

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

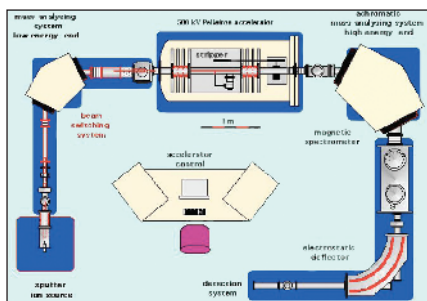
This term is used to describe the relative occurrence of an ion. A mass spectrum is a plot of the ion abundances against the m/z values determined and is normalised to the most abundant ion. This term should be distinguished from intensity which, while appropriate for the signal of the individual ion 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 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.

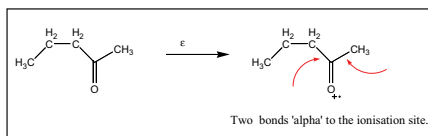
accurate molecular mass

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

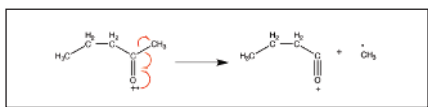
from complex mixtures such as biofluids or peptide digests.

algorithm

A software procedure in a computer program designed to perform a defined task.



Alpha bond



Alpha cleavage

alpha bond

In discussing the fragmentation mechanism of an ion, the bond adjacent to the site of ionisation is frequently referred to as an alpha bond. In the ketone ionised by EI in the figure shown here, the arrows show the two alpha bonds.

alpha cleavage

Fission of the alpha bond by a radical site-driven electron shift. Illustrated here for a ketone ionised by EI. Note the fishhook arrows designating single electron transfers.

alternating current (AC)

An electrical current supply in which the magnitude and sign vary cyclically in the form of a sine wave.

ambient mass spectrometry

A general term describing mass spectrometry in which ionisation takes place at ambient pressure and temperature, usually in the open air. Specific types include DESI and DART.

ammonia

A gas, formula NH_3 , frequently used in CI sources to promote low-energy adduct ion formation. The most common species observed is the ammoniated adduct ion $[\text{M}+\text{NH}_4]^+$. The ionisation is softer than with methane or isobutane, the other two common CI gases. Ammonia is also used to moderate the electrons produced in negative-ion electron capture sources.

analogue ion

Ions with similar chemical valence, such as $[(\text{CH}_3)_2\text{NC}=\text{S}]^+$ and $[(\text{CH}_3)_2\text{NC}=\text{O}]^+$.

analogue signal

A continuous electrical signal which is digitised prior to passing to a computerised data system. To be contrasted with pulse count signal acquisition.
See also pulse count signal

analogue-to-digital converter (ADC)

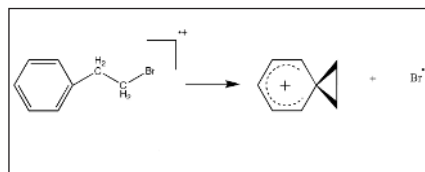
A device, usually based on a semiconductor chip, which samples an analogue signal, e.g. a voltage, and converts it into a digitised form. Important parameters include the number of bits that are output, the speed of conversion and the accuracy and precision. Virtually all signals from mass spectrometers are processed in this way prior to being passed to the data system. The inverse operation is performed by a DAC.

analyser

That part of a mass spectrometer in which ions of differing m/z values are separated and ejected or are detected *in situ*. It can take the form of filters formed by parallel rods to which appropriate RF and DC voltages are applied (quadrupole filters), three-dimensional ion traps, again using RF and DC voltages (Paul trap or Orbitrap) or also with magnetic fields (Penning or ICR trap), magnetic and electrostatic fields (sector instruments) or time of flight arrangements. It is common for more than one analyser to be coupled together in tandem. *See also tandem mass spectrometry*

anchimeric assistance

The participation of a neighbouring group in a molecule in the reaction of an adjacent part, resulting in an increase in the reaction rate. In MS, it is used to describe fragmentation mechanisms assisted in this manner. In the scheme here, the combined participation of the bromine radical loss and the formation of a stable 'phenonium' ion provide the driving force for this rearrangement.



Anchimeric assistance

anion

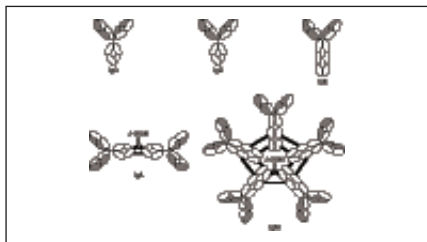
Any atom, molecule, ion or fragment of a molecule carrying a negative charge.

anomeric configuration

A term used in carbohydrate chemistry to define aspects of the stereochemistry of the molecule.

anti-aromatic ion

A planar cyclic ion containing alternating single and double bonds with a total of $4n$ π electrons ($n = 0, 1, 2, 3$ etc.) and it is therefore not aromatic.



