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COMMISSION ON MOLECULAR STRUCTURE AND SPECTROSCOPY*
SUBCOMMITTEE ON MASS SPECTROSCOPY†

RECOMMENDATIONS FOR NOMENCLATURE AND SYMBOLISM FOR MASS SPECTROSCOPY (including an appendix of terms used in vacuum technology) (IUPAC Recommendations 1991)

Prepared for publication by

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Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991)

Abstract - The recommendations contained in this document refer to nomenclature relating to theoretical, technological and experimental aspects of mass spectroscopy, and to the symbolism used when presenting and discussing mass spectral data. In 1974, the Commission on Analytical Nomenclature of IUPAC issued recommendations for nomenclature of mass spectroscopy which are in the form of definitions of some of the terms used in this subject. In 1978 the Commission on Molecular Structure and Spectroscopy updated and extended these recommendations and, in addition, made further recommendations concerning the use of symbols, acronyms, abbreviations and newly invented jargon. Because the subject continues to expand rapidly, a further compilation of defined terms has become necessary, and the opportunity has been taken to incorporate previous relevant recommendations concerning nomenclature and symbolism in order to produce a single comprehensive document. A further set of terms relating to vacuum technology, provided through the generosity of the American Vacuum Society, has been appended. It is therefore intended that this set of Recommendations should replace the earlier publications on the subject.

PREAMBLE

Mass Spectroscopy is the study of systems by causing the formation of gaseous ions, with or without fragmentation, which are then characterized by their mass-to-charge ratios and relative abundances. The recommendations contained in this document refer to nomenclature relating to theoretical, technological and experimental aspects of the subject, and to the symbolism used when presenting and discussing mass spectral data.

The Commission on Analytical Nomenclature of IUPAC has previously issued recommendations for nomenclature of mass spectroscopy [Pure and Applied Chemistry (1974) 37, No. 4, 469]. These are in the form of definitions of some of the terms used in this subject. In formulating the definitions, note was taken of the definitions proposed by the Fachnormenausschuss Vakuumtechnik in Deutsche Normenausschuss and the Editorial Review in Organic Mass Spectrometry (1969) 2, 249. In 1978 the Commission on Molecular Structure and Spectroscopy updated and extended these recommendations and, in addition, made further recommendations concerning the use of symbols, acronyms, abbreviations, and newly invented jargon [Pure and Applied Chemistry (1978) 50, 65].

Because the subject continues to expand rapidly, a further compilation of defined terms has become necessary, and the opportunity has been taken to incorporate previous relevant recommendations concerning nomenclature and symbolism in order to produce a single comprehensive document. It is therefore intended that this set of Recommendations should replace the earlier publications on the subject. Despite its length it is recognized that this present document is in some respects incomplete, and further definitions are currently under consideration.

In drawing together these recommendations, considerable use has been made of a set of proposed terms and definitions prepared by the Nomenclature Committee of the American Society for Mass Spectrometry under the successive chairmanships of Prof. J. H. Beynon, Dr. D. Cameron and Dr. P. Price, and the work undertaken by this group is gratefully acknowledged. A further set of terms relating to Vacuum Technology, provided through the generosity of the American Vacuum Society, has been appended.

The subject matter has been divided into major Sections, as follows:

- I. Introduction
 - II. General Terms
 - III. Ionization Nomenclature
 - IV. Types of Ions
 - V. Scanning of Spectra
 - VI. Sample Introduction and Sensitivity
 - VII. Ion Detection
 - VIII. Signal Recording
 - IX. Ion/Molecule Reactions
 - X. Isotope Mass Spectroscopy
 - XI. Symbolism
- Appendix A: Data Systems
Appendix B: Terms Used in Vacuum Technology

Within each section the terms have been listed alphabetically and have been cross-referenced where possible. Attention is drawn to the communication entitled 'Critical Evaluation of Class II and Class III Electron Impact Mass Spectra. Operating Parameters and Reporting Mass Spectra', by J. G. Dillard, S. R. Heller, F. W. McLafferty, G. W. A. Milne and R. Venkataraghavan, which appeared in Organic Mass Spectrometry (1981) 16, No. 1, 48; IUPAC recommendations concerning this aspect of the subject are currently under consideration.

1. INTRODUCTION

An acronym, abbreviation or invented jargon should only be used after a full explanation of its meaning has been given in the text. It is not sufficient merely to give the expression followed by a literature reference. It is only necessary or desirable to use a special term at all if it allows an appreciable saving of space or prevents repetition of a long or clumsy phrase. The only exceptions, relating to mass spectroscopy, should be the following few commonly accepted initials and symbols that may be used freely and without amplification:

GC/MS (LC/MS)	meaning either the combined techniques of gas (liquid) chromatography and mass spectroscopy or the combination of a gas (liquid) chromatograph with a mass spectroscope
ICR	meaning ion cyclotron resonance (see below)
m/z	meaning mass-to-charge ratio (see below).

[Note: Except in the cases of GC/MS and LC/MS given above, the initials MS should not be used without specific definition. They can mean, for example, mass spectrum, mass spectrometer, mass spectroscopy, metastable, magnetic sector, etc., and their indiscriminate use thus leads to considerable confusion.]

Other terms that have been invented to describe equipment or techniques are often referred to by their initials. This can become confusing when, for example, SID is used regularly to mean specific ion detector, secondary ion detection, single ion detection, and surface-induced dissociation. This emphasizes another aspect of the general undesirability of the proliferation of new terms and acronyms: all acronyms should be defined and used as defined.

Terms peculiar to the discipline of mass spectroscopy should be used only when more generally used and understood terms are either inadequate, ambiguous or very inconvenient. Authors should resist the proliferation of invented words; jargon should be minimized to maximize communication with scientists in other areas. Several special terms are already in widespread use. It is recommended that the lists in the following sections be confirmed as terms of this kind that may be used without explanation.

Proper names should only be used as a shorthand method of referring to an instrument, a theory, a rule or a reaction if there is no other convenient and adequate descriptive method available. Proliferation of the use of names should be discouraged on the grounds that their use can lead to subjective thinking, to lack of recognition of simultaneous work in other laboratories and to confusion when a person extends or changes his ideas or equipment. It is recommended that, in the few cases where the use of proper names is unavoidable, their use should always be accompanied by a literature reference to the original work. Only in this way can ambiguity of meaning be avoided.

It is recommended that three cases of the use of proper names that have already been defined in the earlier IUPAC recommendations should continue to be used as a convenient shorthand. These are:

Mattauch-Herzog geometry

Nier-Johnson geometry

McLafferty rearrangement

In connection with the use of the above terms, it should be noted that they refer only to the defined arrangements and reaction. Thus, the Nier-Johnson geometry necessarily involves a deflection of $\pi/3$ radians in the magnetic field and no other. Precise definitions of these terms are included in the following sections. Terms, such as modified Nier-Johnson geometry or quasi-McLafferty rearrangement are meaningless and should not be used.

In some instances, words that have a recognized meaning in everyday conversation are used (sometimes with inverted commas) to have a somewhat different meaning. Thus, the terms 'loose' and 'tight' transition complex appear in the literature and the meaning to be ascribed to them is not clear. Such terms should never be used without definition or a reference explaining the meaning [see, for example, P. J. Robinson and K. A. Holbrook, 'Unimolecular Reactions', Wiley-Interscience, 1972, pp. 154-156; W. Forst, 'Theory of Unimolecular Reactions', Academic Press, 1973, pp. 363-368].

The parts of a mass spectrometer should be described clearly according to their position within the instrument or the function that they perform. Thus, one should not refer to the α - or β - slits or simply to the 'first' or 'second' field-free regions. Rather, one should use terms such as the source slit, the slit limiting the angular divergence, the energy resolving slit, the field-free region traversed by the ion beam before entering the magnetic sector or the ion repeller plate.

The initials HV or EHT to describe voltages of the order of a few thousand volts should not be used. Rather, one should use the expression accelerating voltage without abbreviation.

To describe the performance of mass spectroscopic equipment it is necessary to specify inter alia the sensitivity and resolving power; definitions of these terms are given in Sections VI and VIII, respectively.

The symbol u has been recommended for atomic mass units using the standard that the mass of ^{12}C is 12 u exactly (see Quantities, Units and Symbols in Physical Chemistry, Blackwell, 1988). In biochemistry this unit is sometimes called the dalton, with symbol Da, although this name and symbol have not been approved by the Conférence Générale des Poids et Mesures (CGPM). The symbol amu is no longer recommended - this was the old unit using the standard based on the mass of ^{16}O .

II. GENERAL TERMS

Charge number (z). This is the total charge on an ion divided by the elementary charge (e).

Crossed electric and magnetic fields. Electric and magnetic fields with the electric field direction at right angles to the magnetic field direction.

Data processing. Once information is obtained with a data system or other output device (oscilloscope or pen recorder), the information must be presented in a form appropriate to the end use of the experiment. Those steps which lead to this appropriate format are of concern to data processing. Note that data processing does not necessarily include application of modern computer techniques (see Appendix A).

Data reduction. The process of transforming the initial representation of a spectrometer output into a form which is amenable to interpretation; for example, a bar graph or a table of ion currents (see Appendix A).

Data system. The components used to record and process information during the analysis of a sample are part of the data system. This may include electronic or other control devices, and recording storage and data manipulation devices (see Appendix A).

Detection of ions. In mass spectroscopy this concerns the observation of the arrival of particular ionic species at a detector under conditions that preclude or minimize ambiguities due to interferences. Ions may be detected by photographic or suitable electrical means (see Section VII).

Electric sector. An arrangement of two conducting sheets forming a capacitor and giving a radial electrostatic field which is used to deflect and focus ion beams of different energies. The capacitor may, for example, be cylindrical, spherical or toroidal.

m/z . This abbreviation is used to denote the dimensionless quantity formed by dividing the mass number of an ion by its charge number. It has long been called the mass-to-charge ratio although m is not the ionic mass nor is z a multiple of the elementary (electronic) charge, e . The abbreviation m/e is, therefore, not recommended. Thus, for example, for the ion $\text{C}_7\text{H}_7^{2+}$, m/z equals 45.5.

