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Negative ions of transition metal-halogen clusters[1] KALPATARU PRADHAN, Department of Physics, VCU, Richmond, VA, 23284, USA, GENNADY L. GUTSEV, Department of Physics, Florida A&M University, FL 32307, USA, PURUSOTTAM JENA, Department of Physics, VCU, Richmond, VA, 23284, USA — A systematic density functional theory based study of the structure and spectroscopic properties of neutral and negatively charged MX_n clusters formed by a transition metal atom M (M=Sc, Ti, V) and up to seven halogen atoms X (X=F, Cl, Br) has revealed a number of interesting features: (1) Halogen atoms are bound chemically to Sc, Ti, and V for $n < n_{max}$, where the maximal valence n_{max} equals to 3, 4, and 5 for Sc, Ti, and V, respectively. For $n > n_{max}$, two halogen atoms became dimerized in the neutral species, while dimerization begins at n = 5, 6, and 7 for negatively charged clusters containing Sc, Ti, and V. (2) Magnetic moments of the transition metal atoms depend strongly on the number of halogen atoms in a cluster and the cluster charge. (3) The number of halogen atoms that can be attached to a metal atom exceeds the maximal formal valence of the metal atom. (4) The electron affinities of the neutral clusters abruptly rise at $n=n_{max}$, reaching values as high as 7 eV. The corresponding anions could be used in the synthesis of new salts, once appropriate counterions are identified.

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