

Abstract Submitted
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Magnetic Properties of Arsenic Cluster Assemblies¹ MEICHUN QIAN, A. C. REBER, S. N. KHANNA, Dept. of Physics, Virginia Commonwealth University, A. SEN, S. MANDAL, N. K. CHAKI, Depts. of Chemistry and Physics, Penn. State University — Clusters have the potential to serve as building blocks of materials, enabling the tailoring of materials with novel properties. Recently, we synthesized a magnetic cluster assembled material using the As₇ cluster and cryptated K, which are the elements from main group. X-ray studies show that the As cluster is distorted to accompany two cryptated K. We have investigated the magnetic properties of As cluster assembly using density functional theory. We found the As₇ cluster has the (-2) valence state and possess one unpaired electron. The magnetic state is stabilized in the crystal and has a lower energy of 90 meV than the nonmagnetic state. The magnetic moments are located on the As₇ cluster and display antiferromagnetic order in the crystal. We also study the magnetic properties of the As cluster assemblies with transition metal as a linker, and these findings are possible to provide a new kind of magnetic materials.

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