

# ANALYTICAL SOLUTIONS FROM A SINGLE SOURCE

Product Line Analytics



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# INTRODUCTION

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## WHAT DO YOU EXPECT FROM A PROVIDER OF ANALYTICAL SERVICES?

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For instance, is there a contact person available to handle your questions personally?

A team with the ability to understand your needs and to find the optimum solution?

We provide analytical solutions with the reliability and necessity of various quality standards, such as ISO 17025 or GMP.

With our techniques and methods, we have been serving our customers successfully for years in the field of specialty chemicals, pharmaceuticals and polymer.

The tests, results and interpretations are naturally treated as highly confidential.

In our laboratories, we offer you analytical services in the field of research, process development, product development, application technology, upscaling and production.

The base is a broad range of modern qualified methods as well as a wide variety of internally developed techniques and procedures.

We draw on decades of experience and highly specialized know-how – let us be your competent partner in analytical questions!

## CUSTOMER FEEDBACK

„Thank you very much for the excellent performance. This helped us a lot!“

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„...your expertise was highly valuable.“

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# QUALITY STANDARD



## EXPERIENCE

For you as our customer, it is truer than ever that time for solutions and projects is getting tighter all the time. So, it is a relief to have a reliable and experienced partner at your side who knows your business and can really help.

## QUALITY

We guarantee the highest level of quality in all test methods. Our quality standards are recognized by various international and independent entities.

Regular participation in proficiency testing is a matter of course for us, as is regular monitoring and validation of our processes.

## CONFIDENTIALITY

The samples, analytical methods and the corresponding results are naturally treated as confidential. Upon request, additional confidentiality agreements can be arranged.

## PROCESSING TIME

We guarantee the fastest possible on-time processing of your order in accordance with your requirements. Because of various accessible techniques, it may even be possible within one day.

# OUR CERTIFICATIONS AND ACCREDITATIONS

- Accreditation according to DIN EN ISO/IEC 17025 (DAkkS)
- Certification according to DIN EN ISO 9001
- Work according to § 67 German Drug Law (AMG) / GMP, FDA-registered
- Environmental management system as per DIN EN ISO 14001
- Handling permittance following the German Narcotics Law (BtMG)

# DEVELOPMENT FOCUS

## GOALS

One of our core competences is to develop, assess and implement new analytical methods, especially on large analytical devices like NMR or mass spectrometers.

It is our goal to provide innovative and required methods at an early stage transferring systematically our empiric knowledge. Here, we focus on a higher selectivity and sensitivity, rapidness, and even new kinds of information.

Our focus is explicitly on specialized analytical services with a selected portfolio.

## EXAMPLES

- CryoProbe Technology in NMR spectroscopy to increase sensitivity and reduce sample volumes
- Modern electron microscopic and spectroscopic methods to characterize various surfaces
- High-resolution mass spectroscopy for structural elucidations, high-throughput screening and bioanalysis
- X-ray micro-computerized tomography ( $\mu$ -CT) for non-destructive analysis of three-dimensional specimen





# INORGANIC ANALYSIS

## QUALITATIVE AND QUANTITATIVE ELEMENT DETERMINATION IN BULK SAMPLES

- **AAS:** atomic absorption spectroscopy generated by flame, graphite furnace, hydrides and cold vapor
- **ICP-OES:** Optical emission spectroscopy with inductively coupled plasma
- **ICP-MS:** Elemental mass spectroscopy with inductively coupled plasma, high and low-resolving, ultra-trace analysis, single element and multielement screening analysis
- **GD-MS:** Multielement analysis, element overview
- **XRF:** X-ray fluorescence analysis, quantitative and qualitative single element analysis, qualitative overview analysis, semiquantitative XRF with fundamental parameter analysis
- Volumetry, gravimetry
- Photometry
- Titrations (complexometric, acid, base, potentiometric, redox, argentometric)
- Ion-sensitive electrodes
- Ion chromatography, quantitative determination of halogenides, anions, and cations
- Combustion analysis, elemental analysis of inorganic and organic samples (determination of C, H, N, O, and S)
- Incineration and ash analysis, loss on ignition and loss on drying





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#### ELEMENTS ON SURFACES AND IN THIN LAYERS

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- GD-MS: Glow discharge mass spectrometry
- Surface analysis, light and electron microscopy, energy dispersive X-ray spectroscopy (EDX)

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#### PHASE ANALYSIS

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- XRD: Qualitative and quantitative phase analysis, including Rietveld refinement
- Quantitative determination of amorphous fractions/determination of crystallinity
- Crystallite size determination and determination of lattice parameters
- Small-angle scattering (SAXS) for determination of particle size distribution
- Temperature-independent (non-ambient) structure characterization
- Polymorphy

#### INFO

By using techniques suitable for solids and liquids, we are able to determine primary and secondary elements in inorganic and organic samples up to the trace and ultra-traces range.

