Analytica Chimica Acta 691 (2011) 18–32

Contents lists available at ScienceDirect

Analytica Chimica Acta

journal homepage: www.elsevier.com/locate/aca

Review

Atomic spectrometry methods for wine analysis: A critical evaluation and discussion of recent applications

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ARTICLE INFO

Article history:
Received 12 January 2011
Received in revised form 15 February 2011
Accepted 17 February 2011
Available online 24 February 2011

Keywords:
Atomic spectrometry
Wine
Elemental analysis
Matrix effects

ABSTRACT

The analysis of wine is of great importance since wine components strongly determine its stability, organoleptic or nutrition characteristics. In addition, wine analysis is also important to prevent fraud and to assess toxicological issues. Among the different analytical techniques described in the literature, atomic spectrometry has been traditionally employed for elemental wine analysis due to its simplicity and good analytical figures of merit. The scope of this review is to summarize the main advantages and drawbacks of various atomic spectrometry techniques for elemental wine analysis. Special attention is paid to interferences (i.e. matrix effects) affecting the analysis as well as the strategies available to mitigate them. Finally, latest studies about wine speciation are briefly discussed.

Guillermo Grindlay was born in Granada (Spain) in 1978. He studied chemistry at the University of Alicante where he obtained his PhD in 2006 working on a microwave fully based sample introduction system atomic spectrometry. He is currently an assistant professor in the University of Alicante. Over the past few years, he has performed several post-doctoral research works at TUDelft and the University of Ghent. His current research interests are focused on the development of new sample introduction systems for plasma based techniques as well as on the origin of non-spectral matrix effects.

Juan Mora obtained his PhD degree in Analytical Chemistry from the University of Alicante (Spain) in 1994. He continued his research work as a post-doctoral fellow at the Delft University of Technology (The Netherlands). Currently, he is teaching Analytical Chemistry and member of the Analytical Atomic Spectrometry Group at the Department of Analytical Chemistry, Nutrition and Food Sciences of the University of Alicante. His research interests are in the field of analytical atomic spectrometry and include the development and characterization of different sample introduction systems and the study of fundamental and applied aspects in plasma based atomic spectrometry techniques.

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doi:10.1016/j.aca.2011.02.050

Luis Gras was born in Elche (Spain) in 1968 and obtained his PhD degree in Chemistry in 1997, after which, he performed a post-doctoral stage at the TUDelft University (Holland). Since 1993 he is part of the Analytical Atomic Spectrometry Group of the University of Alicante and nowadays his main research areas are the design of new instrumentation based on microwave radiation for on-line sample pretreatment and the development of analytical methods for the elemental analysis of foods and the use of chemometrics for sample characterization.

Margaretha de Loos-Vollebregt graduated from Delft University of Technology and obtained her PhD from the same university in 1980 (supervisor Prof. Leo de Galan). She is currently teaching spectroscopy in the Analytical Biotechnology group at Delft University of Technology and she is guest professor in the Atomic and Mass Spectrometry group of the Department of Analytical Chemistry at Ghent University, Belgium. She is editor of Spectrochimica Acta Part B: Atomic Spectroscopy, advisory board member of Journal of Analytical Atomic Spectrometry and editorial board member of Analytica Chimica Acta. Her research interests are in the field of analytical atomic spectroscopy.

1. Introduction

Wine is an alcoholic beverage of a great social and economic significance. This beverage was initially used as mind-altering substance for religious ceremonies in ancient times but, over the years, it has become a standard item in human diet. Nowadays, worldwide wine production and consumption has been estimated over 20,000 million litres per year by the Organisation Internationale de la Vigne et du Vin (OIV) which points out the importance of this product [1].

From a chemical point of view, wine is a complex water–ethanol mixture which contains a great variety of both organic and inorganic substances [2,3]. A brief overview on the chemical composition of wine is shown in Table 1.

