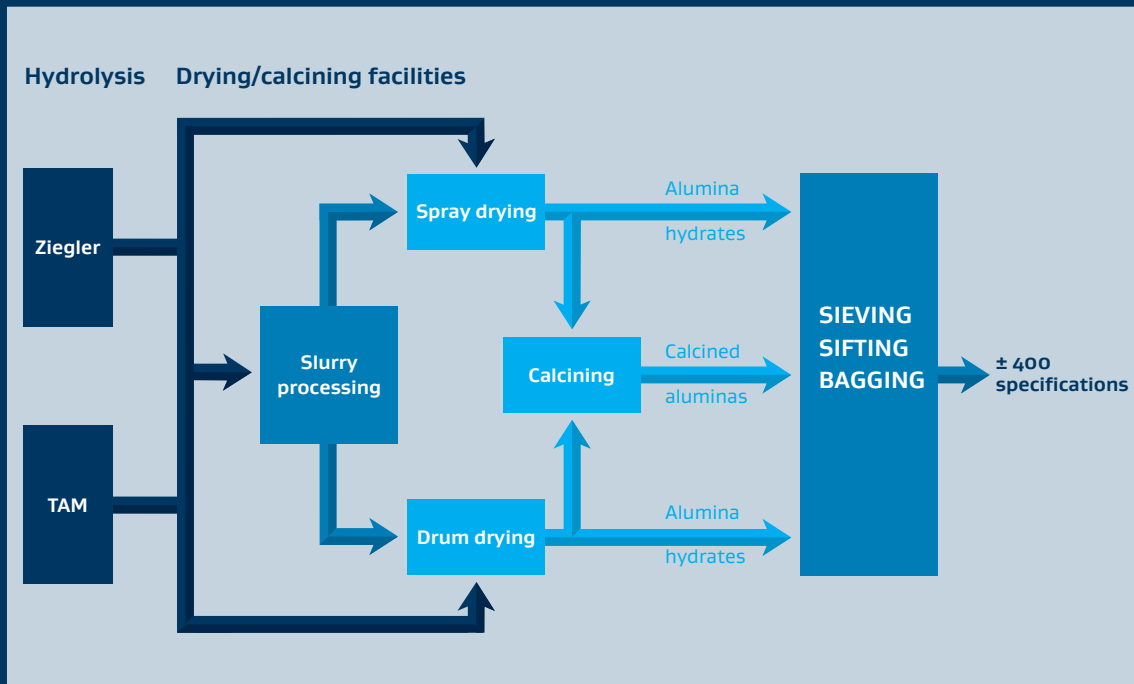


Figure 1: Schematic for the alumina manufacturing process

2. Doped Aluminas and Mixed Oxides

Sasol has manufactured high-purity aluminas and alumina hydrates with tailored physical properties for 50 years. The development of doped aluminas and mixed oxides led to a further diversification of our product portfolio with an even higher level of optimization for final use. The combination of dopants and doping technologies is another important step towards support materials with well-defined phase composition leading to improved properties like thermostability and acidity.

Silica-aluminas exhibit a higher degree of acidity than pure aluminas. The hydrates are sold under the trade name **SIRAL** and the corresponding oxides as **SIRALOX**.

Mg/Al mixed hydroxides and oxides exhibiting more basic surface sites are indispensable support materials for diverse applications. These materials are sold as **PURAL MG** and **PURALOX MG**.

Besides the formation of mixed oxides, also the addition of other elements to the pure alumina, silica-alumina or mixed Al/Mg oxides and hydroxides is a facile way to further improve the properties of the corresponding starting materials for several applications. For example, lanthanum-doped aluminas exhibit a much higher thermostability in comparison to the non-doped counterparts.



2.1 SIRAL/SIRALOX

Silica-alumina hydrates (**SIRAL**) and the corresponding oxides (**SIRALOX**) exhibit characteristics which differ significantly from pure aluminas. One of the key properties of silica-aluminas is their comparatively high level of surface acidity, making them useful catalyst support materials, for example in the field of refinery catalyst or in diesel-engine applications.