Magnetic deflection. The deflection of an ion beam as a result of the motion of the ions in a magnetic field (magnetic sector). Generally the direction of motion of the ions is at right angles to the direction of the magnetic field, and the motion is uniform.

Mass analysis. A process by which a mixture of ionic or neutral species is identified according to the mass-to-charge (m/z) ratios (ions) or their aggregate atomic masses (neutrals). The analysis may be qualitative and/or quantitative.

Mass number (m) (nucleon number). This is the sum of the total numbers of protons and neutrons in an atom, molecule or ion.

Mass spectrograph. An instrument in which beams of ions are separated (analysed) according to the quotient mass/charge, and in which the deflection and intensity of the beams are recorded directly on photographic plate or film.

Double-focusing mass spectrograph. An instrument which uses both direction and velocity focusing, and therefore an ion beam initially diverging in direction and containing ions of different kinetic energies is separated into beams according to the quotient mass/charge, these beams being focused on to a photographic plate or film.

Mass spectrometer. An instrument in which beams of ions are separated (analysed) according to the quotient mass/charge, and in which the ions are measured electrically. [Note: This term should also be used when a scintillation detector is employed.]

Double-focusing mass spectrometer. An instrument which uses both direction and velocity focusing, and therefore an ion beam of a given mass/charge is brought to a focus when the ion beam is initially diverging and contains ions of the same mass and charge with different translational energies. The ion beam is measured electrically.

Dynamic field(s) mass spectrometer. A mass spectrometer in which the separation of a selected ion beam depends essentially on the use of fields, or a field, varying with time. These fields are generally electric.

Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometer. [Sometimes contracted to Fourier transform mass spectrometer (FT-MS)]. A high-frequency mass spectrometer in which the cyclotron motion of ions, having different mass/charge ratios, in a constant magnetic field is excited essentially simultaneously and coherently by a pulse of a radio-frequency electric field applied perpendicular to the magnetic field. The excited cyclotron motion of the ions is subsequently detected on so-called receiver plates as a time domain signal that contains all the cyclotron frequencies that have been excited. Fourier transformation of the time domain signal results in the frequency domain FT-ICR signal which, on the basis of the inverse proportionality between frequency and the mass/charge ratio, can be converted into a mass spectrum. [See also ion cyclotron resonance (ICR) mass spectrometer.]

Ion cyclotron resonance (ICR) mass spectrometer. A high-frequency mass spectrometer in which the ions to be detected, with a selected value of the quotient mass/charge, absorb maximum energy through the effect of a high-frequency electric field and a constant magnetic field perpendicular to the electric field. Maximum energy is gained by the ions which satisfy the cyclotron resonance condition and as a result they are separated from ions of different mass/charge.

Ion trap mass spectrometer. Arrangement in which ions with a desired range of quotients mass/charge are first made to describe stable paths under the effect of a high-frequency electric quadrupole field, and are then separated and presented to a detector by adjusting the field so as to selectively induce path instability according to their respective mass/charge ratios.

Mass spectrometer operating on the linear accelerator principle. A mass spectrometer in which the ions to be separated absorb maximum energy through the effect of alternating electric fields which are parallel to the path of the ions. These ions are then separated from other ions with different mass/charge by an additional electric field.

Prolate trochoidal mass spectrometer. A mass spectrometer in which the ions of different mass/charge are separated by means of crossed electric and magnetic fields in such a way that the selected ions follow a prolate trochoidal path. [Note: The usual term 'cycloidal' used sometimes is incorrect because the path used is not cycloidal. A cycloid is a special case of a trochoid.]

Quadrupole mass analyser. Arrangements in which ions with a desired quotient mass/charge are made to describe a stable path under the effect of a static and a high-frequency electric quadrupole field, and are then detected. Ions with a different mass/charge are separated from the detected ions because of their unstable paths.

Quadrupole ion storage trap (Quistor). Arrangement in which ions with a desired range of quotients mass/charge are trapped by making them describe stable paths under the effect of a static and a high frequency electric quadrupole field.

Single-focusing mass spectrometer. An instrument in which an ion beam with a given value of mass/charge is brought to a focus although the initial directions of the ions diverge.

Static fields mass spectrometer. An instrument which can separate selected ion beams with fields which do not vary with time. The fields are generally both electric and magnetic.

Tandem mass spectrometer. An arrangement in which ions are subjected to two or more sequential stages of analysis (which may be separated spatially or temporally) according to the quotient mass/charge. A hybrid mass spectrometer is an instrument which combines analysers of different types, e.g. magnetic plus electric sector combined with quadrupole. The study of ions involving two stages of mass analysis has been termed mass spectrometry/mass spectrometry.

Time-of-flight mass spectrometer. An arrangement using the fact that ions of different mass/charge need different times to travel through a certain distance in a field-free region after they have all been initially given the same translational energy.

Mass spectrometry. The branch of science dealing with all aspects of mass spectrometers and the results obtained with these instruments.

Mass spectroscopy. A term (now essentially obsolete) which may refer to either a mass spectrometer or a mass spectrograph.

Mass spectroscopy. The study of systems by causing the formation of gaseous ions, with or without fragmentation which are then characterized by their mass-to-charge ratios and relative abundances.

Mattauch-Herzog geometry. An arrangement for a double-focusing mass spectrograph in which a deflection of $\pi/(4\sqrt{2})$ radians in a radial electrostatic field is followed by a magnetic deflection of $\pi/2$ radians.

Nier-Johnson geometry. An arrangement for a double-focusing mass spectrometer in which a deflection of $\pi/2$ radians in a radial electrostatic field analyser is followed by a magnetic deflection of $\pi/3$ radians. The electrostatic analyser uses a symmetrical object-image arrangement and the magnetic analyser is used asymmetrically.

π/n Radian ($180^\circ/n$) magnetic sector. An arrangement in which an ion beam is deflected magnetically through π/n radians, where $n > 1$.

Sample introduction. This refers to the manner in which a material which is to be subjected to analysis is placed in the ion source of a mass spectrometer before and/or during such an analysis (see Section VI).

Scanning method. This term refers to the sequence of control over operating parameters of a mass spectrometer that results in a spectrum of masses, velocities, momenta or energies (see Section V).

Transmission. The ratio of the number of ions leaving a region of a mass spectrometer to the number entering that region.

Vacuum system. Those components used to lower the pressure within a mass spectrometer are all parts of the vacuum system. This includes not only the various pumping components but also valves, gauges and associated electronic or other control devices, the chamber in which ions are formed and detected, and the vacuum envelope (see Appendix B).

III. IONIZATION NOMENCLATURE

Appearance energy. This is the minimum energy which must be imparted to an atom, molecule or molecular moiety in order to produce a specified ion. [Note: The use of the term appearance potential is not recommended.]

Electron affinity. The electron affinity of a species M is defined as the minimum energy required for the process $M^{\cdot-} \rightarrow M + e$ where M and $M^{\cdot-}$ are in their ground rotational, vibrational and electronic states and the electron has zero kinetic and potential energy.

Electron attachment. A resonance process whereby an external electron is incorporated into an atomic or molecular orbital of an atom or molecule.

Electron energy. The potential difference through which electrons are accelerated before they are used to bring about electron ionization.

Field desorption. This term is used to describe the formation of ions in the gas phase from a material deposited on a solid surface (known as an 'emitter') in the presence of a high electrical field. 'Field desorption' is an ambiguous term because it implies that the electric field desorbs a material as an ion from some kind of emitter on which the material is deposited. There is growing evidence that some of the ions formed are due to thermal ionization and some to field ionization of vapour evaporated from material on the emitter. Because there is generally little or no ionization unless the emitter is heated by an electric current, 'field desorption' is a misnomer. The term is however firmly implanted in the literature and most users understand what is going on regardless of the implications of the term. In addition, no better simple term has been suggested to take its place and so, reluctantly, it is recommended that it be retained.

Ionic dissociation. A decomposition of an ion into another ion of lower mass and one or more neutral species.

Ionization. A process which produces an ion from a neutral atom or molecule.

Adiabatic ionization. A process whereby an electron is either removed from or added to the atom or molecule producing an ion in its ground state.

Associative ionization (see also chemi-ionization). Occurs when two excited gaseous atoms or molecular moieties interact and the sum of their internal energies is sufficient to produce a single, additive ionic product.

Atmospheric pressure ionization. An ambiguous term; in essence, it is used to describe chemical ionization at atmospheric pressure. It is recommended that use of the term should be discontinued.

Auto-ionization. Occurs when an internally supra-excited atom or molecular moiety loses an electron spontaneously without further interaction with an energy source. (The state of the atom or molecular moiety is known as a pre-ionization state.)

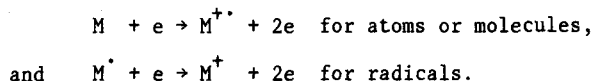
Charge exchange (charge transfer) ionization. Occurs when an ion/atom or ion/molecule reaction takes place in which the charge on the ion is transferred to the neutral species without any dissociation of either.

Chemical ionization. Concerns the process whereby new ionized species are formed when gaseous molecules interact with ions. The process may involve transfer of an electron, proton or other charged species between the reactants. When a positive ion results from chemical ionization, the term may be used without qualification. When a negative ion is involved, the term negative ion chemical ionization should be used; note that negative ion formation by attachment of a free electron does not fall within this definition (see Electron attachment). [Note: Chemical ionization and chemi-ionization are two terms which should not be used interchangeably.]

Chemi-ionization. Refers to a process whereby gaseous molecules are ionized when they interact with other internally excited gaseous molecules or molecular moieties (see also associative ionization). [Note: Chemi-ionization and chemical ionization are two terms which should not be used interchangeably.]

Dissociative ionization. An ionization process in which a gaseous molecule decomposes to form products, one of which is an ion.

Electron ionization. This is the term used to describe ionization of any species by electrons. The process may, for example, be written†



The term 'electron impact' should not be used (see also photo-ionization).

Fast atom bombardment ionization. This term is used to describe ionization of any species by causing interaction of the sample (which may be dissolved in a solvent matrix) and a beam of neutral atoms having high translational energy (see also secondary ionization).

