

hydrogen bond

in theoretical organic chemistry

A particular type of multicenter (three center - four electron) X–H ...Y in which the central hydrogen atom covalently linked to an electronegative atom X (C, N, O, S..) forms an additional weaker bond with atom Y (N, O, S..) in the direction of its lone electron pair orbital. The energy of hydrogen bonds, which is usually in the range of 3 –15 kcal/mol (12 –65 kJ/mol), results from the electrostatic interaction and also from the orbital interaction of the antibonding $\sigma^*(\text{XH})\text{MO}$ of the molecule acting as the hydrogen donor and the non-bonding lone electron pair MO_{NY} of the hydrogen acceptor molecule.

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1945