

# Coordinated Water as Hydrogen Bond Acceptor: Crystallographic and Quantum Chemical Study

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Among the rich variety of noncovalent interactions, hydrogen bond is probably the most famous one. Several studies have shown that metal coordination strengthens hydrogen bonds of water. [1] Most of these studies treated coordinated water as hydrogen bond donor. In this work, we have addressed the possibility of coordinated water as hydrogen bond acceptor. A total of 1229 hydrogen bonds between coordinated water as hydrogen bond acceptor and uncoordinated water as hydrogen bond donor were found in the crystal structures deposited in the Cambridge Structural Database. These hydrogen bonds are somewhat longer and have lower tendency toward linear geometries than hydrogen bonds of donor coordinated water. Due to the close proximity of uncoordinated water to neighboring ligands, the observed hydrogen bonds are in most cases found together with additional interactions, which have a strong influence on the overall strength of the interactions. The B97D/def2-TZVP calculations show wide range of energies of observed hydrogen bonds (Figure 1), that depend on the charge of metal complexes and on additional interactions.

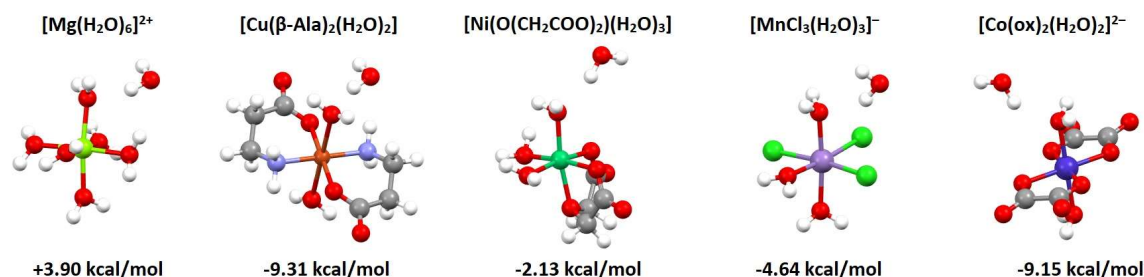


Fig. 1: Hydrogen bonds between coordinated and uncoordinated water and their B97D/def2-TZVP interaction energies.

This study suggests that hydrogen bonds of acceptor coordinated water are important contributors to the overall stability of supramolecular systems, even though they are weaker than hydrogen bonds of donor coordinated water.

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[1] Andrić, J.M.; Misini-Ignjatović, M.Z.; Murray, J.S.; Politzer, P.; Zarić, S.D. *ChemPhysChem* **2016**, *17* (13), 2035–2042.