Mécanismes de fragmentation des bases ionisées d'ADN/ARN

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Résumé

The different fragmentation channels of three ADN and ARN bases, namely cytosine, adenine and guanine have been studied through DFT calculations. The energy dissociation and the fragmentation channels are all calculated from the most stable structure of each base. The elimination of a HCNO molecule is one major dissociation route for all bases, adenine excepted (That last one does not contain an oxygen atom in its structure). The elimination of NH3 (or NH2) molecule is another route common for all studied bases which contain an amino group. However, this last channel is relatively difficult, so that the corresponding peaks in the mass spectra are relatively weakly intense. The CO or HCN (HNC) loss is also investigated for most bases, either directly from the cationic bases or from primary fragments. First results were obtained for uracil [1], and are now comleted for cytosine, adenine and guanine [2].
PCCP, 2012, 14, 9855-9870; CPL, 2013, 165-169.
submitted.

Mots-Clés: DNA, RNA, bases, mass spectra

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