† See Radical ion for a note concerning the symbolic representation of radical ions.

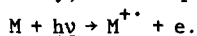
Field ionization. This term relates to the removal of electrons from any species by interaction with a high electrical field (see also field desorption).

Laser ionization occurs when a sample is irradiated with a laser beam. In the irradiation of gaseous samples, ionization occurs via a single- or multi-photon process. In the case of solid samples, ionization occurs via a thermal process.

Multi-photon ionization. Occurs when an atom or molecule and their concomitant ions have energy states whereby the energy in two or more photons is absorbed.

Penning ionization. Occurs through the interaction of two or more neutral gaseous species at least one of which is internally excited.

Photo-ionization. This is the term generally used to describe ionization of any species by photons. The process may, for example, be written



[Note: Electrons and photons do not "impact" molecules or atoms. They interact with them in ways that result in various electronic excitations including ionization. For this reason it is recommended that the terms 'electron impact' and 'photon impact' not be used.]

Plasma desorption ionization (or fission fragment ionization). This term is used to describe the ionization of any species by interacting it with heavy particles (which may be ions or neutral atoms) formed as a result of the fission of a suitable nuclide adjacent to a target supporting the sample.

Secondary ionization. This term is used to describe the process in which ions are ejected from a sample surface (which may be a solid or a substrate dissolved in a solvent matrix) as a result of bombardment by a primary beam of atoms or ions.

Spark (source) ionization. Occurs when a solid sample is vapourized and partially ionized by an intermittent electric discharge. Further ionization occurs in the discharge when gaseous atoms and small molecular moieties interact with energetic electrons in the intermittent discharge. It is recommended that the word 'source' be dropped from this term.

Surface ionization. Takes place when an atom or molecule is ionized when it interacts with a solid surface. Ionization occurs only when the work function of the surface, the temperature of the surface, and the ionization energy of the atom or molecule have an appropriate relationship.

Thermal ionization. Takes place when an atom or molecule interacts with a heated surface or is in a gaseous environment at high temperatures. [Examples of the latter may be a capillary arc plasma, a microwave plasma, or an inductively coupled plasma.]

Vertical ionization. This is a process whereby an electron is removed from a molecule in its ground or an excited state so rapidly that a positive ion is produced without change in the positions or momenta of the atoms. The resultant ion is often in an excited state.

Ionization cross section. This is a measure of the probability that a given ionization process will occur when an atom or molecule interacts with an electron or a photon.

Ionization efficiency is the ratio of the number of ions formed to the number of electrons or photons used.

Ionization efficiency curve shows the number of ions produced as a function of the energy of the electrons or photons used to produce ionization.

Ionization energy. This is the minimum energy of excitation of an atom, molecule or molecular moiety required to remove an electron in order to produce a positive ion. [Note: the use of the term ionization potential is not recommended.]

Ion-pair formation. Involves an ionization process in which a positive fragment ion and a negative fragment ion are among the products.

Proton affinity. The proton affinity of a species M is defined as the negative of the enthalpy change for the reaction $M + H^{+} \rightarrow MH^{+}$.

IV. TYPES OF IONS

Adduct ion. An ion formed by interaction of two species, usually an ion and a molecule, and often within the ion source, to form an ion containing all the constituent atoms of one species as well as an additional atom or atoms.

Cluster ion. An ion formed by the combination of two or more ions or atoms or molecules of a chemical species often in association with a second species. For example, $[(H_2O)_n H]^+$ is a cluster ion.

Daughter ion. An electrically charged product of reaction of a particular parent ion. In general such ions have a direct relationship to a particular precursor ion and indeed may relate to a unique state of the precursor ion. The reaction need not necessarily involve fragmentation. It could, for example, involve a change in the number of charges carried. Thus, all fragment ions are daughter ions, but not all daughter ions are necessarily fragment ions.

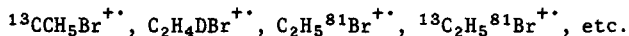
Dimeric ion. An ion formed either when a chemical species exists in the vapour as a dimer and can be detected as such, or when a molecular ion can attach to a neutral molecule within the ion source to form an ion such as $[M_2]^+$ where M represents the molecule.

Even-electron ion. An ion containing no unpaired electrons, for example CH_3^+ in its ground state.

Fragment ion. An electrically charged dissociation product of an ionic fragmentation. Such an ion may dissociate further to form other electrically charged molecular or atomic moieties of successively lower formula weight (see also daughter ion).

Isotopic ion. Any ion containing one or more of the less abundant naturally occurring isotopes of the elements that make up its structure, e.g., CH_2D^+ .

Isotopic molecular ion. A molecular ion containing one or more of the less abundant naturally occurring isotopes of the atoms that make up the molecular structure. Thus, for ethyl bromide there exist isotopic molecular ions such as



Isotopically enriched ions. When the abundance of a particular nuclide is increased above the level at which it occurs in nature and is incorporated in a molecule, the term "isotopically enriched ion" is used to describe any ion enriched in the isotope.

Metastable ion. An ion which is formed with sufficient excitation to dissociate spontaneously during its flight from the ion source to the detector.

Molecular ion. An ion formed by the removal from (positive ions) or addition to (negative ions) a molecule of one or more electrons without fragmentation of the molecular structure. The mass of this ion corresponds to the sum of the masses of the most abundant naturally occurring isotopes of the various atoms that make up the molecule (with a correction for the masses of the electron(s) lost or gained). For example, the mass of the molecular ion of ethyl bromide $C_2H_5^{79}Br$ will be 2×12 plus 5×1.0078246 plus 78.91839 minus the mass of the electron (m_e). This is equal to $107.95751 u - m_e$, u being the unified atomic mass unit based on the standard that the mass of the isotope $^{12}C = 12 u$ exactly.

Negative ion. An atom, radical, molecule or molecular moiety in the vapour phase which has gained one or more electrons thereby acquiring an electrically negative charge. The use of the term anion as an alternative is not recommended because of its connotations in solution chemistry.

Odd-electron ion. This term is synonymous with radical ion.

Parent ion. An electrically charged molecular moiety which may dissociate to form fragments, one or more of which may be electrically charged, and one or more neutral species. A parent ion may be a molecular ion or an electrically charged fragment of a molecular ion.

Positive ion. This is an atom, radical, molecule or molecular moiety which has lost one or more electrons thereby attaining an electrically positive charge. The use of the term cation as an alternative is not recommended (see negative ion). The use of mass ion is not recommended.

Precursor ion. This term is synonymous with parent ion.

Principal ion. This is defined as a molecular or fragment ion which is made up of the most abundant isotopes of each of its atomic constituents. In the case of compounds that have been artificially isotopically enriched in one or more positions such as $\text{CH}_3^{13}\text{CH}_3$ or CH_2D_2 the principal ion may be defined by treating the heavy isotopes as new atomic species. Thus, in the above two examples, the principal ions would be of masses 31 and 18, respectively.

Product ion. This term is synonymous with daughter ion.

Protonated molecule. An ion formed by interaction of a molecule with a proton abstracted from an ion, as often occurs in chemical ionization according to the reaction: $\text{M} + \text{XH}^+ \rightarrow \text{MH}^+ + \text{X}$. The symbolism $[\text{M}+\text{H}]^+$ may also be used to represent the protonated molecule. [Note: The widely used term 'protonated molecular ion' to describe the MH^+ ion is not recommended. It suggests an association product of a proton with a molecular ion.]

Quasi-molecular ion. A term used to represent a protonated molecule or an ion formed from a molecular ion by loss of a hydrogen atom. [Note: The use of the term 'pseudo-molecular ion' is not recommended.]

Radical ion. This is an ion containing an unpaired electron, which is thus both an ion and a radical. In the mass spectroscopy literature the presence of the unpaired electron is normally denoted by placing a superscript dot alongside and following the superscript symbol for the charge, e.g. $\text{C}_2\text{Hg}^{\cdot+}$ and $\text{SF}_6^{\cdot-}$. An alternative form listed in the IUPAC Compendium of Chemical Terminology (1987) and used in the inorganic and organic chemistry literature is that a radical ion be represented as, for example, $\text{X}^{\cdot+}$, with the charge symbol following the dot.

Representations of the type $\text{X}^{\dagger+}$ were also recommended in the Compendium, if typography allowed. This format is now discouraged because of the difficulty of extending it to ions bearing more than one charge and/or more than one unpaired electron. It is essential that such species be symbolized unambiguously, and the styles $\text{X}^{(2+)(2\cdot)}$ or $\text{X}^{(2\cdot)(2+)}$ are recommended.

Rearrangement ion. An electrically charged species, involving a molecular or parent ion, in which atoms or groups of atoms have transferred from one portion of a molecule or molecular moiety to another during the ionization fragmentation processes.

Singly-, doubly-, triply- etc. charged ion. These terms are used to describe an atom, molecule or molecular moiety which has gained or lost respectively one, two, three or more electrons. The term multiply-charged ion is used to refer to ions that have gained or lost more than one electron where the number of electrons lost or gained is not designated.

Stable ion. An ion which is not sufficiently excited to dissociate spontaneously into a daughter ion and associated neutral fragment(s) or to react further in any other way within the time scale of the experiment, e.g. until hitting the detector.

Unstable ion. An ion which is sufficiently excited to dissociate within the ion source.

V. SCANNING OF SPECTRA

(a) General

Accelerating voltage (high voltage, V) scan. This is an alternative method of producing a momentum (mass) spectrum in magnetic deflection instruments by varying the accelerating voltage. This scan can also be used, in conjunction with a fixed radial electric field, to produce an ion kinetic energy spectrum.

Ion kinetic energy spectrum. A spectrum obtained when a beam of ions is separated according to the translational energy-to-charge ratios of the ionic species contained within it. [Note: A radial electric field (E) achieves separation of the various ionic species in this way.]

Magnetic field (B) scan. The usual method of producing a momentum (mass) spectrum in instruments is by varying the strength of the magnetic field.

Mass spectrum. A spectrum which is obtained when a beam of ions is separated according to the mass-to-charge (m/z) ratios of the ionic species contained within it.

