Challenge

Fast and efficient method to determine chromatic properties of wine according to the compendium of international methods of wine and must analysis (International Organisation of Vine and Wine).

Solution

Fast and simple spectrophotometric determination of color intensity, color shade and chromaticity in wine using the spectrophotometer SPECORD 50 PLUS.

Spectrophotometric Determination of Chromatic Characteristics According to Compendium of International Methods of Wine and Must Analysis (Method OIV-MA-AS2-07B and Method OIV-MA-AS2-11) [1, 2]

Introduction

Wine production is a relevant industry sector and economic engine for a wide range of regions in Europe, Americas, Eurasia and Africa. Current customer trends point towards an increased demand for product traceability (e.g., organic and origin traceability) and product diversification (alternative processing and grape varieties). Thus, quality evaluation is a key challenge for all wine stakeholders.

Apart from their organoleptic contribution, anthocyanins, largely abundant in the skin of grapes, have a deep impact on the optical properties of wine, thus directly modulating wine quality and classification. Monitoring anthocyanin concentration based on color leverages a rapid yet reliable indicator, both in the final product and through each stage of the production process: quality for raw materials (grapes), post-harvest processing (fermentation), storage (aging and development) and the overall shelf-life.

During wine processing and ageing anthocyanins (e.g., the malvidin-class) oxidize, forming oligomeric entities. Here, change in molecular structure correlates with the change in color.

The method described in this application note is particularly suitable for rapid evaluation of color. In general, this application note sets the focus on the analysis of color intensity, color shade and chromatic characteristics (CIE L*a*b) in agreement with the analysis method of the International Organisation of Vine and Wine. In a more detailed approach, anthocyanin degradation during storage (ageing) or the optical properties of the various processing steps (e.g., specific use of yeast fermentation) might also be analyzed.

Materials and Methods

Analytik Jena offers high quality spectrophotometers with an application-focused accessories portfolio and an easy-to-use software for fast and efficient absorbance spectra recording and successful evaluation of various parameters. Here we focused on using the standard cuvette holder and the adjustable holder for micro cuvettes, but the SPECORD PLUS series offers a variety of cuvette holders and cuvette changers for higher throughput from 6-fold cuvette changer and 8-fold cuvette changer up to 15 positions with the cuvette carrousel.

Following the International Organisation of Vine and Wine analysis' method for color, shade and chromaticity intensity determination, this current application note focuses on rapid evaluation of optical properties in wine, as well as a rapid assessment of the spectroscopic features as a marker for quality evaluation, here anthocyanin absorption properties.

The intensity of color and shade were measured by using the module spectrum of the ASpect UV software. The colorimetry module of the software leverages the chromaticity coordinates and tristimulus values (CIE L*a*b*), which exactly define the color of the target sample, in this case wine. Values are given using the CIE L*a*b* system, one of the most widely used color systems.

Color intensity [3]
Is the sum of the absorption at 420 nm, 520 nm and 620 nm. These three values represent the optical color perception of brown (420 nm), red (520 nm) and blue (620 nm). Related parameters, such as the color nuance, can be derived from the color intensity.

Color shade [3]
The quotient of the brown (420 nm) and red (520 nm) color provides a statement about the color shade.

CIE L*a*b* [4]
The L*a*b* color space is a color model that describes the range of colors perceptible to the eye. The L* value describes the brightness of a sample (max. bright = 100; max. dark = 0). The a* value describes the red-green components of a sample in more detail (a* values > 0 = red; < 0 = green).
The b* value describes the yellow-blue ratio (b* values > 0 = yellow; < 0 = blue).

Samples and reagents

In line with the wine guidelines in method OIV-MA-AS2-07B and method OIV-MA-AS2-11 distilled water was used as reference. [1, 2] For the samples displayed in table 1, no additional sample preparation was required.
If the wine is turbid, suspended sediments should be removed by centrifugation. Prescence of carbon dioxide in young or sparkling wines must be removed through agitation under vacuum. Micro bubbles might alter the measurement.

Table 1: Wine samples

Types of wine	Specification
Rosé wines	Dornfelder Rosé Primitivo
Red wines	Vino Tinto Portwine

Instrumentation and software settings

The SPECORD 50 PLUS spectrophotometer equipped with the holder for standard cuvettes and a 10 mm glass (OS) cuvette was used to measure the spectra of rosé wine samples, whereas the spectra of red wine samples (higher color density) where recorded using a 2 mm glass (OS) cuvette and the holder for micro cuvettes up to 10 mm pathlength. The holder for micro cuvettes allows easy adjustment to optimize signal recording.

To determine color intensity, color shade and chromaticity, the spectrophotometer software ASpect UV was used. The software settings are listed in table 2.

