

MS14-P24 | PSEUDO-SYMMETRY AND ORDER-DISORDER TRANSITIONS IN METAL HYDRIDES

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Pseudo-symmetry is a well-known phenomenon in inorganic compounds and very common in metal hydrides for various reasons. Metallic hydrides typically exhibit non-stoichiometry by partial occupation of crystallographic sites by hydrogen. Ordered low-temperature modifications often show pronounced pseudo-symmetry, e. g. monoclinic or triclinic pseudo-cubic Laves phase hydrides. In complex hydrides, order-disorder transitions may arise due to rotational degrees of freedom in groups such as BH_4 (NaBH_4), SiH_3 (KSiH_3) or NiH_4 (Mg_2NiH_4). Sometimes, only an ordered arrangement is found showing pseudo-symmetry of a hypothetical disordered polymorph, e. g. IrH_4 and IrH_5 groups in monoclinic pseudo-hexagonal $\text{Mg}_6\text{Ir}_2\text{H}_{11}$. Directional (covalent) bonds are yet another reason for developing pseudo-symmetry. Zintl phases are a good example, since upon formation of Si-H and Si-Si bonds in $\text{CaSiH}_{1.33}$ and $\text{SrSiH}_{1.67}$, a superstructure of the parent hydrogen free phase occurs. Even in mainly ionic compounds like $\text{Eu}_6\text{Mg}_7\text{H}_{26}$ the more covalent nature of metal-hydrogen bonds introduces pseudo-symmetry as compared to more ionic fluorides and chlorides. Pseudo-symmetry in metal hydrides may thus occur for many different reasons. Resulting crystallographic pitfalls will be discussed on examples and advice given for dealing with such problems in structure solution and refinement.