

SUPPORTING INFORMATION

Improved multivariate analysis for fast and selective monitoring of structural dynamics by in situ x-ray powder diffraction.

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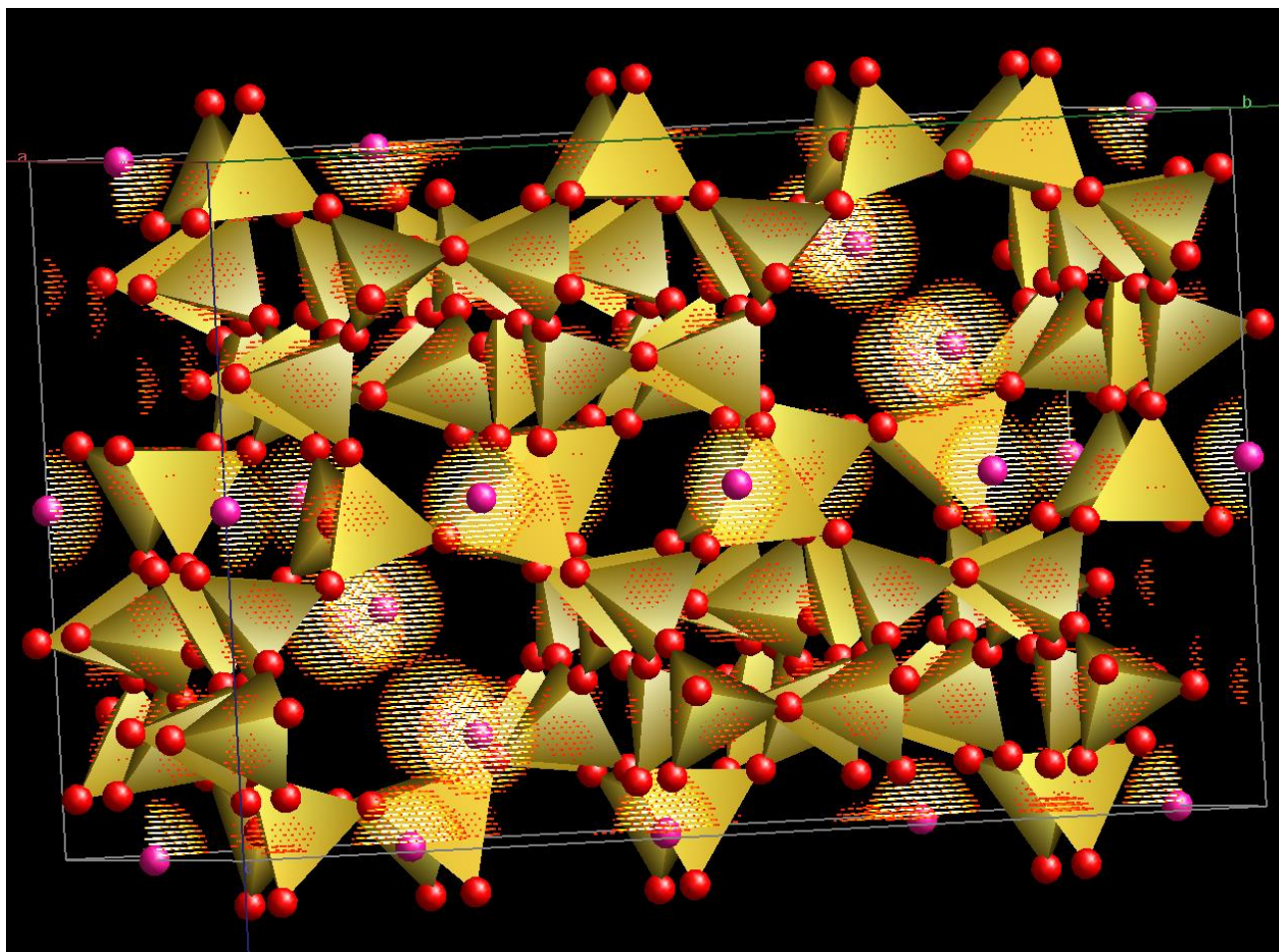


Figure S11 Fourier difference electron density map calculated for the low-T pattern, by using a model with 4 Xe atoms (ref 1). Not clear extra density is seen.

