*12.3.3 Scanning of spectra*

12.3.3.1 General

**Accelerating voltage (*V* ) scan**

A method of producing a momentum (mass) spectrum in a magnetic deflection instrument 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 in it. 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 that is obtained when a beam of ions is separated according to the mass/charge (*m/z* ) ratios of the ionic species contained within it.

**Momentum spectrum**

A spectrum that is obtained when a beam of ions is separated according to the momentum/charge ratios of the ionic species contained within it. 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* produced.

**Selected ion (peak) monitoring**

This term is used to describe the operation of the mass spectrometer in which the intensities of several specific ion beams are recorded arther than the entire mass spectrum. An alternative recommended term is *multiple ion (peak) monitoring*. The

use of the terms “multiple ion detection” and 'mass fragmentography' is not recommended.

12.3.3.2 Tandem Mass Spectrometers

*General*

**Fixed neutral loss (gain) scan**

A scan that determines, in a single instrument, all the parent ion mass/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/charge ratios that react by the loss (gain) of a selected neutral mass.

**Fixed precursor ion scan**

A scan that determines, in a single experiment, all the daughter ion mass/charge ratios that are produced by the reaction of a selected parent ion mass-to-charge ratio.

**Fixed precursor ion spectrum**

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

**Fixed product ion scan**

A scan that determines, in a single experiment, all the parent ion mass/charge ratios that react to produce a selected daughter ion mass/charge ratio.

**Fixed product ion spectrum**

A spectrum obtained when data are acquired that determine all parent ion mass/charge ratios that react to produce a selected daughter ion mass/charge.

*Magnetic Sector Instruments*

**2*E* mass spectrum**

Processes of the partial charge-transfer type:

$$M^{2+} + X \rightarrow M^{+} + X^{+}$$

occurring in collision cell (containing 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 is set to twice the value required to transmit the main ion beam, the only ions transmitted will be those with kinetic energy/charge ratio twice, or almost twice, that of the main ion beam. The product ions of the above charge stripping process fulfil that condition. If the magnetic field, *B*, is scanned, a mass spectrum of such singly-charged product ions and thus of their doubly-charged precursors is obtained. Such a spectrum is termed a *2E mass spectrum*.

***B* (magnetic flux density)**

Refers to the *magnetic flux density* within the magnetic sector of a mass spectrometer. See also 1.3.3.

**Charge inversion mass spectrum**

Charge inversion processes of the types:

$$M^{+} + X \rightarrow M^{-} + X^{2+}$$

or

$$M^{-} + X \rightarrow M^{+} + X + 2e$$

respectively, occurring in a collision cell (containing a gas X) located in a field-free zone 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 respectively will be transmitted. If the magnetic field is scanned a spectrum of such ions will be

obtained and this is termed a *charge-inversion spectrum*. These are sometimes referred to as $-E$ and $+E$ spectra.

Note: The terms '$2E$, $E/2$, $-E$ or $+E$ mass spectrum' should not be used without prior explanation of their meaning.

**$E$ (electric field strength)**

Refers to the *electric field strength* within the electric sector of a mass spectrometer. See also 1.3.3.

**$E/2$ mass spectrum**

Processes of the charge-stripping type:

$$M^+ + X \rightarrow M^{2+} + X + e$$

occurring in collision cell (containing 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 is set to half the value required to transmit the main ion beam, the only ions transmitted will be those with kinetic energy/charge ratio half, or almost half, that of the main ion beam. The product ions of the above charge stripping process fulfil that 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 termed a *$E/2$ mass spectrum*.

**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 predetermined relationship between parameters characterizing these fields. While these parameters are commonly field strengths, they may also be frequencies in analysers where alternating fields are employed.

**Linked scan at constant $B/E$**

This can be performed with a sector instrument incorporating at least one magnetic sector and one electric sector. The magnetic sector field strength, $B$, and the electric sector field strength, $E$, are scanned simultaneously, while holding the accelerating voltage, $V$, constant, so as to maintain the ratio $B/E$ constant. This constant value is

determined by the ratio of the two field strengths required to transmit main-beam ions of predetermined mass/charge ratio. These preselected main-beam ions are the precursor ions whose fragment ion spectrum is required. The term *B/E* linked scan is not recommended.

**Linked scan at constant $B\,[1-(E/E_0)]^{1/2}/E$**

This can be performed with a sector instrument incorporating at least one electric sector plus one magnetic sector. The magnetic sector field strength, *B*, and the electric sector field strength, *E*, are scanned simultaneously, while holding the accelerating voltage , *V*, constant, so as to maintain the ratio $B\,[1-(E/E_0)]^{1/2}$ /E constant. This constant value is equal to $B_3/E_0$, where $E_0$ and $B_3$ are respectively the electric and magnetic sector fields required to transmit $M^{3+}$ ions in the main ion beam; $m_3$ represents the mass ($m_1$-$m_2$) of the selected neutral fragment $M_3$ whose precursor spectrum is required. The fragmentation reactions thus observed occur in a field-free region traversed before the two sectors scanned in this way. The term '$B\,[1-(E/E_0)]^{1/2}/E$ linked scan' is not recommended.

**Linked scan at constant $B^2/E$**

This can be performed with a sector instrument incorporating at least one electric sector plus one magnetic sector. The accelerating voltage is fixed and the magnetic field, *B*, and the electric field, *E*, are scanned simultaneously so as to maintain $B^2/E$ constant. This constant value corresponds to the ratio of the two fields which transmits main-beam ions of predetermined mass/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. The term
'$B^2/E$ linked scan' is not recommended. Note: other examples of linked scan should be defined in a similar way to the examples given here.

**Linked scan at constant $E^2/V$**

This may be performed with a sector instrument incorporating at least one electric sector plus one magnetic sector. The electric sector field, *E*, and the accelerating voltage, *V*, are scanned simultaneously so as to maintain $E^2/V$ ratio at constant value equal to the value of this ratio that transmits the main beam ions through the electric sector. The magnetic sector field is set at a fixed value such that main-beam ions of a predetermined mass/charge ratio are transmitted by the magnetic sector; these preselected main-beam ions are the precursor ions whose fragment ion spectrum is required. The fragmentation reactions thus observed occur in a field-free region

traversed before the two sectors scanned in this way. The term '$E^2/V$ linked scan' is not recommmended.