ALPHA II

- FTIR Must & Wine Analyzer

FTIR

Innovation with Integrity

Explore a new way of controlling the quality of your wine over the complete production process: The ALPHA II FTIR wine analyzer allows to analyze must, must under fermentation and finished wine. With only one measurement you can determine many important quality related parameters within seconds and without the need for an extensive sample preparation. Since no reagents or consumables are needed the method is very cost effective.

- Simultaneous analysis of different parameters with one measurement.
- Reliable measurement results due to robust ATR measurement technique.
- No sample preparation.
- Extensive calibrations for the analysis of finished wines, must under fermentation and must.
- Unrestricted access to set up new calibration databases.
- Easy to use thanks to a software assisted step-by-step analysis.
- Space saving and portable.
- Low maintenance and low running costs.

ALPHA II FTIR Must & Wine Analyzer

Robust measurement principle

The ALPHA II Wine Analyzer analyzes the sample by utilizing the so called ATR (Attenuated Total Reflection) measurement technique. A robust ATR diamond crystal serves as sample interface. It allows measurements without sample preparation and guarantees precise and reproducible analysis results.

The principle of the ATR is shown in the schematic in figure 1. The core of the ATR-technique is a diamond crystal that reflects the incoming light in a right angle to the detector. If a sample is placed on top of the diamond a fraction of the light penetrates into the sample and is attenuated according to the absorption characteristics of the sample. This attenuation is measured by the detector and transformed into a spectrum.

The ATR- measurement principle has many benefits when compared to the transmission technique that is used in other analyzers: The layer thickness remains constant, the cell is resistant to chemicals and scratches and the setup is insensitive against turbid and outgassing samples.

For more details on FTIR analysis, see last page.

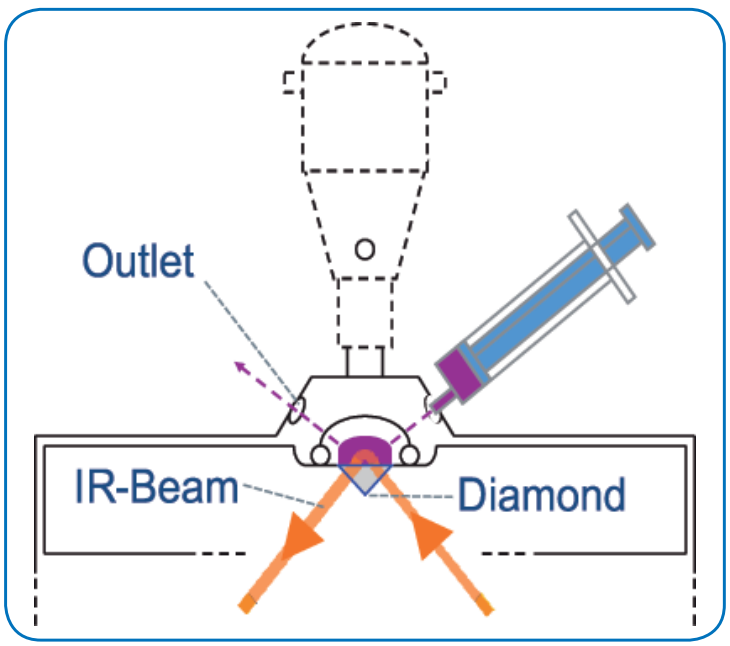


Figure 1: Schematic of the ATR flow-through cell.

Instrumentation and Software

The wine analyzer is based on the well-proven ALPHA II FTIR spectrometer from Bruker and is therefore very robust, space saving and mobile. As an addition to the analysis of liquids, the diamond-ATR unit can also be used without the flow-through cell for the measurement and identification of solid samples like for instance wine lees etc.

Due to its easy to use hard- and software the ALPHA II Wine Analyzer can be operated by inexperienced personnel. As the user is guided through the analysis process with the aid of a special software-wizard (figure 2), operating errors are effectively ruled out.

The manual measurement of a sample with the Wine-Wizard is really simple and takes only a few steps. After the sample is being injected into the flow-through cell the user only needs to enter the sample information and press "OK" (see figure 3).

