NONPLANARITY OF NUCLEIC ACID BASES IN HELIUM NANODROPLETS: A VIBRATIONAL TRANSITION MOMENT ANGLE STUDY

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Mid infrared spectra are reported for Nucleic Acid Bases (NABs), such as adenine, cytosine and guanine, in helium nanodroplets. We show that there are several tautomers of NABs in helium nanodroplets, observed and characterized by using ab initio calculations and the measurement of vibrational transition moment angles (VTMAs) for the various vibrational modes of the NAB monomers. The VTMA analysis on the amide group of NABs gives insights into their nonplanarities. In this study a detailed VTMA study of these amino tautomers of NABs is discussed.