

Analytical Chemistry

Theoretical and Metrological Fundamentals

K. Danzer

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With 138 Figures and 31 Tables

 Springer

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Preface

Analytical chemistry can look back on a long history. In the course of its development, analytical chemistry has contributed essentially to the progress of diverse fields of science and technology. Significant progress in natural philosophy, chemistry and other disciplines has been founded on results and discoveries in analytical chemistry. Well known examples include Archimedes' principle, iatrochemistry, emergence and overcoming of phlogiston theory, basic chemical laws on stoichiometry and mass proportions as well as the discoveries of elements and of nuclear fission.

As chemistry split into inorganic, organic and physical chemistry in the middle of the nineteenth century, the question occasionally arose as to whether analytical chemistry was likewise an autonomous field of chemistry. At the beginning of the twentieth century, analytical chemistry was established by Wilhelm Ostwald and other protagonists on the basis of chemical and physicochemical laws and principles. In addition, analytical procedures and instruments spread into other chemical fields. However, in the 1950s and 1960s a new generation of analysts opened their mind to ideas coming from other scientific fields dealing with measurements from other points of view such as information science, metrology, technometrics, etc.

As a result, efforts made towards the acceptance of analytical chemistry as an autonomous field of chemistry increased. Analysts in USA and Europe founded organisations and forums that focussed ideas and developments in progressive directions. In this way, not only were national and international societies formed but also regular conferences like Pittcon and Euroanalysis. In this connection the so-called Lindau circle should be mentioned where analysts from Germany, Austria and Switzerland made public relevant fundamentals of analytical chemistry derived from statistics, information theory, system theory, signal theory, game theory, decision theory, metrology, etc. In parallel with this, such modern principles have been successfully applied in selected case studies, mainly by scientists from USA, UK, and Canada. From this development, real theoretical and metrological fundamentals of analytical chemistry have crystallized. However, the acceptance of analytical chemistry as an autonomous branch of chemistry has not been realised. Gradually, however, progress in analytical chemistry culminated in the 1990s in the proclamation of a new scientific discipline, *analytical science*. Protagonists of these activities included Michael Widmer and Klaus Doerffel.

Today, analytical chemistry is still a discipline within chemistry. Although characterized as an auxiliary science, analytical chemistry continues to develop and grow just as before. It is no detraction being characterized as an auxiliary discipline as mathematics shows. However, it is likely that efforts to make analytical chemistry a more independent science will be repeated in the future from time to time.

Analytical chemistry possesses today a sound basis of chemical, physical, methodical, metrological, and theoretical fundamentals. The first of these are usually taken as the basis of classical textbooks on analytical chemistry. The others are found in diverse publications in the field of analytical chemistry and chemometrics. It is essential to state that chemometrics *is not* the theoretical basis of analytical chemistry but it contributes significantly to it. Frequently, analytical chemistry is considered to be a measuring science in chemistry. Therefore, its object is the generation, evaluation, interpretation, and validation of measuring signals as well as the characterization of their uncertainty. With this aim, the analyst needs knowledge of the general analytical process, statistics, optimization, calibration, chemometrical data analysis, and performance characteristics.

In this book the attempt is made to summarize all the components that can be considered as building blocks of a theory of analytical chemistry. The “building” constructed in this way is a provisional one. It is incomplete and, therefore, extension, reconstruction and rebuilding have to be expected in the future.

A large number of mathematical formulas will be found in the book. This may be regarded as a disadvantage particularly because some of them are not readily to apply in daily analytical practice. However, great scientists, explicitly Emanuel Kant, said that a scientific branch contains only so much of science as it applies mathematics. Consequently, all the relationships which can be described mathematically should be so described. It is true despite Werner Heisenbergs statement: Although natural processes can be described by means of simple laws which can be precisely formulated, these laws, on the other hand, cannot directly be applied to actions in practice.

Wherever possible, official definitions of IUPAC, ISO and other international organizations have been used, in particular in the “Glossary of Analytical Terms” compiled at the end of the book. However, uniformity could not be achieved in every case. In a few instances, special comments and proposals (characterized as such) have been added. Although progress in the field of harmonization of nomenclature and definitions has been considerable, some things still remain to be done.

