

Abstract Submitted
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Symmetry and Magnetism in Ni₉Te₆ clusters ligated by CO or Phosphine Ligands.¹ VIKAS CHAUHAN, ARTHUR REBER, SHIV KHANNA, Department of Physics, Virginia Commonwealth University — The removal of a single ligand from the magnetic Ni₉Te₆(L)₈ (L=P(CH₃)₃, CO) clusters is found to quench the magnetic moment. The reduction in magnetic moment is caused by a geometric deformation of the Ni₉Te₆ core that breaks the octahedral symmetry of the cluster. This effect is observed in both the CO and phosphine based ligands. The octahedral symmetry bare cluster is also found to have a large magnetic moment. These results highlight the dilemma faced by magnetic ligand protected clusters whose symmetry has been broken: whether to break the spin symmetry as in Hund's rules, or to break the spatial symmetry as in the Jahn-Teller effect. The spatial symmetry breaking is found to be an oblate distortion that forms additional Ni-Te bonds resulting in the enhanced stability of the cluster.

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