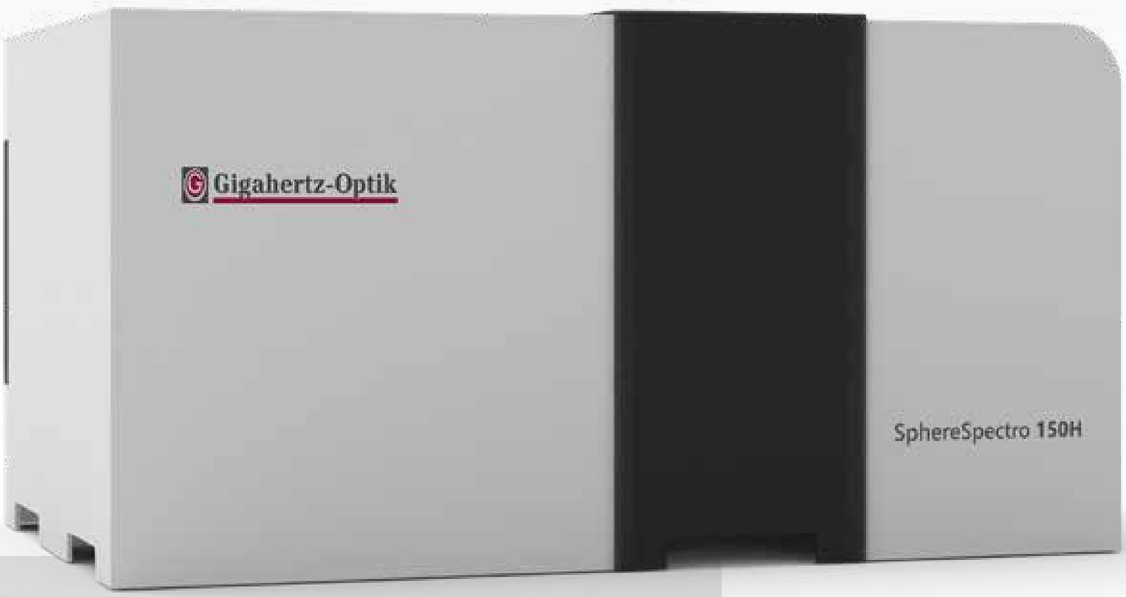
MATERIAL CHARACTERIZATION with SphereSpectro 150H

for scattering samples
from Berghof Gigahertz-Optik



THIS BROCHURE GIVES AN OVERVIEW OF:

Functionality, benefit and comparison to other analytical laboratory equipment on the market such as spectrophotometers.

OVERVIEW
SphereSpectro 150H

- The SphereSpectro 150H
- What do typical spectrophotometers incorporating integrating spheres measure?
- What is different about the SphereSpectro 150H?
- Why can the SphereSpectro 150H deliver such high accuracy for these material parameters that others can´t?
- Why should the whole sample volume be taken into account and what is the resulting benefit?
- What type of samples can be measured?
- For what type of applications is it an advantage to measure both spectral absorption and spectral effective scattering coefficients?
  - CASE STUDY:
    Measurement of chemical substances in quality control
  - CASE STUDY:
    Reproducing the color of any kind of product
  - CASE STUDY:
    Rendering
- Other advantages of the SphereSpectro 150H
- What does „SphereSpectro 150H" stand for?
- Conclusion

SphereSpectro 150H

The **SphereSpectro 150H** is a unique laboratory measurement system for simultaneously quantifying and discriminating two fundamental material properties of **scattering media**, namely the **spectral absorption coefficient** and the **spectral effective scattering coefficient**.

Statement:

"The determination of scattering and absorption coefficients is a challenge for measurement systems, since both effects "overlap" or let's say influence each other. A novel approach was needed to be successful".

R&D Manager of Gigahertz-Optik.

The key to the system, beside its robust and state of the art optical design of the light path, integrating sphere and spectrometers, is an innovation best described as "**a close to reality software model of the whole measurement system in order to determine/derive such physical quantities as the spectral absorption and spectral effective scattering coefficients**".

We can state that the mentioned uniqueness of the implemented software algorithm, which is based on a raytracing algorithm (Monte-Carlo Method) and a solution of the radiation transport theory, allows us a very precise determination of the mentioned material coefficients and that the **SphereSpectro 150H measurement method** is scientifically accepted as the reference method for these quantities.