Momentum spectrum. A spectrum which is obtained when a beam of ions is separated according to the momentum-to-charge ratios of the ionic species contained within it. [Note: A sector magnetic field achieves separation of the various ionic species in this way. If the ion beam is homogeneous in translational energy, as is the case with sector instruments, separation according to the m/z ratios is also achieved and a mass spectrum is obtained.]

Selected ion monitoring. This term is used to describe the operation of the mass spectrometer in which the intensities of several specific ion beams are recorded rather than the entire mass spectrum. An alternative recommended term is multiple ion (peak) monitoring. [Note: The use of the terms multiple ion detection and mass fragmentography are not recommended. This is because, in the case of the former, it is the monitoring of several peaks which should be emphasized rather than the detection of different ions, and in the case of the latter it is often not fragments that are being monitored but peaks from molecular ions.]

(b) Tandem analyser instruments

(i) General

Fixed neutral loss (gain) scan. A scan which determines, in a single experiment, all the parent ion mass-to-charge ratios which react to the loss or gain of a selected neutral mass.

Fixed neutral loss (gain) spectrum. A spectrum obtained when data are acquired that determine all the parent ion mass-to-charge ratios that react by the loss (gain) of a selected neutral mass.

Fixed precursor ion scan. A scan which determines, in a single experiment, all the daughter ion mass-to-charge ratios that are produced by the reaction of a selected parent ion mass-to-charge ratio (sometimes called a 'daughter ion scan').

Fixed precursor ion spectrum. A spectrum obtained when data are acquired that determine all the daughter ion mass-to-charge ratios produced by the reaction of a selected parent ion mass-to-charge ratio.

Fixed product ion scan. A scan which determines, in a single experiment, all the parent ion mass-to-charge ratios that react to produce a selected daughter ion mass-to-charge ratio (sometimes called a 'parent ion scan').

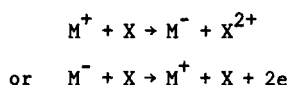
Fixed product ion spectrum. A spectrum obtained when data are acquired that determine all the parent ion mass-to-charge ratios that react to produce a selected daughter ion mass-to-charge ratio.

Linked scan. A scan, in an instrument comprising two or more analysers, in which two or more of the analyser fields are scanned simultaneously so as to preserve a pre-determined relationship between parameters characterising these fields. Often, these parameters are the field strengths, but they may also be the frequencies in the case of analysers in which alternating fields are employed.

(ii) Magnetic sector instruments

NOTE: Special terms have been used to describe particular methods of scanning. For example, one of these has been variously described as 'the Barber-Elliott method', 'metastable defocusing', 'metastable refocusing' and 'scanning in the metastable mode'. All of these expressions are misleading and undesirable and it is recommended that, in all cases, the scanning method should be described by detailing exactly how the scan has been carried out. The above would be described as 'scanning the accelerating voltage with fixed electric sector voltage and fixed magnetic field'. In the definitions which follow, B refers to the magnetic flux density within a magnetic sector, E to the field intensity within an electric sector, and V to the accelerating voltage potential to which the ions have been subjected.

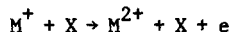
Charge inversion mass spectrum. Charge inversion processes of the types:



respectively, occurring in a collision cell (containing a gas, X) located in a field-free region preceding a magnetic and electric sector combination placed in either order, may be detected as follows.

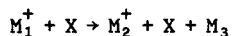
If the instrument slits are wide, and if the connections to the two sectors, appropriate to transmission of either positive or negative main-beam ions, are simply reversed, the negative or positive product ions of the two processes, respectively, will be transmitted. If the magnetic field is scanned, a spectrum of such product ions will be obtained, and this spectrum is called a charge-inversion mass spectrum. These spectra are sometimes referred to as $-E$ and $+E$ spectra, respectively. [Note: The terms ' $2E$, $E/2$, $-E$ or $+E$ mass spectrum' should not be used without prior explanation of the meaning $2E$, E , $+E$ or $-E$.]

$E/2$ Mass spectrum. Processes of the charge-stripping type:



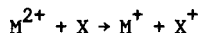
occurring in a collision cell (containing a gas, X) located in a field-free region preceding a magnetic and electric sector combination placed in either order, may be detected as follows.

If the instrument slits are wide and if the electric sector field E is set to half the value required to transmit the main ion-beam, the only ions to be transmitted will be those with a kinetic energy/charge ratio half, or almost exactly half, that of the main ion-beam. The product ions of the charge-stripping process fulfil this condition. If the magnetic field B is scanned, a mass spectrum of such doubly-charged product ions, and thus of their singly-charged precursors, is obtained. Such a spectrum is called an $E/2$ mass spectrum. [Note: Interference from product ions from processes of the type:



where m_1 , m_2 , and $(m_1 - m_2)$ are the masses of M_1^+ , M_2^+ , and M_3 , respectively, and where $m_2 = 0.5 m_1$, can arise in $E/2$ mass spectra.]

$2E$ Mass spectrum. Processes of the partial charge-transfer type:



occurring in a collision cell (containing a gas, X) located in a field-free region preceding a magnetic and electric sector combination placed in either order, may be detected as follows.

If the instrument slits are wide, and if the electric sector field E is set to twice the value required to transmit the main ion-beam, the only ions to be transmitted will be those with a kinetic energy/charge ratio twice, or almost exactly twice, that of the main ion-beam. The product ions of the process shown fulfil this condition. If the magnetic field B is scanned, the mass spectrum of such singly-charged product ions, and thus of their doubly-charged precursors, is obtained. Such a spectrum is called a $2E$ mass spectrum.

Fixed neutral loss (gain) scan:

Linked scan at constant $B[1-(E/E_0)]^{1/2}/E$. A linked scan at constant $B[1-(E/E_0)]^{1/2}/E$ may be performed with a sector instrument incorporating at least one electric sector plus one magnetic sector. It involves holding the accelerating voltage fixed, and scanning the magnetic field B and electric field E simultaneously, so as to maintain the quantity $B[1-(E/E_0)]^{1/2}/E$ at a constant value. This constant value is equal to B_3/E_0 , where E_0 and B_3 are respectively the electric sector field and magnetic sector field required to transmit M_3^+ ions in the main ion-beam; m_3 represents the mass of $(m_1 - m_2)$ of the selected neutral fragment M_3 whose precursor ion spectrum is required. The fragmentation reactions so observed occur in a field-free region traversed before the two sectors scanned in this way. [Note: This term should not be used without prior explanation of the meanings of B , E and E_0 . The term ' $B[1-(E/E_0)]^{1/2}/E$ linked scan' is not recommended.]

Fixed precursor ion scans:

Linked scan at constant B/E . A linked scan at constant B/E may be performed with a sector instrument incorporating at least one magnetic sector plus one electric sector. It involves scanning the magnetic sector field-strength B and the electric sector field-strength E simultaneously, holding the accelerating voltage V constant, so as to maintain the ratio B/E at a constant value. This constant value is determined by the ratio of the two field strengths which transmit main-beam ions of predetermined mass-to-charge ratio; these preselected main-beam ions are the precursor ions whose fragment-ion spectrum is required. The fragmentation reactions so observed occur in a field-free region traversed before the two sectors scanned in this way. [Notes: This term should not be used without prior explanation of the meanings of B and E . The term ' B/E linked scan' is not recommended. It may suggest that the ratio B/E varies during the scan.]

Linked scan at constant E^2/V . A linked scan at constant E^2/V may be performed with a sector instrument incorporating at least one electric sector plus one magnetic sector. It involves scanning the electric sector field E and the accelerating voltage V simultaneously, so as to maintain the ratio E^2/V at a constant value, equal to the value of this ratio which transmits the main beam of ions through the electric sector. The magnetic sector field is set at a fixed value such that main-beam ions of a pre-determined mass to charge ratio are transmitted by the magnet; these preselected main-beam ions are the precursor ions whose fragment-ion spectrum is required. The fragmentation reactions so observed occur in a field-free region traversed before the two sectors scanned in this way. [Notes: This term should not be used without prior explanation of the meanings of E and V . The term ' E^2/V linked scan' is not recommended.]

Mass selection followed by ion kinetic energy analysis. If a precursor (parent) ion is selected, for example by a magnetic sector, all product ions formed from it in the field-free region between the magnetic sector and a following electric sector can be identified by scanning an ion kinetic energy spectrum.

Fixed product ion scan:

Linked scan at constant B^2/E . A linked scan at constant B^2/E may be performed with a sector instrument incorporating at least one electric sector plus one magnetic sector. It involves holding the accelerating voltage fixed, and scanning the magnetic field B and the electric field E simultaneously so as to maintain the ratio B^2/E at a constant value. This constant value corresponds to the ratio of the two fields which transmit main-beam ions of predetermined mass to charge ratio; these preselected main-beam ions are the fragment ions whose precursor-ion spectrum is required. The fragmentation reactions thus observed occur in a field-free region traversed before the two sectors scanned in this way. [Notes: This term should not be used without prior explanation of the meanings of B and E . The term ' B^2/E linked scan' is not recommended.]

Note: The above definitions of linked scans are merely examples of the types of linked scan that might be used. Any other linked scans should be defined in a similar manner.

VI. SAMPLE INTRODUCTION AND SENSITIVITY

Sensitivity. Two different measures of sensitivity are recommended. The first, which is suitable for relatively involatile materials as well as gases, depends upon the observed change in ion current for a particular amount or change of flow rate of sample through the ion source. The recommended unit is coulomb per microgram ($C \mu g^{-1}$). A second method of stating sensitivity, that is most suitable for gases, depends upon the change of ion current related to the change of partial pressure of the sample in the ion source. The recommended unit is ampere per pascal ($A Pa^{-1}$).

It is important that the relevant experimental conditions corresponding to sensitivity measurement should always be stated. These include in a typical case details of the instrument type, bombarding electron current, slit dimensions, angular collimation, gain of the multiplier detector, scan speed and whether the measured signal corresponds to a single mass peak or to the ion beam integrated over all masses. Some indication of the time involved in the determination should be given, e.g., counting time or band width. [Note: The sensitivity should be differentiated from the detection limit. See Section VII.]

