**Description of Additional Supplementary Files**

File name: Supplementary Data 1  
Description: Structure of the bare Model A, used for the SXRD fits.

File name: Supplementary Data 2  
Description: Structure of the bare Model B, used for the SXRD fits.

File name: Supplementary Data 3  
Description: Structure of the bare Model C, used for the SXRD fits.

File name: Supplementary Data 4  
Description: Structure of Model A with one additional O-atom, used for the SXRD fits.

File name: Supplementary Data 5  
Description: Comparison of the measured and calculated structure factors for the full set of CTRs.