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THEORETICAL MASS SPECTROMETRY

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Theoretical mass spectrometry of ESI-MS/MS can be obtained by classical trajectory simulations of collision-induced dissociation of protonated cation or deprotonated anion with Ar atom. This method can record the atomic coordinates of the system as a function of time by solving classical mechanics with forces calculated on the fly from quantum chemistry program. The potential between ion and Ar atom is given by analytical form of Buckingham potential. The coordinates of atoms can be visualized and analyzed to determine the structures and formation mechanisms of the fragment ions. The theoretical mass spectrometry of testosterone, boldenone, and estradiol will be presented with animations.

BIOGRAPHY

Kihyung Song has completed his PhD at the age of 31 years from Texas Tech University, USA. Since 1989, he has been a professor of department of chemistry at Korea National University of Education. He has published more than 110 papers in reputed journals including Science. His h index is 33.

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