VII. ION DETECTION

Detection limit. The detection limit of an instrument should be differentiated from the sensitivity (see Section VI). The detection limit reflects the smallest amount of sample or the lowest partial pressure that gives a signal that can be distinguished from the background noise. It is important to specify the experimental conditions used and also to give the value of signal-to-noise ratio corresponding to the detection limit. It is recommended that a signal-to-noise ratio of 2:1 be used.

Faraday cup (or cylinder) collector. A hollow collector, open at one end and closed at the other, used to collect beams of ions.

Photographic plate recording. The recording of ion beams by allowing them to strike a photographic plate which is subsequently developed.

Secondary electron multiplier. A device to multiply current in an electron beam (or in a photon or particle beam by first conversion to electrons) by incidence of accelerated electrons upon the surface of an electrode which yields a number of secondary electrons greater than the number of incident electrons. These electrons are then accelerated to another electrode (or another part of the same electrode), which in turn emits further secondary electrons so that the process can be repeated.

VIII. SIGNAL RECORDING

Note: It is recommended that one should refer to the abundance of an ion, to the intensity of an ion beam, and to the height or area of a peak.

Abundance sensitivity. The ratio of the maximum ion current recorded at a mass m to the ion current arising from the same species recorded at an adjacent mass ($m \pm 1$).

Background mass spectrum. The mass spectrum observed when no sample is intentionally introduced into the mass spectrometer or spectrograph.

Base peak. The peak in a mass spectrum corresponding to the separated ion beam which has the greatest intensity. This term may be applied to the spectra of pure substances or mixtures.

Intensity relative to base peak. The ratio of intensity of a separated ion beam to the intensity of the separated ion beam which has the greatest intensity. This ratio is generally equated to the normalized ratio of the heights of the respective peaks in the mass spectrum, with the height of the base peak being taken as 100.

Peak height. The height of a recorded peak in a mass spectrum.

Resolution: energy. By analogy with the peak width definition for mass resolution, a peak showing the number of ions as a function of their translational energy should be used to give a value for the energy resolution.

Resolution: 10 per cent valley definition. Let two peaks of equal height in a mass spectrum at masses m and $m - \Delta m$ be separated by a valley which at its lowest point is just 10 per cent of the height of either peak. For similar peaks at a mass exceeding m , let the height of the valley at its lowest point be more (by any amount) than ten per cent of either peak height. Then the resolution (10 per cent valley definition) is $m/\Delta m$. It is usually a function of m . The ratio $m/\Delta m$ should be given for a number of values of m . [Note: see also peak width definition.]

Resolution: peak width definition. For a single peak made up of singly charged ions at mass m in a mass spectrum, the resolution may be expressed as $m/\Delta m$, where Δm is the width of the peak at a height which is a specified fraction of the maximum peak height. It is recommended that one of three values 50%, 5% or 0.5% should always be used. [Note: For an isolated symmetrical peak recorded with a system which is linear in the range between 5% and 10% levels of the peak, the 5% peak width definition is technically equivalent to the 10% valley definition. A common standard is the definition of resolution based upon Δm being Full Width of the peak at Half its Maximum height, sometimes abbreviated 'FWHM'. This acronym should preferably be defined the first time it is used.]

Resolving power (mass). The ability to distinguish between ions differing in the quotient mass/charge by a small increment. It may be characterized by giving the peak width, measured in mass units, expressed as a function of mass, for at least two points on the peak, specifically for fifty per cent and for five per cent of the maximum peak height.

Total ion current.

- (a) After mass analysis. The sum of all the separate ion currents carried by the different ions contributing to the spectrum (this is sometimes called the reconstructed ion current).
- (b) Before mass analysis. The sum of all the separate ion currents for ions of the same sign before mass analysis.

IX. ION/MOLECULE REACTIONS

Collisional activation, collisionally activated dissociation. An ion/neutral species process wherein excitation of a projectile ion of high translational energy is brought about by the same mechanism as in collision-induced dissociation. (The ion may decompose subsequently.)

Collisional excitation. An ion/neutral species process wherein there is an increase in the reactant ion's internal energy at the expense of the translational energy of either (or both) of the reacting species. The scattering angle may be large.

Collision-induced dissociation. An ion/neutral species process wherein the projectile ion is dissociated as a result of interaction with a target neutral species. This is brought about by conversion of part of the translation energy of the ion to internal energy in the ion during the collision.

Note: It is recommended that all three of the above terms should be retained.

Collisions

Elastic collision. A collision resulting in elastic scattering.

Inelastic collision. A collision resulting in inelastic scattering.

Ionizing collision. An ion/neutral species interaction in which an electron or electrons are stripped from the ion and/or the neutral species in the collision. Generally, this term has come to be used to describe collisions of fast-moving ions with a neutral species in which the neutral species is ionized with no change in the number of charges carried by the ion. Care should be taken when this term is used to emphasize if charge stripping of the ion has taken place.

Superelastic collision. A collision in which the translational energy of the fast-moving collision partner is increased.

Elastic scattering. An ion/neutral species interaction wherein the direction of motion of the ion is changed, but there is no change in the total translational energy or internal energy of the collision partners.

Impact parameter. The distance of closest approach of two particles if they had continued in their original direction of motion at their original speeds.

Inelastic scattering. An ion/neutral species interaction wherein the direction of motion of the ion is changed, and the total translational and/or internal energy of the collision partners are also changed.

Interaction distance. The farthest distance of approach of two particles at which it is discernible that they will not pass at the impact parameter.

Ion energy loss spectra. Spectra that show the loss of translational energy of ions involved in ion/neutral species reactions.

Reactions

Association reaction (associative combination). The reaction of a (slow moving) ion with a neutral species wherein the reactants combine to form a single ionized species.

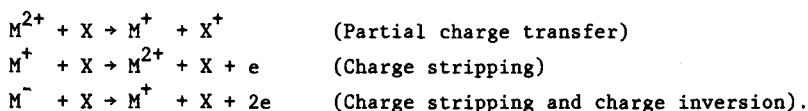
Charge exchange reaction. This term is synonymous with charge transfer reaction.

Charge inversion reaction. An ion/neutral species reaction wherein the charge on the reactant ion is reversed in sign.

Charge permutation reaction. This is a general term to describe an ion/neutral species reaction whereas there is a change in the magnitude and/or sign of the charges on the reactant.

Charge stripping reaction. An ion/neutral species reaction wherein the charge on the reactant ion is made more positive.

Charge transfer reaction. An ion/neutral species reaction wherein the total charge on the reactant ion is transferred initially to the reactant neutral species so that the reactant ion becomes a neutral entity. [Note: Considering some of the possible reactions of ions M^{2+} , M^+ and M^- with a neutral species X, these would be categorized on the basis of the above definitions as follows:



All are ion/neutral species reactions and also charge permutation reactions.]

Ion/molecule reaction. An ion/neutral species reaction in which the neutral species is a molecule. [Note: The use of ion-molecule reaction is not recommended; the hyphen suggests a reaction of a species that is both an ion and a molecule and is not the intended meaning.]

Ion/neutral species reaction. A process wherein a charged species interacts with a neutral reactant to produce either chemically different species or changes in the internal energy of one or both of the reactants. [Note: The contrasting expression ion/neutral reaction is not ideal, simply because the word neutral is not a noun. However, any alternatives such as ion/neutral species reaction are so clumsy as to mitigate against their general acceptance.]

Ion/neutral species exchange reaction. In this reaction an association reaction is accompanied by the subsequent or simultaneous liberation of a different neutral species as product.

Partial charge exchange reaction. This term is synonymous with partial charge transfer reaction.

Partial charge transfer reaction. An ion/neutral species reaction wherein the charge on a multiply-charged reactant ion is reduced.

Translational spectroscopy. A technique to investigate the distribution of the velocity of product ions from reactions of ions and neutral species.

X. ISOTOPE MASS SPECTROSCOPY

See Section IV ('Types of Ions') for definitions of the terms isotopic ion, isotopic molecular ion, isotopically enriched ions, principal ion.

Deuteration. This term is used to represent replacement of protium by deuterium. The use of the word deuteriated is also acceptable.

Isotopic scrambling. This term is only to be used to denote the complete random mixing of isotopes between specified positions in an ion of neutral species. [Note: The term partial scrambling has no meaning and should not be used. One can, however, talk about partial or incomplete isotopic or atomic exchange over specified positions in molecules.]

Monoisotopic mass spectrum. This is a spectrum containing only ions made up of the principal isotopes of atoms making up the original molecule.

XI. SYMBOLISM

$A(X^+)$: appearance energy for the production of a specified ion X^+ .

$I(M)$: ionization energy of an even-electron molecule M (see below).

m/z : mass-to-charge ratio.

15% rel. int.: a separated ion beam whose intensity is 15% of the intensity of the most intense separated ion beam (generally determined from the relative heights of the corresponding mass spectral peaks).

15% Σ_{40} : 15% of total ion current encompassing the range from m/z 40 to the highest value of m/z observed in the mass spectrum.

u: unified atomic mass (1/12 of the mass of an atom of nuclide ^{12}C).

eV: electronvolt.

M_r : relative molecular mass of a substance (also called 'molecular weight').

The superscript symbol $^+$ should be used to represent a positive charge.

The superscript symbol $^-$ should be used to represent a negative charge.

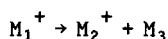
The superscript symbol \cdot should be used to represent an unpaired electron. When used in combination, the above symbols should be written $+\cdot$ and $-\cdot$. The use of \ddagger and $\bar{\cdot}$ is not recommended (see also Radical ion).

The symbol M should be used exclusively to represent an even-electron molecule and M' an odd-electron molecule. The symbol $M^{+\cdot}$ represents the odd-electron ion formed from an even electron molecule by the removal of a single electron (the molecular ion).

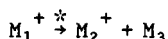
The symbols m_1 , m_2 , m_3 , etc., may be used to represent the mass numbers of neutral species. Ions carrying a single positive or negative charge and having a mass number m_1 may be represented by M_1^+ or M_1^- or by $M_1^{+\cdot}$ or $M_1^{-\cdot}$, if it is desired to emphasize the presence of an odd electron. Ions carrying 2, 3 or 4 charges may be represented as M_1^{2+} , M_1^{3+} , M_1^{4+} , etc., or M_1^{2-} , M_1^{3-} , M_1^{4-} , etc. Alternative symbolism, for example, M_1^{++} , M_1^{+2} , M_1^{--} , M_1^{-3} , is not recommended.