Some of the contents of various sections have been published previously and are, of course quoted verbatim. In this connection the author is grateful to Klaus Doerffel, Karel Eckschlager, Günter Ehrlich, Andrzej Parczewski, Karol Florian, Mikulas Matherny, Günter Marx, Dieter Molch, Eberhard Than, Ludwig Küchler and others for long-standing collaboration resulting in mutually complementary papers and books. A chapter on statistics was previously published in another book (*Accreditation and Quality Assurance*

in Analytical Chemistry edited by Helmut Günzler at Springer). Gratefully I have adapted essential parts of the translation of Gaida Lapitajs here in this book.

Stimulations and ideas have arisen from discussions with William Horwitz, Duncan Thorburn Burns, Alan Townshend, Koos van Staden, and other members of diverse IUPAC Commissions and Task Groups as well as officers of the Analytical Chemistry Division. From a 20-year membership of various IUPAC bodies I have gained a variety of feedback and experience which has proved to be useful in the writing of this book. In particular, I owe Lloyd Currie and Mattias Otto a great debt of gratitude. They have permitted me to use essential parts of common publications on calibration quoted in Chap. 6. Many of the results stem from work carried out with colleagues, collaborators, postdocs and graduate students. All of them are deserving of my thanks but, due to the large numbers involved, this cannot be done here. Some representative colleagues include Jürgen Einax, Hartmut Hobert, Werner Schrön, Manfred Reichenbacher, Reiner Singer, Dietrich Wienke, Christoph Fischbacher, Kai-Uwe Jagemann, Michael Wagner, Katrin Venth, Raimund Horn, Gabriela Thiel, Demetrio de la Calle García, and Balint Berente.

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No book is free of errors and this one will be no exception. Therefore, the author would be grateful to readers who point out errors and mistakes and suggest any improvement.

Jena, July 2006

Klaus Danzer

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Symbols

A	Matrix of sensitivity factors in multicomponent analysis (e.g., absorbance factors)	(6.66)
a	Regression coefficient (calibration coefficient): intercept (general and regression in case of errors in both variables)	
a_x	Regression coefficient a for the estimation of y from x	(6.9)
a_{x_w}	Regression coefficient a in case of weighted calibration	(6.37)
a_y	Regression coefficient a for the estimation of x from y	(6.10)
$acc(x), acc(\bar{x})$	Accuracy of an analytical result x and of a mean \bar{x} , respectively	(7.10) (7.11)
antilog x	$= 10^x$, antilogarithm of x	
b	Regression coefficient (calibration coefficient): slope (general and in case of regression having errors in both variables)	
b_x	Regression coefficient b for the estimation of y from x	(6.8)
b_{x_w}	Regression coefficient b in case of weighted calibration	(6.36)
b_y	Regression coefficient b for the estimation of x from y	(6.10)
$bias(x), bias(y)$	Bias (systematic deviation) of an individual test value x (or y) from the (conventional) true value x_{true} (or y_{true})	(4.1)

$bias(\bar{x}), bias(\bar{y})$	Bias of an average test value \bar{x} (or \bar{y}) from the (conventional) true value x_{true} (or y_{true})	
$cnf(\bar{x}), cnf(\bar{y})$	Total (two-sided) confidence interval of a mean	(4.17)
$cond(A)$	Condition number of the matrix A	(6.80)
$cov(p_i, p_j)$	Covariance of the quantities p_i and p_j	
CB	Confidence band (of a calibration line)	(6.26a)
CR	Concordance rate (proportion of correct test results in screening)	(4.53a)
d_{crit}	Critical diameter (in microprobe analysis)	
d_{ij}	Distance (in multivariate data)	(8.12)
df	Discriminant function	(8.16)
$d\nu$	Discriminant variable	
E	Information efficiency	
E_{in}	Input energy	
E_{out}	Output energy	
E	Residual matrix (in multivariate data analysis)	
e, e_x, e_y	Error term (general, in x , and in y , respectively), in concrete terms, e_y may be the deviation of an individual value from the mean or the residual of a mathematical model, see next line (e_x analogous)	
e_y	$= y_i - \bar{y}$, deviation of an individual measured value from the mean (also d_y)	
e_y	$= y_i - \hat{y}$, deviation of an individual measured value from the estimate of the corresponding mathematical model	
\hat{F}	Test statistic (estimate) of the F test	(4.37)