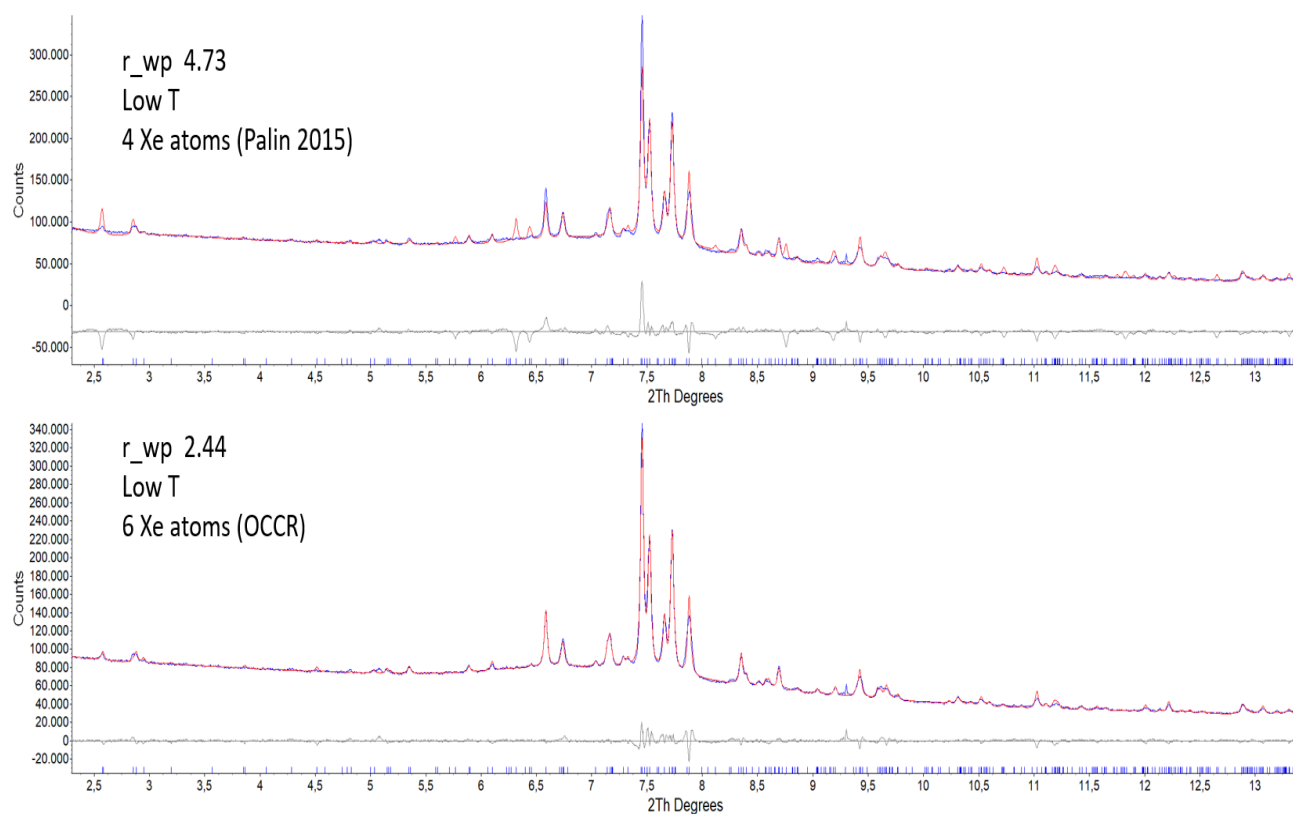


Figure SI2 Results of Rietveld refinement of the low T static pattern with the structural model composed by 4 Xe atoms derived by previous analysis (ref 1) (top) and by 6 Xe atoms derived by the present peak alignment+OCCR analysis (bottom).

