doi:10.1351/goldbook.M03988

molecular ion

in mass spectrometry

An ion formed by the removal from (positive ions) or addition to (negative ions) a molecule of one or more electrons without fragmentation of the molecular structure. The mass of this ion corresponds to the sum of the masses of the most abundant naturally occuring isotopes of the various atoms that make up the molecule (with a correction for the masses of the electron(s) lost or gained). For example, the mass of the molecular ion of ethyl bromide $C_2H_5{}^{79}Br$ will be 2×12 plus 5×1.0078246 plus 78.91839 minus the mass of the electron (m_e). This is equal to 107.95751 u $- m_e$, u being the unified atomic mass unit based on the standard that the mass of the isotope $^{12}C = 12$ u exactly.

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 1549

Orange Book, p. 205