$F_{1-\alpha, \nu_1, \nu_2}$	Quantile of the F distribution at the level of significance $1 - \alpha$ and for the degrees of freedom ν_1 and ν_2	
\hat{F}_{\max}	Test statistic (estimate) of HARTLEY's test	(4.37')
FNR	False negative rate (of screening tests)	(4.51)
FPR	False positive rate (of screening tests)	(4.50)
$f_{det}(\dots)$	Deterministic function of ...	
$f_{emp}(\dots)$	Empirical function of ...	
\hat{G}	Test statistic (estimate) of GRUBB's outlier test	(4.36)
\hat{G}_{\max}	Test statistic (estimate) of COCHRAN's test	(4.38)
$G_{\alpha, n}$	Significance limits of GRUBB's outlier test for a risk of error α and n individual measurements	
$g_{accept}(n)$	Acceptance function in attribute testing	
$g_{reject}(n)$	Rejection function in attribute testing	
$g_{accept}(n, s, \bar{\alpha})$	Acceptance function in variable testing	
$g_{accept}(n, s, \bar{\beta})$	Rejection function in variable testing	
H'	a posteriori information entropy	
H	a priori information entropy	
H_0	Null hypothesis	
H_A	Alternative hypothesis	
$hom(A)$	Quantity characterizing the homogeneity of an analyte A in a sample	(2.9)
I	Information content	(9.1)
I_{Aj}	Specific strength of an influence factor j on the signal of analyte A	
$I(p, p_0)$	Divergence measure of information	(9.9)
J	Information flow	(9.40)

L	Loading matrix (of principal component analysis and factor analysis)	(6.44) (8.19)
LCL	Lower control limit (in quality control)	
LWL	Lower warning limit (in quality control)	
l_x, l_y, l_z	Dimensions (lengths) in x -, y - and z -direction, respectively	
$\text{lb } a$	Binary logarithm of a	
M	Information amount	
$M(n)$	Information amount of multicomponent analysis (of n components)	(9.21)
$\text{mad}\{y_i\}$	Median absolute deviation (around the median), i.e., the median of the differences between an individual measured value and the median of the series: $\text{mad}\{y_i\} = \text{med}\{ y_i - \text{med}\{y_i\} \}$	
$\text{med}\{y_i\}$	Median of a set of measured values	(4.22)
N	Number of repeated measurements for the estimation of x by means of a calibration function	
N_{pp}	Noise amplitude, peak-to-peak noise	
$N(\mu, \sigma^2)$	Normal distribution with mean μ and variance σ^2	
$\overline{N(t)}$	Time average of noise	
NPR	Negative prediction rate (in screening tests)	(4.55)
n	Number of individual measurements (also in establishing a calibration model), number of objects (in a data set)	
$n(t)$	Noise component of a signal function in the time domain	
$\text{net}_i(t), \text{net}^{(i)}$	Net function (propagation function) in a neural network (layer i)	(6.117)
$O_i(t), O^{(i)}$	Output of a layer i of a neural network	(6.119)

P	Two-sided level of significance of statistical tests ($P = 1 - \alpha$)	
\bar{P}	One-sided level of significance of statistical tests ($\bar{P} = 1 - \bar{\alpha}$)	
$P(A)$	Probability of an event A (ratio of the number of times the event occurs to the total number of trials)	
$P(A)$	Probability that the analyte A is present in the test sample	
$P(\bar{A})$	Probability of the opposite of the event A (ratio of the number of times the event does not occur to the total number, $P(A) + P(\bar{A}) = 1$)	
$P(\bar{A})$	Probability that the analyte A is present in the test sample	
$P(A B)$	Conditional probability: probability of an event B on the condition that another event A occurs	
$P(T^+ A)$	Probability that the analyte A is present in the test sample if a test result T is positive	
P	Score matrix (of principal component analysis)	(6.44)
PB	Prediction band (of a calibration line)	(6.26b)
PPR	Positive prediction rate (in screening tests)	(4.54)
PV	Prevalency of screening tests: probability that the analyte A is present in a given number of samples	(4.52)
p	Number of primary samples (in sampling); Number of calibration points	
p_i, p_j, p_{ij}	Influence parameters	(4.25)
$prec(x)$	Precision of an analytical result x	(7.8)
$prd(x), prd(a)$	Prediction interval of a quantity x (and a , respectively)	
q	Number of subsamples (in sampling)	(2.5)
\hat{q}_R	Test statistic (estimate) of the DAVID test	(4.33)

