

## **Supporting Information**

### **Addition of a Thallium Vertex to Empty and Centered Nine-Atom Deltahedral Zintl Ions of Germanium and Tin**

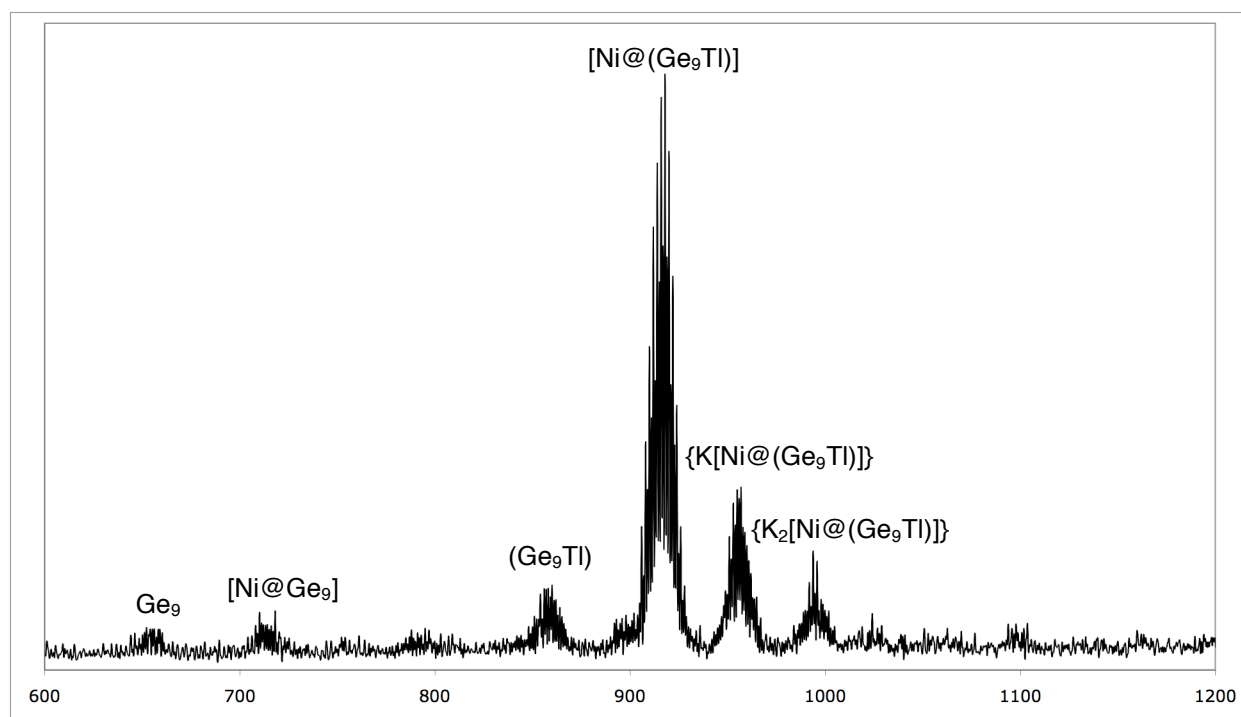
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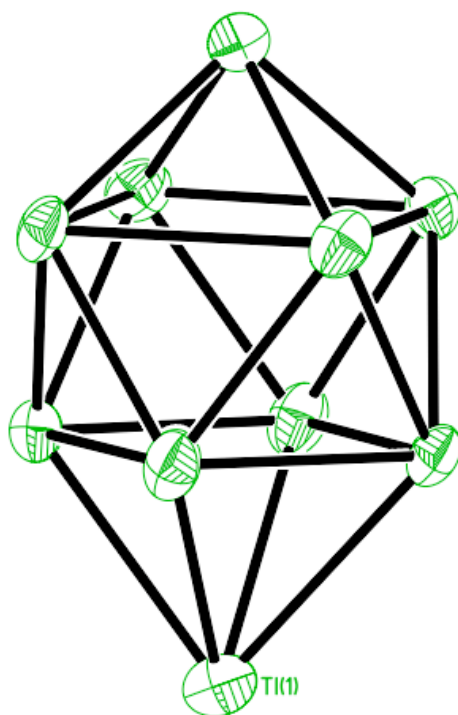
*University of Notre Dame*