The number of charges carried by an ion should be indicated by the symbol z . The ratio of the mass number of an ion to the number of charges carried (commonly referred to as the mass-to-charge ratio) should be written m_1/z , m_2/z , etc. m/e should not be used to indicate this ratio, e (italic) being reserved for the charge upon the electron and e (Roman) for the electron itself when it appears in an equation.

A fragmentation reaction may be written:



The decomposition of a metastable ion of mass-to-charge ratio m_1/z_1 into an ion of mass-to-charge ratio m_2/z_2 after electric acceleration of the metastable ion and before magnetic deflection gives rise to a peak in the mass spectrum at an apparent mass, $m_2^2 z_1 / (m_1 z_2^2)$. The symbol m^* should be used to indicate the apparent mass of the product ions giving rise to this peak. Traditionally, the peak itself has been called a metastable peak and this should preferably be expressed as metastable ion peak. It is nevertheless recommended that the former term should be retained. The word metastable should never be used as a noun. Its use as an adjective should be limited to such terms as metastable ion, where it is used correctly, and to the special case of metastable peak discussed above. It should never be used in such terms as metastable reaction, metastable decomposition, metastable studies, etc. It should be clear that the metastable ion is the ion that undergoes fragmentation; it is not detected. When a reaction is written with an asterisk above the arrow as shown:



this means that the reaction has been confirmed by the observation of a metastable peak.

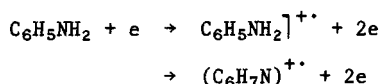
The textual description of such a process may be written as, for example, (m^* , 43 \rightarrow 28, calcd 18.2, obsd 18.3) meaning 'for the fragmentation m/z 43 \rightarrow m/z 28 a metastable peak at m/z 18.3 (calculated 18.2) has been observed'.

Ion structures. Capital letters enclosed in parentheses should be used to represent an ion containing different structural features and the charge should be located outside the parentheses. Thus, one should write, for example, (ABC) $^+$ or (ABC) $^{+\cdot}$ (if it is desired to emphasize that one is dealing with an odd-electron species).

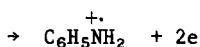
An exception to the above is that an ion may be written, for example, $\overset{\cdot}{A}BC$ or $\overset{\cdot}{A}\overset{\cdot}{B}C$ if it is required to discuss structures in which the charge and odd electron are localized.

When it is required to write the empirical formula of a molecular ion, this may be written in several ways. Thus, for example, the molecular ion of aniline may be written (C₆H₇N) $^{+\cdot}$ or it may be written C₆H₅NH₂ $^{\cdot+}$ to emphasize that one is discussing an ion formed from a molecule with the structure C₆H₅NH₂ by the removal of a single electron, the upper half of a square bracket being used to indicate that the structure of the ion may or may not be the same as that of the molecule from which it was formed. If one wishes to discuss a particular structure in which an odd electron is localized then one can write, for example, C₆H₅NH₂ $^{\cdot}$.

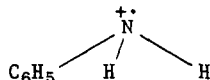
The ionization process, for example, under electron bombardment, may be written:



or (to represent a particular ion structure)

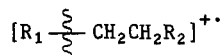


Structural formulae may also be drawn so as to indicate the relative dispositions of the bonds, e.g.,

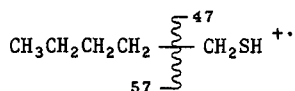


Bond fission. Confusion sometimes arises because of the use of a hyphen or of a dash sign in the symbolism. Thus, $\text{D}(\text{R-X})^+$ has been used to mean the dissociation energy of the bond between R and X while $(\text{X-CH}_2)^+$ might mean the next higher homologue of X^+ or the ion formed from X^+ by removal of a CH_2 group. To overcome some of this confusion, it is recommended that a dash should not be used to indicate a bond, except in a conventional structural formula such as that for the acetone molecular ion. In other cases, the next higher homologue of X^+ should be written $(\text{XCH}_2)^+$, without any dash being used.

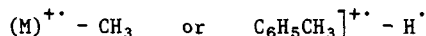
In the event that it is necessary to emphasize that a bond is breaking, then it should be represented by a wavy line between them. Thus we might write



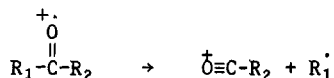
no other bond than the breaking bond being illustrated. When, in addition to indicating fragmentation of the bond, it is necessary to emphasize the mass numbers of the fragments formed, this is done by writing the mass numbers at the top (right-hand fragment) or the bottom (left-hand fragment) as shown





Loss of a particular group should be indicated by the use of a minus sign located outside the parentheses or to the right of the $+\cdot$ sign. Spaces should be left on either side of the minus sign to reduce any confusion as to its meaning. Thus, one would write



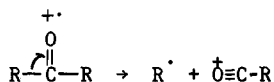
It is recommended that the convention used by Budzikiewicz, Djerassi and Williams ('Mass Spectrometry of Organic Compounds', Holden-Day, Inc., (1967) p. 2) be followed in referring to α -cleavage as 'fission of a bond originating at an atom which is adjacent to the one assumed to bear the charge; the definition of β^- , γ^- , then follows automatically'. The process



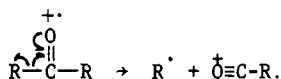
would thus be described as ' α -fission of a ketone with expulsion of a radical R_1^{\cdot} '. The carbon atoms of the radical R_1^{\cdot} are called the α^- , β^- , γ^- , carbons, starting with the atom nearest the functional group.

The symbol  is recommended for indicating the movement of two electrons (heterolysis). The symbol  is recommended for indicating the movement of one electron (homolysis).

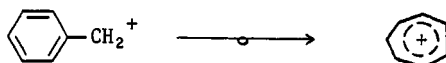
Note: Unless the clarity of presentation might be jeopardized, a 'shorthand' presentation should be used, viz.:



instead of

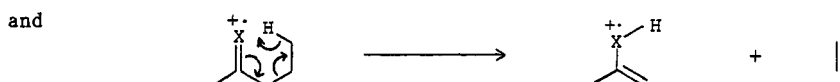
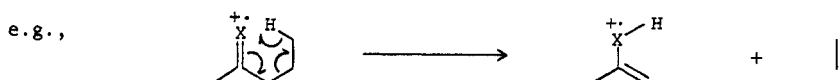


Rearrangement reactions. These may be skeletal, in which case the symbol \rightarrow is employed, e.g.,



or involve the specific transfer of atom(s) within a molecule together with bond fission.

An example of the latter is the McLafferty Rearrangement which is defined as β -cleavage with concomitant specific transfer of a γ -hydrogen atom in a six-membered transition state in mono-unsaturated systems irrespective whether the rearrangement is formulated by a radical or by an ionic mechanism and irrespective with which fragment the charge stays:



APPENDIX A: DATA SYSTEMS

Amplifier bandwidth. The range of signal frequencies over which an amplifier is capable of undistorted or unattenuated transmission. An operational amplifier should transmit DC voltage accurately and the upper (bandwidth) limit is defined as the 3 db point (factor of 2 attenuation). Bandwidth can vary with gain and hence gain-bandwidth product may be a more useful parameter.

Amplifier complex. A number of operational amplifiers arranged for a specific function, connected as a single unit and used as such.

Amplifier noise. This can be of two kinds, white noise which is random signal fluctuations whose power spectrum contains all frequencies equally over a specified bandwidth and pink noise where the frequencies diminish in a specified fashion over a specified range.

Amplifiers

Differential amplifier. An (operational) amplifier which has two inputs of opposite-sense gain polarity with respect to its output. Differential output amplifiers with two opposite-sense outputs also exist.

Operational amplifier. A high gain DC voltage amplifier with high input impedance, low output impedance and the capability of producing a bipolar output from a bipolar input.

Single-ended amplifier. An (operational) amplifier with a single input (or output).

Analogue signal. This is a signal which can be expressed as a continuously variable mathematical function of time or another parameter.

Data acquisition. The process of transforming representations of (spectrometer) signals from their original form into suitable representations, with or without modification.

Data logging. Is a more specific term implying data collection from more than one relatively low frequency source with storage of the collected data for later processing.

Digital signal. This is a signal which represents information in a computer-compatible form as a sequence of (binary) numbers which may describe discrete samples of an analogue signal.

Firmware. Computer programs stored in a semi-permanent form, usually semiconductor memory, and used repeatedly without modification. Firmware can be changed only by exchanging or removing hardware.

Hardware. The term used for the physical components of a computer system.

Hard wired. A preprocessor may be hard wired, that is, capable of performing only certain defined tasks and no others without major physical modification.

Off-line. In this method of data acquisition there is some discontinuity in time and space in the transfer or transformation of the representations.

On-line. In this method of data acquisition there is no discontinuity in time and space in the transfer or transformation of the representations.

Pre-processor. A device in a data acquisition system which performs a significant amount of data reduction, extracting specific information from raw signal representations, in advance of the main processing operation. A preprocessor may constitute the whole of a data acquisition interface, in which case it must also perform the data acquisition task (spectrometer signal to digital representation conversion), or it may specialize solely in data treatment.

Pre-programmed. A preprocessor may be pre-programmed, that is, it can be a general purpose device incorporating specific but readily alterable instructions to perform a particular task.

Real time. In data acquisition in real time the digital representations are generated in step with the time frame of the original experiment.

Signal conditioning. The process of altering the relationship of a transducer (spectrometer) output with respect to time or other parameters (frequency, voltage or current).

Signal processing. The mechanism of analyzing, routing, sampling or changing the representation of a signal.

Software. This term is used to describe computer programs, whether inside or outside a computer, and whether they are machine readable or normally legible.

APPENDIX B: TERMS USED IN VACUUM TECHNOLOGY

(The terms in this section have been contributed, almost entirely, by the American Vacuum Society, to whom grateful acknowledgment is made.)