Q	Categorical variable characterizing chemical entities (species) being investigated, e.g., elements, isotopes, ions, compounds	
\hat{Q}	Test statistic (estimate) of DIXON's outlier test	(4.35)
$Q(z)$	Evaluation relationship (of quantities characterizing qualitative properties) in form of a function, atlas, or table	
$Q = f^{-1}(z)$	Evaluation function of quantities characterizing qualitative properties, viz type of species, Q , in dependence of signal position, z	
R	Range ($R = y_{\max} - y_{\min}$)	
R	Resolution power	
R	Correlation matrix	(6.4)
R_C	Risk for customers (in quality assurance)	(4.56b)
R_M	Redundancy	(9.31a)
R_M	Risk for manufacturers (in quality assurance)	(4.56a)
R_t	Temporal resolution power	(7.57)
R_z	Analytical resolution power	(7.53)
$RMSP$	Root mean standard error of prediction	(6.128)
RR	Recovery rate	
$R\{q\}$	Range of a quantity q	
r	Number of measurements at a subsample	(2.4)
r_M	Relative redundancy	(9.31b)
r_{xy}	Correlation coefficient between the (random) variables x and y	(6.3)
$rob(A/B \dots; f_1 \dots)$	Robustness of a procedure to determine an analyte A with regard to disturbing components (B, \dots) and factors (f_1, \dots)	(7.31)

$rug(A/B \dots; f_1 \dots; u_1 \dots)$	Ruggedness of a procedure to determine an analyte A with regard to disturbing components (B, \dots), factors (f_1, \dots), and unknowns (u_1, \dots)	(7.33)
S	Sensitivity, derivative of the measured quantity (response) y with respect to the analytical quantity x	
S_{total}	Total multicomponent sensitivity	(7.18)
S	Covariance matrix	(6.5)
	Sensitivity matrix	(7.17)
S_{AA}	Sensitivity of the response of the analyte A with respect to the amount x_A of the analyte A (also S_A)	(7.12)
S_{AB}	Cross sensitivity (partial sensitivity) of the response of the analyte A with respect to the amount x_B of the component B	
S_{Ai}	Cross sensitivity (partial sensitivity) of the response of the analyte A with respect to the amount x_i of species i ($i = B, C, \dots N$)	(3.11)
S_{xx}, S_{yy}	Sum of squared deviations (of x and y , respectively)	(6.3')
S_{xy}	Sum of crossed deviations (of x and y)	(6.3')
$S_{\bullet}, S_{\bullet i}$	Sum over a variable index (e.g., at constant i); the dot replaces the index over that the summation is carried out	
$S(x)$	Sensitivity function	(6.64)
s	Estimate of the standard deviation (SD of the sample)	(4.12)
s^2	Estimate of the variance (variance of the sample)	(4.10)
s_N	Standard deviation of noise	(7.5)
$s_{p_i p_j}, s(p_i, p_j)$	Covariance of the quantities p_i and p_j	(4.27)
$s_{y \cdot x}$	Residual standard deviation (of the calibration); estimate of the error of the calibration model	(6.19)

XX		Symbols
$sel(A, B, \dots, N)$	Selectivity of a multicomponent analysis with regard to the analytes A, B, \dots, N	(7.24)
$snr(\bar{y})$	Signal-to-noise ratio of an average signal intensity \bar{y} (related to N_{pp})	(7.6)
$spec(A/B, \dots, N)$	Specificity of the determination of an analyte A with regard to the accompanying components B, \dots, N	(7.26)
S/N	Signal-to-noise ratio of an average signal intensity \bar{y} or a net intensity \bar{y}_{net} (related to s_y)	(7.1)
$(S/N)_c$	Critical signal-to-noise ratio	(7.51)
SS	Sum of squares	
$ssr(y)$	Sum of squares of residuals (of y)	(6.12)
t_w	Test statistic (estimate) of the generalized t test (WELCH test)	(4.43)
TE	Test efficiency of screening tests	(4.53b)
TNR	True negative rate (of screening tests)	(4.49)
TPR	True positive rate (of screening tests)	(4.48)
\hat{t}	Test statistic (estimate) of STUDENT'S t test	(4.41)
$t_{1-\alpha, \nu}$	Quantile of the t -distribution at the level of significance $1 - \alpha$ and for ν degrees of freedom	
UCL	Upper control limit (in quality control)	
UWL	Upper warning limit (in quality control)	
$u(x)$	Combined uncertainty of an analytical value x	(4.31)
$u(x(p_1, p_2, \dots))$	Uncertainty of an analytical value x , combined from the uncertainties of the parameters p_1, p_2, \dots	
$u(y)$	Combined uncertainty of a measured value y	
$u(y(p_1, p_2, \dots))$	Uncertainty of a measured value y , combined from the uncertainties of the parameters p_1, p_2, \dots	(4.25)

