

MS30-O3 Gold as a hydrogen-bond acceptorCatharine Esterhuysen¹

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Although hydrogen bonds are the most common and well-known intermolecular interactions, a wide variety of other, fascinating interactions that play a role in stabilising crystal structure packing have been identified. For instance, Au(I) complexes are well-known for forming aurophilic interactions, which are inter- or intramolecular Au...Au interactions of a similar strength to hydrogen bonds, with Au...Au distances similar to those found in gold metal.[1] In the intervening thirty years since these interactions were identified they have been extensively studied, and are known to have their origin in relativistic effects.[2] They are also of interest since they are often luminescent and exhibit unusual electronic properties. It has recently been shown that the auride ion, Au⁻, can also act as a hydrogen bond acceptor.[3] However there appears to be a lack of experimental evidence for a hydrogen bonding to Au(I) acceptors, since identification of these interactions in crystal structures is complicated by the simultaneous presence of other hydrogen bonding interactions.[4] Here we present quantum mechanical evidence utilising Density Functional Theory confirming that a number of different hydrogen bond donors do form interactions with a variety of Au(I) complexes, which can therefore be classified as Lewis bases.[5] We also show that a secondary interaction (usually a hydrogen bond) is required to fully stabilise the interaction, as observed experimentally.

The nature of these interactions will be described utilising results obtained with the Atoms in Molecules (AIM) and Noncovalent Interactions (NCI) methodologies, while the role that relativistic effects play in stabilising such interactions will be explored.

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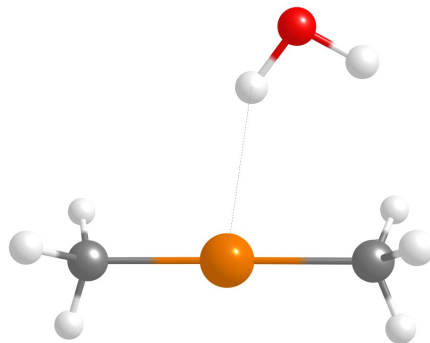


Figure 1. Au(CH₃)₂⁻ forming a hydrogen bond with water

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