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Eu(II) luminescence in the perovskite host lattices $KMgH_3$, $NaMgH_3$ and mixed crystals $LiBa_xSr_{1-x}H_3$

N. Kunkel[a*], A. Meijerink[b], M. Springborg[a] and H. Kohlmann[c*],

Supporting information

I. Characterization

X-ray powder diffraction data were collected on a *Panalytical Philips X'Pert Pro* diffractometer or a *Bruker D8 Advance* (with *Lynxeye*) with focusing Bragg-Brentano geometry and a fine focus X-ray tube ($CuK\alpha_{1,2}$ radiation). Samples were enclosed between kapton foils in apiezon grease, leading to an increased amorphous background below 22° 2θ and the two reflections at 21.53° 2θ and 23.91° 2θ. The data collection time was 60 min, diffraction range 10 – 110° 2θ. Furthermore, temperature-dependent XRD data of $KMgH_3$ were recorded on a *Huber G670* Guinier camera ($CuK\alpha_1$) with cryostat. Crystal structure refinement was carried out via Rietveld analysis using TOPAS 4.2 (Bruker AXS, Karlsruhe, Germany)[1] and the fundamental parameter approach[2]. The instrumental function was determined empirically by means of a reference scan of LaB_6. Typically, complete structures including hydrogen positions from literature were taken as starting structures and scale factors, lattice parameters, atomic positions of the metal atoms and microstructural parameters were refined. Standard deviations in the lattice constants are given as calculated by the program TOPAS 4.2 and might be underestimated, as can be often seen in Rietveld refinement programs[3].
Some $KMgH_3$ samples contained K_2MgH_4, however, since the $KMgH_3:Eu^{2+}$ sample used for temperature-dependent measurements did not contain impurity phase, the luminescence emission originates from $KMgH_3:Eu^{2+}$.

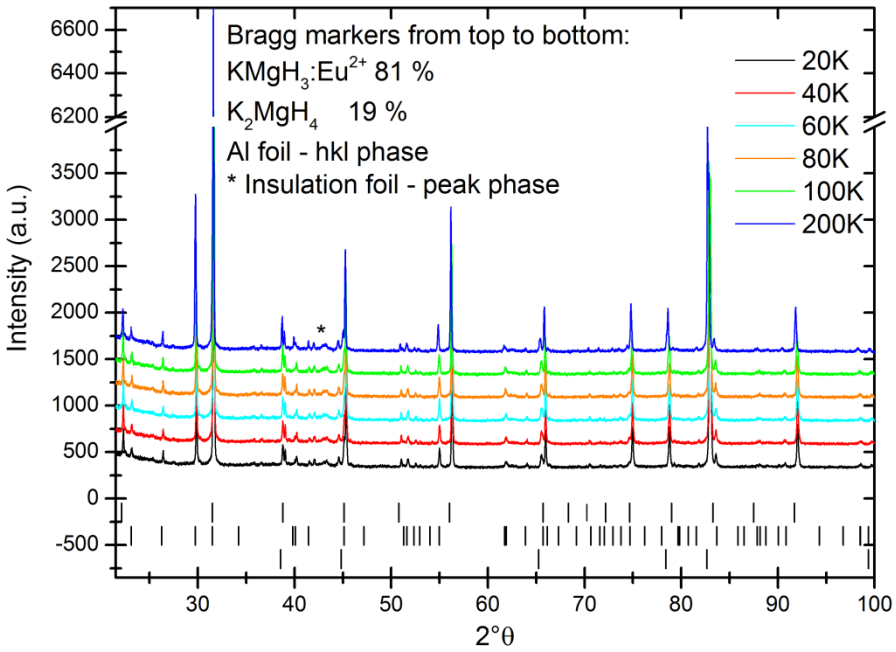

Figure 1: Temperature-dependent XRD data of $KMgH_3$.