$U(x)$	Extended combined uncertainty (limit) of an analytical value x	
$U(y)$	Extended combined uncertainty (limit) of a measured value y	(4.29)
$unc(\bar{x})$	Uncertainty interval of a mean \bar{x}	(4.32)
$unc(\bar{y})$	Uncertainty interval of a mean \bar{y}	(4.30)
w_{y_i}, w_i	Weight coefficient (in weighted calibration)	(6.34)
x	Analytical value: analyte amount, e.g., content, concentration	
x_{LD}	Limit of detection	(7.44)
x_{LQ}	Limit of quantitation	(7.48)
x_Q	Analytical value (amount) of a species Q	
x_{test}	Analytical value of a test sample	
x_{true}	(Conventional) true value of a (certified) reference sample	
\bar{x}	Arithmetic mean of x (of the sample)	
\hat{x}	Estimate of x	
$x(Q)$	Sample composition (function)	
$x = f(Q)$	Analytical function in the sample domain, sample composition function	
$Y(\omega)$	Signal function in the frequency domain, FOURIER transform of $y(t)$	
y	Measured value, response (e.g., intensity of a signal)	
y_c	Critical value	(7.41)
y_{z_i}	Measured value (e.g. intensity) of a signal at position z_i	
\bar{y}	Arithmetic mean of y (of the sample)	
$\overline{\bar{y}}$	Total mean of several measured series	
\bar{y}_{BL}	Blank	
\bar{y}_{geom}	Geometric mean of y (of the sample)	
\hat{y}	Estimate of y	

y^*	Outlier-suspected value among the measured values	
$y(t)$	Signal function in the time domain	
$y_{true}(t)$	Component of the signal function in the time domain that is considered being true (influenced by noise)	
$y(z)$	Signal record (spectrum, chromatogram, etc.)	
$y = f(x)$	Calibration function (in the stricter sense, i.e. of quantities characterizing quantitative properties, e.g., signal intensity vs analyte amount)	
$y = f(z)$	Signal function (measurement function, analytical function in the signal domain)	
z	Signal position: measuring quantity that depends on a qualitative property of the measurand. Therefore, analytes may be identified by characteristic signal positions. The z -scale may be directly or reciprocally proportional to an energy quantity or time	
z	z -scores, standardized analytical values	(8.9)
$z(Q)$	Signal assignment function (table, atlas etc.)	
$z = f(Q)$	Calibration function of quantities characterizing qualitative properties, viz signal position as a function of the type of species	
α	Risk of the error of the first kind (two-sided)	
α	Regression coefficient (intercept)	(4.2)
α_i	Coefficient characterizing influences	(5.3)
$\bar{\alpha}$	Risk of the error of the first kind (one-sided)	
β	Risk of the error of the second kind (two-sided)	

β	Regression coefficient (slope)	(4.3)
β_j	Coefficient characterizing influences	(5.4)
$\bar{\beta}$	Risk of the error of the second kind (one-sided)	
$\hat{\chi}^2$	Test statistic (estimate) of the χ^2 test	
$\chi^2_{1-\alpha, \nu}$	Quantile of the χ^2 distribution at the significance level $1 - \alpha$ and for ν degrees of freedom	
$\Delta \bar{x}_{cnf}$	Confidence limit of a mean \bar{x}	
$\Delta \bar{x}_{prd}$	Prediction limit of a mean \bar{x}	
$\Delta \bar{y}_{cnf}$	Confidence limit of a mean \bar{y}	
Δ^2	Test statistic (estimate) for VON NEUMANN's trend test	(4.34)
$\mathcal{F}\{x(t)\}$	FOURIER transform of the time function $x(t)$ into the frequency function $X(\omega)$	
$\mathcal{F}^{-1}\{X(\omega)\}$	FOURIER backtransform of the frequency function $X(\omega)$ into the time function $x(t)$	
γ	Exponent characterizing nonlinear errors	(4.5)
λ	Eigenvalue (characteristic root) of a matrix	
\mathcal{M}	Multiplet splitting according to relevant rules	
μ_x	Mean of x of the population	
μ_y	Mean of y of the population	
ν	Number of the statistical degrees of freedom	
ν	Dispersion factor	(4.20)
σ	Standard deviation (of the population)	
σ^2	Variance (of the population)	(4.8)
Ξ	KAISER's selectivity	(7.21)

