12.5 Applications

12.5.1 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.

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 reactant species.

Collision-induced dissociation

An ion/neutral species interaction 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 collision.

Elastic scattering

An ion/neutral species interaction in which the direction of motion is changed but there is no change in the total translational 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 speed.

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 discernable 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.

**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 neutral species in the collision. Generally this is used to describe collisions of fast-moving ions with a neutral species in which the latter is ionised with no change in the number of charges carried by the ion.

**Superelastic collision**

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

**Reactions**

**Association reaction**

The reaction of a (slow-moving) ion with a neutral species in which the reactants combine to form a single ionized species.

**α - cleavage**
Fission of a bond originating at an atom which is adjacent to the one assumed to bear the charge; the definition of $\beta$ - cleavage etc follows automatically.

$\beta$ - cleavage

See $\alpha$ - cleavage.

Charge exchange reaction

See synonymous term 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 wherever there is a change in the magnitude and/or sign of the charges on the reactant.

Charge stripping reaction

An ion/neutral species reaction in which the charge on the reactant is made more positive.

Charge transfer reaction

An ion/neutral species reaction in which the total charge on the reactant ion is transferred initially to the reactant neutral species so that the reactant ion becomes a neutral entity. Some of the possible reactions of ions $M^{2+}$, $M^+$ and $M^-$ with a neutral species $X$ are categorized in terms of the above definitions as follows:

$$M^{2+} + X \rightarrow M^+ + X^+ \quad \text{(Partial charge transfer)}$$

$$M^+ + X \rightarrow M^{2+} + X + e \quad \text{(Charge stripping)}$$

$$M^- + X \rightarrow M^+ X^- + 2e \quad \text{(Charge stripping & charge inversion)}$$

These are all 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.

**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 a product.

**McLafferty rearrangement**

This is an example of a rearrangement reaction and is defined as $\beta$ - cleavage with concomitant specific transfer of a $\gamma$ - hydrogen atom in a six-membered transition state in mono-unsaturated systems, irrespective of whether the rearrangement is formulated by a radical or by an ionic mechanism and irrespective of with which fragment the charge stays.

**Partial charge exchange reaction**

See the synonymous term *partial charge transfer reaction*.

**Partial charge transfer reaction**

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