Abstract Submitted
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Zinc in +III oxidation state DEVLEENA SAMANTA, PURU JENA, Virginia Commonwealth University — The possibility of Group 12 elements, such as Zn, Cd, and Hg existing in an oxidation state of +III or higher has fascinated chemists for decades. Significant efforts have been made in the past to achieve higher oxidation states for the heavier congener mercury (since the 3^{rd} ionization potential of the elements decrease as we go down the periodic table). It took nearly 20 years before experiment could confirm the theoretical prediction that Hg indeed can exist in an oxidation state of +IV. While this unusual property of Hg is attributed to the relativistic effects, Zn being much lighter than Hg has not been expected to have an oxidation state higher than +II. Using density functional theory we show that an oxidation state of +III for Zn can be realized by choosing specific ligands with large electron affinities i.e. superhalogens. We demonstrate this by a systematic study of the interaction of Zn with F, BO_2, and AuF_6 ligands whose electron affinities are progressively higher, namely, 3.4 eV, 4.4 eV, and 8.4 eV, respectively. Discovery of higher oxidation states of elements can help in the formulation of new reactions and hence in the development of new chemistry.

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