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Gas phase fragmentation mechanisms of protonated testosterone as revealed by chemical dynamics simulations

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We have studied the fragmentation mechanisms leading to ions produced by collision-induced dissociation of protonated testosterone in the gas phase. At this aim we have used QM+MM chemical dynamics simulations with semi-empirical Hamiltonian for the description of testosterone ion fragmentation. Results show that MSINDO method is able to correctly produce the typical peaks obtained experimentally for protonated testosterone. Simulations also provide mechanisms. In particular we discussed those providing the typical testosterone peaks, *m/z* 97, 109 and 123 and compare with what suggested experimentally. Finally, we rationalized the appearance of different peaks in terms of their dynamical behavior. This study shows for the first time that chemical dynamics can be used to rationalize steroid gas phase fragmentation, thus paving the way for using this approach as complementary tool in doping detection.

Biography

Kihyung Song has completed his PhD at the age of 39 years from Texas Tech University. Since 1989, he have been a Professor of Department of Chemistry at Korea National University of Education. He is the chairman of the department now. He has published more than 100 papers in reputed journals.

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