

Description of Additional Supplementary Files

File name: Supplementary Data 1

Description: Structure of the bare Model A, used for the SXR D fits.

File name: Supplementary Data 2

Description: Structure of the bare Model B, used for the SXR D fits.

File name: Supplementary Data 3

Description: Structure of the bare Model C, used for the SXR D fits.

File name: Supplementary Data 4

Description: Structure of Model A with one additional O-atom, used for the SXR D fits.

File name: Supplementary Data 5

Description: Comparison of the measured and calculated structure factors for the full set of CTRs.