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Electron affinities of d1 transition metal chloride clusters and onset of super halogen behavior SWAYAMPRABHA BEHERA, JORLY JOSEPH, PURUSOTTAM JENA, VCU — Geometry, electronic structure, and electron affinity of d1 transition metal chloride clusters (MCl_n, M = Sc,Y, La; n = 1–5) have been calculated using density functional theory. Chlorine atoms are chemically bound in all cases except for MCl_5. The electron affinities of MCl_n (n = 1–3) are small and increase only marginally as a function of n until the valence of the metal atom is consumed. Beyond this, they rise sharply and reach a value of 5.96, 6.03 and 5.90 eV for $ScCl_4$, YCl_4 and $LaCl_4$, respectively and remain high for n = 5. MCl_n, (n = 4,5) clusters, therefore, behave as superhalogens. Results are compared with available experimental data

Swayamprabha Behera
VCU

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