The concentration and type of acidic sites (Lewis-acidic sites versus Brønsted-acidic sites) present in the materials strongly depends on $\text{Al}_2\text{O}_3/\text{SiO}_2$ ratio as it can be seen from figure 1. In general, the total acidity is governed by the Lewis-acidic sites. The highest concentration of Lewis-acidic sites is observed for **SIRAL 5** while the highest amount of Brønsted-acidic sites is found in **SIRAL 30** and **SIRAL 40**.

The more recently developed **SIRAL HPV** series provides even higher acidity and exhibits a larger pore volume. The higher acidity is shown by NH_3 -TPD curves in figure 2 for **SIRAL 40**.

Figure 1:
Acidity of SIRAL
after calcination at 900 °C

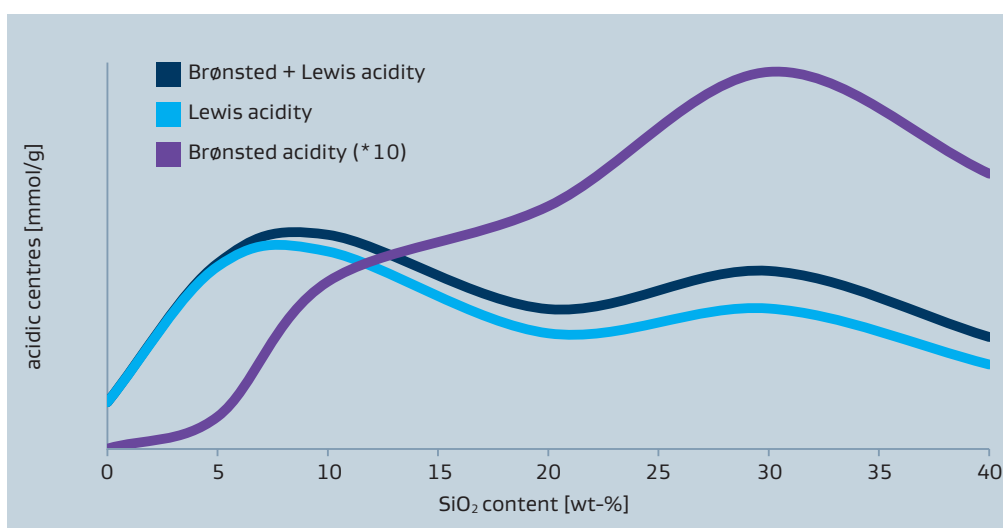
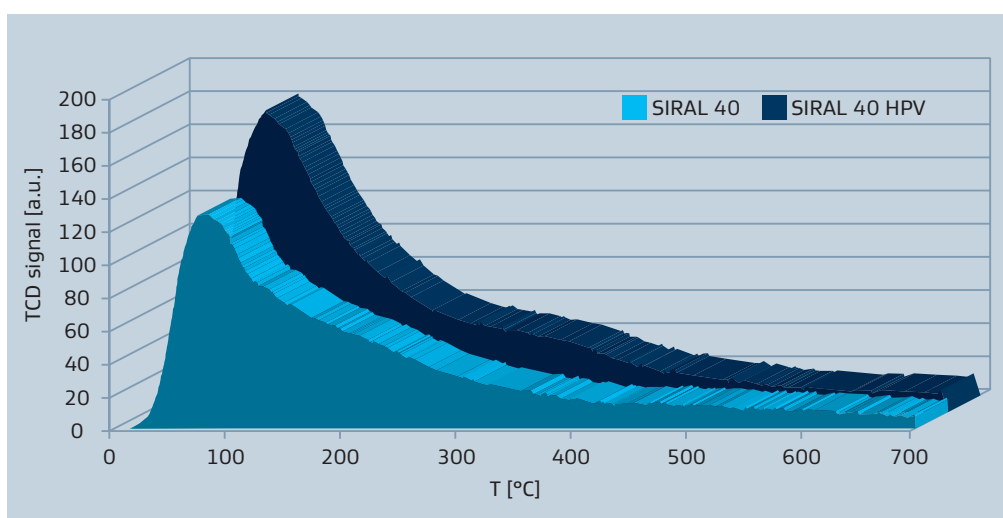


Figure 2:
 NH_3 -TPD of SIRAL 40 types
after calcination at 900 °C



Besides differences in the chemical properties, also some physical characteristics like surface area are in marked contrast to pure aluminas as illustrated in figure 3.

As different applications also demand for different physical properties, these can be tailored by varying the base alumina.