Organic substances in wine can be divided in two groups: volatile and non-volatile compounds. Among the volatile group, ethanol is the most abundant compound ranging from 8% to 19% (v/v). There are other volatile compounds (e.g. methanol, esters and terpenes) which are directly responsible for wine organoleptic properties but their concentration levels are rather low compared to ethanol. Non-volatile organic compounds include low-volatile alcohols, sugars and organic acids as well as their conjugated salts. They may be present at concentrations above 1.0 $g\,L^{-1}$. Wine also contains small quantities of other substances (<1.0 $g\,L^{-1}$) such as amino acids, polyphenols, flavonoids, etc. As regards the inorganic fraction, wine is rich in Cl^-, PO_4^{3-}, SO_4^{2-} and SO_3^{2-} salts. The most abundant counter ions (i.e. major elements) for both inorganic and organic salts are those related to grape physiological processes such K, Ca, Na and Mg. Among them, K shows the highest concentration levels between 500 and 1500 $mg\,L^{-1}$ followed by Ca, Mg and Na around 10–200 $mg\,L^{-1}$. The elements usually present in concentrations ranging from 0.1 to 10 $mg\,L^{-1}$ (i.e. trace elements) are Al, B, Cu, Fe, Mn, Rb, Sr and Zn. Finally, ultratrace elements are those below 0.1 $mg\,L^{-1}$ such as Se, Pb and Cd.

The great number of parameters affecting wine quality has initiated the development of different protocols for analysis [4]. In fact, wine constituents are strictly regulated by international organizations [5] or government agencies [6] to avoid fraud and health risks. Luque de Castro et al. [7] have recently reviewed methods of analysis for the most commonly determined parameters in wine such as ethanol, sulphur dioxide, reducing sugars, polyphenols, organic acids, total and volatile acidity, Fe, soluble solids, pH and color.

Wine elemental composition provides additional important information about the quality or characteristics of the wine [8,9]. Pohl has summarized what metals tell us about wine in an article focused on the role of metals in wine and processes involved in winemaking [10]. Elements in wine can be classified into two groups: endogenous and exogenous. Wine endogenous elements, the most abundant, are related with the type of soil in the vineyard, the grape variety and maturity and the climatic conditions. Exogenous elements are associated with the external impurities which may reach wine during the growth of grapes. Thus, differences in the content of K, Ca or Cu in different wines can be due to the use of fertilizers for cultivation. Application of pesticides, fungicides and fertilizers during the growing seasons of wines can lead to an increased amount of Cd, Cu, Mn, Pb or Zn in the resulting wine. The environmental pollution of the vineyards may also enhance the concentration of some elements [11]. Thus, wines from vineyards close to the coast show a relatively high concentration of Na whereas high concentrations of Pb or Cd are found in wines from vineyards located close to road traffic or industrial areas. In addition, exogenous metals are related with winemaking (from harvesting to bottling and cellaring) such as: (i) process equipment. The long contact of wine with materials such as Al, brass, glass, stainless steel, wood, etc., used to build pipes, casks and barrels is the usual source for Al, Cd, Cr, Cu, Fe and Zn; or (ii) the addition of different substances at different steps of wine production [12]. Thus, contamination with Na, Ca or Al can be associated with the use of fining and clarifying substances (flocculants such as bentonites) added to the wine to remove suspended solids after fermentation and to reduce turbidity. Ca contamination can also arise from the addition of $CaCO_3$ or $CaSO_4$ or de-acidification of must and wine or enhancement of acidity of grape juices, respectively. The main source of Cu in wine is the $CuSO_4$ added to remove H_2S and other sulphidic compounds.

From the statements made above, it is obvious that monitoring elemental wine composition has a great importance for winemaking industry as well as customers. Fig. 1 summarizes the main objectives accomplished with wine elemental analysis. Wine elemental analysis has been employed in the literature for different purposes:

1. Bioavailability/toxicity. It has been demonstrated that daily consumption of wines in moderate quantities significantly contributes to the requirements of the human organism for essential elements such as Ca, Co, Cr, Cu, Fe, K, Mg, Mn, Mo, Ni or Zn, among others [13,14]. In fact, it can be assumed that wine constitutes a very significant contribution to the total diary intake of elements such as V [15] or Al [16]. Its nutritional effect depends on the physicochemical form and concentration of the elements. In fact, some of the above mentioned essential elements are harmful for human health in case of excessive intake. To prevent health damage, wine analysis on the metals' content and tolerable concentrations are regulated. In addition, according to the different health-protection laws in different countries, it is required to detect the presence of hazardous species (e.g., Cd, Pb, Hg, Al, Tl, As, Sb, S, different organometallic compounds of Pb, As, etc.) [17,18]. Hence, there is an increasing interest in wine speciation analysis to evaluate the toxicity, bioavailability, bioaccumulation and transport of specific elements (Pb, As).