Ψ_A	KAISER's specificity with regard to an analyte A	(7.22)
$\Psi_{xx}(\tau)$	Autocorrelation function (ACF) of a function $x(t)$ with time lag τ	(2.11)
$(\alpha\beta)_{ij}$	Coefficient characterizing interactions of influences α and β	(5.4)
$(\alpha\beta\gamma)_{ijk}$	Coefficient characterizing interactions of influences α , β , and γ	(5.5)
$\{x_i\}$	Set (series, sequence) of analytical results whose terms are $x_1, x_2, \dots, x_i, \dots$	
$\{y_i\}$	Set of measured values (observations of a measurement series) whose terms are $y_1, y_2, \dots, y_i, \dots$	
\hat{a}, \hat{b}, \dots	Estimates of the quantities a, b, \dots	

In general, variables are expressed by italics, vectors by bold small letters, and matrices by bold capital letters.

Abbreviations and Acronyms

This list of abbreviations contains both acronyms which are generally used in analytical chemistry and such applied in the book. In addition to terms from analytical methods, essential statistical and chemometrical terms as well as acronyms of institutions and organizations are included. Terms of very particular interest are explained on that spot.

2D	Two-Dimensional (e.g., 2D-NMR)
3D	Three-Dimensional
AA	Activation Analysis
AAS	Atomic Absorption Spectrometry
ACF	Autocorrelation Function
ACV	Analytical value at critical (measuring) value
AEM	Analytical Electron Microscopy
AES	Auger Electron Spectroscopy
AES	(Atomic Emission Spectrometry) → OAES, OES
AFM	Atomic Force Microscopy
AFS	Atomic Fluorescence Spectrometry
ANN	Artificial Neural Networks
ANOVA	Analysis Of Variance
AOAC	Association of Official Analytical Chemists
ARM	Atomic Resolution Microscopy
ARUPS	Angle Resolved Ultraviolet Photoelectron Spectrometry
ASV	Anodic Stripping Voltammetry
ATR	Attenuated Total Reflectance
BASIC	Programming language: <u>B</u> eginners <u>A</u> ll-purpose <u>S</u> ymbolic
BCA	Beckman Glucose Analyzer
BIPM	Bureau International des Poids et Mesures
CA	Chemical Analysis
CARS	Coherent Anti-Stokes Raman Spectrometry
CCC	Counter Current Chromatography
CCD	Charge-Coupled Device
CE	Capillary Electrophoresis

C-E-R	Calibration-Evaluation-Recovery (Function)
CFA	Continuous Flow Analysis
CGC	Capillary Gas Chromatography
CMP	Chemical Measurement Process
CPAA	Charged Particle Activation Analysis
CRM	Certified Reference Material
CV	Critical value
CV-AAS	Cold Vapour Atomic Absorption Spectrometry
DCM	Dielectric Constant Measurement (Dielcometry)
DENDRAL	Expert system: <u>Dendritic Algorithm</u>
DIN	Deutsches Institut für Normung
DSC	Differential Scanning Calorimetry
DTA	Differential Thermal Analysis
DTG	Differential Thermogravimetry
EBV	Errors in Both Variables (Model, Procedure)
ECA	Electrochemical Analysis
ECD	Electron Capture Detector
ED	Electron Diffraction
EDX	Energy-Dispersive X-Ray (Spectrometry)
ED-XFA	Energy-Dispersive X-Ray Fluorescence Analysis
EDL	Electrodeless Discharge Lamp
EELS	Electron Energy Loss Spectrometry
EM	Electron Microscopy
EMP	Electron Microprobe
EN	European Norm
EPA	Environmental Protection Agency (USA)
EPH	Electrophoresis
EPMA	Electron Probe Microanalysis
ESAC	Expert Systems in Analytical Chemistry
ESCA	Electron Spectroscopy for Chemical Analysis
ESD	Estimated Standard Deviation
ESR	Electron Spin Resonance (Spectroscopy)
ETA	Electrothermal Atomizer
ETA-AAS	Electrothermal Atomizing Atomic Absorption Spectrometry
EXAFS	Extended X-Ray Absorption Fine Structure (Spectrometry)
FAB	Fast Atom Bombardment
FANES	Furnace Atomization Non-Thermal Emission Spectrometry
FD	Field Desorption
FEM	Field Electron Microscopy