The flexibility which is possible in case of the silica-aluminas is represented in figure 4. The different physical properties of SIRALOX 5 depend on the corresponding starting alumina.

Figure 3:
Surface area of SIRALOX Effect
of silica content and temperature

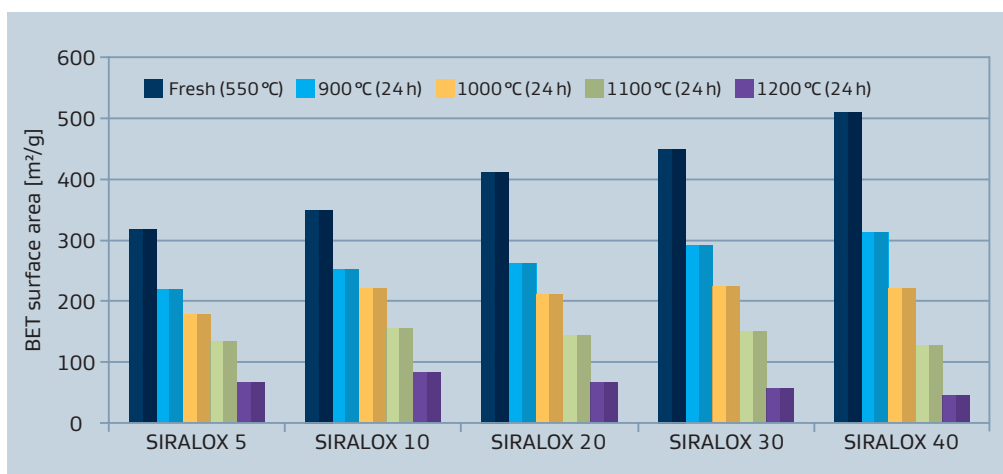
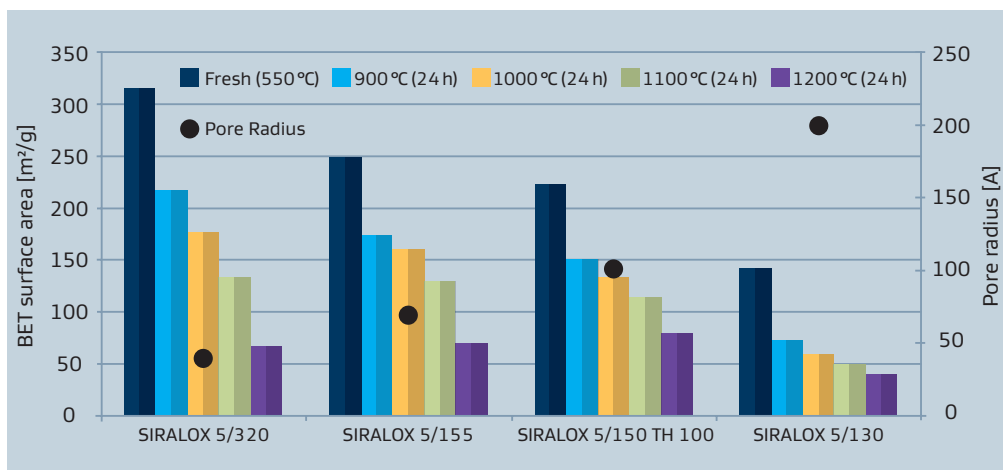