# CHROMATOGRAPHY

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## GAS CHROMATOGRAPHY (GC)

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- Detectors: Flame ionization, heat conductivity, mass spectrometry
- Special injection techniques: Split/splitless, on-column, headspace, thermodesorption, pyrolysis
- Gases and liquified gases
- Gas sampling, also under GMP
- Compressed gas analytics in the field of pharmaceuticals (identity, composition, oil traces, particle content)
- GC after derivatization
- Headspace analysis (headspace GC, headspace trap GC/MS)
- High-temperature GC
- Pyrolysis GC/MS, multistage possible

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## HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY (HPLC)

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- Various separation selectivities, such as reversed phase, normal phase, ion exclusion and ion pair chromatography, etc.
- Various Detectors such as UV, diode array, fluorescence, refraction index, mass spectrometry, conductivity, light scattering (ELSD), charged aerosol, etc.
- Pre-column and post-column derivatization
- Separation of enantiomers, analytical racemate separation, determination of enantiomeric purity
- Micro preparative and preparative isolation of unknown components from products or product mixtures (identification, isolation of reference materials, recovery of pure product)

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## GEL PERMEATION CHROMATOGRAPHY (GPC)

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- GPC with RI and UV detection in different organic solvents and water

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## ION CHROMATOGRAPHY (IC)

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- Determination of inorganic and/or organic anions and cations (including carbohydrate analysis)
- In addition to the usual HPLC detection types, the main methods used are conductivity detection (with and without suppression technique) and electro-chemical detection

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## AMINO ACID ANALYSIS (AAA)

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- Qualitative and quantitative amino acid determination, trace determination, amino acid analysis following hydrolysis (e.g., for peptide quantification and characterization)
- Determination as per EP "Ninhydrin-positive substances and ammonia"

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## BIOANALYTICS

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- Gel electrophoresis (e.g., SDS-PAGE, Western Blotting)
- Assays with photometric detection (e.g., ELISA, kinetic analysis, end point analysis)





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### CAPILLARY ELECTROPHORESIS (CE)

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- Direct and indirect detection by UV, diode array
- Capillary zone electrophoresis (CZE) and micellar electrokinetic chromatography (MEKC)

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### THIN-LAYER CHROMATOGRAPHY (TLC)

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Qualitative determination of main and secondary components

### INFO

Various chromatographic separation techniques are available to determine the purity, to quantify secondary components and determine organic trace components.

# POLYMER ANALYSIS

## ANALYSIS OF PLASTICS

- Deformulation of polymer materials
- Mechanical/physical and chemical separation methods
- Extraction techniques (microwave extraction, Soxhlet, etc.)
- Identification of components (e.g., additives, emulsifiers)
- Separation and identification of material inclusions, impurities, and surface coatings or deposits

## DISC CENTRIFUGE

- Particle size distribution in aqueous dispersions from 10 nm to approx. 10  $\mu\text{m}$
- Identification of particulate impurities in dispersions

## POLYMER CHARACTERIZATION

- Determination of the chemical heterogeneity via gradient HPLC
- Various types of 2D chromatography
- Micro preparative isolation of unknown components
- Determination of conversion and polymer content



## THERMOGRAVIMETRY

- Thermostability, decomposition, and degradation of polymers
- Identification of decomposition products
- Content of carbon black
- Volatilization loss as per ASTM D6375

## DIFFERENTIAL CALORIMETRY

- Determination of the glass temperature
- Melting and crystallization temperatures
- Thermal capacity

## GPC

- Determination of polymer content
- Polymer concentration by RI, UV, and viscosity
- Eluent systems: THF, THF with addition of base and acid, DMAC with addition of base and acid
- Calibration via PMMA, PS, and polybutadiene standards
- Solvent-enhanced GPC
- Preparative isolation of molar mass fractions
- Determination of polymer content

## INFO

As a rule, to characterize polymer compounds, several, often complicated methods must be applied. The polymers have to be disjoint, additives, fillers or excipients to be identified. This approach of reversed engineering following by the testing of the components creates a huge benefit to understand and develop innovative polymer compounds.

