

Hydrogen bonding between simple hydrides

M. Simončič and T. Urbič

*University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, 1000 Ljubljana, Slovenia,
E-mail: matjaz.simoncic@fkkt.uni-lj.si*

The hydrogen bond (HB) is one of the most important intermolecular interactions which gives a lot of substances its characteristic and also anomalous properties. Its effects can be observed from large biomolecules like nucleic acids, proteins, cellulose and other polymers, to simpler substances like liquid water where its effects are still quite complex. The common ground of all hydrogen bonded systems is the interaction between an electronegative element and a hydrogen atom which is bonded to another electronegative element. If we want to understand the HB on the macroscale we start with simpler systems and because it is not just a simple electrostatic interaction it should be evaluated on a quantum level (*ab initio* calculations).

In this work we calculated the HB strength of different dimere hydrides (HCl, HF, HBr, H₂O, H₂S, H₂Se, NH₃, PH₃, AsH₃ and CH₄) using the MP2 method and Aug-cc-pVTZ basis set. The aim was to determine what influences the strength of strong as well as weak hydrogen bonds between those molecules. Various relationships were checked. A relation between the strength of the bond and the electronegativity of the participating atoms was found. We also observed a correlation between the strength of hydrogen bonds and the inter-atomic distances, along with the dependence on the charge transfer on the atom of the donor. We also provide characteristic geometries of evaluated dimers.

