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Effect of Charge and Composition on the Structural Fluxionality and Stability of Nine Atom Tin-Bismuth Zintl Analogues[1] PENEE CLAYBORNE, Virginia Commonwealth Univeristy, UJJWAL GUPTA, Pennsylvania State University, ARTHUR REBER, Virginia Commonwealth University, JOSHUA MELKO, A.W. CASTLEMAN, Pennsylvania State University, SHIV KHANNA, Virginia Commonwealth University — Synergistic studies of bismuth doped tin clusters combining photoelectron spectra with first principles theoretical investigations establish that highly charged Zintl ions, observed in the condensed phase, can be stabilized as isolated gas phase clusters through atomic substitution that preserves the overall electron count but reduces the net charge. Mass spectrometry studies reveal that Sn_8Bi^-, $Sn_7Bi_2^-$, and $Sn_6Bi_3^-$ exhibit higher abundances than neighboring species, and photoelectron spectroscopy show that all of these heteroatomic gas phase species have high adiabatic electron detachment energies. $Sn_6Bi_3^-$ is found to be a particularly stable cluster, having a large highest occupied molecular orbital (HOMO)-lowest unoccupied molecular orbital (LUMO) gap. Theoretical calculations demonstrate that Sn_8Bi^-, $Sn_7Bi_2^-$, and $Sn_6Bi_3^-$ are deltahedral clusters and isoelectronic to the Zintl polyatomic clusters Sn_9^{2-}, Sn_9^{3-} and Sn_9^{4-}, respectively. However, the fluxionality reported for tin-Zintl clusters is suppressed by substituting Sn atoms with Bi atoms in Sn_8Bi^- and $Sn_6Bi_3^-$. The similarities between bismuth doped deltahedral tin clusters and deltahedral Zintl polyanions, suggest these gas phase Zintl clusters (GPZC) may find use for building blocks of cluster assembled materials.

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