Statement:

"The combination of high quality opto-mechanics with software modelling and a deep understanding in physics makes this an accepted reference system."

R&D Engineer of Gigahertz-Optik.

This clearly shows the difference to classical spectrophotometers which just measure energy ratios (transmission and remission). The SphereSpectro 150H goes one step further and uses physics to determine real material properties.

Measurement Output Values:

- Material parameter: Spectral Absorption Coefficient
- Material parameter: Spectral Effective Scattering Coefficient
- Classical Remission and Transmission data in 8:d measurement geometry (illumination under 8° and diffuse measurement)

The **spectral absorption coefficient** gives information on the interaction between optical radiation and the material (molecules) of the sample. Since the possible vibrational states in the molecule depend on the molecule structure and on the wavelength of the incident light, the absorption coefficient generally shows a strong wavelength dependency and characteristic shape for each molecule and is ideally suited for analytical analysis like concentration determination, etc..

In conventional spectrophotometer systems, the absorption coefficient is determined for clear samples (no scattering, just specular reflection and absorption) like colored glasses, etc. in order to perform these analytical investigations.

However with diffuse samples this classical measurement approach introduces significant measurement uncertainties since scattering effects influence the measurement results. Hence an improved approach is needed, e.g. the SphereSpectro 150H method.

In typical spectrophotometry many application oriented databases are available to do chemical analysis based on the spectral absorption coefficients (UV-VIS-IR). Since the degree of spectral absorption is determined with the **SphereSpectro 150H** with the same accuracy even for scattering samples, such databases can also be used in a similar way for measurement results from the SphereSpectro 150H.

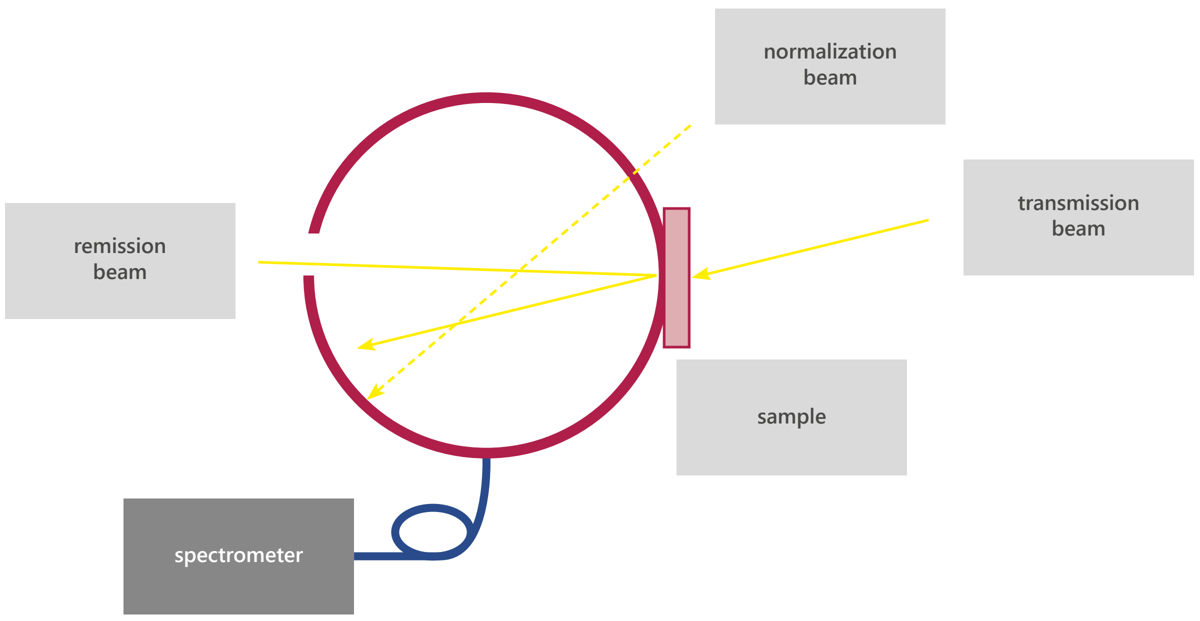
The **effective scattering coefficient** gives information on the inner structure of the sample such as the free distance between scattering molecules. It is crucial to distinguish and separate the effective scattering from absorption in order to determine the absorption with high accuracy. If this is not done, as with classical photometers, then a high uncertainty is introduced in the determination of the spectral absorption coefficient.