Figure 4:
Characteristics of SIRALOX Effect
of different starting aluminas



2.2. PURAL MG/PURALOX MG

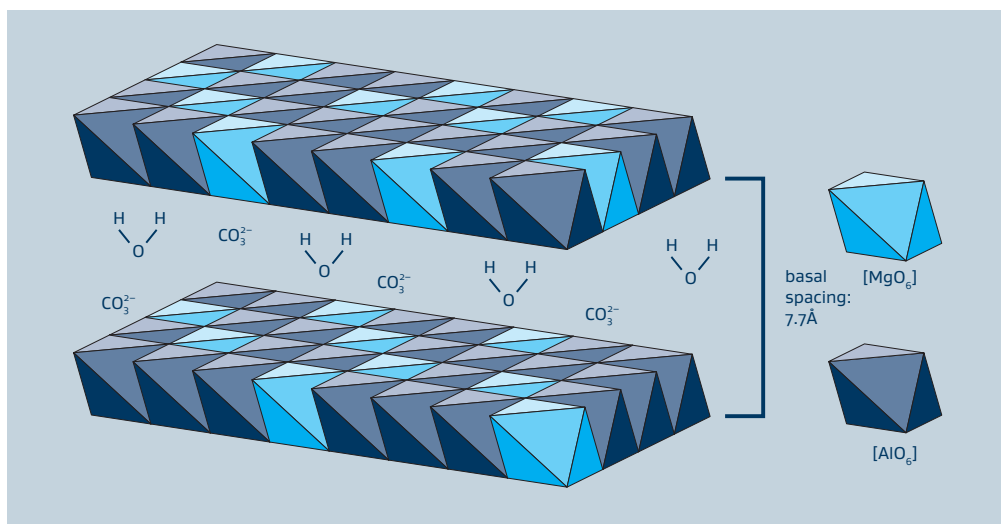
The collected and refined know-how to produce alumina hydrates via the sol-gel technique is used by Sasol to prepare other inorganic oxides or mixed oxides. The properties of these inorganic specialty materials are leading Sasol into new, interesting fields of research and application. One of these specialties is the hydrotalcite family (aluminium-magnesium compounds) which is obtained by hydrolysis of mixed alcoholates.

Compared to alumina hydrates, hydrotalcites are even more alkaline in nature. Basicity is adjustable by increasing the Mg/Al ratio and/or incorporating anions other than OH^- . As shown below, hydrotalcites have a double-layered metal hydroxide structure. The layers consist of magnesium and aluminium hydroxide octahedra sharing edges. Additional interstitial anions between the layers compensate the charge of the crystal and determine the size of the interlayer distance (basal spacing)(figure 5).

While hydrotalcites are accessible through the corresponding metal salts [Miyata et al., Clay and Minerals, 25, 14–18 (1977)], the metal alcoholate route, patented by Sasol, has advantages over other synthesis routes. Most important is that the Al/Mg ratio can be varied over a wide range. In addition, it is now possible to obtain hydrotalcites with a purity and a controlled anion content that have to date been unavailable.

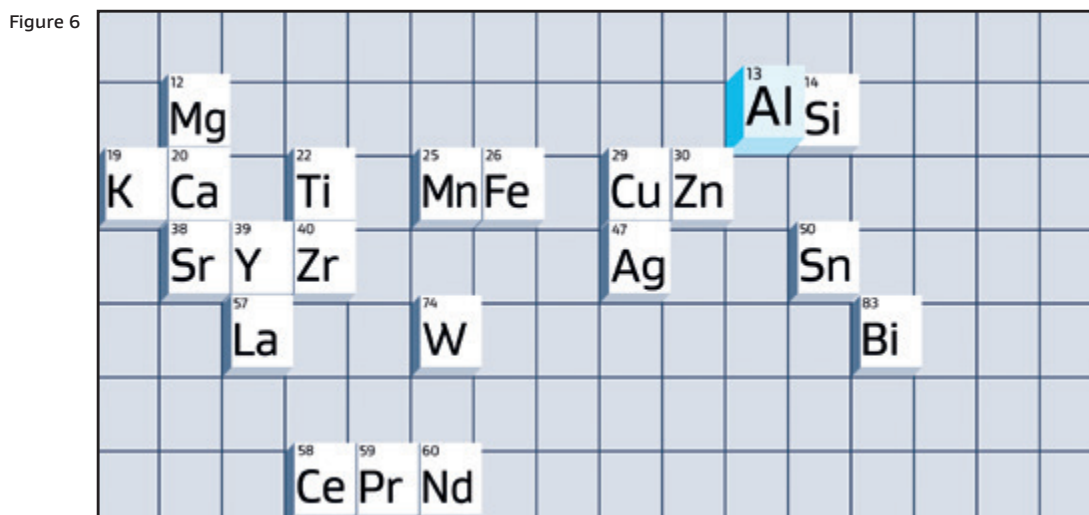
The calcined version **PURALOX MG 28** consists of the spinel phase MgAl_2O_4 . This oxide is another attractive catalyst support material for applications which require a lower degree of surface acidity than obtained in pure alumina. The advantage of **PURALOX MG 28** is its high surface area of $100 \text{ m}^2/\text{g}$ in combination with its high phase purity. Also versions with an excess of Al_2O_3 (**PURALOX MG 20**) or MgO (**PURALOX MG 30**) are available.