Table 2: Software settings for measurement according to method OIV-MA-AS2-07B and method OIV-MA-AS2-11

	Method OIV-MA-AS2-07B	**Method OIV-MA-AS2-11**
Module	Spectrum	Colorimetry
Measurement mode	Absorbance	Transmittance
Wavelength [nm]	360 – 830	360 – 830
Measuring points [nm]	1	1
Speed [nm/s]	10	10
Integration time [s]	0.1	0.1
Evaluation	Values of defined Wavelength [nm]: 420, 520, 620	Color coordinates: CIE-Lab according to EN ISO 11664 Observer [°]: 10 Light type: CIE illuminant D65 according to EN ISO 11664

The color intensity (I) and color shade (N) were calculated according to the method OIV-MA-AS2-07B. The intensity is given as the sum of the absorbance at 420 nm, 520 nm and 620 nm (formula 1) and the shade is the quotient of the absorption value 420 nm to 520 nm (formula 2):

$$I = A_{420} + A_{520} + A_{620} \quad (1)$$

$$N = \frac{A_{420}}{A_{520}} \quad (2)$$

With the build-in formula editor of the software ASpect UV the color intensity (Figure 1) and color shade (Figure 2) can be easily calculated.

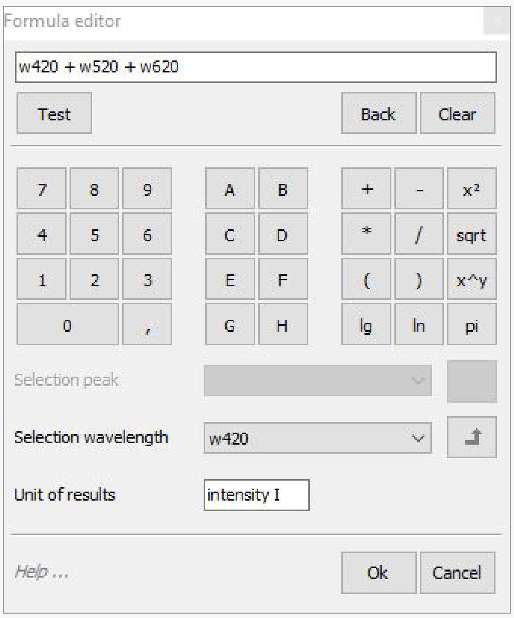

Figure 1: ASpect UV formula editor
– evaluation of color intensity

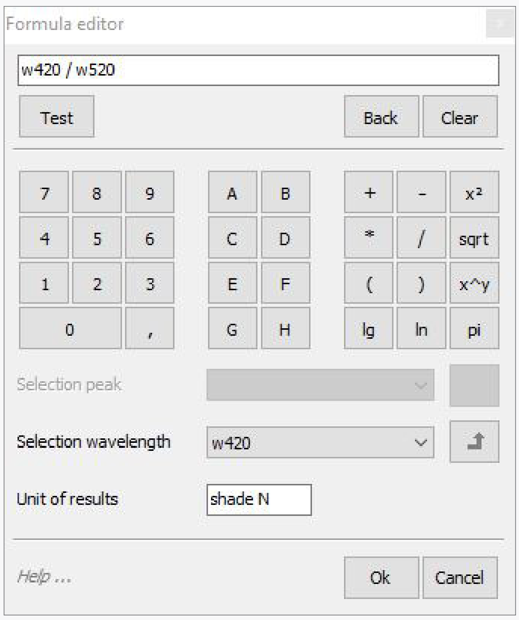

Figure 2: ASpect UV formula editor
– evaluation of color shade

Results and Discussion

While wine contains a large range of aromatic compounds, color can be traced to a relatively small group of molecules, such as anthocyanins, flavanones, and tannins. The corresponding structural formula are shown in figure 3.A, 3.B and 3.C, respectively. The contribution of anthocyanin is rather specific, it spans from 400 nm up to 600 nm and it is sensitive to changes in the pH value. On the other hand, flavanones, while related to anthocyanins, lack the large aromatic structure. Thus, they tend to absorb below 400 nm. Finally, tannins tend to absorb light below 300 nm with broad absorbance features. Both molecular classes have a negligible contribution to the absorption range relevant for color analysis.

