Fuzzy versus AIM schemes in hydrogen bonds

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Hydrogen bonds (HB) are essential to understand the interactions of some of the most important biological systems. The formation of two HB between two molecules leads to a creation of an extra ring in the complex, with a cooperativity between bonds, which will result in a change of the stabilization of the system. For this reason, the subject of this study is based on using different model compounds (with a donor and an acceptor atom in each molecule) which will be gathered in pairs in order to form two hydrogen bonds and, consequently, a new cycle.

There is not a unique method to calculate the strength of a HB when having a complex with two or more HB. Different parameters can be correlated with their strength, being one of them delocalization indexes. As it was previously demonstrated, the strength of a HB is related to the delocalization index between its atoms. Atomic charges can also help to classify HB complexes.

In order to lower the computational cost of delocalization indexes calculations, Fuzzy atoms definition can be used. The main goal of this talk will be the study of different 3D partition schemes to calculate atomic charges and delocalization indexes. For this purpose, and by using B3LYP/6-311++G(d,p), we will analyse the behaviour of these two concepts.

The extra stabilization when forming a new cycle will be analysed using the previously mentioned delocalization indexes. A rotation of monomers 90º will help us to compare the energies and to calculate the cooperative one. A comparison between delocalization indexes before and after rotating will give us a deeper insight into the electronic distribution when forming the new cycles.