To make this breakthrough technology and measurement method better understandable, see the most important questions answered in the following.

This picture shows the measurement output values of a typical sample in the intutitive touchscreen ready application software of the SphereSpectro 150H.
This software can be extended with application tools in order to best meet the application.

What do typical spectrophotometers incorporating integrating spheres measure?

- The transmission is measured by typical 8:d optical path through the sample
- The remission/reflection (no differentiation) is measured by typical 8:d reflection beams from the sample
- The "degree" of absorption is determined by a comparison to a reference standard (relative measurement method)



Principle setup of the measurement light path (remission and transmission) and the normalization beam.

What is different about the **SphereSpectro 150H**?

In addition to the functions of conventional Spectrophotometer Systems, the **SphereSpectro 150H** offers the already briefly explained enhanced functionality based on the software algorithm.

The hardware setup of the **SphereSpectro 150H** is in principle comparable and consists of similar components, such as a light source, an integrating sphere and a spectral measurement unit. Unlike many systems, we are not using a scanning monochromater (long measurement times of minutes to hours).

We are using fast solid-state spectroradiometers, which allow measurements within a couple of seconds. This is possible since Gigahertz-Optik developed innovative spectroradiometers which can compete with double monochromator in the UV in e.g. stray light reduction.

(link paper https://iopscience.iop.org/article/10.1088/1361-6501/aada34)

The SphereSpectro 150H measures the following:

- The transmission is measured by illumination through the sample volume (8:d) into the integrating sphere
- The remission (called remission since it is reflection signal and signal which is scattered in the media and re-enters the integrating sphere) is measured by illumination through the sphere in 8:d on the sample's inner surface
- The "degree" of absorption can be determined by comparison to a reference standard (relative measurement method)
- The spectral absorption coefficient is determined additionally with help of the implemented model solution (absolute measurement method)
- The spectral effective scattering is determined additionally as well with the help of the implemented model solution (absolute measurement method)

The **SphereSpectro 150H** includes an algorithm that makes it possible to determine the complete light propogation through the whole sample volume.

This algorithm, developed in conjunction with Institut für Lasertechnologien in der Medizin und Meßtechnik (ilm) - Universität Ulm, is based on a solution of the radiative transport equation and a raytracing method (Monte-Carlo) which determines the propagation of light (millions of rays) inside of the sample volume therefore making it possible to do an absolute determination of both coefficients separately, the coefficients of absorption and effective scattering. In order to be successful with such a method the model needs to be perfectly adapted to the used integration sphere, measurement geometry and all the relevant physics to allow accurate measurement results.

Every single influence of the knife-edged detector port of the integrating sphere, needs to be considered and corrected.
Without going into detail, we can say that many years, almost centuries, of applied science are in this mentioned model solution.
Results have been published and are scientifically accepted as the reference method meanwhile, which shows this success.

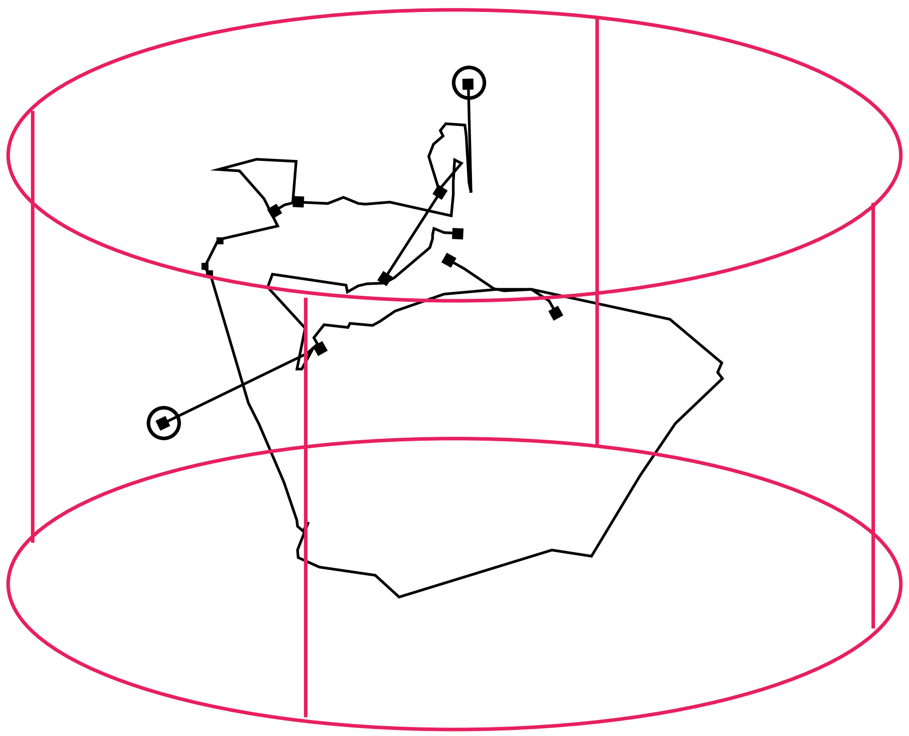
Why can the **SphereSpectro 150H** deliver this high accuracy for these material parameters which others can't?

