THE MAGIC GOLD CLUSTER Au20(TD) AND ITS LOW-ENERGY FULLERENE-TYPE ISOMERS

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The 20-nanogold cluster Au20 exhibits a large variety of two- and three-dimensional isomeric forms. Among them is the ground-state isomer Au20(Td) representing the stable cluster with a unique tetrahedral shape, with all atoms on the surface, and large HOMO-LUMO gap which even slightly exceeds that of the buckyball fullerene C60. The anionic cluster Au20-(Td) holds its parent tetrahedral symmetry features a high catalytic activity. The list of the properties of the 20-nanogold clusters surveyed in the present work ranges from the energetic order of stability of its isomers to the optical absorption and excitation spectra of the Au20(Td) cluster. We also report the structures and the properties of its doubly charged clusters Au202+ and Au202- and computationally confirm that Au202- is indeed stable. The zero-point-energy-corrected adiabatic second electron affinity of Au20(Td) amounts to 0.43 . 0.53 eV that is consistent with the experimental data. In addition, we provide computational evidence of the existence of the novel, hollow cage isomers of Au20 and analyze their key properties. These 20-nanogold low-energy hollow cages are thoroughly examined: their structures and stabilities, their key properties are revealed and compared with Au20Z(Td) in the different charge states Z=+1,0,-1, and -2. Their void reactivity are investigated at the DFT level. Special attention is devoted to the bifunctional reactivity of the studied Au20 hollow cages, the outer or exo-reactivity and the inner, void, or endo-reactivity. We analyze the general features of the voids of the reported golden fullerenes. The values of ionization potentials and electron affinities, the molecular electrostatic potential and HOMO-LUMO patterns are compared with those of C60 that has a similar void size.