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Anion Photoelectron Spectroscopy and Density Functional Investigation of Diniobium-Carbon Clusters¹ P.A. CLAYBORNE, Virginia Commonwealth University, K.L. KNAPPENBERGER, JR., University of California, Berkeley and Lawrence Berkely National Laboratory, J.U. REVELES, Virgina Commonwealth University, M.A. SOBHY, C.E. JONES, JR., U.U. GUPTA, I. IOR-DANOV, J. SOFO, A.W. CASTLEMAN, JR., Pennsylvania State University, S.N. KHANNA, Virginia Commonwealth University — Experimental photoelectron and computational results show diniobium-carbon (Nb_2C_n) clusters to coexist in multiple structural isomers: three-dimensional geometries, planar rings and linear chains. Three-dimensional clusters having up to five carbons are formed preferentially with Nb-Nb bonding, whereas only Nb-C bonding is observed experimentally at six carbons. Clusters consisting of an odd number of atoms are also observed with linear geometries. The larger binary clusters ($n \geq 7$) display properties similar to pure carbon clusters. We provide evidence for niobium substitution of carbon atoms.

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