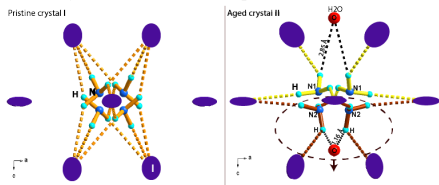


[6] J. Xie *et al.*, *Journal of Power Sources*, **285**, 349 (2015).

[7] T. Baikie *et al.*, *J. Mater. Chem. A1*, 5628 (2013).

[8] A. Arakcheeva, D. Chernyshov, M. Spina, L. Forro, E. Horvath. *CH<sub>3</sub>NH<sub>2</sub>PbI<sub>3</sub>: precise structural consequences of water absorption at ambient conditions* *Acta Cryst. B*. (Submitted in April, 2016).



**Figure 1.** The N-H...I H-bonds in the pristine and the aged crystals. Four shown NH<sub>3</sub> groups conform to four orientations of MA<sup>+</sup>. In I, all NH<sub>3</sub> groups are statistically present with probability of 25% for each one. In II, N2H<sub>3</sub> and N1H<sub>3</sub> are present with probability of 29.5% and 16.5%, respectively.

**Keywords:** crystal structure, hybrid organic-inorganic lead iodide, aged MAPbI<sub>3</sub>

## MS20-P2 Thermoelectric transport properties in magnetically ordered crystals

Hans Grimmer<sup>1</sup>

<sup>1</sup>. Laboratory for scientific developments and novel materials, Paul Scherrer Institut, WHGA/342, Villigen PSI, CH-5232, Switzerland

email: hans.grimmer@psi.ch

Thermoelectric transport properties of magnetically ordered crystals in an external magnetic field  $\mathbf{H}$  were investigated in [1, 2] from a space-time symmetry point of view. Crystals belonging to any of the 122 point groups may show electric resistivity, thermal conductivity, Seebeck and Peltier effect for  $\mathbf{H}=0$ , as well as the following effects linear in  $\mathbf{H}$ : Hall, Righi-Leduc, Nernst and Ettingshausen. The tensors describing these effects are invariant under space inversion  $I$  and time inversion  $I'$ ; their form can be found using Neumann's principle and the Onsager relations  $\Gamma_{\mu\nu}(\mathbf{H}) = \Gamma_{\nu\mu}(-\mathbf{H})$ , where  $\Gamma$  is a  $6 \times 6$  matrix giving the gradient of the electrochemical potential and the heat current as functions of the electric current and the temperature gradient in the crystal.

Magnetically ordered crystals belong to one of the 90 magnetic point groups (MPGs) that do not contain time inversion  $I'$  as a separate element. For  $\mathbf{H}=0$ , spontaneous Hall and Righi-Leduc effects appear for the 31 MPGs allowing ferromagnetism; spontaneous Nernst and Ettingshausen effects appear for 58 MPGs. Whereas magneto-resistance, magneto-heat-conductivity, magneto-Seebeck and magneto-Peltier effect are of even order in  $\mathbf{H}$  in magnetically unordered crystals, such effects linear in  $\mathbf{H}$  appear in case of magneto-resistance and magneto-heat-conductivity for the 66 MPGs allowing piezomagnetism, and in case of magneto-Seebeck and magneto-Peltier effect for all 69 MPGs that do not contain space-time inversion  $I'$  as a separate element.

To find the forms of the tensors describing the effects in magnetically ordered crystals, Onsager relations were used in [1] as formulated in [3]:  $\Gamma_{\mu\nu}(\mathbf{H}, \mathbf{M}) = \Gamma_{\nu\mu}(-\mathbf{H}, -\mathbf{M})$ , where  $\mathbf{M}$  denotes the time averaged magnetization field describing the magnetic configuration.

Whereas the results of [1] and [2] agree for  $\mathbf{H}=0$ , some of the results obtained in [2] for the effects linear in  $\mathbf{H}$  are at odds with generally accepted results. The procedure used in [1] makes it easy to separate tensors into two parts being invariant and changing sign under  $I'$ , respectively. Whereas [2] considers both parts as forming a single tensor, it will be shown that considering the two parts (which can be measured separately) as independent tensors leads to simpler and stronger results.

### References:

- [1] H. Grimmer (1993). *Acta Cryst. A49*, 763-771.
- [2] M. Seemann, D. Ködderitzsch, S. Wimmer & H. Ebert (2015). *Phys. Rev. B*, **92**, 155138.
- [3] S. Shtrikman & H. Thomas (1965). *Solid State Commun.* **3**, 147-150.

**Keywords:** Thermoelectrics, Transport properties, Onsager relations, Magnetic order