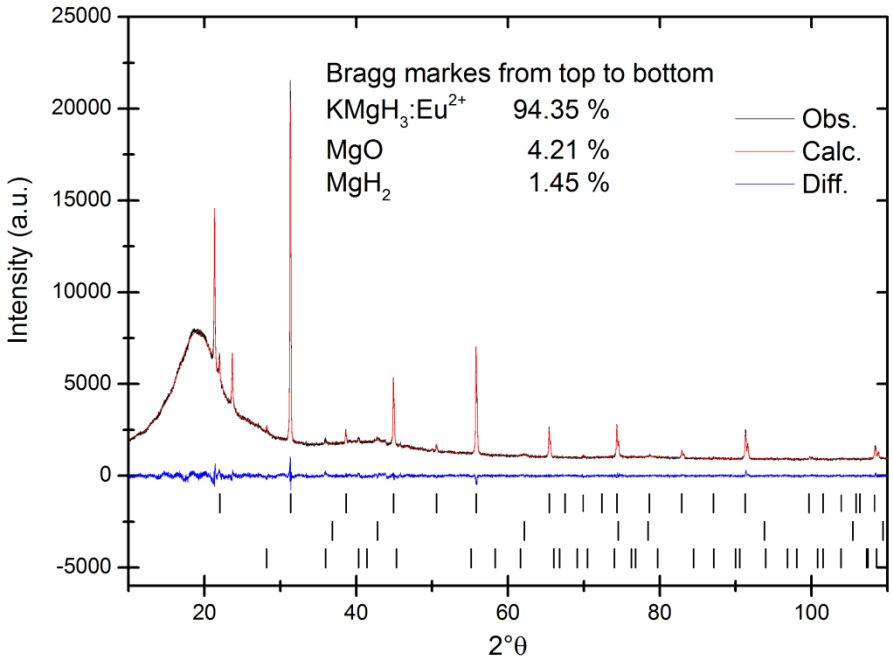

Figure 2: Refinement of the crystal structure of $KMgH_3:Eu^{2+}$ (1.0 mol%).

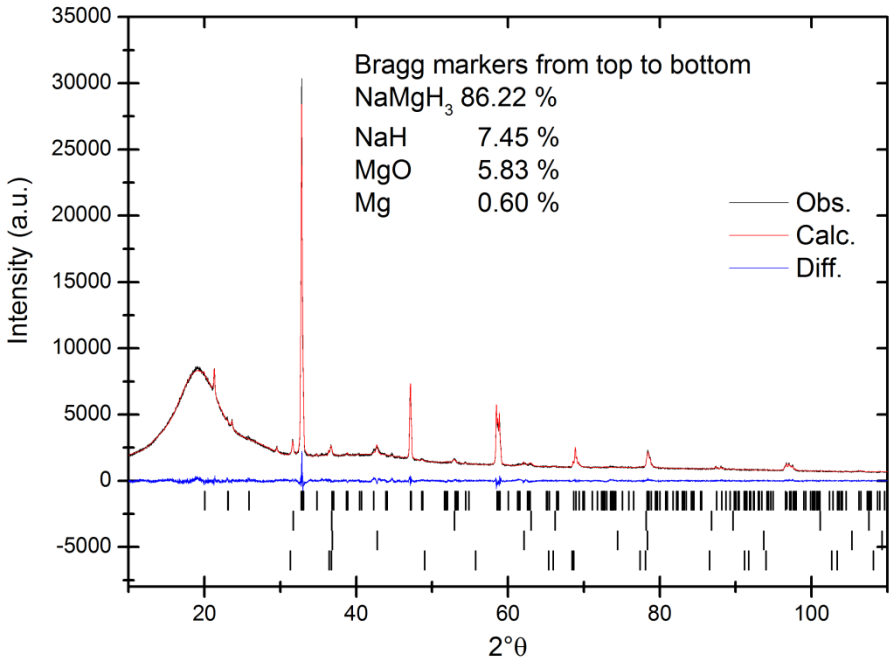

Figure 3: Refinement of the crystal structure of $NaMgH_3$.