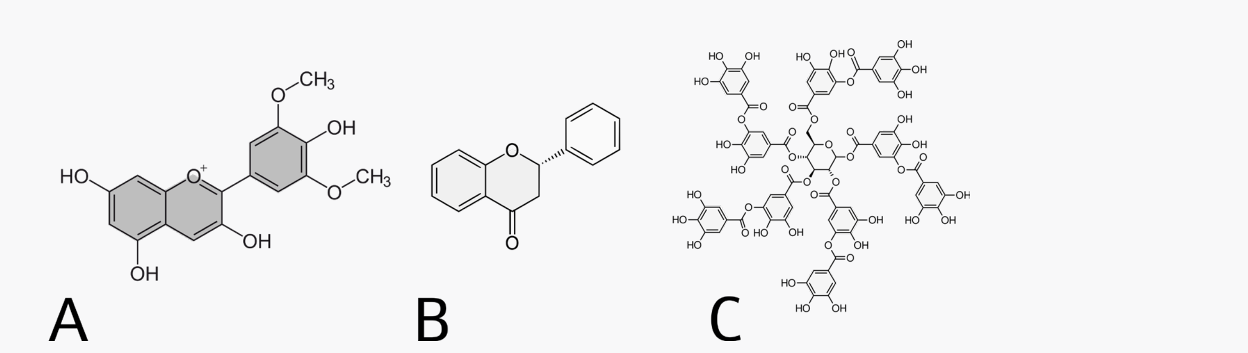

Figure 3: Chemical structure of (A) malvidin, a type of anthocyanin, (B) basic flavanone and (C) representation of a tannin structure. As an example, the aromatic moiety is shown in the anthocyanin class (Figure 3. A).

The recorded spectra of the four wine samples are shown in figure 4 in the range from 360 nm up to 830 nm. Main features are an increased absorption towards 400 nm and a broad asymmetric absorption peak around 520 nm with a bathochromic shoulder between 560 nm to 585 nm. This multi-peak feature rises from the absorption of anthocyanins and/or anthocyanin-derivates. The spectra of the rosé wine samples (Dornfelder Rosé and Primitivo) and Vino Tinto (red wine) show an overall similar band profile, however the Portwine spectrum shows a rather broad feature, characteristic for polymerized anthocyanins.

Finally, a detailed inspection of the anthocyanin absorption profile in Vino Tinto, Primitivo and Dornfelder Rosé clearly shows that each sample has a very characteristic maxima and band profile (red shifted shoulder). The distinct spectral feature derives from distinct anthocyanin concentration, potentially providing a spectroscopic marker. This however requires further analysis, as well as correlation with other measurements such as pH determination.

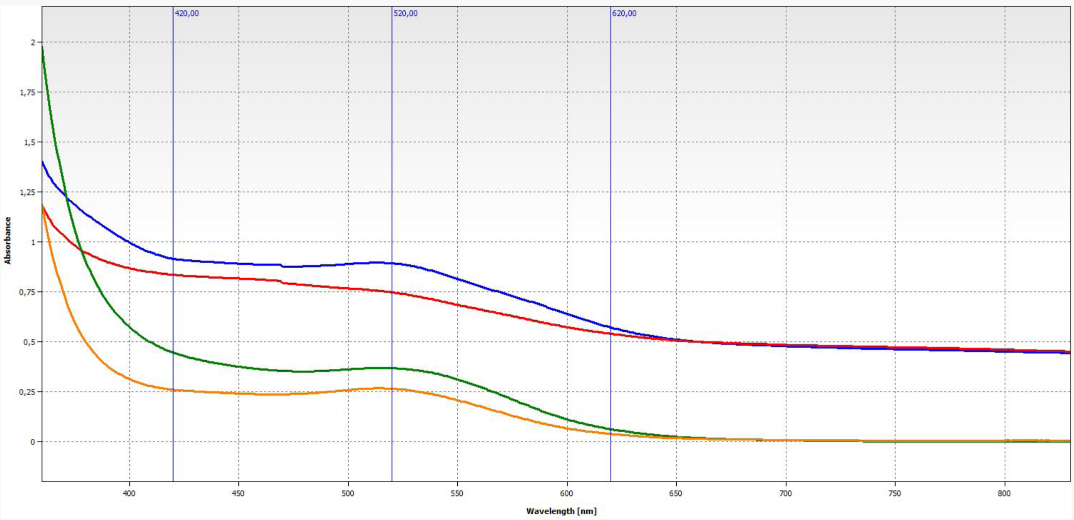

Figure 4: ASpect UV screenshot of the measured spectra of wine samples (blue: Vino Tinto, red: Portwine, green: Dornfelder Rosé, orange: Primitivo)

The expected difference between red and rosé wine is clearly shown at an absorbance of 520 nm. In table 3, the results of the defined wavelengths and the automatically calculated CIE L*a*b* color coordinates as well as color intensity (I) and color shade (N) are displayed.

