Negative ions of transition metal-halogen clusters\textsuperscript{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\textsubscript{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 \( n < n_{\text{max}} \), where the maximal valence \( n_{\text{max}} \) equals to 3, 4, and 5 for Sc, Ti, and V, respectively. For \( n > n_{\text{max}} \), 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 \( n=n_{\text{max}} \), 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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