

Understanding the Structure and Chemical Bonding of Copper Iodide Clusters

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A series of copper iodide clusters is an important class of bi-elemental clusters. In this present work, we have explored the structure and bonding pattern of a selected series of copper iodide clusters. The ground state geometries of each cluster are predicted and electronic and geometric properties are studied. A regular trend between the calculated properties with the number of iodine atoms is observed. In addition, similar properties for an experimentally synthesized cluster containing coordination polymer are evaluated and compared with the respective pristine cluster.