Figure 5:
Crystal structure of hydrotalcite



2.3. Doped Aluminas

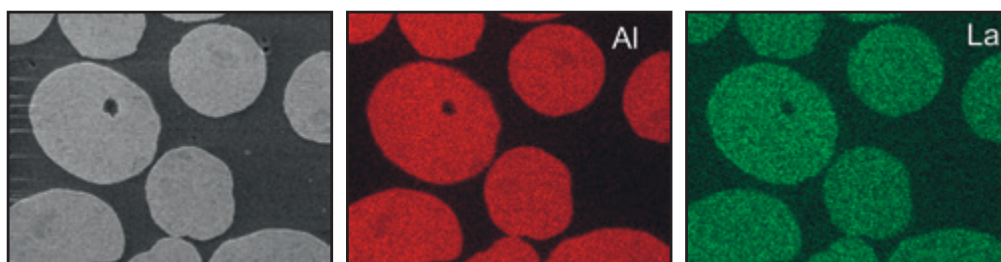
Our PURALOX, SIRALOX and PURALOX MG grades are also available as doped or even multidoped versions with a large flexibility regarding the dopants.



Furthermore, even the homogeneity of the dopant distribution among the base support can be adjusted due to our flexible doping technologies. As an example, figure 7 shows an SEM-EDX intersection image of a lanthanum-doped alumina with a very homogeneous distribution of lanthanum among the alumina particles.

These materials can be tailored according to customer request. In case of interest, please contact a representative.

Figure 7:
SEM-EDX illustration
of a La-doped alumina



2.4 Surface-Modified Alumina

Apart from homogeneous element doping, Sasol also offers the possibility to deposit dopants on the surface of the pure or already doped alumina. This allows to adjust surface chemical properties like acidity or even to combine the beneficial physical properties of alumina with chemical properties of other oxides. The technologies used for the preparation also allow surface modification of shaped carriers like spheres and extrudates.

3. Technical Data

3.1 Silica-Aluminas

Typical chemical and physical properties		SIRAL 1	SIRAL 5	SIRAL 10	SIRAL 20	SIRAL 30	SIRAL 40	SIRAL 40 HPV	SIRAL 70
Al ₂ O ₃ / SiO ₂	[%]	99 / 1	95 / 5	90 / 10	80 / 20	70 / 30	60 / 40	60 / 40	30 / 70
LOI	[%]	25	25	25	25	20	20	20	25
Loose bulk density	[g/l]	600–800	450–650	400–600	300–500	250–450	250–450	100–300	400–600
Particle size (d ₅₀)	[µm]	35	35	35	35	35	35	35	35
Surface area (BET)*	[m ² /g]	280	350	370	420	380	480	500	450
Pore volume*	[ml/g]	0.5	0.7	0.75	0.8	0.9	1.0	1.5	0.3

3.2 Doped Aluminas

Typical chemical and physical properties		PURALOX SCFa-160 Ce20	PURALOX SCFa-190 Zr20	PURALOX SCFa-140 L3	PURALOX TH 100/150 L4
Al ₂ O ₃	[%]	80	80	97	96
Na ₂ O	[%]	0.002	0.002	0.002	0.002
La ₂ O ₃	[%]	–	–	3	4
CeO ₂	[%]	20	–	–	–
ZrO ₂	[%]	–	20	–	–
L.O.I.	[%]	3	3	2	2
Loose bulk density	[g/l]	600–800	600–800	500–700	300–500
Particle size (d ₅₀)	[µm]	30	30	30	40
Surface Area (BET)	[m ² /g]	160	190	140	150
Pore volume	[ml/g]	0.5	0.5	0.5	0.8–1.0
Pore radius	[nm]	8	5	8	11
Thermal stability:					
Surface area: 24h/1100 °C	[m ² /g]	–	–	80	80
Surface area: 24h/1200 °C	[m ² /g]	–	–	40	50

*After activation at 550 °C for 3 hours.

Above Silica-Aluminas are also available as calcined materials under the trademark SIRALOX.

Further specialty grades are available upon request.

Analytical methods see page 14.