Accumulation leak detection technique. A leak detection technique in which tracer gas (e.g., helium) enters the part under test and is allowed to accumulate within the part, or within a system containing the part, for a period of time. The part or system is then opened to the leak detector. The system may include the leak detector sensing element.

Adsorption. The process by which gas or vapour is bound on a solid or liquid surface.

Aperture impedance. The additional resistance encountered by gas flowing through a tube with an abrupt reduction in cross-section. For molecular flow, it is the product of the molecular effusion impedance of an orifice with a cross-sectional area A_2 and the aperture correction factor $(1 - A_2/A_1)$, where A_1 is the cross-sectional area of the larger tube and A_2 that of the smaller tube.

Background spectrum. A mass spectrum of residual gas species in a system. It is usually obtained before a sample of interest is introduced and analyzed in order to deduce by subtraction of spectra the true mass spectrum of the sample.

Backing space leak detection technique. A leak detection technique in which the leak detector is connected to the forevacuum side of a pump attached to the vacuum system or element undergoing leak test. A tracer gas is sampled at a higher pressure after compression by the diffusion pump or other type of pump operating at high speed relative to its backing pump.

Backstreaming. The flow of charged and/or neutral particles emanating from a pump and moving counter to the intended flow of the gases being pumped.

Baffle. A series of surfaces placed in the line of gas or vapour flow to prevent linear flow.

Bagging. A jargon term for a leak detection technique in which the part under test is enclosed in a bag (or other enclosure) which is filled with a tracer gas to slightly more than atmospheric pressure. A tracer gas is applied to the entire surface of the part to

determine the total leakage from all leaks in the part.

Collision frequency. The number of molecules or atoms striking a unit area of surface per unit time; also, the number of collisions between the molecules or atoms in a gas per unit volume and unit time. The collision frequency per molecule is equal to the probability per unit time that a molecule will collide with a surface or another molecule.

Collision rate. The collision probability per unit time for an atom or molecule travelling at a specified speed through a gas.

Conductance. The ratio of throughput, under steady-state conservative conditions, to the pressure differential between two specified cross-sections within a pumping system.

Critical inlet pressure. The inlet pressure of a vapour pump above which an abrupt decrease in pumping speed occurs.

Cryosorption pumping. A technique of producing vacuum by physical adsorption of gases on solid adsorbents cooled to low temperatures.

Evaporation. The conversion of a substance from the liquid state into the gaseous state by absorption of energy.

Exhaust port. An opening in a vacuum pump or stage from which gases are ejected either to a succeeding stage or to the atmosphere.

Feedthrough. A device for transmitting electrical current, fluids or mechanical motion through the wall of a vacuum system.

Flange. A (projecting) rim usually in the form of an annulus intended for fastening and sealing one part of the vacuum system to another.

Flow (gas). The motion or passage of a gas. A description of gas flow may be characterized by the Knudsen number into three ranges.

Knudsen flow. The flow of gas through a pump or system under transition flow conditions which are intermediate between viscous flow and molecular flow.

Molecular flow. The flow of gas through a channel under conditions such that the mean free path is much greater than the largest dimension of a transverse section of the channel. At these pressures, the flow characteristics are determined by collisions of the gas molecules with the channel surfaces and flow effects from molecular collisions are insignificant.

Transition flow. The flow of a gas through a channel under conditions that the mean free path is of the same order as the transverse dimensions of the channel. In this pressure range, the flow characteristics are determined by collisions of the gas molecules with surfaces as well as with other gas molecules. Also called Knudsen flow.

Viscous flow. The flow of a gas through a channel under conditions such that the mean free path is very small in comparison with the smallest dimension of a transverse section of the channel. At these pressures the flow characteristics are determined mainly by collisions between the gas molecules, i.e., the viscosity of the gas. The flow may be laminar or turbulent.

Gauges

Bayard-Alpert gauge. A hot-cathode ionization gauge in which a fine wire ion collector is positioned on the axis of a cylindrical grid functioning as the anode. The cathode is mounted outside the grid.

Hot-cathode ionization gauge. An ionization gauge in which pressure is measured in terms of the current of positive ions produced by electrons emitted from a heated cathode.

Knudsen gauge. A vacuum gauge which indicates pressure by responding to the net rate of transfer of momentum by molecules moving between two surfaces maintained at different temperatures and separated by a distance smaller than the mean free path of the gas molecules. Various types of Knudsen gauges differ mainly in the shape and method of suspension of the movable element.

McLeod gauge. A liquid level manometer in which a known volume of the gas, whose pressure is to be measured, is compressed by the movement of a liquid column and confined in a small measurable volume. Corrections need to be made for any appreciable change in gas pressure in the system caused by the movement of the liquid.

Thermal conductivity (Pirani) gauge. A vacuum gauge containing two surfaces at different temperatures between which heat can be transported by gas molecules. Changes in the temperatures, or in the heating power required to maintain constant temperature of one of the surfaces can be correlated with the gas pressure. Thermal conductivity gauges differ in the method of indicating the temperature change. (See: thermocouple gauge.)

Thermistor gauge. A form of thermal conductivity gauge in which the temperature-sensitive elements are made of semiconducting material instead of metal.

Thermocouple gauge. A thermal conductivity gauge which contains a heated filament and a thermocouple for measuring the filament temperature as a function of gas pressure.

Holding time (pump). The time required for the forepressure of an isolated vapour or diffusion pump to reach the limiting forepressure.

Impedance. The reciprocal of conductance.

Incidence rate. The number of molecules striking a unit area of surface per unit time.

Knudsen number. The ratio of the mean free path of a gas molecule to a characteristic dimension of the channel through which gas is flowing. For a cylindrical tube, the diameter is a characteristic dimension.

Leak. A hole or permeable element through which leakage may occur under the action of a pressure difference. This includes a device used to introduce gas into a vacuum system at a controlled rate.

Calibrated leak. A leak which has a known leakage rate for a specific gas under specific conditions.

Capillary leak. A leak having a small cross-section dimension and length many times its cross-section dimension.

Diffusion leakage. A leakage resulting from the temperature-dependent diffusion of a specific gas through a membrane. Examples are the diffusion of hydrogen through palladium and helium through glass or teflon.

Membrane leak. A leak which permits gas flow by permeation through a thin non-porous wall.

Molecular leak. A leak of such a size that the flow through it is predominantly molecular for a given pressure.

Variable leak. A leak with an adjustable leakage rate which can be controlled.

Virtual leak. An apparent leak because of the presence of contaminants which outgas very slowly within a vacuum system.

Viscous leak. A leak of such a size that the flow through it is predominantly viscous for a given pressure.

Leakage (leak) rate. The quantity of gas passing through a leak per unit time (see throughput).

Load (vapour pump). The quantity of gas, not including pump fluid vapour, in mass units, flowing through the pump per unit time. It is also called capacity or mass flow.

Manometer. An instrument for measuring the pressure of gases and vapours.

Mean free path. The average distance a particle travels between successive collisions with the other particles of an ensemble.

Mean path. The mean distance a particle travels between successive collisions with other particles or surfaces. When the pressure is high or the vessel dimensions are large, so that the mean path is small with respect to the vessel dimensions, the mean path and mean free path become numerically identical.

Molecular effusion. The molecular flow of gas from a region at one pressure to one at a lower pressure through an orifice in a wall of negligible thickness and with a diameter much less than the mean free path of the molecules.

Molecular flux. The net number of gas molecules crossing a specified surface in unit time. Those having a velocity component in the same direction as the normal to the surface at the point of crossing are counted as positive and those having a velocity component in the opposite direction are counted as negative.

Molecular velocity distribution. The average value of the fraction of the molecules in a small volume, $d\mathbf{r}$, surrounding a given point, located by the radius vector \mathbf{r} in a fluid medium, which have velocity vectors lying within an infinitesimal volume, $d\mathbf{v}$, surrounding the point in velocity space. The averaging process is carried out over a time long enough to smooth statistical fluctuations in the molecular populations, but short compared with the time required for significant variations in the macroscopic properties. For a gas in equilibrium at rest, the distribution of the velocity vectors with a given magnitude is uniform over a sphere about the origin in velocity space. The distribution known as Maxwell's law of velocity distribution is $f_{\mathbf{v}}d\mathbf{v} = 4\pi v^2 [m/(2\pi kT)]^{3/2} \exp[-mv^2/(2kT)]d\mathbf{v}$, where m is the mass of a molecule, T is the absolute temperature, k is the Boltzmann constant, and $4\pi v^2 dv$ is the volume of a spherical shell of radius equal to the magnitude of \mathbf{v} and of thickness dv equal to the increment in this magnitude and gives the fraction of molecules having speeds between v and $v + dv$. The function $f_{\mathbf{v}}$ is the Maxwellian distribution function.

Net speed (vacuum pump). The throughput across a section remote from the pump inlet divided by the pressure as measured at that section. The net speed can be calculated when the pumping speed is known by adding to the sum of all the impedances between the pump inlet and the given cross section, the reciprocal of the measured pumping speed and then taking the reciprocal of the result.

Pascal (symbol Pa). The SI base unit of pressure recommended for general use in vacuum technology. It is one newton per square meter. (See also: Torr)

Permeability coefficient. The rate of flow of gas through a unit area and a unit thickness of a solid barrier per unit differential pressure at a given temperature.

Permeation. The passage of gas through a solid. The process always involves diffusion through the solid and may involve surface phenomena such as sorption, dissociation, migration and desorption.

Physical adsorption. An adsorption process caused by van der Waals forces between adsorbent and adsorbate. Typical binding energies are less than 40 kJ mol⁻¹. Synonym: physisorption. (See adsorption.)

Pressure (gas). The average normal force per unit area exerted by gas molecules impacting on a surface.

Forepressure. The pressure measured downstream from the outlet or foreline of a vacuum pump.

Inlet pressure. The gas pressure at the entrance to a pump.

Interstage pressure. The gas pressure at any point between the exhaust port of the low-pressure stage and high-pressure or roughing stage of a compound pump.

Limiting forepressure. The pressure at the discharge side of a vacuum pump, at a stated throughput, above which the pumping action of the pump rapidly deteriorates, evidenced by a sudden increase of inlet pressure. Synonym: critical backing pressure.