FFT	Fast Fourier Transform
FIA	Flow Injection Analysis
FI-AP	Field Ion Atom Probe
FID	Flame-Ionization Detector
FIM	Field Ion Microscopy
<i>fn</i>	false negative (decisions in screening tests)
<i>fp</i>	false positive (decisions in screening tests)
FNAA	Fast Neutron Activation Analysis
FORTRAN	Programming language: <u>F</u> ormula <u>T</u> ranslation
FT	Fourier Transform
FT-ICR-MS	Fourier Transform Ion Cyclotron Resonance Mass Spectrometry
FT-IR, FTIR	Fourier Transform Infrared (Spectrometry)
FT-MS	Fourier Transform Mass Spectrometry
FT-NMR	Fourier Transform Nuclear Magnetic Resonance Spectrometry
FWHM	Full Width at Half Maximum
GA	Genetic Algorithm
GC	Gas Chromatography
GC-IR	Gas Chromatography Infrared Spectrometry Coupling
GC-MS	Gas Chromatography Mass Spectrometry Coupling
GDL	Glow Discharge Lamp
GDMS	Glow Discharge Mass Spectrometry
GDOS	Glow Discharge Optical Spectrometry
GF-AAS	Graphite Furnace Atomic Absorption Spectrometry
GLC	Gas Liquid Chromatography
GLS	Gaussian least squares (regression)
GLP	Good Laboratory Practice
GMP	Good Manufacturing Practice
HCL	Hollow Cathode Lamp
HEED	High Energy Electron Diffraction
HEIS	High Energy Ion Scattering
HG-AAS	Hydride Generation Atomic Absorption Spectrometry
HPLC	High Performance Liquid Chromatography
HPTLC	High Performance Thin-Layer Chromatography
HR	High Resolution
HRMS	High Resolution Mass Spectrometry
IC	Ion Chromatography
ICP	Inductively Coupled Plasma (Spectrometry)

ICP-MS	Inductively Coupled Plasma Mass Spectrometry
ICP-OES	Inductively Coupled Plasma Optical Emission Spectrometry
ICR	Ion Cyclotron Resonance
ID	Ion Diffraction
IDMS	Isotope Dilution Mass Spectrometry
IEC	Ion Exchange Chromatography
IEC	International Electrotechnical Commission
IFCC	International Federation of Clinical Chemistry
IM	Ion Microscopy
IMS	Ion Mobility Spectrometry
INAA	Instrumental Neutron Activation Analysis
INDOR	Internuclear Double Resonance
INS	Inelastic Neutron Scattering
IR, IRS	Infrared Spectroscopy
IRM	Infrared Microscopy
ISE	Ion-Selective Electrodes
IRS	Internal Reflectance Spectroscopy
ISO	International Organisation for Standardization
ISS	Ion Surface Scattering, Ion Scattering Spectrometry
IU	Insulin unit
IUPAC	International Union of Pure and Applied Chemistry
IUPAP	International Union of Pure and Applied Physics
LAMMS	Laser (Ablation) Micro Mass Spectrometry
LASER	Light Amplification by Stimulated Emission of Radiation
LC	Liquid Chromatography
LC-MS	Liquid Chromatography Mass Spectrometry Coupling
LD	Limit of Detection
LDMS	Laser Desorption Mass Spectrometry
LEED	Low Energy Electron Diffraction
LEIS	Low Energy Ion Scattering
LEMS	Laser Excited Mass Spectrometry
LIDAR	Light Detection And Ranging (analogous to RADAR)
LIMS	Laboratory Information Management Systems
LISP	<u>List</u> Processing
LLC	Liquid Liquid Chromatography
LM	Light Microscopy
LMA	Laser Microspectral Analysis
LM-OES	Laser Micro Optical Emission Spectroscopy
LOD	Limit Of Detection

