Different Cerium Valence Transitions Observed by Hydrogenation of the Ternary Germanides CeRhGe and CeIrGe – Structure, Physical Properties and Chemical Bonding

Bernard Chevalier\textsuperscript{a}, Etienne Gaudin\textsuperscript{a}, Adel F. Al Alam\textsuperscript{a}, Samir F. Matar\textsuperscript{a}, François Weill\textsuperscript{a, b}, Birgit Heying\textsuperscript{c}, and Rainer Pöttgen\textsuperscript{c}

\textsuperscript{a} ICMCB, CNRS, Université Bordeaux 1, 87 Avenue du Docteur Albert Schweitzer, 33608 Pessac Cedex, France
\textsuperscript{b} Centre de Ressource en Microscopie Electronique et Microanalyse, CREMEM, Université Bordeaux 1, Avenue des Facultés, Batiment B8, F-33400 Talence Cedex, France
\textsuperscript{c} Institut für Anorganische und Analytische Chemie, Universität Münster, Corrensstraße 30, D-48149 Münster, Germany

Reprint requests to Dr. B. Chevalier. E-mail: chevalie@icmcb-bordeaux.cnrs.fr or Prof. Dr. R. Pöttgen. E-mail: pottgen@uni-muenster.de


\textit{Dedicated to Professor Gérard Demazeau on the occasion of his 65\textsuperscript{th} birthday}

The ternary germanides CeRhGe and CeIrGe which crystallize in the orthorhombic TiNiSi-type structure, absorb hydrogen at 523 K. X-Ray powder diffraction and transmission electron microscopy indicate that the hydrides CeRhGeH\textsubscript{1.8} and CeIrGeH\textsubscript{1.8} adopt the hexagonal ZrBeSi-type structure. Magnetization, electrical resistivity and thermoelectric power measurements reveal that these hydrides are intermediate-valence compounds. An unusual transition from antiferromagnetic to spin fluctuation behavior occurs upon hydrogenation of CeRhGe, while on the contrary, CeIrGeH\textsubscript{1.8} presents a Kondo temperature of 285 K smaller than that observed for CeIrGe (610 K). In order to explain these opposite valence transitions, the electronic structures of the hydrides have been self-consistently calculated within the local spin density functional theory (LSDF). The structures are compared to those reported previously by us for CeRhGe and CeIrGe.

\textit{Key words:} Hydrogenation, Structural Transition, Intermediate-valence Compounds, Electronic Structure Calculation