The Casa Cookbook

Part 1: Recipes for XPS Data Processing

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Foreword

CasaXPS is designed to take data from a wide range of instruments and their data systems using native file formats wherever possible, convert these formats to the ISO 14976 ("VAMAS") format and provide a single environment in which to process XPS and AES data. For many analysts problem solving using multiple techniques is common-place and while the origins of CasaXPS are clearly XPS the expansion of the system to cover AES (and, in Part II of this Series, SIMS) is both natural and desirable. In addition, XPS image processing has also become increasingly important, and to fulfil the potential of the modern imaging instruments, new features and new algorithms have been added to CasaXPS.

Many of the capabilities of CasaXPS require an understanding of why as well as how an operation is performed and therefore a large part of this CasaXPS manual is devoted to explaining the context for a sequence of data reduction steps. Procedures for these steps are addressed within sections describing specific examples, but the essential functions of CasaXPS routines and options and the overall structure of the program are presented in separate reference chapters. The practical examples are necessarily wordy and to compensate to some degree the reference section is pictorial in essence.

Seasoned Auger and XPS practitioners may wonder at the apparent omission of separate chapters dealing with topics such as "Depth Profiling". The approach is deliberate as it is felt more appropriate to cover issues of quantitation vs depth in relation to the (more fundamental) processing mechanisms of peak fitting, PCA, SVD, and the like. It is hoped that the index will provide an adequate guide to specific applications orientated questions in this regard.

It is also important to note that Chapter 19 does not intend to supplant existing excellent books which deal in detail with all aspects of XPS as an analytical technique (some of which are listed in the Bibliography), but simply to provide a convenient introduction to the basics for those from disciplines such as biochemistry, earth sciences, and so on who may not otherwise have easy access to this information.

Acknowledgement

CasaXPS wishes to thank all those connected with the production of this manual and the software system it describes.

Section 1 - Quick Summary

CHAPTER 1

Introduction

Computer Aided Surface Analysis for X-ray Photoelectron Spectroscopy (CasaXPS) has been designed and written for analysts and research scientists who use XPS for surface characterisation.

In contrast to the special purpose control systems that form part of commercial XPS instruments, CasaXPS offers a compact, portable, efficient and user-friendly processing system to anyone with an IBM compatible (Pentium) PC running Microsoft Windows 95 (or later) or a suitable emulator[1]. It incorporates much of - and in most cases more than - the processing functionality of the instrument-linked packages without recourse to unfamiliar operating systems or hardware or proprietary file formats. It is designed from the outset on the basis of the ISO 14976 Surface Chemical Analysis Standard Data Transfer Format and so by design has a universal, manufacturer-independent, "cross platform" approach, relying on nothing other than a reasonable adherence to the ISO standard. Spectra collected in the standard format may be selected, viewed and processed in a simple yet powerful way and the results of CasaXPS data reduction, presented in a variety of graphical and tabular formats, are available for incorporation into and use as data by other popular Microsoft pack-

1. Microsoft XP systems are the most likely platform (in 2005) for CasaXPS, but in these days of affordable high performance systems, such as the Macintosh G5, emulators such as Virtual PC (for Mac OS X) should be seriously considered

ages such as “Word” or “Excel”. Additional spectrum input filters for other commercial file formats are also provided, supplementing the ISO standard and broadening its usefulness.

Casa XPS has been written entirely in native C++ using the Microsoft Developers Studio programming environment. It employs Microsoft Foundation Class (MFC) libraries to provide a standard graphical user interface as well as much of the data management required by the system.
The software suite as a whole may be regarded as being structured from five interacting components:

- Data display and browser (an “experiment window”)
- Element library (a “dialog window” as are the others)
- Graph annotation
- Data processing
- Quantification.

This publication provides a detailed description of the system, its operation, command and function set, and its use in practice in “real life” analytical applications.

The CasaXPS Cookbook’s objectives are to provide both a guide to the software and its use and some background to the techniques of surface analysis as well as the principle behind the mathematics used in the evaluation of the analytical data.

