Solution of the heavily stacking faulted crystal structure of the honeycomb iridate $H_3LiIr_2O_6$
- Supporting Information -

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Solid-State NMR-spectroscopy

^{7}Li and ^{1}H solid-state NMR measurements were performed with a standard superheterodyne pulsed spectrometer. The frequency-swept NMR spectra were composed using Fourier-step-sum technique and each Fourier-transform spectrum has been acquired by standard spin echo with pulse-pulse periods of 40-50 μs. The powder samples were put into Fluorinert and shaken by motors under a field before a low-temperature measurement to align crystal orientations along the magnetic easy axis.

Figure S 1 shows ^{7}Li- and ^{1}H-NMR spectra of the partially field-oriented sample under fields 5T and 2T, respectively. The linewidths in the current experiment are mainly governed by spin-spin relaxation and demagnetization fields, not by the quadrupole shifts even for ^{7}Li signals. The Knight shifts are temperature dependent, mostly proportional to the bulk uniform magnetization. The data point to one crystallographically distinct Li-site and to H-sites with nearly identical chemical environment. If there were more than one crystallographic Li-site and if the H-sites exhibited vastly different chemical environments, there would be multiple distinguishable singles NMR spectra.

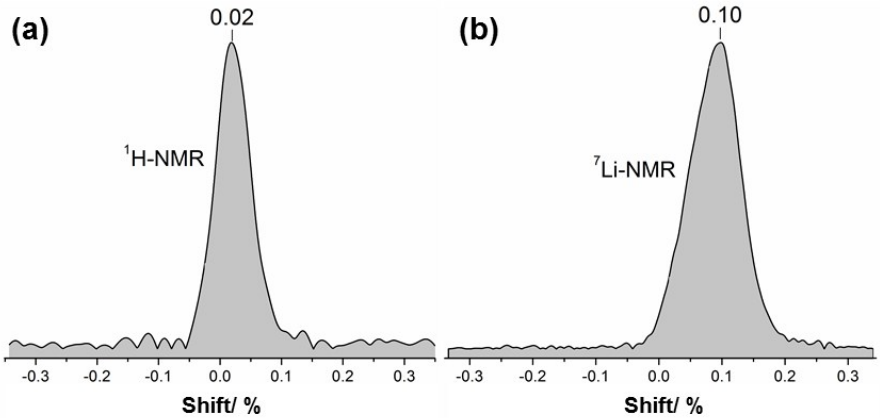

Figure S 1. (a) ^{1}H- and (b) ^{7}Li-solid state NMR spectra of $H_3LiIr_2O_6$.

Pseudosymmetries in the lattice of $H_3LiIr_2O_6$

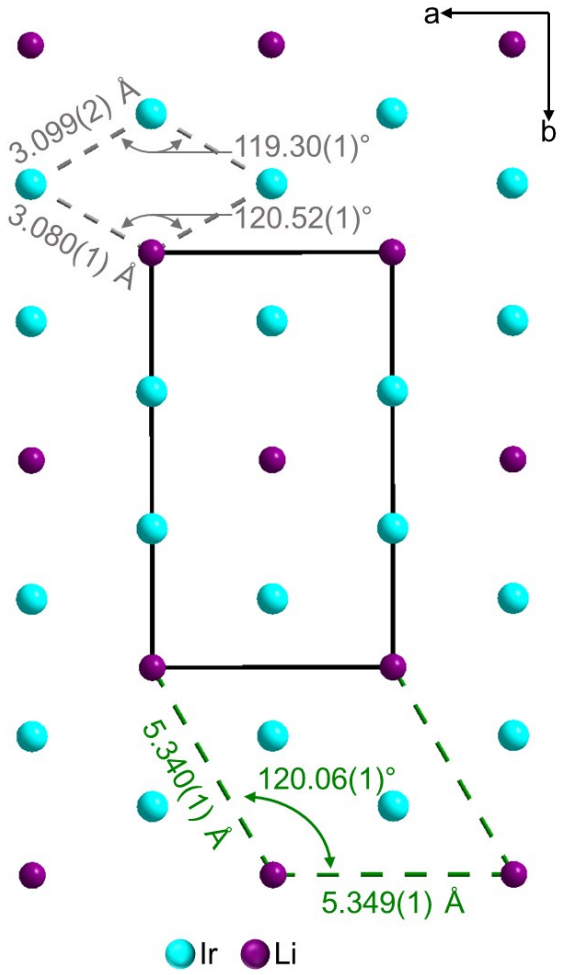

Figure S 2. Cation layer in the crystal structure of $H_3LiIr_2O_6$, the unit cell edges are presented as black lines, the *ab*-plane of a pseudo-trigonal unit cell as found by O'Malley et al.[1] are given as dashed grey lines, the translational symmetry is broken by the ordering of the cation sublattice, the *ab*-plane of a pseudo-hexagonal unit cell is indicated by dashed green lines, the symmetry is broken by the predominance of the **S1**-stacking vector (Fig. 9a in the manuscript).