

LICa₇Si₃H₃ AND LICa₇Ge₃H₃: NEW COMPLEX SILICIDE AND GERMANIDE HYDRIDE PHASES GROWN IN METAL FLUX. David A. Lang, Thomas E. Gedris, Susan E. Lattuner. Department of Chemistry and Biochemistry, Florida State University, 95 Chieftan Way, Tallahassee, FL 32306.

LiCa₇Si₃H₃ and LiCa₇Ge₃H₃ are produced from reactions of Si or Ge with CaH₂ in Ca/Li flux. These phases crystallize in orthorhombic space group *Pnma*. Unit cell parameters are $a = 9.8371(36) \text{ \AA}$, $b = 13.7352(50) \text{ \AA}$, $c = 8.7191(32) \text{ \AA}$ for LiCa₇Si₃H₃ and $a = 9.8599 \text{ \AA}$, $b = 13.7716 \text{ \AA}$, $c = 8.7430 \text{ \AA}$ for LiCa₇Ge₃H₃. These structures feature isolated Si⁴⁻ or Ge⁴⁻ anions and three crystallographic hydride sites. The Si⁴⁻ anions form silane during the protolysis reaction with NH₄Cl. ²⁹Si, ⁷Li, and ¹H MAS NMR spectra show Knight shifts in the semiconducting range. This agrees with density of states calculations which show a band gap of ~0.5 eV, supporting the identification of these compounds as charge-balanced Zintl phases. The presence of hydride anions makes these phases of interest as hydrogen storage materials. The hydrogen storage properties and thermal decomposition are being investigated using a custom-built thermovolumetric apparatus.

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