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Degree:MS

Title: Ammonia Elimination from Protonated Nucleobases

Chapter 1: The dediazoniations of the diazonium ion 1 of 4-aminopyrimidine and of the tautomeric cytosinediazonium ions 2 and 3 are facile and result in the formations of cations 4, 5, and 6. The pyrimidine ring-opening of 4, 5 and 6 form their acyclic isomers 7 – 9, respectively. The stability of (E)- and (Z)-isomers is studied.

Chapter 2: The results are discussed of mass-spectrometric studies of the nucleobases adenine 1h (1, R = H), guanine 2h, and cytosine 3h. The protonated nucleobases are generated by electrospray ionization of adenosine 1r (1, R = ribose), guanosine 2r, and deoxycytidine 3d (3, R = deoxyri-bose) and their fragmentations are studied with tandem mass spectrometry. Possible NH3 elimination fragmentation paths for all the ions are given.

Chapter 3: The conformational and isomer preferences of cyanoamine 1 and carbodiimide 2, their conjugate acids and the formation of isoguanosine are discussed. Possible NH3 elimination paths from the protonated cyanoamine 1 and carbodiimide 2 are studied.