

fragmentation reaction (in mass spectrometry)

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’.

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