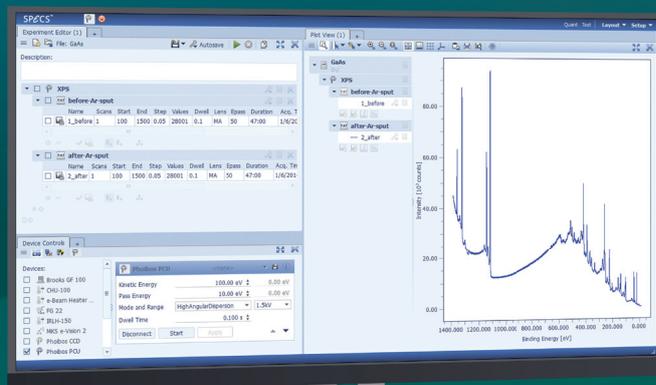


Prodigy ISQAR

IDENTIFICATION OF SAMPLES BY QUANTITATIVE ANALYSIS AND REPORTING

KEY FEATURES

- Fully integrated module
- User-friendly handling
- State-of-the-art models for background subtraction, curve fitting and chemical composition
- Comprehensive functionalities
- Data export and reporting included

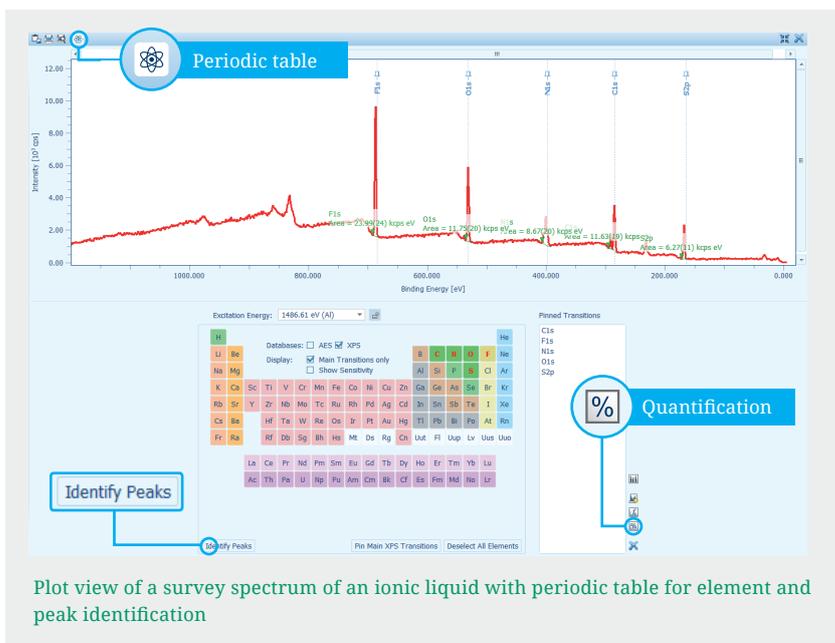


SPECS™

Prodigy ISQAR

IDENTIFICATION OF SAMPLES BY QUANTITATIVE ANALYSIS AND REPORTING

The quantification feature ISQAR in Specs-Lab Prodigy allows for reliable quantification of the chemical composition of sample surfaces, multipeak identification by curve fitting and calculation of angle profiles or sputter depth profiles.



Plot view of a survey spectrum of an ionic liquid with periodic table for element and peak identification

Introduction

Quantification of XPS data for precise determination of the chemical surface composition is still a complex procedure: after taking the significant sets of data, they have to be exported into the correct data format together with important machine parameters like transmission functions and then reimported into a completely different software package. In contrast, the ISQAR module of SpecsLab Prodigy is completely integrated into the data acquisition package. It allows for precise determination of relative quantities of each element in selected peak areas of the photoelectron spectrum. All technical parameters, like transmission functions, lens modes, geometrical parameters and X-ray source settings are considered during the quantification. ISQAR is designed for easy handling. It is comprehensive with respect to models, features and parameter settings.