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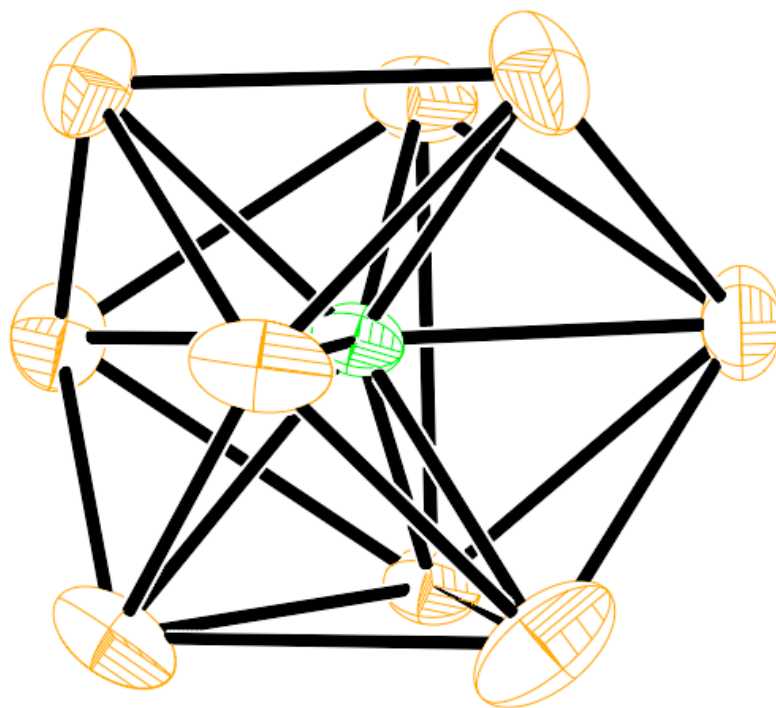
ssevov@nd.edu



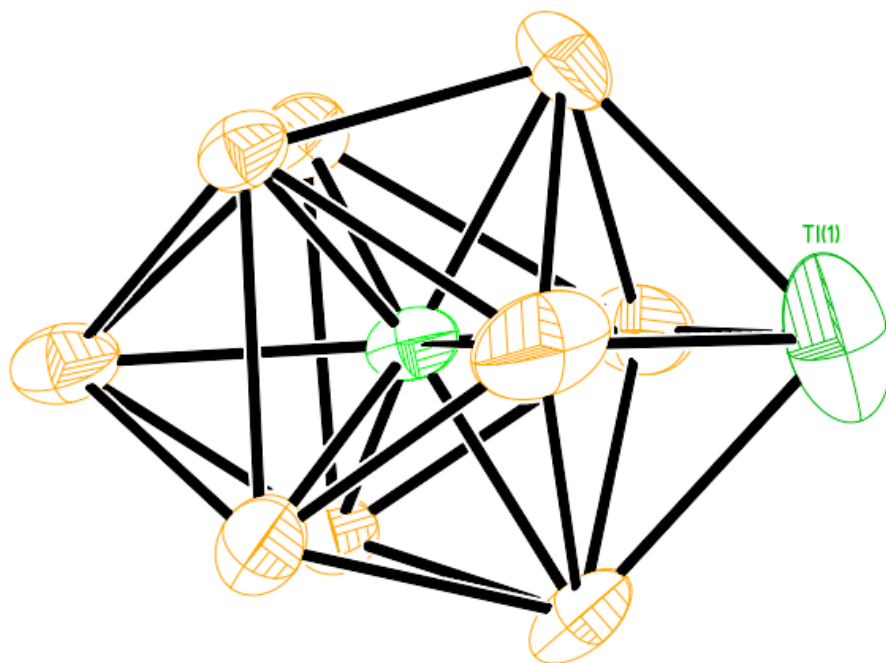
**Figure S1.** The full electrospray mass spectrum ( $m/z$ : 600 – 1200) in negative ion mode of the reaction solution producing  $[\text{Ni} @ (\text{Ge}_9\text{Tl})]^{3-}$ . Notice that the uncapped  $[\text{Ni} @ \text{Ge}_9]$  clusters are in only negligible amount which indicates that the Tl-atom in the capped clusters is an integral part of the cluster and is not simply  $\text{Tl}^+$  cation.



**Figure S2.** An ORTEP view of the *closo*-[Ge<sub>9</sub>Tl]<sup>3-</sup> cluster with the shape of a bicapped square antiprism where one of the caps is the thallium atom (thermal ellipsoids at the 70 % probability level).



**Figure S3.** An ORTEP view the Ni-centered [Ni@Sn<sub>9</sub>]<sup>3-</sup> with the shape of a distorted tricapped trigonal prism (thermal ellipsoids at the 70 % probability level).



**Figure S4.** An ORTEP view the Ni-centered Tl-capped cluster  $[\text{Ni}@\text{Sn}_9\text{Tl}]^{3-}$  with the shape of a bicapped square antiprism (thermal ellipsoids at the 70 % probability level).