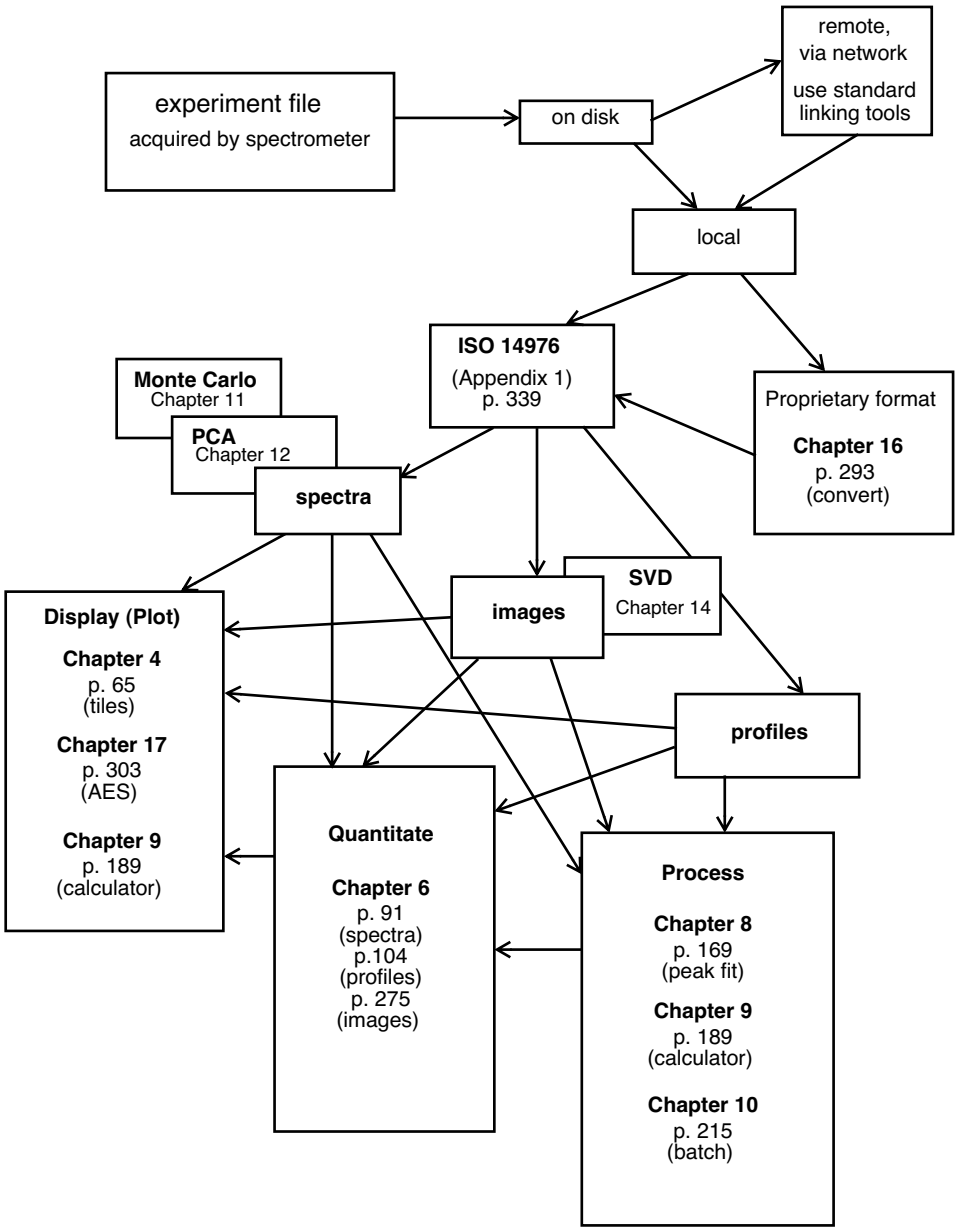
CasaXPS is more than “just another data system”: it is hoped that, similarly, this “Cookbook” provides more than just “recipes”, provoking serious thought about procedures and possibilities in one of the most challenging of experimental disciplines.

Getting Started

Installing CasaXPS

You must install the application from the CasaXPS CD onto your hard disk. “Drag and Drop” installation is all that is required for Windows XP or ‘98. Instructions are available, if required, in the “Read Me” file on the installation CD and some further details in “Appendix 6: CasaXPS Installation Notes” on page 358. Make sure that you have your serial number to hand when you install the application, or else the package will revert to “Demonstration Mode” and will not allow you to save the results of your work. The serial number is available from your registration documents (which may be e-mailed to you or included with the CD). You can “validate” a registration at any time after installation, turning a “demo” version into a fully licensed product, by using the “About” button in the Toolbar.

CasaXPS - Organisation, work flow, and information



If you are using an emulator package on a processor other than an Intel Pentium, ensure that you obey the emulator's instructions for installation of applications packages, that you understand the limitations (if any - e.g. mouse button availability) of the system, and that you have sufficient space and processing power for the convenient use of CasaXPS.
There is further, more detailed, information on program installation (and removal) in "Appendix 6: CasaXPS Installation Notes" on page 358

Starting CasaXPS

Simply click on the desktop short-cut (if, as recommended, you installed one) or double click on the programme icon in "Windows Explorer". Ensure that you have stored your ISO 14976 data files in an easily accessible directory (or have the demo data on the installation CD available) Ensure also that you have an appropriate element library available (one needs to be installed before the first use of "Library" system - see "Element Library Files" on page 320 - a simple "generic" version is available on the installation disk, but check with your instrument operator which is the most appropriate file for the data acquired by that particular instrument). At some point you may wish to install and use the on-line "help" files (see note on your CD inlay) and you should have a ".def" directory prepared if you wish to store configuration files for future use (see e.g. p. 79, p. 143).

