**Elucidation of Structural and Optical Properties of Metal Cation (Na+, K+, and Bi3+) Incorporated Cs2AgInCl6 Double Perovskite Nanocrystals**

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**XRD Data**

This contains 3 subfolders of Cs2AgInxBi1-xCl6, Cs2NaxAg1-xInCl6:Bi, and Cs2KxAg1-xInCl6:Bi nanocrystals labelled as In-Bi, Na incorporated and K incorporated, respectively. In each subfolder, the XY notepad file of each composition is presented, which can be processed using Origin or Excel software.

**TEM Data**

This contains TEM Tiff image of Cs2AgIn0.90Bi0.10Cl6, Cs2Ag0.60Na0.40InCl6:Bi, and Cs2Ag0.60K0.60InCl6:Bi nanocrystals. Each sample has a low resolution and high resolution micrograph.

**UV-Vis absoption Data**

This contains CSV file of Cs2AgInxBi1-xCl6, Cs2NaxAg1-xInCl6:Bi, and Cs2KxAg1-xInCl6:Bi nanocrystals labelled as In-Bi, Na incorporated, and K incorporated. CSV file can be processed using Excel or Origin software.

**Photoluminescence (PL) Data**

This folder contains the sample photo and PL data of Cs2AgInxBi1-xCl6, Cs2NaxAg1-xInCl6:Bi, and Cs2KxAg1-xInCl6:Bi nanocrystals in CSV format, which can be processed using Excel or Origin software.

**NMR Data**

The NMR folder contains the raw data acquired for 133Cs, 23Na and 39K MAS NMR data for Cs2AgInxBi1-xCl6, Cs2NaxAg1-xInCl6:Bi, and Cs2KxAg1-xInCl6:Bi nanocrystals along with their corresponding *T*1 saturation recovery data. This raw data (.1r files) can be opened and fully processed using the Bruker software, ‘Topspin’ and then exported to origin as an ASCII file for further analysis.

**DFT calculations**

The folder for DFT calculations contains all the output files (.magres) obtained from the CASTEP DFT software for the Cs2KxAg1-xInCl6:Bi nanocrystal system and the DOS data from the OptaDOS postprocessing tool. The .dat and .magres file formats can be opened using a standard editor such as notepad, notepad++, vim or emacs. The .magres files can be processed using the Atomic Simulation Enviroment (Ask Hjorth Larsen et al 2017 J. Phys.: Condens. Matter 29 273002) or visualised using [MagresView](https://www.ccpnc.ac.uk/magresview/magresview/magres_view.html).

All text documents and the .xy XRD data can be opened using Excel, OriginPro or any text editor. OPJU files can be opened in Origin or OriginPro. .Tiff files can be opened using Photo Viewer. .Csv file can be opend using Excel. .1r files can be opened using the Bruker software Topspin. .magres files can be opened using an editor.