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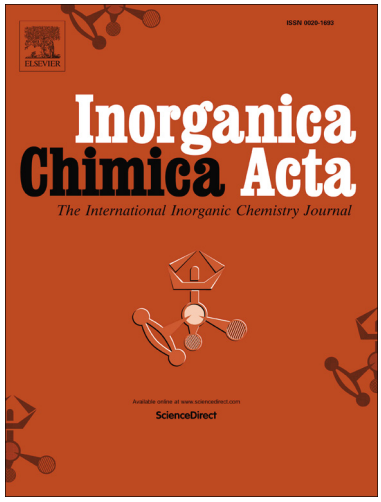

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PII: S0020-1693(17)30930-1
DOI: http://dx.doi.org/10.1016/j.ica.2017.07.052
Reference: ICA 17775

To appear in: *Inorganica Chimica Acta*

Received Date: 15 June 2017
Revised Date: 24 July 2017
Accepted Date: 26 July 2017

Please cite this article as: F.V. Escobedo-Cruz, T.R. Hughbanks, Synthesis and characterization of a new cubic structure in the reduced zirconium iodide chemistry, *Inorganica Chimica Acta* (2017), doi: http://dx.doi.org/10.1016/j.ica.2017.07.052

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Synthesis and characterization of a new cubic structure in the reduced zirconium iodide chemistry

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Abstract

The solid-state synthesis and characterization of a new reduced zirconium iodide are reported. Black cubic-like crystals with twinning characteristics and suitable for single crystal X-ray diffraction were obtained when equimolar amounts of Zr, ZrI_4 and MnI_2 were reacted for the nominal composition of Zr_6MnI_{12}. The compound $[Zr_6MnI_{12}]_4[MnI_4]_3$ crystallizes in the cubic space group $I\bar{4}3d$ with the lattice parameter a = 23.1879(6) Å. Magnetic susceptibility measurements confirm the presence of Mn in tetrahedral cavities, making it the first compound to have the same element as interstitial and as a cation. This new compound features clusters with two different electronic configurations and with three I^a. The structural and electronic features of $[Zr_6MnI_{12}]_4[MnI_4]_3$ are unprecedented in the chemistry of reduced zirconium clusters.

Keywords: `Zirconium`, reduced clusters, iodides, X-Ray diffraction, crystal structure, solid-state synthesis

1. Introduction

Since the discovery that reduced zirconium clusters are stabilized by interstitial atoms, an ample variety of new compounds and structures have been found.[1] The reduced zirconium halides are characterized by octahedra of zirconium encapsulating an interstitial atom, and the octahedra have their vertices and edges capped by halogens. The bridging properties of the halogenido ligands allow the zirconium octahedra to interconnect and arrange in varying motifs.[2] In addition, the intercalation of counterions, usually alkali-metals, influence the electronic and structural configurations of the resulting compounds.[3] The reduced zirconium halides, with some exceptions, [4, 5] can be described by the general formula $A_x[Zr_6ZX^i_{12}]X^a_n$ in which A is a cation from group 1 or 2, X^i are edge-capping halides, X^a are axial halides, $0 \leq x$, and $n \leq 6$. From the halides, the chlorides and the bromides, to certain extent, have shown to be versatile

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