The measurement and analysis are then performed fully automatically. The analysis process needs about two minutes; the cleaning of the cell is done by the injection of water. The analysis result is shown on the display and additionally a detailed measurement report is being created (pdf and/or csv format, figure 4).

The ALPHA II Wine Analyzer allows to expand the set of analysis parameters by adding user made calibrations. Moreover the user can extend the range of analyzed products to juices, beer and other beverages.

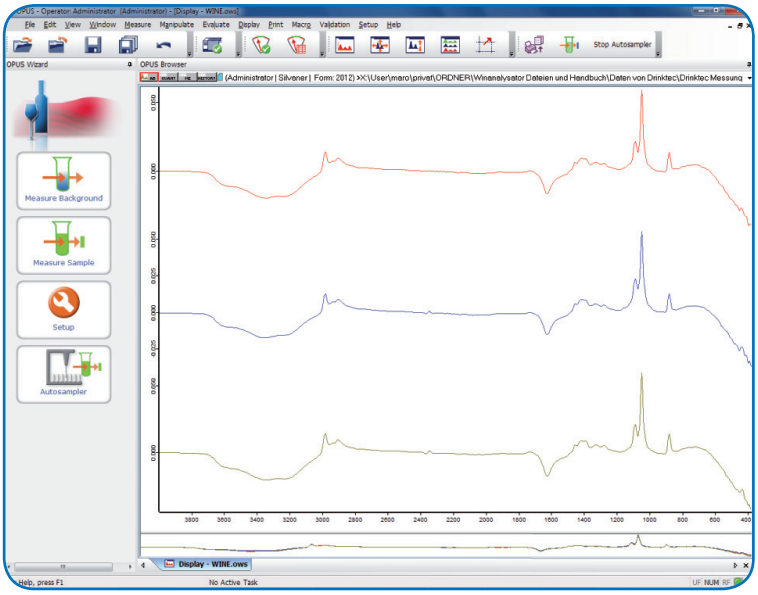


Figure 2: User interface of the ALPHA II Wine Analyzer.

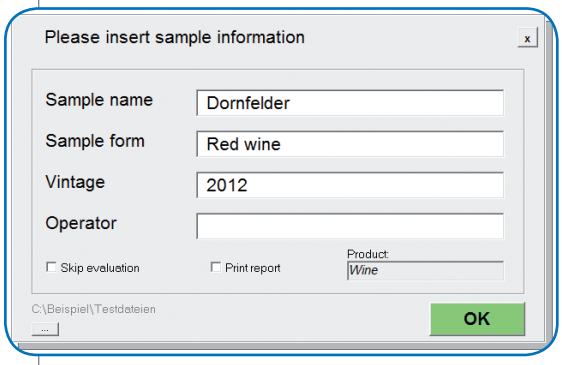


Figure 3: Dialogue with sample information.

