

# **La<sub>2</sub>MgNi<sub>2</sub>H<sub>8</sub>, the first mixed polyanionic transition metal hydride**

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Following our discovery of a hydrogen induced insulating state in the LaMg<sub>2</sub>Ni-H system [1] we have investigated the closely related La<sub>2</sub>MgNi<sub>2</sub>-H system. Hydrogenation of tetragonal La<sub>2</sub>MgNi<sub>2</sub> at 10 bar and 100°C leads to a complex metal hydride of composition La<sub>2</sub>MgNi<sub>2</sub>H<sub>8</sub> having monoclinic symmetry. In contrast to LaMg<sub>2</sub>NiH<sub>7</sub> which displays tetradedral [NiH<sub>4</sub>]<sup>4-</sup> complexes that are isolated from each other, La<sub>2</sub>MgNi<sub>2</sub>H<sub>8</sub> displays two types of polyanionic hydrido complexes having novel geometries. The complexes are ordered and represent the first case of a mixed polyanionic metal hydride system in the literature. The metal and deuterium atoms were located by collecting high resolution synchrotron and neutron powder diffraction data, respectively. The structure (26 independent atoms) was solved by a direct space method and then refined by the Rietveld method. The Ni-H distances vary from 1.43 to 1.91 Å. Some hydrogen atoms are coordinated by La and Mg atoms only in octahedral [La<sub>4</sub>Mg<sub>2</sub>]-type or tetrahedral [La<sub>2</sub>Mg<sub>2</sub>]-type configurations. The hydride does not desorb hydrogen below 190°C and 1.10<sup>-1</sup> mbar pressure and segregates into LaH<sub>3</sub> and other unidentified phases above 300°C.

[1] K. Yvon, G. Renaudin, C. M. Wei, and M.Y. Chou, Phys. Rev. Lett. **94**, 066403 (2005)