# METHACRYLATE CHEMISTRY



## INFO

We focus on typical research topics of methacrylates chemistry and provide tailor-made solutions to meet specific customer needs.

## GAS CHROMATOGRAPHY

- GC overview analyses
- Purity check and determination of the C-number distribution of the monomers
- Determination of residual monomers, volatile components, and polymerization excipients via GC headspace

## LIQUID CHROMATOGRAPHY

- Determination and identification of stabilizers
- Determination of residual monomers and characterization of low molecular components in polymer compounds

## WET-CHEMICAL ANALYSIS

- Potentiometric titrations
- Water contain via Karl Fischer method (coulometry, volumetry, KF oven)
- UV spectra, determination of the color index
- Dry contents
- Viscosity due to Brookfield
- Determination of the viscosity number
- pH value, index of refraction
- Various methods to determine the density
- pH microwave digestion

## ATOMIC SPECTROSCOPY

- Detection of various elements in the ppm range via ICP-OES and AAS (flame, graphite furnace)
- Digestion via microwaves (solubilization)
- Pressure-less acidulation /acidic digestion

# MASS SPECTROMETRY



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## GENERAL ORGANIC MASS SPECTROMETRY

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- Ionization techniques: Electron impact (EI), chemical ionization (CI), electrospray ionization (ESI), nano-ESI, atmospheric pressure chemical ionization (APCI), matrix assisted laser desorption/ ionization (MALDI)
- Positive and negative ions
- Combination with gas chromatography (GCMS) or liquid chromatography (LCMS)
- Quantification with triple stage quadrupole mass spectrometry
- Qualitative measurements for structural determination with high-resolution mass spectrometry
- High resolution and maximum resolution with Orbitrap mass spectrometry
- Multidimensional mass spectrometry (MS-MS, MS<sup>n</sup>)
- Accurate masses for determination of the element composition/empirical formula

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## COUPLING TECHNIQUES

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- Direct vaporization
- Coupling with gas chromatography (GC)
- Static/dynamic headspace GC-MS (HS-GC-MS)
- Thermodesorption GC-MS (TD-GC-MS)
- Pyrolysis GC-MS
- Liquid chromatography (HPLC, micro-HPLC, nano-HPLC, UPLC)
- Coupling of liquid or gas chromatography with MS for determination of accurate masses

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## SPECIAL TECHNIQUES

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- Analysis of technical polymers and bio-polymers
- Qualitative and quantitative proteomics
- Enzymatic protein digestion and peptide mapping
- Identity and purity testing of proteins
- Sequence analyses of polypeptides/proteins using MS/MS techniques
- High-throughput quantification using single reaction monitoring (SRM) techniques
- LC-MS in chiral phases

## INFO

Mass spectrometry allows the identification and quantification of single components in complex mixtures of substances. The high sensitivity of this method enables to detect substances even at trace levels.

# COMPUTATIONAL CHEMISTRY

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## MOLECULAR SIMULATION WITH QUANTUM-CHEMICAL FORCE FIELD AND STATISTICAL METHODS

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- Molecule configurations and crystal structures
- Crystal morphology
- Chemical reactions, catalysis, surface processes
- Substance data
- Polymer properties
- Correlation of a substance's structure and its properties
- Reaction kinetics, molecular dynamics
- Phase equilibria and solubilities



# MICROSCOPY



## ELECTRON MICROSCOPY

- Scanning electron microscopy (SEM) and field emission scanning electron microscopy (FE-SEM) with, among other things, secondary electron detector, material contrast back scatter detector, various sample preparation techniques, among others (cryo-)microtomy, embedding, grinding, polishing, cryo-fracture, selective etching, low-vacuum unit for sensitive samples and “gentle beam” with in lens-detector (both possible without sample sputter/carbon coating)
- Transmission electron microscopy (TEM) with various sample preparation techniques, among others (cryo-)ultramicrotomy, contrasting methods
- Analytical TEM with maximum resolution (HR-TEM, 200 kV field emission, resolution down to 1.2 angstroms)
- X-ray micro-analysis (EDS) on SEM and TEM, integral analyses (point, area), line spectra (line scan), element distribution images (mapping, quantitative mapping)
- Electron diffraction, determination of lattice constants
- Particle size distributions
- Primary particle size determination (as per ASTM, by means of particle sizing technique)