Basic Quantification: Element Identification and Chemical Composition

By using templates and proven databases, the user gets an initial set of useful quantification results in only a few quick steps. As part of the quantification procedure, Prodigy's ISQAR module automatically performs peak area operation on the selected peaks. Afterwards the quantification operation is performed on the group of selected spectra. For the very first quantification of elements in an unknown sample the respective spectrum in the Plot View Data Browser is selected and the periodic table is activated. Then

Quantification

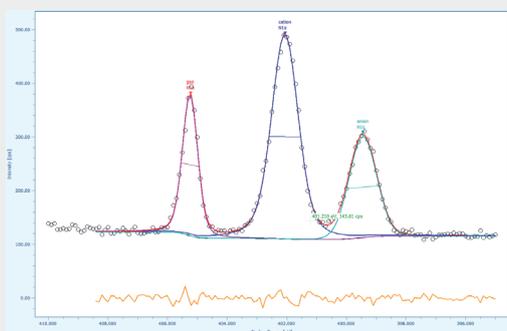
Included Angle (θ) = 54.74, Electron Emission Angle (θ) = 0

Peak	at%	Eb [eV]	σ [Mb]	β [a.u.]	L [a.u.]	λ [nm]	Q [a.u.]	s [norm.]	A [cps eV]	An [cps eV]	$\Delta A/A$ [%]
<input checked="" type="checkbox"/> C1s	35.84 ± 0.42	284.64	0.01	2.00	1.00	2.93	92.01	1.00	11625.45	126.35	1.64
<input checked="" type="checkbox"/> N1s	15.93 ± 0.32	400.23	0.02	2.00	1.00	2.72	92.32	1.67	8667.04	56.18	2.28
<input checked="" type="checkbox"/> O1s	14.6 ± 0.23	530.89	0.04	2.00	1.00	2.47	92.21	2.48	11747.54	51.46	1.66
<input checked="" type="checkbox"/> F1s	22.75 ± 0.24	687.10	0.06	2.00	1.00	2.17	91.08	3.28	23987.64	80.22	0.99
<input checked="" type="checkbox"/> S2p	10.88 ± 0.18	167.66	0.02	1.15	1.00	3.13	91.42	1.79	6273.85	38.36	1.65

Show Details

Quantification table with all parameters for an ionic liquid

you use the Identify Peaks button to automatically find and display excitations that match the peaks in the selected spectrum. Choose the peaks that you want to use for quantification either by selection of the spectra or the transitions of the element in the periodic table. Starting the procedure will finally calculate the area of the selected peaks and add a quantification section to the browser. The results of the quantification are shown in a table at the bottom of the quantification section. By default, only the peaks and the calculated atomic percentages are shown. Further details can be added into the table or become visible as mouse-over information in the tooltip. In particular, the tooltip discloses the database, model and interpolation used for the quantification.



Multi Peak Fit of a Near Ambient Pressure XPS N 1s spectrum of an ionic liquid in 1 mbar of N₂ atmosphere

Multi Peak Fit

Parameters

Range 408.49 eV 395.00 eV

	Peak 1	Peak 2	Peak 3
Transition	N1s	N1s	N1s
Label	cation	gas	anion
C	0	0	0
A	0	0	0
a	+++	+++	+++
s	+++	+++	+++
FL	+++	1 +++	1 +++
FG	+++	1 +++	1 +++
k	0.0075	0.0075	0.0075

Add Peak Remove Peak

Input parameters of the Multi Peak Fit

Advanced Quantification: Database choices and Multipeak Curve Fitting

For a more sophisticated analysis there are many ways to refine the procedure and improve the quantification, for instance by variations of the Inelastic Mean Free Path (IMFP) calculation method, background subtraction methods and numerical separation of overlapping peaks by using a multipeak curve fit routine. Advanced users can refine all integrated databases easily by extension or addition with user databases to properly reflect material specific properties deviating from the standard references given in literature. Also XPS data intentionally taken at different emission angles can be used for quantification by taking into account the actual measurement geometry.

Peak Function	Gauss, Doniach-Sunjic Gauss, Gauss Lorentz Product, Gauss Lorentz Sum, Voigt
Background	None, Linear, Tougaard, Shirley
Photoionization Cross Section	Scofield, Yeh/Lindau
Inelastic Mean Free Path (IMFP)	Exponential, TPP-2M

Reporting

The result of the quantification can be exported as data. Also publication-ready graphics can be designed and exported from ISQAR. Even full reports with customized templates and contents can be edited inside the software and also been exported. For all three purposes common file formats can be chosen.

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