Simply said, it´s because of the introduced **model-based software algorithm**.
In the following picture the propagation of one ray is illustrated in the sample in order to get an appreciation of how the fundamental principle of the algorithm works.

The coefficients of spectral absorption and spectral effective scattering are determined with this algorithm based on the remission and transmission measurement data and material properties like sample thickness, refractive index and asymmetric factor.

This is achieved without the need of any application based calibration procedure, as is often required, since absolute measurement results are determined. The system just needs one reference measurement with a reference standard which is supplied as part of the measurement system.

It should be mentioned that similar kind of ray-tracing algorithms are already proofed over many years in other type of applications such as computer rendering software of products in different lighting conditions. The **SphereSpectro 150H** is another step further.

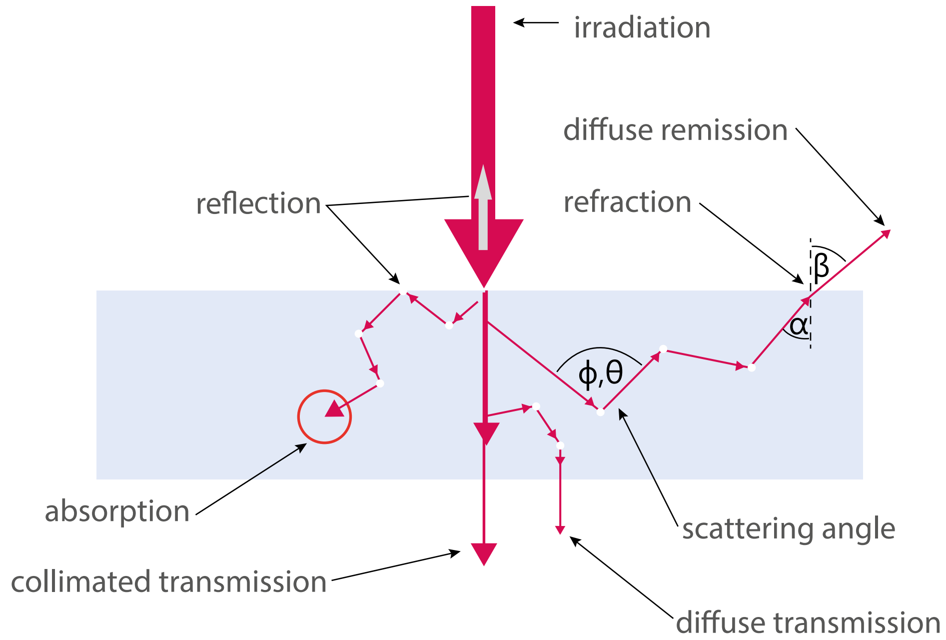


Why should the whole sample volume be taken into account and what is the resulting benefit?

Typically, if you do conventional measurements with spectrophotometers (incl. integrating sphere) you perform transmission and reflection measurements with specular components included and excluded. This is perfectly suited for surface scattering samples and transparent samples.

However for volume scattering diffuse samples this methods reaches its limits. Since without further knowledge no precise differentiation of scattered, absorbed, reemitted or transmitted radiation can be done. This is physically not possible.

