Defining the Bounds of Chemical Coupling Between Covalent and Hydrogen-bonds in Small Water Clusters

Zi Li[1], Yong Yang[1], Xing Nie[1], Tianlv Xu[1], Steven Kirk[1], and Samantha Jenkins[1]

[1]Hunan Normal University

July 14, 2021

Abstract

We seek to determine the two-way transfer of chemical character due to the coupling occurring between hydrogen-bonds and covalent-bonds known to account for the unusual strength of hydrogen-bonds in water. We have provided a vector-based quantification of the chemical character of uncoupled hydrogen-bonds and covalent-bonds and then determined the effects of two-way coupling consistent with the total local energy density H(rb) < 0 for hydrogen-bonds. We have calculated the precessions K' of the eigenvectors around the bond-path for the Ehrenfest Force F(r) and compared with the corresponding QTAIM K'. In doing so we explain why the Ehrenfest Force F(r) provides insights into the coupling between the hydrogen and covalent bonds whilst QTAIM cannot. Conditions for favorable transfer of electron momentum from the hydrogen atom of a sigma bond to the hydrogen-bond are found, with excellent agreement with the hydrogen-bond BCP and covalent-bond BCP separations providing the theoretical bounds for coupling.

Hosted file

`ms_water_precession_K'_2021_06_25_V3.docx` available at https://authorea.com/users/420357/articles/530386-defining-the-bounds-of-chemical-coupling-between-covalent-and-hydrogen-bonds-in-small-water-clusters