

## PROTON, HYDRIDE, OR NEITHER? THE IDENTITY OF H IN THE $\text{Au}_9(\text{PPh}_3)_8\text{H}^{2+}$ CLUSTER

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The diverse tunability of gold nanoclusters via size, geometry, and ligand chemistry allows them to be optimized for greater catalytic activity, selectivity, and optoelectronic properties. The binding of a hydride to  $\text{Au}_9(\text{PPh}_3)_8^{3+}$  to form  $\text{Au}_9(\text{PPh}_3)_8\text{H}^{2+}$  has raised the question of whether the hydride behaves as a metal dopant which donates its two electrons to the Au core or whether it behaves as an electron-withdrawing ligand such as  $\text{Cl}^-$  and  $\text{Br}^-$ . We previously showed significant similarities between its electronic absorption spectrum to that of  $\text{Au}_9(\text{PPh}_3)_8\text{Cl}^{2+}$  and  $\text{Au}_9(\text{PPh}_3)_8\text{Br}^{2+}$ , but follow-up theoretical work suggested that this was a coincidence. Here we analyze the infrared absorption spectra of  $\text{Au}_9(\text{PPh}_3)_8\text{H}^{2+}$  with a single  $\text{N}_2$  or  $\text{H}_2\text{O}$  molecule physisorbed onto the cluster to further elucidate the role of the hydride in  $\text{Au}_9(\text{PPh}_3)_8\text{H}^{2+}$ .