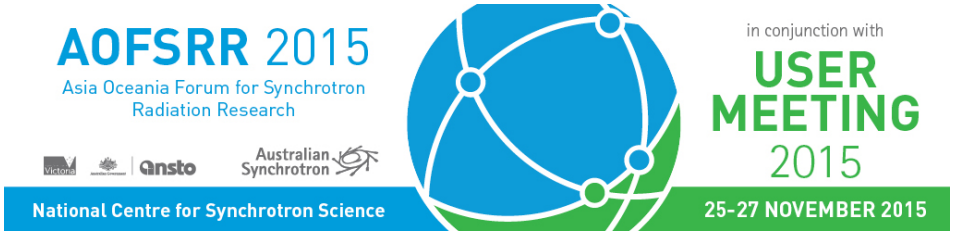

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Why only pyrimidine serves in DNA amongst its diazine isomers?

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X-ray photoemission spectra (XPS), their nuclear magnetic resonance (NMR) spectra and solvent effects of pyrimidine (1,3-diazine) and its other diazine structural isomers (1,2-diazine and 1,4-diazine) are studied using density function theory (DFT) based B3LYP/aug-ccVTZ quantum mechanical calculations, in order to reveal the structure and property information why only pyrimidine serves in DNA, i.e., cytosine (C), thymine (T) and uracil (U) are pyrimidine derivatives, amongst its diazine isomers (Pyridazine (1,2-), Pyrazine (1,4-)). To further elucidate the effects of the structural and the properties differences when interaction with environment, the present work also studies the effect of the solvents (i.e. carbon tetrachloride (CCl4) and water (H2O)) on the structure and vibrational spectra of the diazine isomers along. The preliminary results indicate that the C1s and N1s spectra of the diazine isomers indeed show apparent differences reflecting their nitrogen positions in the ring, which agrees with the calculated molecular electrostatic potentials (MEPs) and NMR chemical shift. Significant blue shifts of the vibrational spectra of the tautomers were observed in the vibrations of C-H bonds due to structures of the N-positions. Finally, the chemical graph LU decomposition matrix from graph theory also indicates that the connection of pyrimidine is quite different from its diazine isomers.

Keywords

DNA base pair, X-ray photoemission spectra (XPS), NMR

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