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Isomers and Isomags in MnnX (n = 5-6, X=N, O) Clusters[1] W.-J. ZHENG, J.M. NILLES, K.H. BOWEN, Department of Chemistry, Johns Hopkins University, Baltimore, MD 21218, N.O. JONES, S.N. KHANNA, P. JENA, Physics Department, Virginia Commonwealth University, Richmond, VA 23284-2000, T. BARUAH, M.R. PEDERSON, Complex Systems Theory, Naval Research Laboratory, Washington, D. C. 20375 — It is shown that the addition of N or O to pure Mn_n clusters can lead to situations where the ground state is marked by configurations having comparable binding energies, same total spins but differing distribution of local moments. We call these "isomags" and demonstrate their existence through a synergistic approach combining negative ion photo-detachment spectra and theoretical investigations. In the case of Mn_5O and Mn_6O clusters show that the O atom occupies either bridge or hollow sites. While it occupies a bridge site with a binding energy of 6.88 eV in Mn_5, it prefers a hollow site with a binding energy of 7.18 eV in Mn_6 clusters. Further, Mn_5O is shown to possess two magnetic isomers with total spins of 13 and 5 μ_B that contain three and five isomags respectively. Mn_6O possesses three isomers, two with moments of 8 and 2 μ_B in addition to a non-magnetic state. It is shown that the isomags, although undetected in magnetic deflection experiments, can be traced via their electronic structure in experimental photoelectron spectra. Corresponding results on Mn_nN will also be presented.

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