

Preface

This book is rooted in an informal discussion with three researchers, Dr Alatzne Carlosena, Dr Mónica Felipe and Dr María Jesús Cal, after they had some problems measuring antimony in soils and sediments by electrothermal atomic absorption spectrometry. While we reviewed the results and debated possible problems, much like in a brainstorming session, I realized that some of their difficulties were highly similar to those found in molecular spectrometry (mid-IR spectroscopy, where I had some experience), namely a lack of peak reproducibility, noise, uncontrollable amounts of concomitants, possible matrix interferences, *etc.*

As many of these difficulties are currently overcome in molecular spectroscopy using multivariate regression methods (or multivariate chemometrics), I proposed that these three ladies should apply them to their spectra. The first reaction on their faces seemed something like ‘ . . . this crazy chemometrician guy . . . ’, but after some discussions we agreed to work together and see what might be achieved. It was not easy to get the spectral raw data that we needed from our old Perkin-Elmer device and Mónica and María spent much time on this until they found a way to do it.

The number of papers we found reporting on the use of multivariate regression in atomic spectrometry was small, and we guessed that this might be because of either a lack of general awareness of the huge potential capabilities of these techniques and/or the difficulties in extracting the spectral data from the spectrometers, something trivial with most instruments dedicated to molecular spectrometry.

We obtained some good results and one morning I read an e-mail from Dr Merlin Fox (Commissioning Editor at the RSC) with a totally surprising proposal: to prepare a monograph on the subject. After reading his e-mail several times and asking him if that was true (some electronic ‘spam’ seemed very possible), Dr Carlosena and I contacted several good scientists in the two fields of atomic spectrometry and chemometrics. I am indebted to all authors

for their constructive words and immediate collaboration, although, maybe, it was the first one we contacted, Professor Alfredo Sanz-Medel (a worldwide-reputed atomic spectroscopist, with several international awards, including the 2007 Robert Kellner Lecture), who really fuelled us to go on. I really want to express my deep and sincere gratitude to each participant in this exciting project. You are not only skilful scientists but also nice persons, enthusiastic workers and, first of all, good friends. Joan, thanks for the nice photograph on the cover, you have a marvelous hobby. Recognition is also due to Merlin Fox for his continuous support and encouragement.

Finally, our thanks to you, the reader. It is the honest desire of the authors to hear from you. We would like to receive your feedback. It is impossible to produce a text like this that satisfies everyone, their expectations and needs. Many things were left out of the book, but if you feel that some more explanations, reviews or information are required, please do not hesitate to contact us. If a new version comes with the winds of the future, your suggestions will be greatly appreciated and, as far as possible, included (and publicly acknowledged, of course).

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