

Bonding in gold-rare earth [Au₂M] (M = Eu, Yb, Lu) ions. A strong covalent gold-lanthanide bond

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The electronic structure and bonding nature of a series of intermetallic gold-lanthanide [Au₂Ln] molecules, where Ln = Eu, Yb, Lu is predicted via the DFT and CASSCF/CASPT2 calculations. The 2c-2e bond model shows a good description of the intermetallic bonding which have a large covalent component with important contribution from bonding interaction between the 6s-Au and the 6s-Ln shell of orbitals. © 2017 Elsevier B.V.