In order to solve this challenge, the ray-tracing-algorithm comes into play, in addition to the physical measurements.



What type of samples can be measured?

All samples which show significant diffuse scattering like milk, cheese, cosmetic cream, medication tablets, plastics, human teeth, skin, etc..

For transparent samples such as water (with almost zero scattering ingredients) classical spectrophotometers are sufficient.

Since the measurement performs remission and transmission measurements, the sample thickness must be appropriate in order that a transmission measurement is possible. The measurement system's software guides the user in optimizing this by analyzing the signal ratios.

The sample should be homogeneous over the size of the detector port (25 mm diameter in standard configuration) in order to achieve lowest measurement uncertainties

The sample can either be solid or liquid. For liquid samples some standard cuvettes are available. For solids the sample just needs cutting to size with an appropriate thickness that fits in the sample chamber.

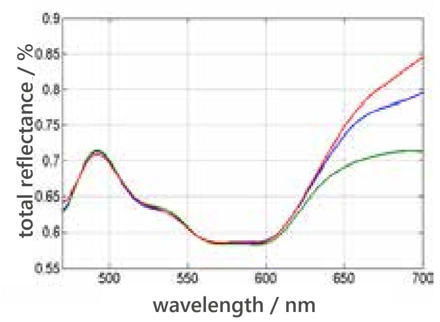
This picture shows the sample chamber where either solid or fluid samples (in cuvettes) could be mounted/clamped quickly and easily

This picture shows some of the cuvettes for liquid samples. Solid samples should have similar geometry.

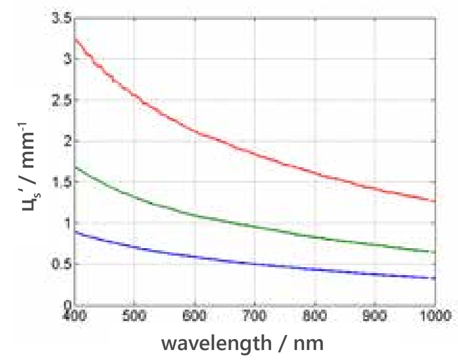
For which type of applications are both - spectral absorption and spectral effective scattering coefficients – an advantage?

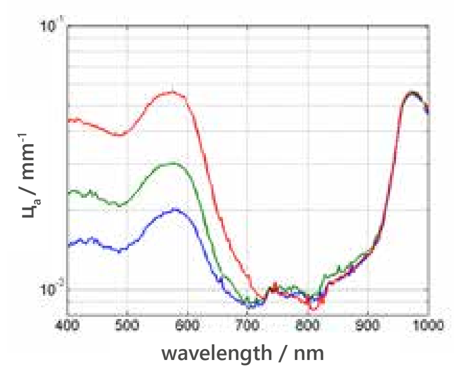
Explanation by example using different ingredients in a basic sample (absorption and dispersion components added):

In the picture three different diffuse samples are shown. From left to right the absorption and scattering is enhanced up to a factor of 4. If scattering and absorption cannot be distinguished, as with classical spectro-photometers, no difference can be determined in the VIS spectral range, see the following measurement result:



The **SphereSpectro 150H** is able to separate these effects and determines the measurement results as expected. This can be achieved by the mentioned separation of scattering and absorption by the developed sophisticated algorithm:





