Key:

Tdt	Drift tube temperature
Pdt	Drift tube pressure
E	Electric field strength around the drift tube
Vdrift	Voltage applied to the drift tube
ldt	Drift tube length
N	Number density of particles in the drift tube
FA	Flowing afterglow
SIFT	Select Ion Flow Tube mass spectrometry
VT-SIFT	Variable Temperature Select Ion Flow Tube mass spectrometry
SIFDT	Select Ion Flow Drift Tube mass spectrometry
PTR-MS	Proton Transfer Reaction Mass Spectrometry
PTCIMS	Proton Transfer Chemical Ionisation Mass Spectrometry (a variation of PTR-MS with an electron impact He/ H2O ion source and 70 cm drift tube (C.F. 9.5 cm in PTR-MS). H3O+ count rates are typically ~ 5 x 10^5 cps to 1x 10^6 cps (C.F. 1 x 10^7 cps in PTR-MS))
PTR-TOF-MS	Proton Transfer Reaction Time-of-Flight Mass Spectrometry (note since only H3O+ reactions are considered here PTR-TOF-MS is used to describe measurements made with a Chemical Ionisation Reaction Time-of-Flight Mass Spectrometer - CIR-TOF-MS)
PTR-IT-MS	Proton Transfer Reaction Ion Trap Mass Spectrometry
EI-MS	Electron Ionisation Mass Spectrometry
KE_{cm}^{r}	Ion-neutral reactant centre-of-mass kinetic energy

Note:

This is not a comprehensive list of possible contributors and does not consider all measurements of product distributions from reactions of H3O+ with trace gas species

Minor product ions are included, where information is available some indication of ion abundance under given reaction chamber conditions is discussed in the "notes" column, refer also to Chapter 3.

The presence of product ions from a partciular compound will vary with E/N and temperature in the drift tube at fixed E/N (neutral as well as ion energy elevated by temperature increases, and internal energy of the ion to a greater extent), E at fixed E/N (ion energy selectively elevated while neutral remains approximately unaffected), and possibly pressure at fixed E/N (for example, increased collisional stabilisation at increased pressure may result in increased association complex formation) in different ways. Ideally mass lists would be compiled for a range of drift tube conditions there is as yet insufficient product distribution data with specified measurement conditions.

Due to the relatively small number of measurements of product distributions in PTR-MS based techniques the products of H_3O^+ reactions with trace gas species in SIFT are discussed. However product distributions in PTR-MS are highly likely to differ from those in SIFT. At the elevated energies in PTR-MS (available due to the electric field) the level of fragmentation is increased and new reaction pathways may become energetically accessible. The polyatomic nature of buffer in PTR-MS compared to helium in SIFT and generally reduced pressure may also effect product distributions observed.

In addition to application of an electric field, as in PTR-MS, the energy available for reaction may be increased by increasing the temperature as in VT-SIFT. Product distributions from H3O+ reactions at elevated temperatures in VT-SIFT are considered. It should be noted that the distribution of the energy in VT-SIFT differs to that in PTR-MS and again a monatomic buffer (helium) and reduced pressure is typically employed in VT-SIFT measurements as opposed to air in PTR-MS.

A lower proton affinity reagent ion also results in increased energy available for reaction (increased exoergicity) and products of reaction of trace gases with some other reagent ions in SIFT are discussed. Again this neglects energy distribution, buffer and pressure changes.

Where EI-MS are discussed in the notes the conclusions are drawn from EI-MS spectra available in: Mallard, W. G., P. J. Linstrom (2005) NIST Chemistry WebBook, NIST Standard Reference Database Number 69, February 2000, National Institute of Standards and Technology, Gaithersburg, MD and discussion is therefore referenced to Mallard and Linstrom (2005). EI-MS percentage product distributions were calculated from peak tables given in JCAMP-DX EI-MS in Mallard and Linstrom (2005) to one decimal place. Although EI-MS data may be helpful in identifying possible fragments it should be used with caution due to the large energies involved in EI-MS, many of the fragments will not be observed in PTR-MS

Proton affinities and gas basicities to calculate enthalpies and Gibbs free energies of reaction discussed in the notes were taken from: Hunter, E. P. L., S. G. Lias (1998) Evaluated gas phase bascities and proton affinities of molecules: An update. *Journal of Physical Chemical Reference Data*, **27** (3): 413-656.

Here normally operated PTR-MS generally refers to E/N of ~120 - 140 Td.

The products resulting from the presence of water in the drift tube; MH$^+$(H$_2$O) ions and the products of reactions with H$_3$O$^+$(H$_2$O)$_n$ (n>1)clusters, are not considered in the mass list.

Dimers, trimers and fragments of them are not included in the mass list.

Contributions of e.g. ^{13}C, ^{18}O, ^{34}S isotopes to m/z are not included in the mass list except those of the H$_3$O$^+$(H$_2$O)$_n$ reagent ions.

References in the "notes" column are given in full in the "some relevant references" column in some instances other relevant references are also given in the "some relevant references" column.

A general discussion of the products of chemical ionisation of a range of compounds with various reagent ions can be found in Harrison, A. G (1992) Chemical Ionization Mass Spectrometry, CRC Press, Inc., Florida.