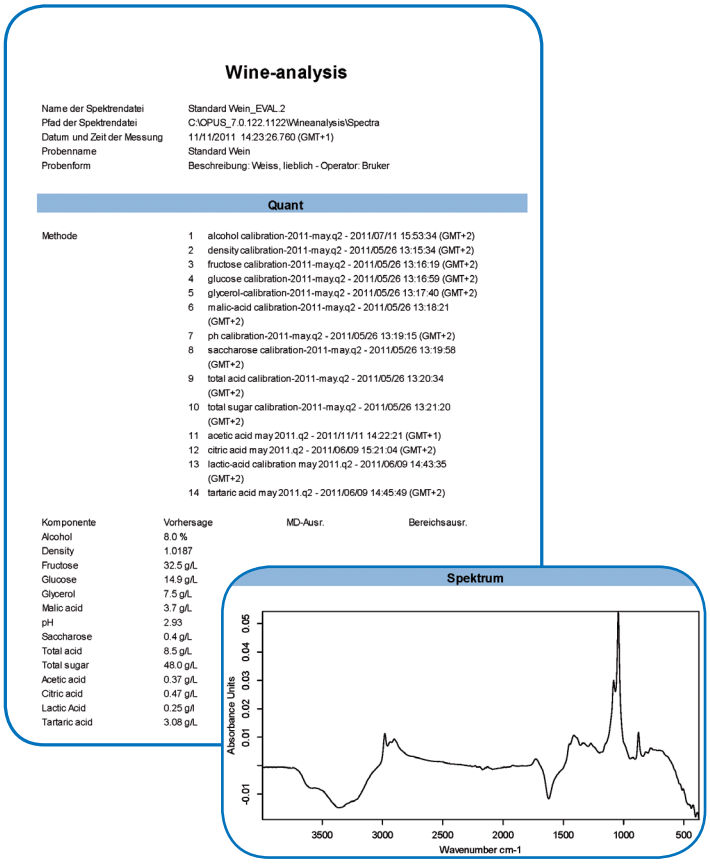


Figure 4: PDF-report of the analysis result.

Calibration Sets

Bruker offers starter calibrations for the analysis of finished wine, must and must under fermentation. The calibrated parameters are listed in the grey box on the right side. These starter calibrations can be expanded by the user with own sample-spectra and reference values for future optimization. Customized calibrations can be created as well.

Wine

The measurement of the wine calibration spectra and the determination of the according reference values were performed by the accredited (DAkkS) Institute Heidger (Osann Monzel, Germany).

The calibration data consists of over 2000 red and white wines from more than 60 different grape varieties. Wines from wine producing countries all over the world (South, Middle and East Europe, North and South America, Australia, South Africa) are included. A subset of the wine calibrations is suitable for the analysis of must under fermentation.

Table 1 lists the parameters that are included in the wine starter calibrations and specifies their individual calibration ranges.

The given Root Mean Square Error of Prediction (RMSEP) has been determined by analyzing more than 3000 independent samples. It shows the average accuracy achieved for the analysis of any wine sample including matrix dependent deviations. To rate the value of the IR-method it is important to note that the average total error of the IR-analysis is almost independent from the concentration range.

The typically achieved precision of the wine calibration-set is shown in Table 2. The standard deviations were calculated from about 70 repeated measurements of one wine over the course of several weeks.

Calibrated Parameters

Finished Wine:

- Alcohol
- Density
- Fructose
- Glucose
- Glycerol
- pH
- Saccharose
- Total acid
- Total sugarr
- Acetic acid
- Citric acid
- Lactic acid
- Malic acid
- Tartaric acid

Must:

- Brix
- Density
- Fructose
- Glucose
- Malic acid
- pH
- Probable Alcohol
- Total acid
- Total sugar

Must under Fermentation:

- Alcohol
- Fructose
- Glucose
- Malic acid
- Total acid
- Total sugar

	Unit	Conc. Range	RMSEP
Alcohol	%	0.12 - 20.48	0.27
Density	n/a	0.9116 - 1.1742	0.0014
Fructose	g/l	0.1 - 111.5	0.71
Glucose	g/l	0.2 - 125.6	0.87
Glycerol	g/l	0.1 - 25.9	0.64
pH	n/a	2.75 - 4.05	0.11
Saccharose	g/l	0.5 - 178.4	0.80
Total acid	g/l	2.9 - 13.5	0.31
Total sugar	g/l	0.0 - 199	1.48
Acetic acid	g/l	0.1 - 1.5	0.14
Citric acid	g/l	0.0 - 6.5	0.27
Lactic acid	g/l	0.0 - 4.3	0.31
Malic acid	g/l	0.1 - 4.7	0.40
Tartaric acid	g/l	0.5 - 5.4	0.43

Table 1: Concentration ranges and average errors of prediction of the analysis parameters available in the starter calibration.

