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Gold Clusters: Non-Classical Hydrogen Bonds with Gold and Nano-Biophysics Applications, and Golden Fullerenes

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We summarize the computational evidence that gold clusters can behave as 'nonconventional' proton acceptors and form a new type of 'nonconventional' hydrogen bonding with the conventional proton donors, which satisfies all necessary and sufficient conditions of the classical or conventional hydrogen bonding and the new features of 'golden' fullerenes.

The origin of this nonconventional hydrogen bonding interaction is investigated on the complexes which gold clusters $Au_{1\leq m\leq 8,20}$ (including the nanosized tetrahedral cluster Au_{20}) form with water clusters $(H_2O)_{1\leq n\leq 6}$, hydrogen fluoride clusters $(HF)_{1\leq n\leq 4}$, DNA bases and Watson-Crick base pairs, formamide and formic acid, amino acids, and ammonia clusters $(NH_3)_{1\leq n\leq 3}$. The application of the multi-faceted bonding patterns between gold cluster in different charge states and oligomers of water, ammonia, and hydrogen fluoride for implementing molecular logic gates is also discussed.

This work is also about the neutral tetrahedral ground-state cluster $Au_{20}(T_d)$ and low-energy hollow cages of 20-nanogold, their structures and stability, and their void reactivity in the different charge states. The undertaken approach is illustrated by encaging H, Li, and rare-gas atoms into the novel golden fullerenes which demonstrate quite different features in comparison with C_{60}.