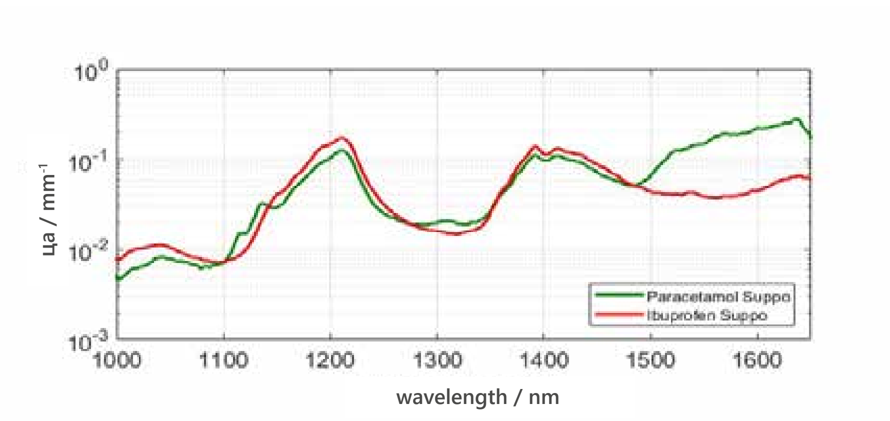
CASE STUDY:
MEASUREMENT OF CHEMICAL SUBSTANCES IN QUALITY CONTROL

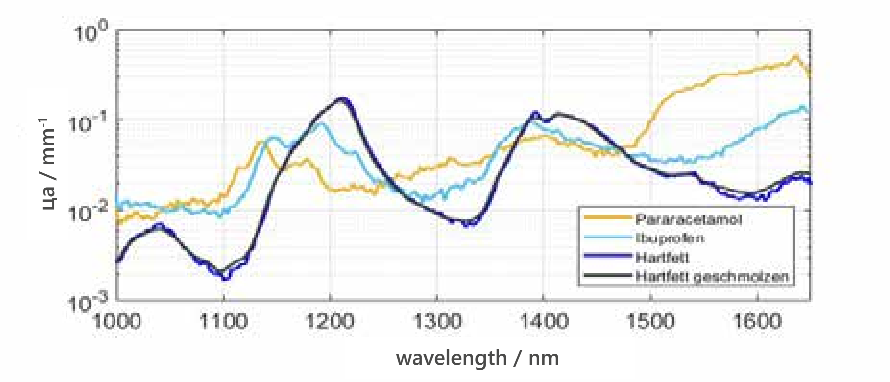
The **SphereSpectro 150H** can be used to determine the concentration of chemical substances based on the linear superposition of the individual absorption coefficient and the effective scattering coefficient spectra. In the example below it shows the measurement of Paracetamol and Ibupropfen.

The **SphereSpectro 150H** can clearly distinguish between absorption and scattering inside of the sample and therefore makes it possible to take the measurement data of the spectral absorption coefficient to analyze the content of Paracetamol and Ibuprofen individually.

A database of the pure content is needed and, based on superposition, the pure concentration of the substance is determined.

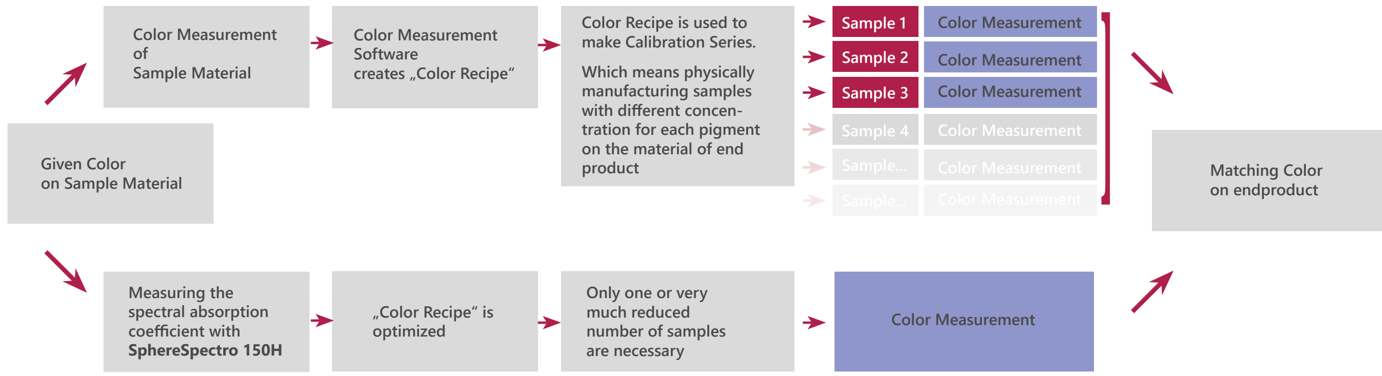
Such types of measurement are of importance in production control.





Paracetamol = 0.379 g/g
Ibuprofen = 0.243 g/g

CASE STUDY:
REPRODUCING COLOR ON ANY KIND OF PRODUCTS



This shows the procedure when (any kind of) products needs to be manufactured and should match to a given color based on a „color sample".

