The Stannide $LiRh_3Sn_5$ – Synthesis, Structure, and Chemical Bonding

Puravankara Sreeraj[a], Dirk Johrendt[b], Helen Müller[b], Rolf-Dieter Hoffmann[a], Zhiyun Wu[a], and Rainer Pöttgen[a]

[a] Institut für Anorganische und Analytische Chemie, Sonderforschungsbereich 458 and NRW Graduate School of Chemistry, Westfälische Wilhelms-Universität Münster, Corrensstraße 36, D-48149 Münster (Germany)
[b] Department Chemie und Biochemie, Ludwig-Maximilians-Universität München, Butenandtstraße 5 – 13 (Haus D), D-81377 München, Germany

Reprint requests to R. Pöttgen. E-mail: pottgen@uni-muenster.de

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The lithium rhodium stannide $LiRh_3Sn_5$ was synthesized from the elements in a sealed tantalum tube and investigated *via* X-ray powder and single crystal diffraction: *Pbcm*, $a = 538.9(1)$, $b = 976.6(3)$, $c = 1278.5(3)$ pm, $wR2 = 0.0383$, 1454 F^2 values, and 44 variables. Refinement of the occupancy parameters revealed a lithium content of 92(6)%. $LiRh_3Sn_5$ crystallizes with a new structure type. The structure is built up from a complex three-dimensional $[Rh_3Sn_5]$ network, in which the lithium atoms fill channels in the *b* direction. The $[Rh_3Sn_5]$ network is governed by Rh–Rh (274 – 295 pm), Rh–Sn (262 – 287 pm), and Sn–Sn (289 – 376 pm) interactions. The lithium atoms have CN 13 (4 Rh + 9 Sn). Electronic band structure calculations and the COHP bond analysis reveal strong Rh−Sn bonds and also significant Rh−Rh bonding within the Rh_3Sn_5 network, which is additionally stabilized by weak but frequent Sn−Sn interactions.

Key words: Lithium Stannide, Crystal Chemistry, Chemical Bonding