	Unit	Average	Std. dev.
Alcohol	%	8.7	0.09
Density	n/a	1.0181	0.00038
Fructose	g/l	34.4	0.49
Glucose	g/l	15.3	0.58
Glycerol	g/l	7.1	0.25
pH	n/a	3.0	0.05
Saccharose	g/l	0.5	0.31
Total acid	g/l	8.6	0.18
Total sugar	g/l	49.5	0.91
Acetic acid	g/l	0.3	0.03
Citric acid	g/l	0.7	0.13
Lactic acid	g/l	0.3	0.09
Malic acid	g/l	3.5	0.17
Tartaric acid	g/l	3.1	0.16

Table 2: Precision of the repeat analysis of one wine using the ALPHA II Wine Analyzer in combination with the starter calibrations.

Must

The must starter calibrations contain up to 2600 different calibration samples and comprise altogether nine different parameters. Table 3 lists the parameters that are included in the must-starter calibrations and specifies their individual concentration ranges. The root mean square error of cross validation (RMSECV) shows the average measurement error of the calibration method.

	Unit	Concentration Range	Error of cross validation (RMSECV)
Brix	%	11.0 - 30.7	0.263
Density	g/cm³	1.068 - 1.135	0.0022
Fructose	g/l	54 - 134	2.93
Glucose	g/l	53 - 136	2.98
Malic acid	g/l	0.34 - 7.4	0.343
pH	n/a	2.21 - 4.23	0.0486
Probable Alc.	%	7.3 - 15.95	0.184
Total acid	g/l	2.43 - 19.5	0.412
Total sugar	g/l	159 - 306	2.92

Table 3: Concentration ranges and average errors of cross validation of the analysis parameters from the starter calibration.

Applicability

The wine calibrations are delivered with a bottle of a standard wine (figure 5) that allows a check of the system's performance.

Figure 5: Standard wine.

The parameters of the standard wine are printed on the label and were measured with both FTIR and reference methods like HPLC or titration. In order to evaluate the measurement results allowed maximum deviation values are given.

Measurement of trub substances

Since the liquid cell of the ALPHA II can easily be removed it is also possible to measure solid substances with the diamond ATR without any further hardware changes. Using this option, trub substances found in wine can easily be identified. Furthermore the identity of any raw material used in wine production can quickly be verified. The substance simply needs to be pressed onto the crystal with the aid of the included one finger pressure clamp. A sample measurement takes only a few seconds. For identification, the measured spectrum is automatically compared against the spectra of known substances. Bruker offers a dedicated library with 30 common trub substances, an example search result is shown in figure 6.

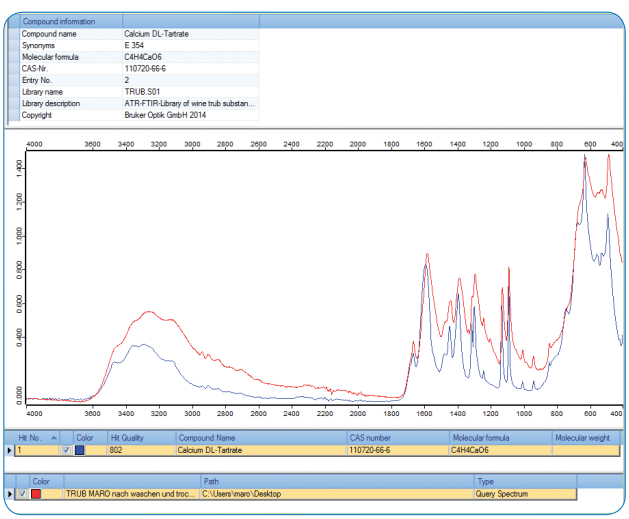


Figure 6: Search result of a trub sample (identified as Calcium-DL-Tartrate).

Fermentation Monitoring

To be able to produce a high quality wine it is important to monitor the fermentation process closely. The optionally available OPUS-DATABASE package allows to store all measured spectra in a database and offers a "Trend-View" that allows monitoring changes in different measurement parameters graphically. Up to four trend lines can be displayed simultaneously.