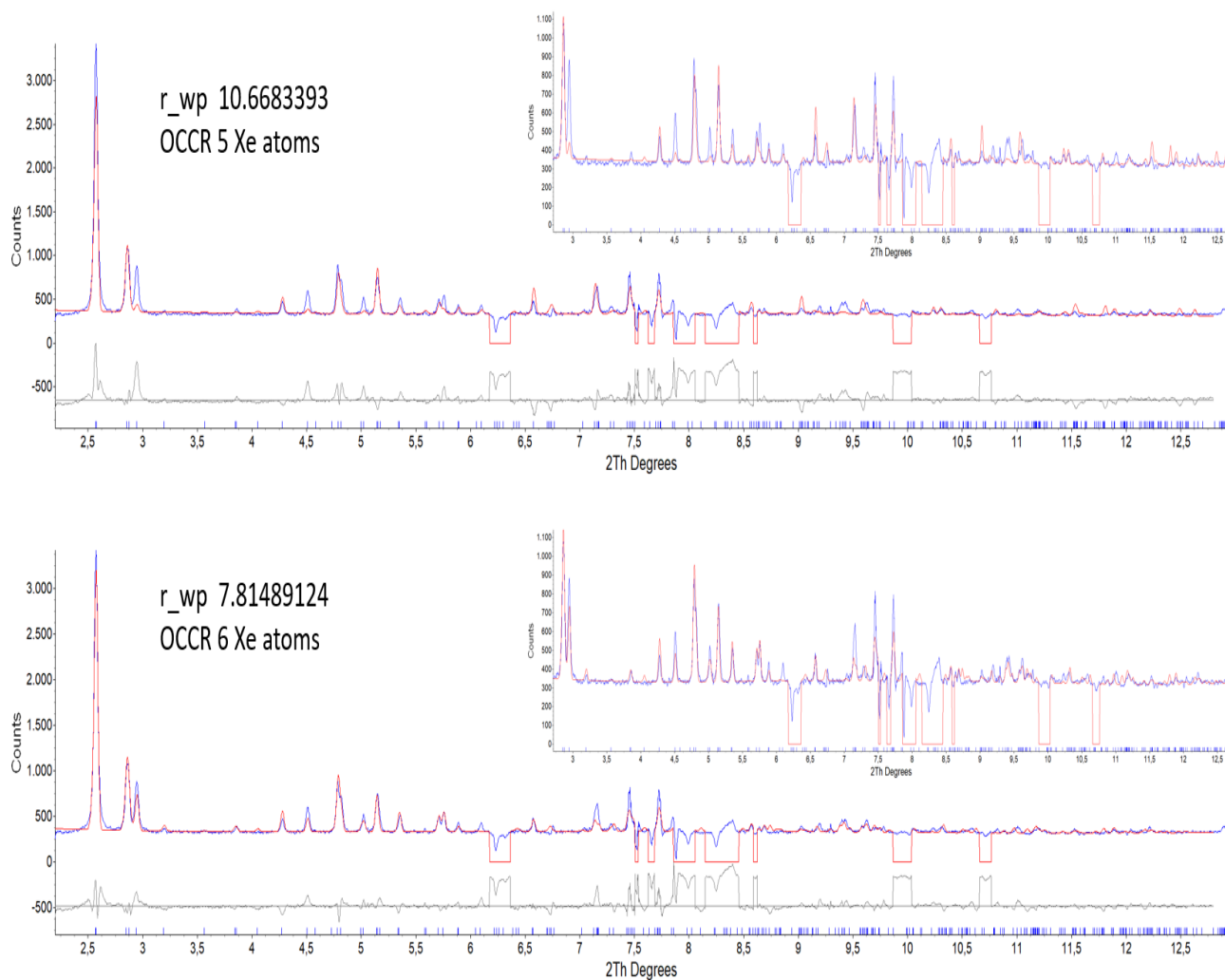


Figure SI3 Results of Rietveld refinement of the pattern obtained by the peak alignment+OCCR procedure with the structural model composed by 5 (top) or 6 (bottom) Xe atoms. Regions with intensities under the background are excluded from the analysis.