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FAMSEC-based insight on the chemical nature of the XH...HY (X,Y = C,N) intramolecular interactions

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HPC content

The diatomic H...H intramolecular interactions in CH...HC, NH...HN and CH...HN molecular fragments in deprotonated, singly protonated and di-protonated conformers of 2,2'-bipyridyl will be discussed. Main focus will be on the chemical nature of these interactions, these fragments energy change and their energy contribution to molecular energy on a structural transformation from a reference (no interaction) to a final state (with interaction of interest) of a molecular. From that, the role played by these interactions, in terms of relative (in)stability of the conformers, will be explored.

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