

principal ion

in mass spectrometry

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.

Source:

PAC, 1991, 63, 1541 (*Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology)*). (*Recommendations 1991*) on page 1550