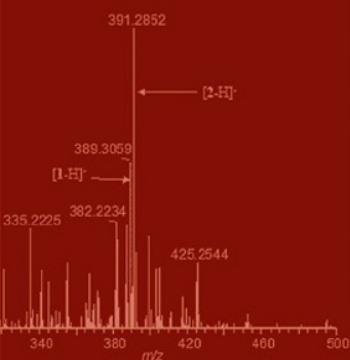


Dictionary of Mass Spectrometry

A.I.Mallet and S.Down

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A.I. Mallet and S. Down



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Preface

The *Dictionary of Mass Spectrometry* is intended to act as a first point of reference for explanations of the common terms and acronyms used in current practice of mass spectrometry. It is aimed at newcomers to mass spectrometry as well as experienced practitioners, covering new and established terminology that is encountered in the literature.

The book follows the format of the *Dictionary of Microscopy*, the entries being accompanied by many illustrations, diagrams and photographs for clarification. The entries are explanations, not definitions, and a deliberately non-judgemental approach has been followed. For an account of the preferred or accepted terms, there are a number of texts, some listed in the suggested reading list, which fulfil this purpose.

This content of this book is not exhaustive. New terms and techniques will appear in the future and the authors welcome suggestions for additions, as well as any corrections and comments on the existing entries.

The authors are indebted to their colleagues and especially to Dr Bob Boyd and Dr Gareth Brenton for their helpful comments.

Tony Mallet
Steve Down
July 2009

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Acronyms

This list contains many of the acronyms encountered in mass spectrometry. They are also defined at the appropriate entry in the listings.

AC	alternating current
ADC	analogue-to-digital converter
AMDIS	automated mass spectral deconvolution and identification system
AMS	accelerator mass spectrometry
AP	atmospheric pressure
APCI	atmospheric pressure chemical ionisation
API	atmospheric pressure ionisation
APPI	atmospheric pressure photoionisation
BIA	biomolecular interaction analysis
BIRD	blackbody infrared radiative dissociation
CAD	collisionally activated dissociation
CE	capillary electrophoresis
CI	chemical ionisation
CID	collision-induced dissociation
CNL	constant neutral loss
CRIMS	chemical reaction interface mass spectrometry
CRM	certified reference material
DAC	digital-to-analogue converter
DAD	diode array detector
DART	direct analysis in real time
DBDI	dielectric barrier discharge ionisation
DBE	double bond equivalent
DC	direct current
DCI	desorption chemical ionisation
DEI	desorption electron ionisation
DEP	direct exposure probe
DESI	desorption electrospray ionisation
DIOS	desorption/ionisation on silicon
DLI	direct liquid introduction
DMS	differential mobility spectrometry
DNA	deoxyribonucleic acid
ECD	electron capture dissociation

acronyms

EI	electron ionisation
EM	electron multiplier
ESA	electrostatic energy analyser
ESI	electrospray ionisation
ESSI	electrosonic spray ionisation
ETD	electron transfer dissociation
FAB	fast atom bombardment
FAIMS	high-field asymmetric waveform ion mobility spectrometry
FD	field desorption
FFR	field-free region
FI	field ionisation
FIA	flow injection analysis
FID	free induction decay
FNF	filtered noise field
FT	Fourier transform
FTICR	Fourier transform/ion cyclotron resonance
FWHM	full width at half-maximum height
GC	gas chromatography
GC-C-IRMS or GCC-IRMS	gas chromatography-combustion-isotope ratio mass spectrometry
GC/MS	gas chromatography/mass spectrometry
GDMS	glow discharge mass spectrometry
GPC	gel permeation chromatography
HDX	hydrogen/deuterium exchange
HPLC	high performance liquid chromatography
ICAT	isotope-coded affinity tag
ICP	inductively coupled plasma
ICPMS	inductively coupled plasma mass spectrometry
ICR	ion cyclotron resonance
IDA	information-dependent acquisition
IKES	ion kinetic energy spectrometry
IMS	ion mobility spectrometry
IR	infrared
IRMPD	infrared multiphoton dissociation
IRMS	isotope ratio mass spectrometry
JeDI	jet desorption ionisation
LAMMA	laser-activated microprobe mass analysis

LC	liquid chromatography
LC/MS	liquid chromatography/mass spectrometry
LC/MS/MS	liquid chromatography/mass spectrometry/mass spectrometry
LDI	laser desorption/ionisation
LIT	linear ion trap
LLOD	lower limit of detection
LLOQ	lower limit of quantitation
LOD	limit of detection
LOQ	limit of quantitation
LSIMS	liquid secondary ionisation mass spectrometry
MALDI	matrix-assisted laser desorption/ionisation
MECA	multiple excitation collisional activation
MIKES	mass-analysed ion kinetic energy spectrometry
MIMS	membrane introduction mass spectrometry
MRM	multiple reaction monitoring
MS	mass spectrometry
MS/MS	mass spectrometry/mass spectrometry
MudPIT	multidimensional protein identification technology
NALDI	nano-assisted laser desorption/ionisation
NICI	negative ion chemical ionisation
NIST	National Institute of Standards and Technology
PA	proton affinity
PAD	post-acceleration detector
PBM	probability based matching
PCA	principal components analysis
PCR	polymerase chain reaction
PDA	photodiode array detector
PICI	positive ion chemical ionisation
PID	photon-induced dissociation
PSD	post-source decay
PTM	post-translational modification
PTR	proton transfer reaction
QIT	quadrupole ion trap
QTOF	quadrupole time-of-flight
QUISTOR	quadrupole ion storage trap
RDBE	rings and double bond equivalents
REMPI	resonance-enhanced multiphoton ionisation

