Ferromagnetic Ordering in CeZnSn

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Dedicated to Professor Ingo-Peter Lorenz on the occasion of his 65th birthday

The stannide CeZnSn was obtained in X-ray-pure form by induction-melting of the elements in a sealed tantalum ampoule. CeZnSn crystallizes with the YPtAs-type structure, space group $P6_3/mmc$, $a = 456.7(3)$, $c = 1673.8(5)$ pm, $wR2 = 0.0862$, 259 $F^2$ values, and 12 variables. The zinc and tin atoms build up puckered Zn$_3$Sn$_3$ hexagons (Zn–Sn 271 pm) with weak interlayer Zn–Zn interactions (323 pm). Susceptibility measurements of CeZnSn reveal modified Curie-Weiss behavior above 50 K with an experimental magnetic moment of 2.77(1) $\mu_B$ / Ce atom. The cerium magnetic moments order ferromagnetically at $T_C = 5.2(1)$ K. $^{119}$Sn Mössbauer spectra show a single tin site at an isomer shift of $\delta = 1.967(4)$ mm/s subjected to a small quadrupole splitting of $\Delta E_Q = 0.41(2)$ mm/s at 40 K. At 4.2 K a magnetic hyperfine field of 0.872(5) T is transferred to the tin site. From DFT scalar relativistic calculations of the electronic and magnetic structures, chemical bonding analysis reveals on one hand a weaker bonding of Zn than of Sn with the cerium substructures with a twice stronger Ce1–Sn bond compared to Ce2–Sn. On the other hand, a ferromagnetic ground state is identified from total energy differences in agreement with experiment.

Key words: Intermetallics, Stannide, Crystal Chemistry, Chemical Bonding (COOP), DFT, Spin Polarized Calculations, DOS, ELF