- Aggregate size distributions and classification analyses (form factors, branching, etc.)
- Plasma preparation techniques, incl. surface cleaning/etching and cross section polishing
- Digital image processing, evaluation (statistics) and documentation

## LIGHT MICROSCOPY

- Light microscopy (reflected/transmitted light, polarization, fluorescence) DIC (differential interference contrast)
- Contrasting of organic matter (regular and fluorescent dyes)
- Digital image processing, evaluation (statistics) and documentation

## X-RAY MICRO COMPUTED TOMOGRAPHY

- 2D and 3D-datasets of material with low to medium density (organic matter, polymers, ceramics, thin metal layers)
- Evaluation of virtual planes in any possible direction of a 3D-reconstruction
- Evaluation of volume-based parameters (defects/inclusions, distribution/orientation of filler materials, phase boundaries, etc.)
- Statistics and non-destructive inspection as a basis for target preparation

# MOLECULAR SPECTROSCOPY

## NMR SPECTROSCOPY

- Digital 400-, 500- and 600-MHz NMR spectrometers, i.e., with CryoProbe Technology (500 and 600 MHz) for maximum sensitivity at  $^1\text{H}$  and hetero nuclei
- $^1\text{H}$ -,  $^{13}\text{C}$ -,  $^{29}\text{Si}$ - and  $^{31}\text{P}$ -NMR spectroscopy in routine operations
- NMR-active hetero nuclei possible ( $^{11}\text{B}$ ,  $^{15}\text{N}$ ,  $^{27}\text{Al}$ ,  $^{119}\text{Sn}$ ,  $^{195}\text{Pt}$ , ...)
- Determination of identity and molecular structure
- Special pulse techniques, multidimensional NMR for structural determination
- Content determinations via certified internal standards (qNMR)
- Kinetic measurements, molecular dynamics
- Solid-state NMR (400 MHz), MAS/CP-MAS

## INFRARED/NEAR-INFRARED/FAR-INFRARED SPECTROSCOPY (IR/FIR), RAMAN SPECTROSCOPY

- Fourier transform infrared spectroscopy (FT-IR)
- Surface and (micro)particle analysis with attenuated total reflection (ATR, diamond ATR, germanium ATR)
- Identity check using spectroscopy
- Infrared (IR) and raman microspectroscopy and particle analysis
- Confocal raman spectroscopy (excitation with different laser wavelengths, surface mapping)

## INFO

Due to the spectroscopic properties of their consisting atoms, molecules can easily be characterized via NMR spectroscopy, just like an identification by fingerprints. We can determine the purity of a substance and identify impurities or byproducts as well as monitor the turnover of chemical reactions .

## SPECTROSCOPY IN THE ULTRAVIOLET AND VISIBLE RANGE (UV/VIS)

- UV/VIS spectrometer



# ANALYSIS OF ORGANIC SUBSTANCES

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## CHEMICAL PARAMETERS

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- Pharmacopoeia tests (e.g., USP, Ph. Eur., DAB, among others)
- Bromine, iodine, carbonyl, ester, hydroxyl, acid, base, saponification numbers
- Water determinations (in solid, liquid, and gaseous samples)
- Evaporation residue, residual moisture, dry, and extract contents
- Ash, volatility
- Color numbers, colorimetry, photometry (APHA, Gardner, Sayboldt, iodine, among others)
- Angle of rotation (polarimeter, (heat able) microcuvettes)

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## ELECTROCHEMICAL METHODS

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- Conductometry, coulometry
- Potentiometry (mass analyses)
- Voltammetry

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## WET ANALYSES, TITRATIONS

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- Neutralization, precipitation, redox titration, complexometry, potentiometry
- Titration in nonaqueous media
- Two-phase titrations for surfactants
- Water determination as per Karl-Fischer (coulometric, volumetric, and by means of the KF oven)

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## PHOTOMETRY, UV/VIS SPECTROSCOPY

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- Anions, cations, stabilizers, aldehydes, phenols
- Spectroscopic determination of color numbers (APHA, Gardner, yellowness index, etc.)
- UV/VIS applications with/without derivatization, color reactions, and derivative spectroscopy
- UV/VIS spectrometer (registering and diode array), transmission and reflection measurements

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## COMBUSTION ANALYSIS, ELEMENTAL ANALYSIS

