

Where The H Is the Interstitial: Single Crystal Neutron Diffraction Studies of Complex Metal Hydrides

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Metal flux reactions in lanthanide-rich eutectics such as La/Ni or Ce/Cu have yielded a variety of complex intermetallics that form as large crystals. We have found that carrying out flux reactions in the presence of anthracene (C₁₄H₁₀) results in the incorporation of both carbon and hydrogen into the growing products. While the position of carbon atoms can be determined using X-ray diffraction, neutron diffraction is crucial to locating and refining the positions of interstitial hydrides surrounded by heavy lanthanide atoms. Single crystal neutron diffraction data collected using the TOPAZ diffractometer at ORNL enabled the refinement of the hydride sites in La₁₅(FeC₆)₄H, La₃BC₂H_{1.7}, and Ce₄B₂C₂H_{2.4}. We were also able to refine H/F mixing on a fluoride-substituted variant of Ce₄B₂C₂(H/F)_x.