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Borane derivatives: A New Class of Superhalogens DEVLEENA SAMANTA, Virginia Commonwealth University, BISWARUP PATHAK, RAJEEV AHUJA, Uppsala University, PURUSOTTAM JENA, Virginia Commonwealth University — Halogens have the largest electron affinities of all elements in the periodic table, that of Cl being the highest, namely 3.6 eV. Superhalogens have electron affinities that far exceed that of halogens. Based on density functional theory calculations, we show that the Wade-Mingo's rule, well known for describing the stability of *closo*-boranes ($B_nH_n^{2-}$), can be used to design a new class of superhalogens by tailoring the size and composition of borane derivatives. These superhalogens do not have to have either a metal or a halogen atom unlike conventional superhalogens. We show this by taking $B_{12}H_{13}$ and $CB_{11}H_{12}$ as examples. Also, these superhalogens can be used as building blocks of hyperhalogens of the form $M(B_{12}H_{13})_2$ and $M(CB_{11}H_{12})_2$ (M=Li, Na, K, Rb, Cs). This finding opens the door to an untapped source of superhalogens and weakly coordinating anions with potential applications.

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