Status quo is that the color of this „color sample" is measured and based on these measurement data a color recipe is created (by software connected to the color measurement system).

This color recipe gives information how the different samples on the end product material needs to be manufactured. There are many samples needed with different color concentrations per each color pigment because the color on the end-product needs to be matched to the color of the sample as good as possible – therefore some trials are needed to achieve the required color match finally.
A lot of manpower and time needs to be invested. Each sample is measured and in the end after a lot of measurements are done the color on the end-product hopefully matches to the given color.

With the **SphereSpectro150H** the spectral absorption coefficient and the spectral effective scattering coefficient are directly measured. With that data, the color recipe is optimized and ideally only one sample needs to be manufactured and measured. This reduces the manpower and time of the whole process considerably.

CASE STUDY:
RENDERING

The image compares two approaches:

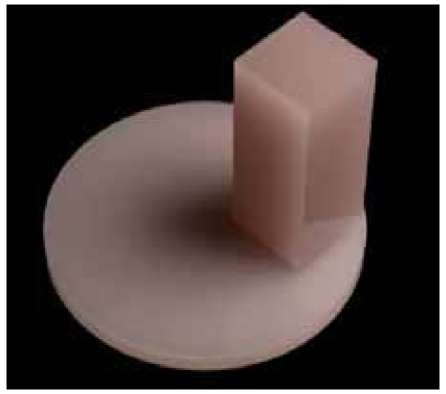
- A picture taken with the camera (reality)
- A virtual picture calculated by computer (rendered picture)

The lighting conditions are the same in both cases i.e. same position of light source relative to the plastic sample, same light spectrum and same intensity of light. The information on these lighting conditions are put into the rendering program on the PC. In order to render the appearance of this sample some further information is needed.

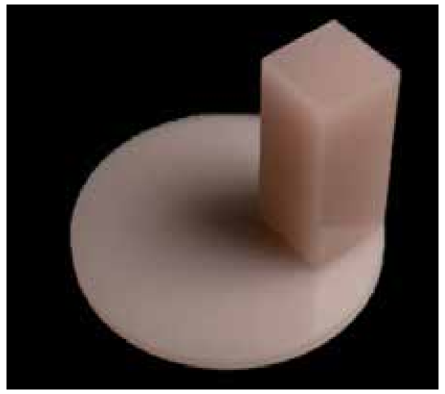
This is the geometry of the sample and the material of the sample. The geometry can be measured and designed (usually done by CAD programs). However, the material of the sample needs to be known in detail. There is no literature existing where this information could be taken from.

The light absorption characteristic and also the light scattering characteristic of this sample material (whole volume) is needed to render this sample as accurately as possible to make it look as the „real“ picture. The **SphereSpectro 150H** is measuring the spectral absorption coefficient and the spectral effective scattering coefficient and with these measurement values entered into the rendering program the virtual sample (rendered on PC) looks very similar to the real picture taken by camera.

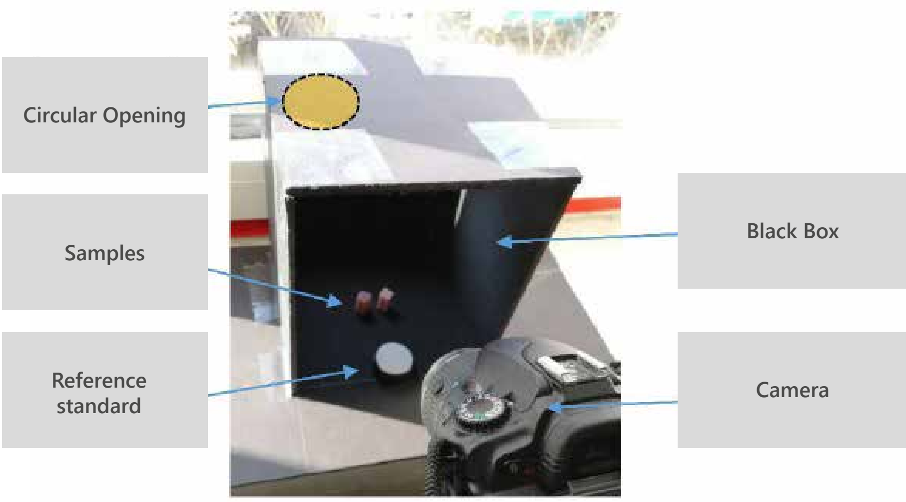
Rendered Image



Real Image



This picture shows the two pieces of plastic in real environment (left) and the two pieces of plastic rendered by using of the material coefficients (spectral effective scattering and spectral absorption coefficient) measured by SphereSpectro 150H (right).