Maximum pressure ratio (vacuum pump). The maximum value of the ratio of forepressure to inlet pressure which a pump can maintain at zero gas flow. In vapour pumps, this term is usually significant only for light gases such as hydrogen and helium.

(Saturated) vapour pressure. The pressure of a vapour in thermodynamic equilibrium with a condensed phase at a fixed temperature. The definition applies to single components as well as to multicomponent systems. In the latter case, it is necessary to distinguish between the total pressure over the condensed phase and the partial pressure of a given component. Synonym: saturation pressure.

Ultimate pressure. The limiting low pressure approached in a vacuum system after a sufficient pumping time has elapsed to establish that further reductions in pressure

will be negligible. Sometimes called the ultimate vacuum, or blank-off pressure, or base pressure when referred to a pump under test.

Ultimate partial pressure. The part of the ultimate pressure in a vacuum system caused by the partial pressure of a specific gas.

Pump fluid. A liquid, usually having a low vapour pressure, used as the working fluid in a mechanical or vapour pump.

Pumps

Cryopump. A vacuum pump which operates by the condensation and/or sorption of gas at surfaces maintained at temperatures sufficiently low for the vapour pressures of the condensed gases to be insignificant.

Cryosorption pump. A vessel containing an adsorbent which can be refrigerated for the cryosorption pumping of gases.

Differential sputter pump. A sputter-ion pump having two cathodes for which materials and sputtering rates differ.

Diffusion pump. A vapour pump in which the pumped gas flows into a vapour stream under conditions in which molecular flow predominates. Momentum is transferred from the vapour to the gas, carrying it along in the direction of the stream. Pump fluid is heated in vacuum to generate the vapour which is directed through a nozzle. It expands freely in the stream before it reaches a cool wall where it condenses and is returned to the boiler to begin a new cycle.

Diode pump. An ion pump containing two uniquely shaped electrodes, viz., a cathode and anode. Two-electrode ion pumps are also referred to as diode getter and diode sputter ion pumps.

Ejector pump. A vapour pump in which the pumped gas enters the pump and the vapour stream under predominantly viscous flow conditions.

Electrostatic pump. An ion pump having only electrostatic fields rather than both electric and magnetic fields to generate the ionizing discharge. The getter material is sublimed by electron heating or by ohmic heating into the discharge space.

Electrostatic getter pump. An electrostatic-ion pump in which a getter material is made to sublime and react with the gas molecules being pumped.

Evaporation pump. A getter-ion pump in which the getter is evaporated from a molten surface rather than sublimed or sputtered from a solid source.

Fore pump. A vacuum pump for maintaining the forepressure of another pump below its critical value.

Fractionating pump. A diffusion pump whose design allows the more volatile impurities in the pump fluid resulting from decomposition or contamination of pumping fluid to be either ejected out of the foreline or trapped within the pump in such a manner as to reduce effectively their change of backstreaming through the pump inlet.

Getter-ion pump. A pump which combines the pumping mechanisms used in the ion pump and the getter pump. (See sputter-ion pump and electrostatic pump).

Ion pump. An electronic device in which ionization produces a significant rate of gas removal by reaction of ions with the cathode material.

Magnetic pump. An ion pump usually with multiple anode cells immersed in a magnetic field parallel to the cell axes with two cathode end plates of reactive material spaced from the ends of the anode cells which terminates the discharge space.

Mechanical pump (vacuum). A device with moving parts such as rotating vanes, a piston, or eccentric rotary members used for pumping gas or vapour.

Noble gas pump. A magnetic-ion pump with novel cathode geometries to enhance the pumping of noble gases.

Positive displacement pump. A mechanical vacuum pump in which the pumping action is provided by displacement or trapped volume of gases typically by a rotating or reciprocating piston, sliding vane, or intermeshing lobes.

Sputter-ion pump. A getter-ion pump in which the getter surfaces are continuously renewed by sputtering.

Triode pump. An ion pump usually of the sputter-ion type, containing three uniquely shaped electrodes; an anode, a sputter cathode, and an ion collector electrode.

Triode getter pump. A triode-ion pump in which gettering is a part of the pumping.

Turbomolecular pump. An axial flow turbine for operation in the molecular flow range consisting of a series of alternate circular rotor and stator disks both of which have inclined blades designed to impart momentum change to gas molecules in a preferential direction from the pump inlet to the outlet.

Pump speed. The volumetric rate of gas flow across a section at the pump inlet. It can be obtained from the ratio of the throughput of a gas to the partial pressure of that gas at a specific point near the inlet port of the pump. (Often called pumping speed.)

Seals

Bakeable seal. A seal which can be baked at elevated temperatures.

Break seal. A seal consisting of a thin glass membrane separating adjacent sections of a vacuum system. The membrane is broken to connect the two sections.

Demountable seal. A seal between two elements designed for disassembly without resort to cutting, fracturing, or melting, which is effective in maintaining the desired vacuum.

Gasket seal. A demountable seal which employs a closed loop of deformable material pressed between two harder members. It may be reusable. The gasket may be fabricated from metal washers, wire rings, elastomers or other materials.

O-Ring seal. A demountable, elastomer, gasket seal made with a toroidal gasket of circular cross section.

Vacuum seal. A joint between two elements of a vacuum system which is effective in maintaining leakage at or below a required level.

Speed factor. The ratio of the speed to the product of the vacuum pump inlet cross section area and the maximum flow rate per unit area as given by the effusion law. It is also called efficiency, or speed efficiency.

Speed of exhaust. The instantaneous rate of reduction of pressure in a system multiplied by its volume and divided by its pressure.

Sticking coefficient. The ratio of the number of molecules which are adsorbed on a surface for a finite period of time to the number of molecules striking that surface.

Sublimation. The process of transition directly from the solid phase to the vapour phase without passing through the intermediate liquid phase by the absorption of energy. Synonym: sublime.

Throat (vacuum component). (a) (Nozzle or Diffuser). The smallest cross section of an expanding nozzle, converging diffuser or converging/diverging nozzle or diffuser. (b) (Vapour Pump). The smallest clearance area between the pump casing and the nozzle nearest the inlet port.

Throughput. The quantity of gas in pressure-volume units, at a specified temperature, flowing per unit time across a specified open cross section. Throughput may be referred to a specific constituent of a gas in which case the partial pressure of that constituent and the associated flow rate are the relevant quantities.

Torr. A unit of pressure defined as 1/760 of a standard atmosphere. It replaced the term millimeter of mercury (mmHg), and has now been replaced by the pascal as a preferred unit of pressure. (1 mmHg = 1.000 000 14 Torr = 133.322 386 7 Pa).

Trap (vacuum system). A device used in a vacuum pumping line to reduce vapour pressure in a vacuum system or prevent backstreaming and migration of vacuum pump fluids such as mercury and/or oil.

Anti-migration trap. A trap which includes a chilled surface or other means to prevent surface migration of oil from a source into the vacuum system.

Cold trap. A trap with a refrigerated surface used to condense various vapours present in the vacuum system.

Molecular sieve trap. A trap containing molecular sieve material that has a high specific surface area and that adsorbs hydrocarbon and water vapours at or below room temperature.

U-Tube trap. A trap in the form of a U-shaped tube which is immersed in a coolant.

Vacuum. The condition of a gaseous environment in which the gas pressure is below atmospheric pressure.

Extreme ultrahigh vacuum. A vacuum in which the pressure is less than 10^{-10} Pa (7.5×10^{-13} Torr).

High vacuum. A vacuum in which the pressure is less than or equal to 10^{-1} Pa (7.5×10^{-4} Torr) and greater than 10^{-4} Pa (7.5×10^{-7} Torr).

Low vacuum. A vacuum in which the pressure is less than 10^5 Pa (750 Torr) and greater than 3.3×10^3 Pa (25 Torr).

Medium vacuum. A vacuum in which the pressure is less than or equal to 3.3×10^3 Pa (25 Torr) and greater than 10^{-1} Pa (7.5×10^{-4} Torr).

Ultrahigh vacuum. A vacuum in which the pressure is less than or equal to 10^{-7} Pa (7.5×10^{-10} Torr) and more than 10^{-10} Pa (7.5×10^{-13} Torr).

Very high vacuum. A vacuum in which the pressure is less than or equal to 10^{-4} Pa (7.5×10^{-7} Torr) and greater than 10^{-7} Pa (7.5×10^{-10} Torr).

Valves

Angle valve. A valve in which the ports are not in line, as, for example a right angle valve.

Butterfly valve. A valve which is opened or closed by rotating a disk 90° about an axis through the centre of the disk.

Diaphragm valve. A valve in which the valve stem is mounted in a bonnet which is isolated from the rest of the valve by using a diaphragm to divide the space inside the valve body. Either metal, elastomer or plastic is commonly used for the diaphragm. An elastomer or plastic diaphragm sometimes functions also as a gasket. In any case, motion is limited to avoid exceeding the elastic limit of the diaphragm material.

Flapper valve. A thin spring steel plate fastened on one end to the pump housing which seals the exhaust port of a mechanical pump from the oil reservoir or atmosphere. During the exhaust cycle, gas pressure is sufficient to deflect the plate from its seat and gas is discharged from the pump. Synonym: flutter reed valve.

Leak valve. A valve for admitting air or gas at a precisely determined rate into a vacuum system.

Needle valve. A leak valve in which a tapered needle is moved along its axis against a seat which may also be tapered.

Relief valve. A valve which will automatically open when the pressure on the seat side rises above a specific pre-set valve. It is generally regarded as a safety device.

Sealed bellows valve. A valve usually for high vacuum applications, in which the stem is sealed by a flexible metal bellows. One end of the bellows is attached to the valve body and the other end to the disk part of the valve stem.

Solenoid valve. A valve in which the movable member is actuated electrically by an electromagnet.

Straight through valve. A valve in which the ports are in line, or coaxial, and for which the internal construction is such that line-of-sight flow occurs when the valve is open.

Vacuum valve. A mechanical device by which the flow of gas or vapour may be started, stopped or regulated by a moving part which opens or obstructs a passage.

Vacuum baffle. A valve containing a shield which remains in line with the valve port and can thus act as a baffle.