acronyms

RF	radiofrequency
RGA	residual gas analyser
RIC	reconstructed ion chromatogram
RMM	relative molecular mass
RNA	ribonucleic acid
RRKM	Rice, Ramsperger, Kassel, Marcus
SALDI	surface-assisted laser desorption/ionisation
SDS-PAGE	sodium dodecyl sulfate polyacrylamide gel electrophoresis
SELDI	surface-enhanced laser desorption/ionisation
SIC	selected ion chromatogram
SID	surface-induced dissociation
SIFT	selected ion flow tube
SILAC	stable isotope labelling of amino acids in cell culture
SIM	selected ion monitoring
SIMION	simulated ion trajectory algorithm
SIMS	secondary ion mass spectrometry
SIR	selected ion recording
SIRA	stable isotope ratio analysis
SNMS	secondary neutral mass spectrometry
SORI	sustained off-resonance irradiation
SPR	surface plasmon resonance
SQUID	superconducting tunnel junction detector
SRM	selected reaction monitoring
SSI	sonic spray ionisation
SWIFT	stored waveform inverse Fourier transform
TDC	time-to-digital converter
TES	translational energy loss spectrometry
TIC	total ion current or total ion chromatogram
TICC	total ion current chromatogram
TLC	thin-layer chromatography
TOF	time of flight
TSP	thermospray ionisation
UV	ultraviolet
XIC	extracted ion chromatogram

A

a_n ion

An N-terminal ion formed by fission of a peptide ion at the C-C peptide bond. *See peptide sequencing*

a_u

Parameter in the Mathieu equation. *See Mathieu stability diagram*

abundance

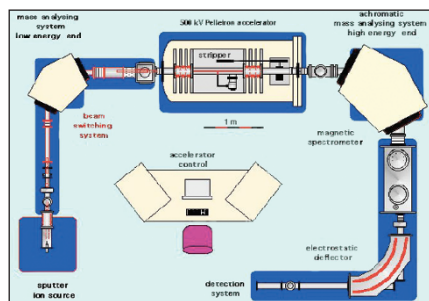
This term is used to describe the relative occurrence of an ion. A mass spectrum is a plot of the ion abundances against the m/z values determined and is normalised to the most abundant ion. This term should be distinguished from intensity which, while appropriate for the signal of the individual ion peak detected, is not used in spectra.

accelerating voltage (V)

The potential applied to newly formed ions in the mass spectrometer source to direct them into the analyser.

accelerating voltage scan

A scan mode for relatively rapid scanning of a magnetic sector instrument where, over a limited m/z range, the accelerating voltage is scanned while the magnetic field is held constant. This obviates the problems associated with hysteresis and inherent resistance to rapid changes in the magnetic field but also defocusses the ion source. *See also defocussing voltage scan*



Accelerator MS, National Electrostatics Corporation

accelerator MS (AMS)

A technique for the determination of precise isotope ratios for elements of very low abundance, principally ^{14}C isotopes but increasingly also ^3H , ^{41}Ca and ^{26}Al . The element to be analysed is extracted from the sample and inserted in the ion source in a metal holder. It is bombarded with a beam of caesium ions (Cs^+) to produce negative ions which are passed through a magnetic field for ion selection. The resultant ions are accelerated to high energy, typically $>1\text{ MeV}$, in a tandem accelerator in which charge stripping occurs to convert the negative ions to positive ions. This will minimise cross talk from other isobaric ions. A sequence of analyser elements is employed to produce signals of high specificity. The method is used in archaeology, geophysics and clinical chemistry.

accuracy

The accuracy of a mass measurement or concentration from a quantitative determination is a measure of how close the value obtained is to the true value. *See also precision*

accurate mass measurement

An experimental determination of the accurate and precise value of m/z for an ion, usually with a view to suggesting elemental composition.

accurate molecular mass

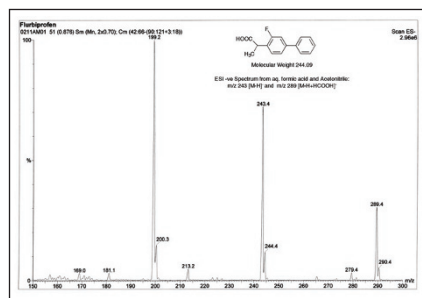
The measured mass of a molecule or ion determined with sufficient accuracy to allow the determination of a probable elemental composition.

acidic residue

An amino acid residue in a peptide or protein that has an acidic nature, such as aspartic acid or glutamic acid.

adduct ion

An electrically charged species formed by non-covalent attachment between an ion and a neutral species. These are most commonly observed in desorption and API and CI ion sources where a molecule of a component in the solvent or reagent gas remains attached to the ion. The illustration shows the formation of a formic acid adduct ion from the negative ESI of a carboxylic acid.



Adduct ions in an ESI spectrum

adiabatic

A term used in thermodynamics which describes an event in which no energy (heat) is transferred to or from the environment.

adiabatic ionisation

Ionisation which takes place so rapidly that the newly formed ion remains in its lowest energy state, as occurs during electron ionisation.

aerosol

A stable suspension of fine particles in a vapour, typically that formed in a pneumatically assisted electrospray ion source.

aerosol mass spectrometry

The measurement of organic aerosol compositions in real time, generally by sampling at ambient pressure. Particle sizes are almost always determined at the same time and the technique has been applied to atmospheric aerosols, bioaerosols and aerosols from human breath.

affinity chromatography

Liquid chromatography in which a particular compound or class of compounds is concentrated or purified by specific interaction with an immobilised ligand attached to the packed column stationary phase. The ligands include a wide variety of compounds but when antigens or antibodies are used the technique is often referred to as immunoaffinity chromatography. It is commonly used to purify biological molecules