Table 3: Results of defined wavelengths, color intensity, color shade and color coordinates

Sample	A420 [nm]	A520 [nm]	A620 [nm]	I	N	L*	a*	b*
Dornfelder Rosé	0.446	0.368	0.063	0.876	1.211	83.21	24.77	21.09
Primitivo	0.260	0.265	0.038	0.564	0.982	88.92	18.91	14.59
Vino Tinto	0.917	0.893	0.572	2.381	1.026	53.42	17.98	15.27
Portwine	0.836	0.748	0.540	2.124	1.118	56.28	11.64	15.68

Consistent with the previous spectroscopic evaluation, color analysis (Figure 5) shows a significant difference between two groups comprising on one side Dornfelder Rosé and Primitivo and on the other side Vino Tinto and Portwine, as expected.

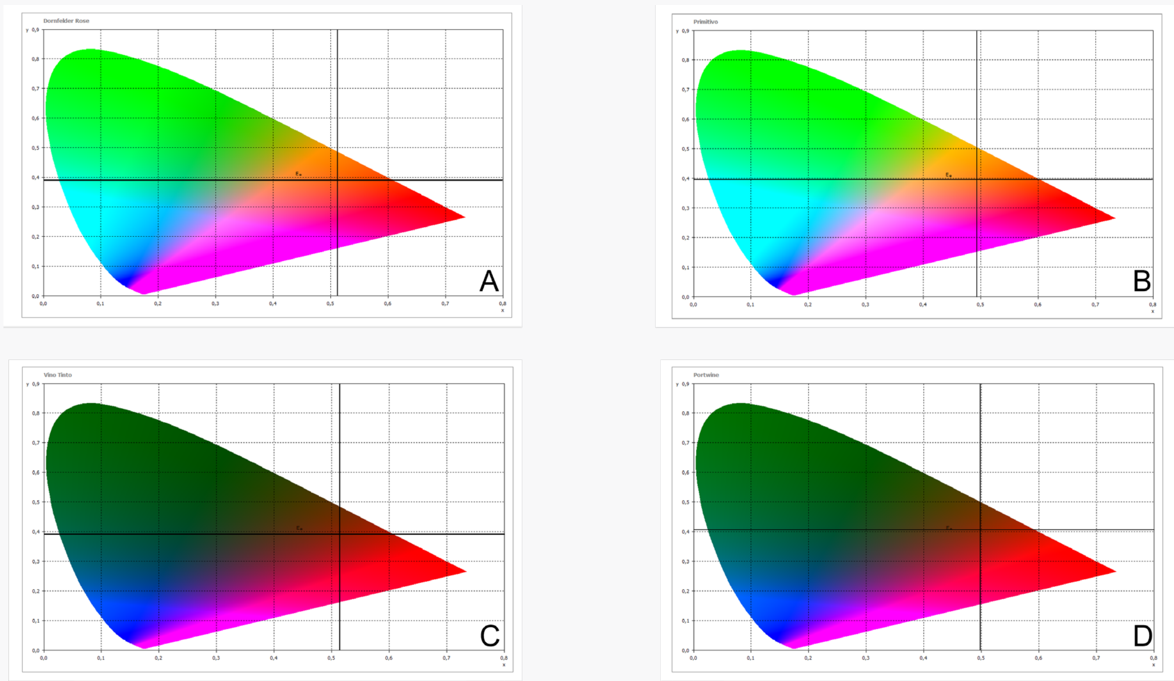

Figure 5: Color view of the four wine samples. A: Dornfelder Rosé, B: Primitivo, C: Vino Tinto, D: Portwine

Conclusion

The overall expertise of Analytik Jena in the field of UV/Vis spectroscopy in combination with the SPECORD 50 PLUS spectrophotometer (Figure 6), accessories and the colorimetry module in the ASpect UV software are suitable tools for the application in the wine industry, especially regarding rapid color-related quality control.

A special focus is set on the potential for the rapid assessment of wine color in accordance with the International Organisation of Vine and Wine standards. Furthermore, a detailed spectroscopic analysis targets the optical properties of anthocyanin as marker for relevant quality insights to support wine production in assessing quality in final products and potentially along the value chain.

Figure 6: SPECORD 50 PLUS spectrophotometer

References

[1] Compendium of International Methods of Wine and Must Analysis - Method OIV-MA-AS2-07B

[2] Compendium of International Methods of Wine and Must Analysis - Method OIV-MA-AS2-11

[3] Journal of Agricultural Sciences (Vol. 61, No. 3, 2016) Spectrophotometric Characterization of red wine from the vineyard region of metohia

[4] Kellerwirtschaft das deutsche Weinmagazin (April, 20th 2013): Schau mir in die Küvette, Bleichgesicht!

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