3.3 PURAL MG/PURALOX MG

Typical chemical and physical properties		PURAL MG 5	PURAL MG 20	PURAL MG 30	PURAL MG 63 HT	PURAL MG 70	PURALOX MG 28/100
Al ₂ O ₃ *	[%]	95	80	70	37	30	72
MgO *	[%]	5	20	30	63	70	28
CO ₃ ²⁻	[%]	–	–	–	10	–	–
LOI	[%]	25	35	35	40	40	max. 5
Loose bulk density	[g/l]	300–600	300–600	300–600	100–300	350–500	250–400
Particle size (d ₅₀)	[µm]	40	40	40	3–9	40	30
Surface Area (BET) *	[m ² /g]	250	250	250	15	180	100
Pore volume *	[ml/g]	0.5	0.5	0.5	n.a.	0.2	0.5
Speciality		Basic Al ₂ O ₃ precursor	Al-rich spinel precursor	Mg-rich spinel precursor	Hydrotalcite	Hydrotalcite	Phase pure spinel

*After activation at 550 °C for 3 hours.

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Analytical methods see page 14.



4. Product Information

4.1 Storage and Transfer

Alumina powders are mildly abrasive materials having a Mohs hardness of 3.5 to 4.0. Therefore, handling and storage equipment should be designed for such materials. Examples are aluminium, abrasion resistant carbon steel and polypropylene or epoxy-lined steel. Blower or vacuum systems can be used to move the powders. A minimum of 4,000 ft/min fluidizing velocity is recommended. Alumina powders will absorb atmospheric moisture, and facilities should be designed appropriately. The liquids are readily pumpable using standard centrifugal or positive displacement pumps. Due to the pH range of available products, recommended materials for process equipment include stainless steel, or polymeric-lined steel.

4.2 Safety and Handling

Pure alumina powders are classified as non-toxic nuisance dusts. Exposure to high concentrations of dust may cause physical irritation and drying of skin and eye tissues. Repeated or prolonged contact with alumina sols may cause irritation as well. Handling and shipping procedures should be designed to avoid such contact and to minimize the inhalation of airborne dust. Normal good laboratory practices and operating procedures should ensure personnel safety. For handling of different doped aluminas please see corresponding material data safety sheet.

4.3 Technical Support

The Sasol alumina organization is committed to offering the technical service necessary to ensure customer satisfaction. Technical support is available worldwide to aid you in choosing the best alumina for your needs, as well as for providing advice on safe and efficient use. The products described in this brochure give some indications of our total capability. We look forward to discussing specific technical requirements with you.



5. Certifications

All Sasol Performance Chemicals locations worldwide are certified to DIN ISO 9001/14001 and to OHSAS 18001 standards (Occupational, Health and Safety Assessment Series), and the German plants additionally comply with EMAS III (Eco Management and Audit Scheme).

Our production sites operate according to an internationally recognised, integrated quality, environmental and safety management system that has been established at the sites for many years.

6. Analytical Methods

6.1 Element Analysis

Alumina powder is quantitatively brought into solution by using acids and then analyzed by ICP, atomic emission. Additionally, X-ray fluorescence spectroscopy is used.

6.2 Crystallite Type and Average Crystalline Phases

Powdered samples of the alumina are analyzed by using X-Ray Diffractometry (XRD) on either a Siemens D5000 or a Philips X'Pert diffractometer. The resulting diffractogram enables the laboratory to identify the crystal structure of the material.

6.3 Particle Size Distribution

The particle size distribution of alumina may be measured by various instruments, namely, Cilas Granulometer 1064 supplied by Quantachrome, Malvern Mastersizer or Luftstrahlsieb (air sieve) supplied by Alpine.

6.4 Surface Area Analysis

The surface area of the alumina is measured by using an instrument supplied by Quantachrome (Nova series) or by Micromeritics (Gemini series). The method entails low temperature adsorption of nitrogen at the BET region of the adsorption isotherm.

6.5 Pore Volume and Pore Size Distribution

The boehmite is first calcined at 550 °C for three hours in preparation for analysis. The porosity is measured by nitrogen desorption using Autosorb instruments supplied by Quantachrome.

6.6 Differential Scanning Calorimetry (DSC)

Netzsch STA 449C Jupiter, Setaram 92 or Perkin Elmer instruments may be used with a selected heating rate to obtain the exothermic and endothermic transitions of alumina. Additional test methods are available for other physical properties upon request.





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