

# [(Me<sub>3</sub>Si)Si]<sub>3</sub>EtGe<sub>9</sub>Pd(PPh<sub>3</sub>), a Pentafunctionalized Deltahedral Zintl Cluster: Synthesis, Structure, and Solution Dynamics

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The title compound, which has a ten-atom deltahedral cluster core of Ge<sub>9</sub>Pd, was synthesized through insertion of Pd(PPh<sub>3</sub>) into the tetrasubstituted nona-germanium cluster [(Me<sub>3</sub>Si)Si]<sub>3</sub>EtGe<sub>9</sub> through a reaction of the latter with Pd(PPh<sub>3</sub>)<sub>4</sub>. This first reaction of neutral tetrasubstituted nine-atom clusters shows that they retain reactivity despite their neutral charge. The Ge<sub>9</sub>Pd core is the first that incorporates a 5-connected transition metal other than from Group VI, a noble metal in this case. Single-crystal X-ray diffraction shows that the ten-atom core is a closo-cluster with the expected shape of a bicapped square antiprism. <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy show that, in contrast to the parent tetra-substituted [(Me<sub>3</sub>Si)Si]<sub>3</sub>EtGe<sub>9</sub>, the new compound does not exhibit dynamics. Relativistic DFT calculations are used to explain the differences. © 2016 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

cluster compounds

germanium

molecular dynamics

palladium

Zintl anions

Atoms

Germanium

Molecular dynamics

Precious metals

Reaction kinetics

Silicon

Silicon wafers

Single crystals

Transition metals

X ray diffraction

Cluster compounds

Deltahedral clusters

DFT calculation

Germanium clusters

Single crystal x-ray diffraction

Solution dynamics

Title compounds

Zintl anions

Palladium