Antibody

antibody

A large protein from the immunoglobulin family (IgA, IgD, IgE, IgG, IgM) which the immune system employs to recognise foreign molecules in the organism prior to their destruction and removal. Each immunoglobulin has two variable regions at the tips of the molecule that are designed specifically to bind to the target antigen.

antigen

A foreign substance which elicits a response from the immune system. This molecule binds to the variable region of the antibody.

apparent mass

The m/z value measured for metastable ions detected with double focussing magnetic analysers. The apparent mass is defined by the equation

$$m^* = m_2^2/m_1$$

where an ion of mass m_1 produces a fragment with mass m_2 .

appearance energy

In EI sources, the minimum electron energy at which an ion can be observed in the spectrum. Sometimes determined by the potential (volts) which is applied to the filament in an EI source relative to the source block.

appearance potential *see* appearance energy

aptamer

A synthetic small oligonucleotide or peptide molecule with an overall three-dimensional structure designed to bind strongly to a target molecule such as a protein, lipid or viral complex. Immobilised aptamers have been used to perform highly specific target molecule extraction and purification prior to MALDI-TOF MS.

argon

An inert gas, symbol Ar, frequently used in low-energy collision cells for tandem mass spectrometric experiments and to form the plasma in ICPMS experiments.

argon plasma

Argon is used in ICPMS to form the ionising plasma as this has the advantage of forming multiply charged elemental ions, simplifying the resulting spectra.

aromatic ion

A planar cyclic ion containing alternating single and double bonds with $(4n + 2)$ electrons (n is a positive number representing the number of conjugated π electrons).

array detector

A device in which a number of ion-detecting elements are arranged in a linear or two-dimensional arrangement. This detector was designed to provide a modern digital version of the old photoplate detector with which an entire spectrum could be recorded without the need to mass scan a sector analyser.

associative ionisation

A cooperative ionisation process in which two excited atoms or molecules react together to form a single adduct ion and an electron.

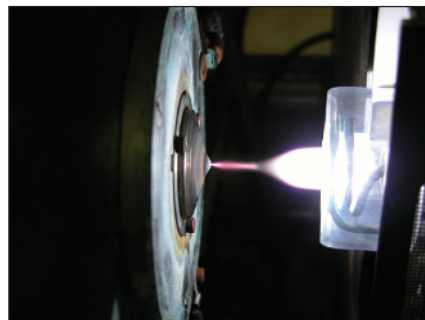
asymmetric field ion mobility spectrometry *see* high-field asymmetric waveform ion mobility spectrometry

atmospheric pressure

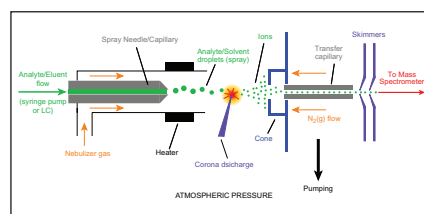
Atmospheric pressure varies with weather and altitude. Standard atmospheric pressure is defined as 1.01325 bar and 760 mm mercury or 760 Torr.

atmospheric pressure chemical ionisation (APCI)

A form of API in which a high voltage applied to a fine needle produces a corona discharge in a heated spray of dissolved analyte, nitrogen gas and air. The plasma so formed contains solvent as well as oxygen and nitrogen radical ions which react with



Argon plasma. Courtesy of Clarisse Mariet, CEA Saclay, France



Atmospheric pressure chemical ionisation (APCI). Reproduced from 'Mass Spectrometry Ionisation Techniques and Applications for the Analysis of Organic Compounds', P. J. Gates et al, in "Current Methods in Medicinal Chemistry and Biological Physics", Carlton A. Taft and Carlos H. T. P. Silva, Research Signpost 2007, 81-308-0141-8

atmospheric pressure ionisation (API)

traces of water to form H_3O^+ and OH^- as well as other ions. These undergo ion/molecule reactions with the analyte to form $[\text{M}+\text{H}]^+$ and $[\text{M}-\text{H}]^-$ species. When employed in LC/MS, higher HPLC flow rates can be accepted than for ESI. Multiply charged species are not common. The abbreviation APCI is a commercial term.

