

Unusual Bonding in Ternary Nitrides: Preparation, Structure and Properties of Ce_2MnN_3 .

Rainer Niewa^a, Grigori V. Vajenine^a, Francis J. DiSalvo^{*,a},
Haihua Luo^b, William B. Yelon^b

^a Department of Chemistry, Cornell University, Ithaca, NY 14853-1301, USA

^b University of Missouri Research Reactor, Columbia, MO 65211, USA

Z. Naturforsch. **53 b**, 63–74 (1998); received September 17, 1997

Ternary Nitride, Crystal Structure, Magnetic Susceptibility, Electrical Resistivity, Extended Hückel Method

Ce_2MnN_3 was prepared by reaction of cerium nitride and manganese with nitrogen gas at 900 °C. It crystallizes isotypic to Ac_2MN_3 (Ac = U, Th; M = Cr, Mn) and Ce_2CrN_3 , space group *Immm* (No. 71), $a = 3.74994(6)$ Å, $b = 3.44450(6)$ Å and $c = 12.4601(2)$ Å. The manganese atoms are coordinated in a nearly square planar fashion by four nitrogen atoms. These corner-connected MnN_4 units form infinite ${}^1_{\infty}[\text{MnN}_2\text{N}_{2/2}]$ chains, which run parallel to each other along the crystallographic *a*-axis, forming the motif of hexagonal rod packing. Cerium atoms connect the chains into a three-dimensional network. The results of measurements of the magnetic susceptibility, as well as of the electrical resistivity suggest metallic behavior. Electronic effects leading to shorter bonds between manganese and bridging nitrogen atoms than between manganese and terminal nitrogen atoms in the ${}^1_{\infty}[\text{MnN}_2\text{N}_{2/2}]$ chains were investigated through extended Hückel and LMTO band structure calculations. Issues pertaining to stability of this and some other nitridometallate structures are discussed.

Reprint requests to F. J. DiSalvo.