A Solid State NMR, Powder XRD Study of Phase Evolution in Mechanochemically Prepared Mixed Cation Lead Halide Perovskites (Cs-CH3NH3)PbX3

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**Guide for data processing**

**Laboratory XRD**

The ‘room temperature’ folder contains powder XRD data collected at ambient temperature in xy format (ASCII). The file names are denoted as Cs%X.xy where Cs% is the nominal composition and X denotes chloride or bromide. These can be imported as standard ASCII files for plotting and analysis.

The ‘variable temperature’ folder contains powder XRD data in xye format (ASCII). The folder names follow Cs%X where Cs% is the nominal composition and X denotes chloride or bromide. Each file contains the temperature of data collection (K) in the file name.

**Synchrotron XRD data**

The datasets in ‘Synchrotron XRD’ folder are named as Cs%X where Cs% is the nominal composition and X denotes chloride or bromide. Each folder has a corresponding text file with the same name and .log extension containing the file number and the corresponding temperature of acquisition (K). Individual data sets are in xye format (ASCII) for further processing and analysis.

**NMR data**

The NMR folder contains sub-folders named ‘Hand grinding vs Mechanochemical’ and ‘CsxMA1-xPbX3’ which contain folders for each sample/composition. These can be opened and processed using Bruker Topspin software. The title file provides the details of target nuclei, MAS rate and sample composition for each dataset.

**TEM**

The TEM folder contains images (HRTEM and SAD) with Cs%X filename. .scdx files can be opened with SingleCrystal software from Crystal Maker for indexing.

**DSC**

DSC folder contains the DSC data in .opju format compatible with Origin software from Originlab.

**UV-Vis**

UV­\_Vis folder contains the absorption data in .opju format compatible with Origin software from Originlab.