atmospheric pressure ionisation (API)

A general term for all forms of ionisation which can take place at atmospheric pressure including ESI, APCI, APPI and MALDI.

atmospheric pressure ion source

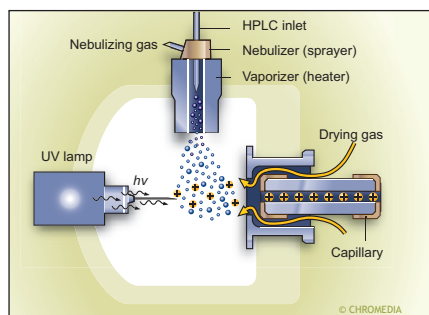
Any ion source operating at atmospheric pressure.

atmospheric pressure MALDI

MALDI can take place at AP, reduced pressure or in a high vacuum. The AP MALDI sources are easily interchanged with ESI or APCI ion sources.

atmospheric pressure photoionisation (APPI)

A form of API in which the analyte is sprayed into the source, as in ESI and APCI sources, in a solvent frequently containing a dopant molecule such as toluene or acetone. The spray is irradiated by a powerful UV source that forms excited species which undergo secondary ion/radical-molecule reactions with the analytes to cause ionisation. It is claimed to be the method of choice for detection of non-polar molecules in HPLC eluates. Protonated or deprotonated molecules or radical molecular ions can be formed, according to the mechanisms and thermodynamics involved.



Atmospheric pressure photoionisation (APPI), courtesy of Chromedia. This source is mounted in front of the entrance capillary to the mass spectrometer

atom gun

A device designed to produce a collimated beam of energetic atoms from a heated source. In MS, this is the prime source for the formation of ions in a FAB source. Most SIMS and FAB sources use atom as well as ion guns, commonly with xenon atoms or caesium ions.

atomic mass

The mass of an atom. The mass scale is a relative one based upon an agreed definition of the mass of an elemental isotope standard. Modern scales are

based on the assumption that ^{12}C has a mass of exactly 12.0000 and are expressed in unified atomic mass units.

atomic mass unit (amu)

A term for atomic weight, originally based on the assumption of a mass of 16.0000 exactly for the ^{16}O isotope of oxygen. Now replaced by unified atomic mass unit (u). $1 \text{ u} = 1 \text{ Da} = 1.665 \times 10^{-27} \text{ kg}$.

atomic weight

A commonly used term for the average atomic weight of an element, calculated from the average of the constituent stable isotope masses of that element using the unified atomic mass scale. *See average atomic weight*

atto

Abbreviation for 10^{-18} . As in attomole.

autodetachment

The spontaneous loss of an electron from an anion to produce a neutral species.

autoionisation

The spontaneous loss of an electron from a neutral species via a radiationless transition from a discrete electronic level to an ionized continuum level of the same energy.

auxiliary gas

An inert gas, usually nitrogen, added to an AP ion source to create an aerosol spray, to assist in solvent evaporation and to minimise access of the atmosphere to the source. Increased gas flow rates are required at higher solvent flows.

average atomic weight

The average mass of an atom taking into account the masses of its constituent stable isotopes and their naturally occurring abundances using data on the unified atomic mass scale.

average molecular mass

The mass of an ion or molecule calculated from the average atomic weights of the constituent isotopes and their natural abundances based on the unified atomic mass scale.

Avogadro number

The number of atoms in 12 g, i.e. one mole, of ^{12}C . This is currently accepted as $6.02214199 \times 10^{23}$.

axial ejection

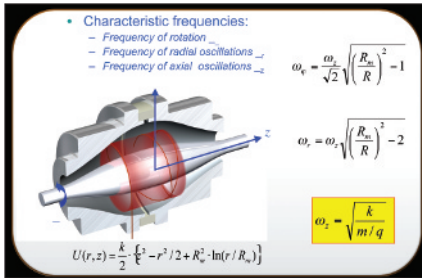
The application of a supplementary electric field to induce the ejection of ions from a trap.

axial oscillation

Together with cyclotron and magnetron motion, a packet of ions in an ICR cell undergoes an oscillatory motion axial to the direction of the magnetic field. Also, for ions in an Orbitrap, a detection principle relies on the image current of the axial motion of ion packages orbiting the inner electrode.

axialisation

The effect of retarding electric fields or of multiple collisions of ions and molecules to induce cooling and congregate the ions in a defined space, such as in an ion trap or an RF-only multipole element.



A diagram illustrating the axial and radial oscillations present in an Orbitrap.
Courtesy of Thermo Scientific