Report for the experiment HC-3840

Cs_4PbBr_6 emissive and non emissive powder were analysed.

Data for PDF analysis were collected ID22 beamline of the European Synchrotron Radiation Facility (ESRF; Grenoble, France) at 300 K and 90 K using a wavelength λ = 0.2065 Å. Data from an empty borosilicate capillary were collected to subtract the container scattering; moreover, a standard LaB_6 sample was analyzed using the same experimental conditions in order to describe the experimental resolution effects. Reduction of the total scattering data to obtain G(r), the reduced PDF, and S(Q), the total-scattering structure function, was achieved by the PDFgetX3 software[37] using Qmax = 25.0 Å-1, a range sufficient for an accurate analysis. Full-profile fitting of the G(r) function was carried out using the PDFgui software.

All inspected samples crystallize in the $R\bar{3}c$ space group (space group number: 167) at 300 K. Figure 1 shows a fitting of a PDF function for one of the analysed samples, selected as representative.

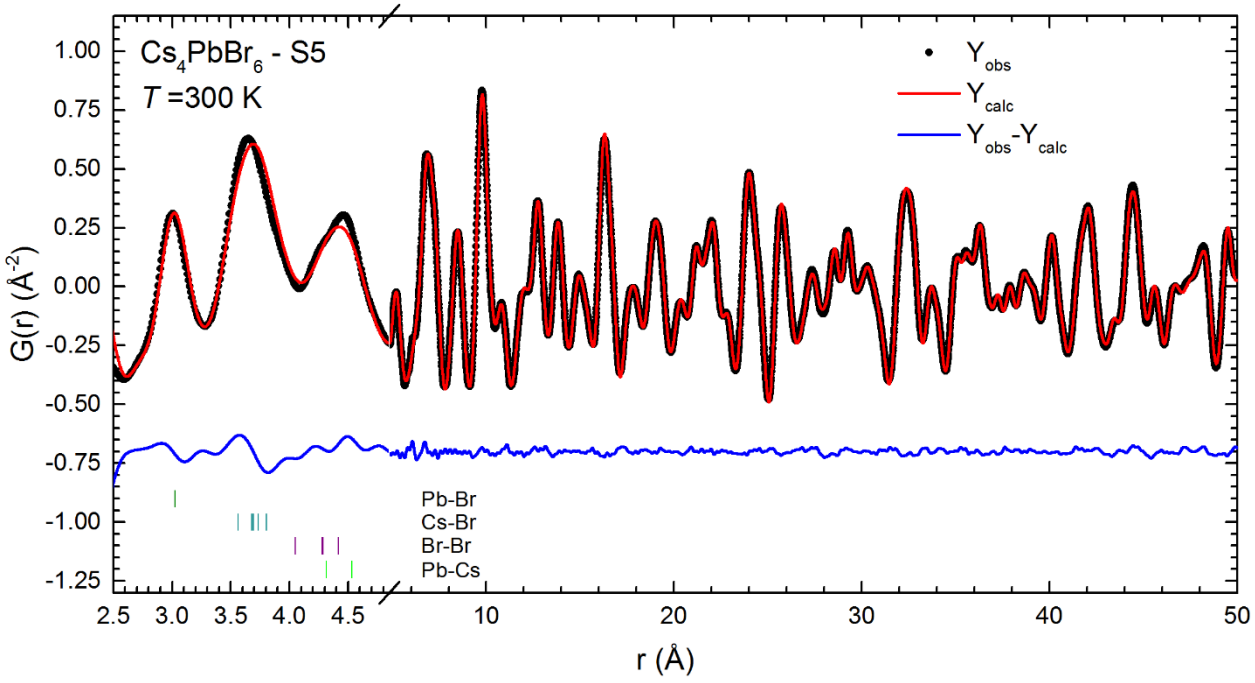

Figure 1: PDF data of a Cs_4PbBr_6 sample collected at 300 K and fitted with the $R\bar{3}c$ structural model (the difference between observed data and fitted PDF is reported in the lower field; the vertical bars indicate the bond lengths with r < 5 Å).

The thermal displacement parameters display higher values measured at the positions of the Cs and Br atoms. On the contrary, Pb atoms display lower values, indicating that lone pairs are steroinactive with the valence charge equally distributed between the Pb-Br bonds. Moreover, the G(r) fitting

evidences the strong anisotropic nature of the atomic displacement parameters. The atomic displacements are strongly anisotropic for Cs(1) as well as, on a less amount, for Cs(2) and Br ions; conversely, atomic displacements for Pb are rather isotropic.

Moreover, structural data indicate that the Cs_4PbBr_6 non-emissive powders are characterized by notably larger cell sizes than the emissive ones; this behaviour has been related to the occurrence of structural H_2O (or OH- units) in the structural voids. Analysis are still in progress in order to ascertain how structural H_2O can quench the emission properties in this material.