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X-ray production cross section measurements for the analysis of metal halide perovskite thin films using heavy ion PIXE spectroscopy

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Abstract.

The use of perovskites for the development of solar cell devices continues to gain traction due to their high light absorption efficiency and tuneable bandgap. Unfortunately, well studied high efficiency organic perovskites contain lead halide compounds in their composition, such that wide-scale commercialisation may not be feasible due to environmental risks and the associated resource access limits. The alternative and more environmentally friendly inorganic metal halide perovskites however have a lower band gap and similarly low light absorption efficiencies compared to their organic counterparts, which negatively affects their performance. Current efforts aimed at achieving higher absorption efficiencies requires better understanding of their structural complexity, including quantitation of both light and heavy elemental impurities within the perovskite matrix. The concurrent use of Ion Beam Analysis (IBA) techniques such as Heavy Ion Particle Induced X-ray Emission (HI-PIXE) spectroscopy together with Time of Flight- Elastic Recoil Detection Analysis (ToF-ERDA) may be an effective method for studying these properties. For instance, PIXE can be used to provide information on the relative concentration of heavy elements, while ToF-ERDA can provide information on the relative concentration of light elements (from H up to O), along with elemental depth profiles of a material (as well as its thickness).

However, unlike with protons, using heavy ion probes like presents a challenge for PIXE due to the unavailability of X-ray production cross section data needed for atomic quantitation. This also extends to the analysis of heavy element targets such as Sn and Cs, which are typically found in metal halide perovskites like . Large discrepancies between theoretical predictions and experimental X-ray production cross section data exacerbate this limitation, requiring additional and substantial experimental measurements. This study therefore presents measurements of X-ray production cross sections of Sn and Cs induced by ⁶³Cu^{q+} ion beams within the (20 –34) MeV ion energy range.

The measurements were carried out using CsBr and thin films prepared using spin coating on Fluorine doped Tin Oxide (FTO) substrates. The cross section data is compared to conventional theoretical models such as the ECPSSR, developed from the binary encounter approximation, and is discussed in terms of the prominent ionisation mechanisms.

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