pyLIB

* collection of functions for my PhD-project

Emil Andreasen Klahn, [eklahn@chem.au.dk](mailto:eklahn@chem.au.dk)

Last updated: 31-03-2018

**projectData 🡪 PND\_susceptibility.py**

Holds susceptibility tensors, susceptibility tensor errors and unit cell parameters of the two compounds in the study

**atomicInfo.py**

Only holds a dictionary of information about atoms. Not complete at all.

**crystalStructure.py**

class crystalStructure

Input

params: the unit cell parameters for the crystal structure in question