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Heterborane Analogs of Silicon clusters: Experimental and Theoretical Studies on Bi_2Si_n KIRAN BOGGAVARAPU, McNeese State University, MILEY JACKSON, McNeese Sate University, XIANG LI, ANDREJ GRUBISIC, DI WANG, KIT BOWEN, Johns Hopkins University, ANIL KANDALAM, McNeese State University, HAOPENG WANG, Johns Hopkins University — Despite numerous studies, silicon clusters continue to fascinate. Part of the intrigue comes from the fact that, unlike metallic clusters which have strongly delocalized electrons and prefer to follow simple electron counting rules such as those originating from Jellium models, there are no simple rules of thumb that can be used to understand the diverse structures of silicon clusters. However, over the last couple of decades, there have been attempts to connect the structure and bonding of silicon clusters to a large class of well-studied three dimensional boron hydride compounds namely, *closo*-boranes, $B_nH_n^{2-}$. By equating the σ-lone pair of divalent silicon to a B-H bond, it was shown that the frontier orbitals of both units are similar. Theoretical studies have concluded that the silicon clusters (Si_n^{2-}) adopt similar structural patterns to those of boranes, when n = 5, 6, 7, 8, 10 and 13. The question then arises, whether neutral analogs of Si_n^{2-} and neutral heteroboranes, $X_2B_nH_n$ (X = N, P, Sb, Bi), can be envisioned. Here, we present the scope and limitation such analogy based on our recent theoretical (DFT) and experimental (anion-photoelectron spectroscopy) studies on Bi_2Si_n (n = 4-8). In particular, we show that that both Bi_2Si_5 and $Bi_2B_5H_5$ adopt similar pentagonal bipyrmidal (PBP) geometries and have analogous orbital energy patterns.

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