

# Structure, Chemical Bonding and $^{119}\text{Sn}$ Mössbauer Spectroscopy of $\text{LaRhSn}$ and $\text{CeRhSn}$

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The rare earth (*RE*) stannides  $\text{LaRhSn}$  and  $\text{CeRhSn}$  were prepared from the elements by arc-melting or by reactions in sealed tantalum tubes in a high-frequency furnace. The structures have been refined from X-ray single crystal diffractometer data:  $\text{ZrNiAl}$  type,  $P6_2m$ ,  $a = 748.74(5)$ ,  $c = 422.16(3)$  pm,  $wR2 = 0.0307$ , 310  $F^2$  values for  $\text{LaRhSn}$  and  $a = 745.8(1)$ ,  $c = 408.62(9)$  pm,  $wR2 = 0.0397$ , 354  $F^2$  values for  $\text{CeRhSn}$  with 14 variables per refinement. The structures contain two crystallographically different rhodium sites which both have a tricapped trigonal prismatic coordination:  $[\text{Rh1Sn}_3\text{RE}_6]$  and  $[\text{Rh2Sn}_6\text{RE}_3]$ . Together the rhodium and tin atoms (280–288 pm Rh–Sn distances in  $\text{LaRhSn}$  and 277–285 pm in  $\text{CeRhSn}$ ) build up three-dimensional  $[\text{RhSn}]$  networks in which the rare earth atoms fill distorted hexagonal channels. DFT band structure calculations reveal a large cerium  $4f$  contribution at the Fermi level and a strong mixing of cerium  $5d/4f$  with rhodium  $4d$  orbitals. These results are in agreement with the short Ce–Rh bonds (304 and 309 pm) and also with the electronic and magnetic properties.  $^{119}\text{Sn}$  Mössbauer spectra of  $\text{LaRhSn}$  and  $\text{CeRhSn}$  show a single tin site at isomer shifts of  $\delta = 1.98(2)$  ( $\text{LaRhSn}$ ) and  $1.79(1)$  mm/s ( $\text{CeRhSn}$ ) subject to quadrupole splitting of  $\Delta E_Q = 0.79(4)$  ( $\text{LaRhSn}$ ) and  $1.12(3)$  mm/s ( $\text{CeRhSn}$ ). The 1.8 K data show no transferred hyperfine field at the tin site for  $\text{CeRhSn}$ .

**Key words:** Intermetallics, Crystal Structure, Chemical Bonding, Mössbauer Spectroscopy