Terminology

CasaXPS components and windows appear on screen as shown in Figure 1•1, where the annotation defines their names as used throughout this book.
It is assumed always that the user is familiar with the "normal" IBM PC and Microsoft Windows operation and terminology.
The following section should be used as a "hands on" introduction to CasaXPS to provide an overview of key features. Subsequent sections enlarge briefly on the role of the system modules, and the remaining chapters deal in depth with specific topics and applications.

The Program Frame

1. The program frame contains experiment frame windows.
2. Each experiment frame is divided into to two splitter windows.
3. The left-hand-side displays the spectra while the right-hand-side offers a data array (data browser) showing the logical structure of the experiment.

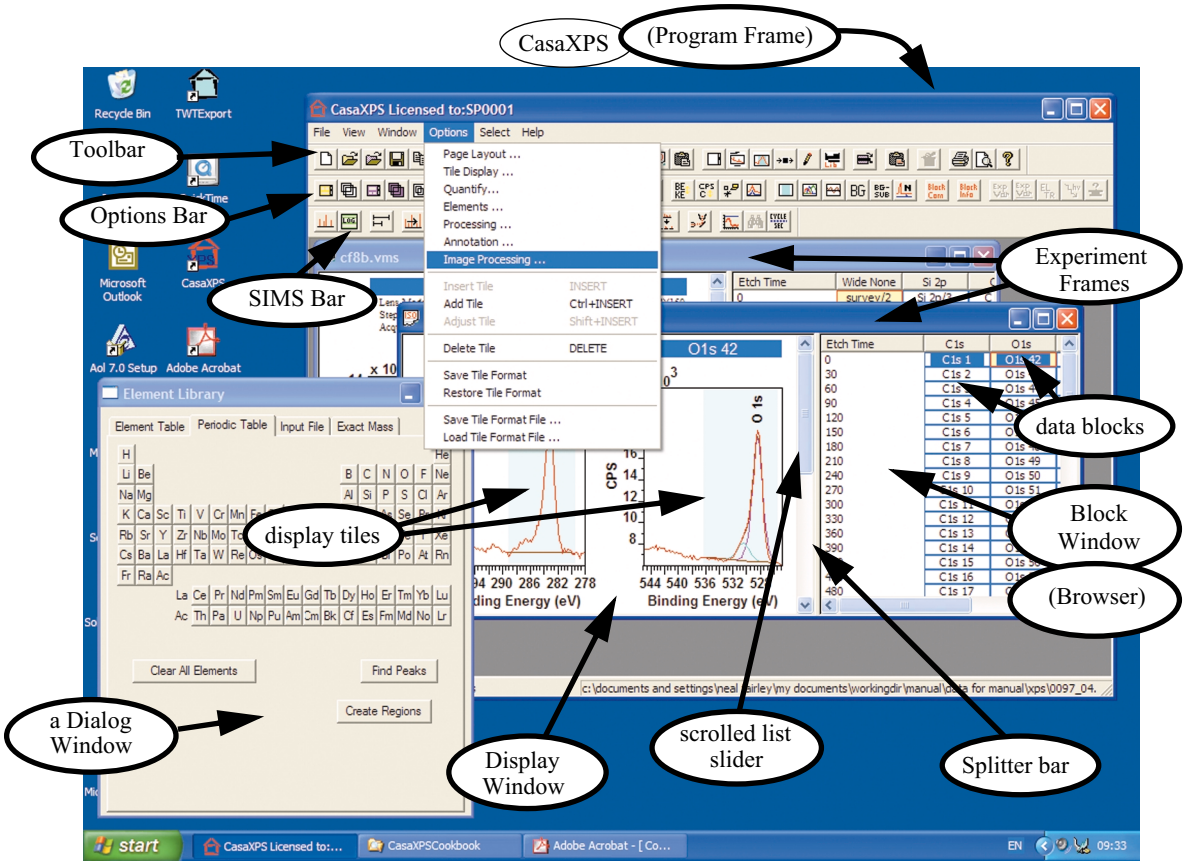


FIGURE 1•1 A Windows XP™ screen showing CasaXPS in operation

How do I....?

(These commands are cross referenced to fuller descriptions in Chapter 3 starting on page 49: U = Upper (main) Toolbar, L = Lower (Options Bar) , 2•3 indicates 3rd button in 2nd group, and so on)

Display spectra

L 1•1-5 (page 58)

Select spectrum block(s) in right-hand-side splitter window (browser - Figure 1•1)

- Press a toolbar button