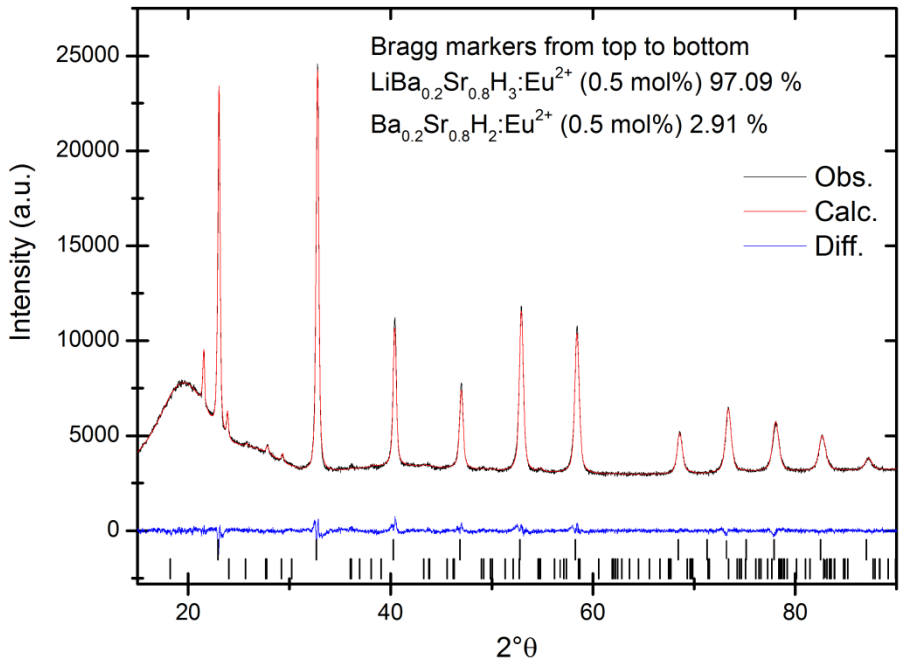

Figure 4: Refinement of the crystal structure of $LiBa_{0.2}Sr_{0.8}H_3:Eu^{2+}$ (0.5 mol%).

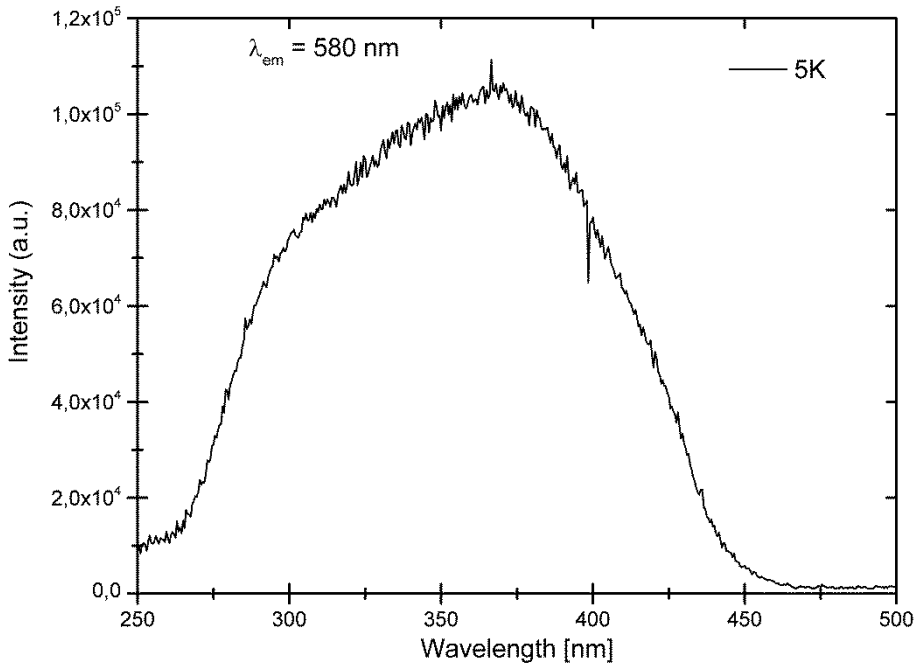

Figure 5: Excitation spectrum of $KMgH_3:Eu^{2+}$ (1.0 mol%) at 5 K.

II. References

1 Bruker, AXS, Karlsruhe, TOPAS V4.2, Gerneral profile and structure analysis software for powder diffraction data, Users's Manual, 2009.

2 A. A. Coelho, *J. Appl. Crystallogr.* 2003, **36**, 86-95.

3 B. H. Toby, *Powder Diffr.* 2006, **21**, 67-70.