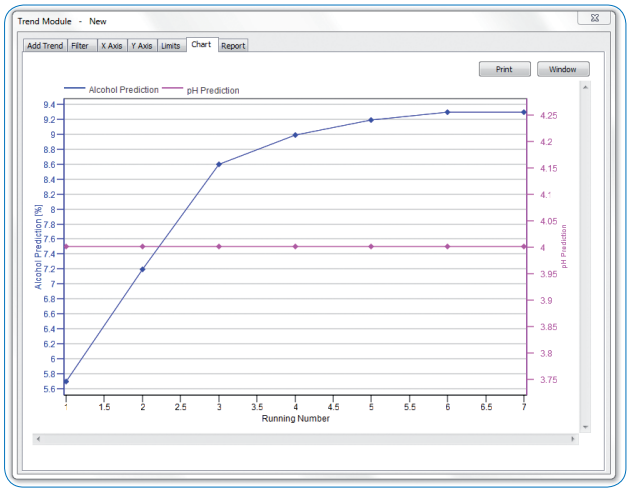


Figure 7: OPUS Trend-Viewer: Analysis results are plotted against running sample number or time.

Automated measurement

An optionally available autosampler (figure 8) facilitates fully automated measurements of up to 63 samples in a row. The samples are tightly sealed in glass vessels with septa caps to prevent evaporation. The autosampler is further equipped with a fixed wash reservoir that always provides clean water for background measurements and an integrated tow channel peristaltic pump.

Figure 8: Autosampler for the ALPHA II Wine Analyzer.

Summary and Conclusion

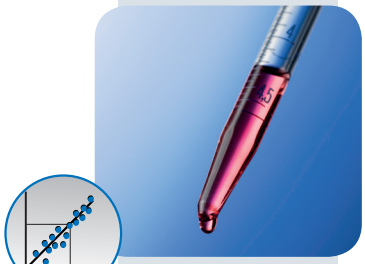
With the ALPHA II Wine Analyzer you are able to reliably monitor the ripening process and quality of your wine, must and must under fermentation. The ATR measurement principle makes the wine analyzer suitable for turbid and outgassing samples. Since the flow-through cell is removable, it is also possible to measure solid samples such as wine lees.

Several parameters that are crucial for wine-making are acquired in parallel with one single measurement without the need for an extensive sample preparation or consumables. The measurement itself is wizard guided and can be performed even by inexperienced personnel. Extensive starter-calibrations are available and can be adapted to specific demands. It is possible to expand and optimize the calibration database as well as to add new calibration parameters.

Basics of FTIR spectroscopy

analyze

identify



quantify

Every chemical substance has an individual spectral signature, just like a fingerprint. The Fourier Transform Infrared (FTIR-) Spectroscopy is widely used to analyze organic and inorganic substances. It uses invisible infrared light of which certain wave lengths are absorbed by the sample, depending on its characteristics. The position and intensity of the measured absorption bands can be utilized both for the identification and quantification of pure substances and mixtures.

The ATR (Attenuated Total Reflection) measurement technique mostly is applied without any sample preparation and allows a quick and simple measurement of liquids and solids. It is nondestructive and requires only a very little sample amount for the analysis.

FTIR does not require any consumables or chemical kits. As the FTIR method does not produce any waste it is environmentally friendly and sustainable. These properties and a long life time of all spectrometer components result in low running costs.

Bruker is the leading manufacturer and worldwide supplier of Infrared and Raman spectrometers. It offers the world's most comprehensive FTIR product line that includes routine to research grade FTIR spectrometers; from very compact to the highest resolution spectrometers for various quality control and research applications.

Customer support is provided worldwide by qualified and experienced application and service personnel.

Technologies used are protected by one or more of the following patents:
DE 102004025448; DE 19940981; US 5923422; DE 19704598

Bruker Optics is ISO 9001 and ISO 13485 certified.

Laser class 1 product.

www.bruker.com/optics

Bruker Optics Inc.
Billerica, MA · USA
Phone +1 (978) 439-9899
Fax +1 (978) 663-9177
info.bopt.us@bruker.com

Bruker Optik GmbH
Ettlingen · Germany
Phone +49 (7243) 504-2000
Fax +49 (7243) 504-2050
info.bopt.de@bruker.com

Bruker Shanghai Ltd.
Shanghai · China
Phone +86 21 51720-890
Fax +86 21 51720-899
info.bopt.cn@bruker.com