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Al_nBi Clusters: A Transition from Aromatic to Jellium Stability[1]

PENEE CLAYBORNE, Virginia Commonwealth University, J.U. REVELES, Virginia Commonwealth Univeristy, S.N. KHANNA, Virginia Commonwealth University, C.E. JONES, JR., U. GUPTA, J. MELKO, A.W. CASTLEMAN, JR., The Pennsylvania State University — Through a synergetic effort using density functional theory and negative ion photodetachment studies we have investigated multiple aluminum-bismuth clusters. Our studies show that Al_3Bi and Al_5Bi are two very stable clusters. Further investigation of their electronic structure reveal that their stability can be explained using the aromatic and Jellium models, respectively. The Al_3Bi cluster has a large ionization potential of 7.1 eV, a low electron affinity of 1.4 eV and a HOMO-LUMO gap of 1.7 eV. The molecular orbitals of the cluster are reminiscent of an aromatic system and the cluster has a nucleus independent chemical shift (NICS) value of -32.19 ppm confirming its aromatic character. The Al_5Bi cluster has a HOMO-LUMO gap of 1.2 eV and a large ionization potential of 6.5 eV. The compact structure of Al_5Bi has 20 electrons, which indicates that this cluster's stability could be accounted for by the Jellium model.

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