LOS, LoS	Level of significance
LQ	Limit of quantitation
LRMA	Laser Raman Micro Analysis
MALDI	Matrix-Assisted Laser Desorption and Ionization
MALDI-TOF	MALDI Time-Of-Flight (Mass Spectrometry)
MEIS	Medium Energy Ion Scattering
MES	Mössbauer Effect Spectroscopy
MIP	Microwave-Induced Plasma
MLD	Measured value at Limit of Detection
MLQ	Measured value at Limit of Quantitation
MORD	Magneto Optical Rotary Dispersion
MÖS	Mössbauer Spectrometry
MS	Mass Spectrometry
MS-MS	Tandem Mass Spectrometry
MS ⁿ	<i>n</i> -fold Tandem Mass Spectrometry
M-OES	Micro(spark) Optical Emission Spectroscopy
MWS	Microwave Spectroscopy
NAA	Neutron Activation Analysis
NBS	National Bureau of Standards, USA (today: NIST)
ND	Neutron Diffraction
NEXAFS	Near-Edge X-Ray Absorption Fine Structure (Spectroscopy)
NIR, NIRS	Near Infrared (Spectrometry)
NIST	National Institute of Standards and Technology, USA
NMR	Nuclear Magnetic Resonance (Spectroscopy)
NOE	Nuclear Overhauser Effect
NQR	Nuclear Quadrupole Resonance
OAES	Optical Atomic Emission Spectroscopy
OCS	Out-of-control situations (in quality control)
OES	Optical Emission Spectroscopy
OIML	Organisation Internationale de Métrologie Légale
OLS	Ordinary least squares (regression)
ORD	Optical Rotary Dispersion
PARC	Pattern Recognition
PAS	Photo Acoustic Spectroscopy
PASCAL	Programming language called by BLAISE PASCAL (1623–1662)
PC	Paper Chromatography
PCR	Principal component regression
PES	Photoelectron Spectrometry
PIXE	Particle Induced X-Ray Emission

PLS	Partial least squares (regression)
PMT	Photomultiplier Tube
ppm	part per million (10^{-6} corresponding to 10^{-4} per cent)
ppb	part per billion (10^{-9} corresponding to 10^{-7} per cent)
ppt	part per trillion (10^{-12} corresponding to 10^{-10} per cent)
ppq	part per quadrillion (10^{-15} corresponding to 10^{-13} per cent)
PROLOG	Programming language: <u>Program</u> ming in <u>Logic</u>
QCC	Quality control charts
QMS	Quadropol Mass Spectrometer
R&D	Research and Development
RADAR	Radiowave Detection And Ranging
RBS	Rutherford Backscattering Spectrometry
REELS	Reflection Electron Energy Loss Spectrometry
REM	Reflection Electron Microscopy
RHEED	Reflection High Energy Electron Diffraction
RF	Refractometry
RIMS	Resonance Ionization Mass Spectrometry
RM	Reference Material
RMSP	Root mean standard error of prediction
RPC	Reversed Phase Chromatography
RPLC	Reversed Phase Liquid Chromatography
RRS	Resonance Raman Scattering
RS	Raman Spectroscopy
SAM	Scanning Auger Microscopy
SAM	Standard Addition Method
SEC	Size Exclusion Chromatography
SEM	Scanning Electron Microscopy
SERS	Surface Enhanced Raman Scattering
SFC	Supercritical Fluid Chromatography
SI	Système International (d'Unités)
SIMS	Secondary Ion Mass Spectrometry
SNMS	Sputtered Neutrals Mass Spectrometry
SNR	Signal-to-Noise Ratio
SOP	Standard Operating Procedure
SPE	Solid Phase Extraction
SPME	Solid Phase Micro Extraction
SRM	Standard Reference Material
SSMS	Spark Source Mass Spectrometry
STEM	Scanning Transmission Electron Microscopy

STM	Scanning Tunneling Microscopy
SV	Standard value
TA	Thermal Analysis
TCD	Thermal Conductivity Detector
TEELS	Transmission Electron Energy Loss Spectrometry
TEM	Transmission Electron Microscopy
TG	Thermogravimetry
TGA	Thermogravimetric Analysis
THEED	Transmission High Energy Electron Diffraction
TIC	Total Ion Chromatogram
TID	Thermoionic Detector
TLC	Thin-Layer Chromatography
TMA	Thermomechanical Analysis
<i>tn</i>	true negative (decisions in screening tests)
TOF-(MS)	Time-Of-Flight (Mass Spectrometry)
<i>tp</i>	true positive (decisions in screening tests)
TXRF	Total Reflection X-ray Fluorescence (Spectrometry)
UPS	Ultraviolet Photoelectron Spectrometry
UV	Ultraviolet (radiation)
UV-VIS	Ultraviolet-Visible (Spectrometry)
VIS	Visible (radiation)
WD-XFA	Wavelength-Dispersive X-Ray Fluorescence (Spectrometry)
XAS	X-Ray Absorption Spectrometry
XD	X-Ray Diffraction
XFA	X-Ray Fluorescence Analysis
XFS	X-Ray Fluorescence Spectrometry
XPS	X-Ray Photoelectron Spectrometry
XRD	X-Ray Diffraction
XRF	X-Ray Fluorescence (Spectrometry)
ZAF	Z (stands for atomic number) Absorption Fluorescence (Correction) (XFA)
ZAAS	Zeeman Atomic Absorption Spectrometry