

# DEFINITION OF THE HYDROGEN BOND

Hydrogen bonding may be to some extent within the eye of the beholder. If the “hydrogen bond” is worth less than a single  $\text{kcal mol}^{-1}$ , how does that really differ from van der Waals interactions or London dispersion? If the interaction is upwards to  $40 \text{ kcal mol}^{-1}$ , do we benefit from not simply calling that a *bond*? Further complexity comes in the nature of the hydrogen bond: is it simply strong dipole-dipole attraction? Does it possess some covalent character? What is its dispersion component? And can it have some charge transfer character? Is it perhaps some or all of these? Or does the particular environment dictate the nature?

Under certain conditions an atom of hydrogen is attracted by rather strong forces to two atoms, instead of only one, so that it may be considered to be acting as a bond between them and in a dash of the Pimentel and McClellan definition:

(1) There is evidence of a bond and (2) there is evidence that this bond specifically involves a hydrogen atom already bonded to another atom to come up with

The hydrogen bond is an attractive interaction between a hydrogen atom from a molecule or molecular fragment X-H in which X is more electronegative than H, and an atom or a group of atoms in the same or different molecule, in which there is evidence of bond formation. A typical hydrogen bond may be depicted as X-H $\cdots$ Y-Z, where the three dots denote the bond. X-H represents the hydrogen bond donor. The acceptor may be an atom or an anion Y or a fragment or molecule Y-Z, where Y is bonded to Z. In specific cases X and Y can be the same with both X-H and Y-H bonds being equal. In any event, the acceptor is an electron-rich region such as, but not limited to, a lone pair in Y or a  $\pi$ -bonded pair in Y-Z.

Broad enough to cover just about everything! But it demands “evidence of bond formation” and the commission spells out a series of experiments/computations that might provide this evidence. One might wonder if this list is acceptable and complete.

Source: <http://comporgchem.com/blog/?p=1402>