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The crystal structure of ${}^7\text{Li}_2\text{ND}$ MASAMI TSUBOTA, Institute for Advanced Materials Research, Hiroshima University, MAGNUS H. SORBY, Institute for Energy Technology, Department of Physics, SATOSHI HINO, Graduate School of Advanced Sciences of Matter, Hiroshima University, TAKAYUKI ICHIKAWA, Institute for Advanced Materials Research, Hiroshima University, BJORN C. HAUBACK, Institute for Energy Technology, Department of Physics, YOSHITSUGU KOJIMA, Institute for Advanced Materials Research, Hiroshima University — Recently much attention has been given to reversible hydrogen storage materials possessing high gravimetric capacity. Lithium amide/imide systems are promising candidates. Chen *et al.*[1] found that a mixture of lithium amide and lithium hydride can reversibly store hydrogen up to 6.5 mass% forming lithium imide (Li_2NH). Among them, the crystal structure of Li_2NH is still controversial. Balogh *et al.*[2] have reported a cubic structure model. However, this model differs significantly from theoretical structure models. In this work, the crystal structure of the isotopically substituted ${}^7\text{Li}_2\text{ND}$ has been investigated by powder neutron and synchrotron X-ray diffraction experiments. In our data some peaks, which should be a single peak for cubic symmetry, were obviously split indicating a lower symmetry than cubic for lithium imide. The structure of ${}^7\text{Li}_2\text{ND}$ will be described. [1] P. Chen *et al.*, J. Phys. Chem. B **107** (2003) 10967. [2] M.P. Balogh *et al.*, J. Alloys Compd. **420** (2006) 326.

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