

Crystal Structure of a Zirconium Based Hydrogen Storage Material

N Garcia¹, K Falcon², C J Thomas³, J Robledo⁴, S Rocha⁵, M Yousufuddin⁶

¹UNT Dallas ²University of North Texas at Dallas, ³University of North Texas at Dallas, ⁴University of North Texas at Dallas, ⁵University of North Texas at Dallas, ⁶NA

nayeligarcialopez@my.untDallas.edu

Metal borohydride (MBH₄) compounds have been studied thoroughly for their potential as hydrogen storage materials. Zirconium borohydrides are one such class of metal borohydrides with hydrogen storage potential, however the interaction between the hydrides from BH₄⁻ and Zr is another fascinating feature worth exploring. Cp₂Zr(BH₄)₂ has been investigated for its potential as a hydrogen storage material and as a precursor for other hydrogen storage materials. But, to our knowledge, the structure of Cp₂Zr(BH₄)₂ showing the position of the hydrides is unknown. We present here the synthesis and crystal structure of Cp₂Zr(BH₄)₂ showing, for the first time, the position of the hydrides in relation to Zr.

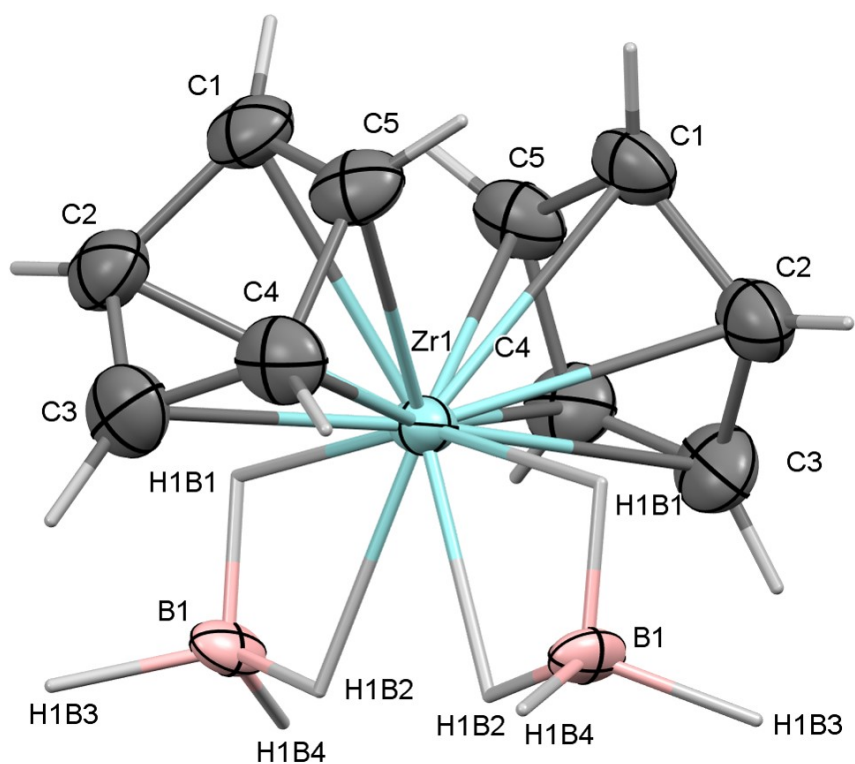


Figure 1