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On the Stability of Sodium-Tin Zintl Ions in Gas phase experiments A. REBER, J.W. GARBUS, S.N. KHANNA, Virginia Commonwealth University, W.J. ZHENG, O.C. THOMAS, J.M. NILLES, K.H. BOWEN, Johns Hopkins University — A synergistic effort combining negative ion photoelectron spectroscopy of $Na_nSn_m^-$ clusters along with the first principles electronic structure studies has been used to demonstrate that Zintl ions found in solutions also exist as stable species in free clusters. The theoretical investigations are carried out within a gradient corrected density functional approach. Our studies on $Na_nSn_4^-$ clusters where n=0-4 and $NaSn_m^-$ clusters where m=4-7 show that $Na_3Sn_4^-$ is a very stable cluster marked by a distorted tetrahedral tin core and can be regarded as $(Na+)_4(Sn_4)^{-4}$ gas phase analogue of the Na:Sn tetrahedral Zintl phase. In addition, the $NaSn_5^-$ cluster is shown to be the most abundant species in the mass spectrum in the $NaSn_m^-$ series and its stability can be reconciled with Sn_5^{2-} Zintl ions. The existence of stable Zintl ions in the gas phase can provide an alternate approach to look for possible Zintl phases.

Arthur Reber

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