SECTION E_2

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Investigation of structure and properties of Cu_n (n=2-6) clusters using Density Functional Theory methods

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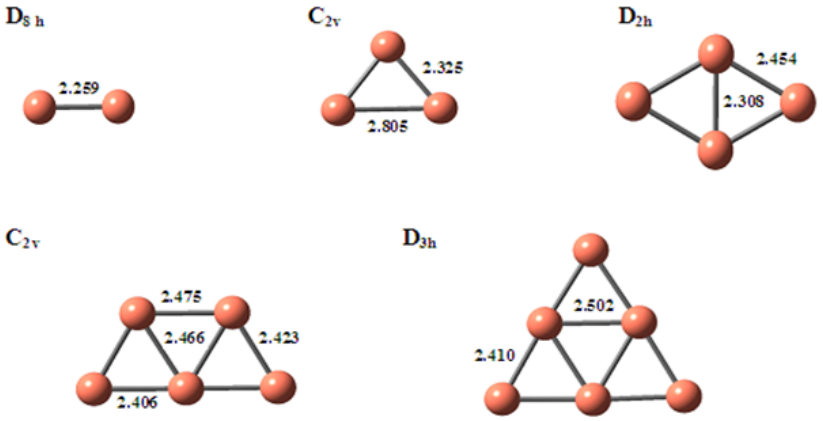
Study of small metal clusters has become interesting in the last few years. Cluster properties are very sensitive to the number of atoms in a small cluster and they can sometimes change dramatically with the addition or removal of one atom from the cluster. Transition metal clusters are particularly interesting for their potential applications in heterogeneous catalysis, new electronic materials and optoelectronic materials etc. Small copper clusters (Cu_n n=2-6) were theoretically investigated using the Density Functional Theory (DFT) at B3LYP/Lanl2DZ level using GAUSSIAN 03.Geometry optimizations of Cu_n (n=2-6) clusters were systematically performed using the DFT method. Vibrational analysis was performed to conform if the optimized structures actually correspond to local minima or the global minimum.



Ground state structures of small copper clusters (Cu_n n=2-6).

Different molecular properties such as total energies, binding energies, ionization potentials, electronic affinities, polarizabilities and hyperpolarizabilities were calculated at the same level of theory. Chemical reactivity of stable copper clusters were described using the Principle of Minimum Polarizability (PMP). Calculated properties show reasonable agreement with available experimental data and with other theoretical results. Cu_3 is the most reactive cluster based on the PMP and it may show catalytic properties due to its reactivity. Hyperpolarizability results help to investigate Non-Linear Optical (NLO) properties of the ground state Cu_n clusters. Cu_3 shows highest hyperpolarizability value of the studied clusters. There may be some applications in the development of non linear optical materials that can be used in many industrial processes.