This picture explains the measurement setup to take the picture.

This is an example of how accurate the measurement results of the **Sphere-Spectro 150H** match the reality and hence it makes completely new applications possible.

You might ask yourself why such things are needed. There are many examples, one of which is the rendering task in dental applications. If a tooth needs to be replaced then it is usually prefered by the patient to have the new tooth of same color as the still existing teeth. For that application the spectral absorption coefficient and the spectral effective scattering coefficients need to be measured.

Real Image

Rendered Image

This picture shows the rendering on teeth, medical application.

Other advantages of the **SphereSpectro 150H**

- Easy sample handling. No need of complex sample preparation. Just fill the liquid samples into the cuvette or cut the solid sample to the needed geometry. Even some solid samples such as tablets could be processed into homogeneous powders and put into cuvettes.
- Measurement time is very short – within seconds
- Plug & Play with intuitive user software
- Large sample compartment with several probe fixing options
- Reduced maintenance costs

Plug & Play with intuitive user software

What does **SphereSpectro 150H** stand for?

Sphere:	Integrating Sphere System
Spectro:	Optical measurement system including different types of Spectroradiometers (UV-VIS-IR)
150:	Diameter of the Integrating Sphere
H:	Halogen Lamp is used as the light source

Conclusion:
The **SphereSpectro 150H** is a device that has **EXTENDED** function to a typical spectrophotometer, which allows the user to apply well known investigations now as well to diffuse scattering samples.

The implemented software algorithm allows highest accuracy and makes this type of measurement to be the reference method for scattering diffuse media.

As a result, this measurement system opens the door to many new applications. Even in established laboratory applications advantages can be expected.

Gigahertz-Optik
Member of the Berghof Group

SPECIFICATIONS: SphereSpectro 150H

General	
Short description	Laboratory measurement system for determining the spectral absorption coefficient and spectral effective scattering coefficient of scattering media
Main features	• Simultaneous determination of scatter and absorption (unique feature) • Measurement on diffuse sample, solid or liquid (unique feature) • Simple sample handling • Measurement within seconds • Table top device • UV, VIS and IR spectral range possible • Large sample compartment with several sample fixing options • Precise and absolute measurements with low measurement uncertainty • Minimal noise and stray light due to use of high end spectrometers • Maximum light throughput based on imaging mirror optics • Easy to change light source • Plug & play with intuitive software package
Measurement ranges	UV, VIS to IR (depends on version)
Typical applications	• Material analysis • Concentration determinations • Quality assurance • Biophotonics • Active ingredient determinations • Chemometrics • Food analysis • Pharmacy, cosmetics • Physical parameter based rendering • etc.
Spectral Detector	
Spectral range	Version 1: VIS (350 nm to 1050 nm) Version 2: VIS and IR (350 nm to 2150 nm) Version 3: UV, VIS and IR (200 nm to 2150 nm)
Measurement time	Typical measurement time is within a few seconds. The measurement time of the high resolution mode is within 2 minutes.

SphereSpectro 150H

If you have any questions or ideas, do not hesitate to contact us.

Our **technical sales team** is always available for further information.

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For more information, please visit our website. **www.gigahertz-optik.com**

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With its innovative and high-quality products as well as application solutions, Gigahertz-Optik enjoys a high regard from its international customers within the field of optical radiation measurement technology. As a manufacturer, Gigahertz-Optik offers standard and custom-made solutions. Regular investments in new technologies ensure that Gigahertz-Optik is able to offer modern measuring solutions to its customers in industry and science.

Broadband light measurement devices

- UV radiometers
- Photometers
- Light hazard meters

Spectral light meters

- Handheld devices
- High-end devices
- UV-VIS-IR Spectroradiometer
- Weather-proof devices
- Light transmission

Complementary products

- Integrating spheres
- Integrating sphere light sources
- Calibration standards
- Electronics, optomechanics
- Optically diffuse materials

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