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- C/H/N/S/O determination
- Oxygen content determination in high-temperature oven, even in metal/metalloid oxides and in samples containing fluorine or phosphorous
- Total content of sulphur, chlorine, bromine, iodine after Wickbold or Schöniger digestion
- Content of inorganic carbon (TIC)
- Content of organic carbon (TOC, DOC)
- Total of carbon (TC)
- Total of nitrogen and nitrogen in ammonium as per Kjeldahl
- Nitrogen determination by chemiluminescence detection



#### INFO

Organic-analytical techniques enable to get the total of elements and functional groups of compounds. In combination with highly selective analytical methods (separation methods, spectroscopy), the composition of the sample can be fundamentally investigated and analytically split up to its smallest units.



# TESTING OF SURFACES, INTERFACES, AND DEPTH PROFILES

## SOLID STATE SURFACE ANALYSES

- X-ray photoelectron spectroscopy (XPS) / electron spectroscopy for chemical analysis (ESCA), monochromatized and non-monochromatized X-radiation
- Small spot XPS, spatially-resolved
- Chemical surface mapping, parallel imaging by XPS
- Determination of electrostatics of powders via XPS
- Cryo-XPS
- Ultraviolet photoelectron spectroscopy (UPS)
- Residual gas and desorption mass spectrometry
- In situ reduction and/or thermal pretreatment

## SORPTION ANALYSIS AND POROSIMETRY

- Specific surface (BET)
- Determination of pore sizes via gas adsorption (micropores: T-plot, Horvath-Kavazoe, mesopores: Barrett, Joyner and Halenda)
- Hg-porosimetry
- Determination of the dispersion of metals (Pt, Pd, Rh, Ni, Cu, ...) on substrates via chemisorption methods
- Dynamic vapor sorption (DVS)

## TENSIOMETRY AND CONTACT ANGLE

- Surface and interface tension measurements on liquids (ring, plate, pendant drop, spinning drop method)
- Critical micelle formation concentration (CMC)
- Contact angle (sessile drop)
- Wetting and wetting angle on level surfaces, fibers and powders



## INFO

Physical investigation tests provide essential information for the characterization of substances and materials.

It is essential to know the physical properties of a material e.g. to develop products with high-quality applications properties or to design, optimize, and control production processes.



# PHYSICAL PROPERTIES



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## PARTICLE SIZE DISTRIBUTION

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- Laser diffraction spectroscopy (wet and dry dispersion method)
- Evolved gas analysis (EGA)
- Optical single particle counter
- Sieve analysis (dry sieving)

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## THERMAL ANALYSES AND CALORIMETRY

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- Thermogravimetry (TG, thermal stability)
- Differential scanning calorimetry (DSC)
- Simultaneous thermoanalysis (TG / DSC)

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## RHEOLOGY AND VISCOMETRY

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- Rotational and oscillating methods (flow curves, flow limit, viscoelastic behavior, structure determination)
- Capillary viscometry

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## PHYSICAL AND OTHER PARAMETERS

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- Density measurements via pycnometers (solids, liquids and gases), oscillating U-tube (liquids)
- Determination of the bulk density and tapped density
- Powder flow behavior (angle of repose, flow index, Hausner ratio)
- Melting point (capillary method, DSC)
- Boiling point (DSC)
- Sieve analysis
- Vapor pressure (static, dynamic)
- Surface tension
- Refractive index
- Specific heat measurements
- Calorific value, heating value
- Water activity ( $A_w$ ), dynamic vapor sorption (DVS)
- Conductivity of aqueous solutions

# MATERIAL TESTING

## MECHANICAL TESTS on

- Tensile strength
- Compression
- Bending/flexural test
- Peel tests
- Shear tests
- Relaxation tests
- Impact or notched impact strength as per Charpy and Izod
- Tensile impact tests
- All the methods above are also available at various temperatures
- Ball indentation hardness
- Shore hardness
- Ball drop test

## PREPARATION OF SPECIMENS by

- Sawing
- CNC milling
- Polishing
- Drilling
- Grinding
- Constructions made of PLEXIGLAS® or aluminum



## RHEOLOGY AND THERMAL TESTING

- Melt mass flow rate MFR/MVR
- Flow/ viscosity curves
- Rotation and oscillation rheology
- Dynamic mechanical thermoanalysis and torsional vibrations (DMTA)
- Minimum film forming temperature (MFFT)



## **EVONIK OPERATIONS GMBH**

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