

Supporting Information

Noncovalent bonding assessment by Pair Distribution Function

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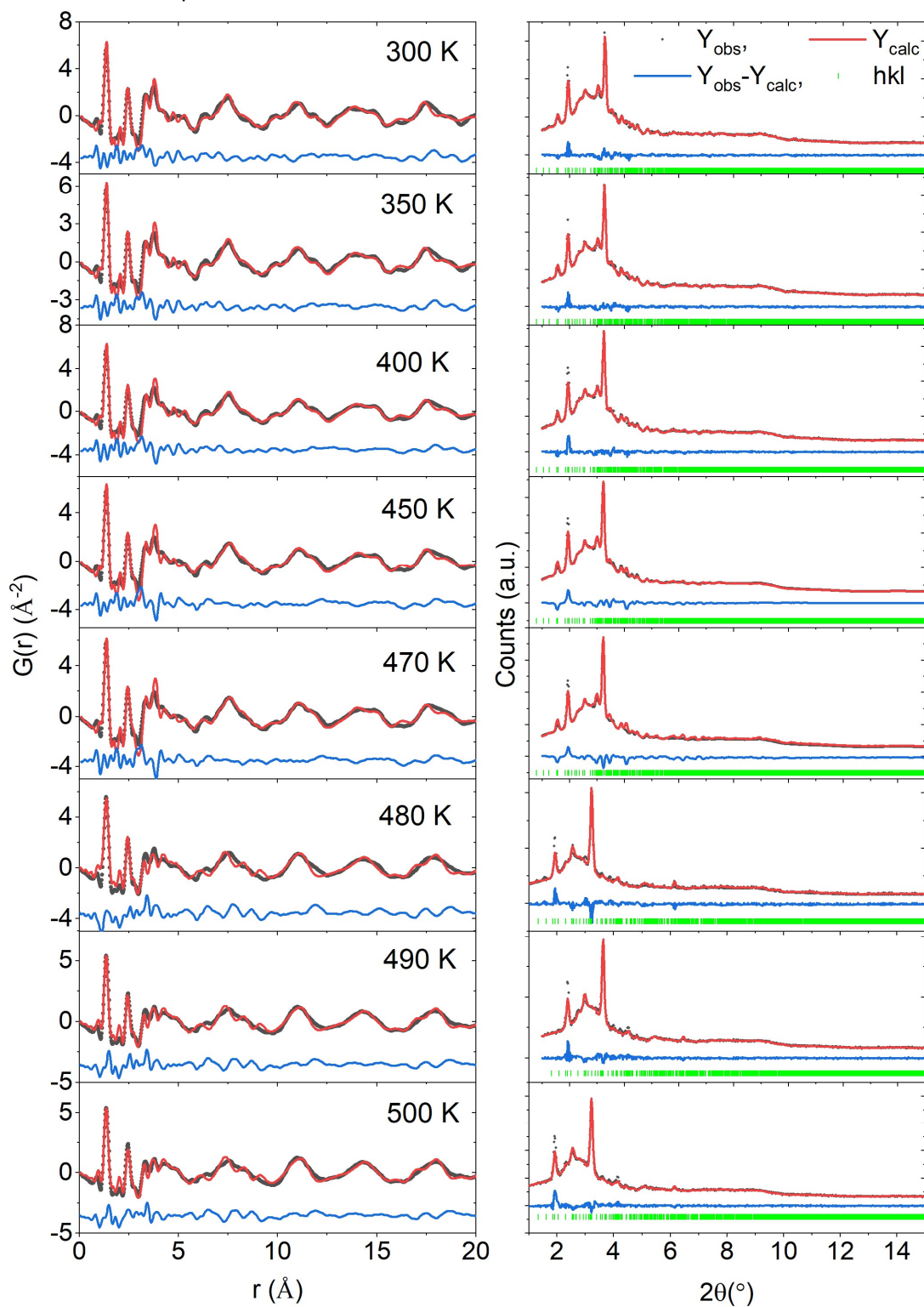


Figure S1. Magnified view of the Joint PDF (left) and Rietveld fits (right) using the HAZFAP01 model (350-470 K) and HAZFAP07 (480-500 K). The fits were done in the 0-50 \AA and 1-60 $^\circ$ range.

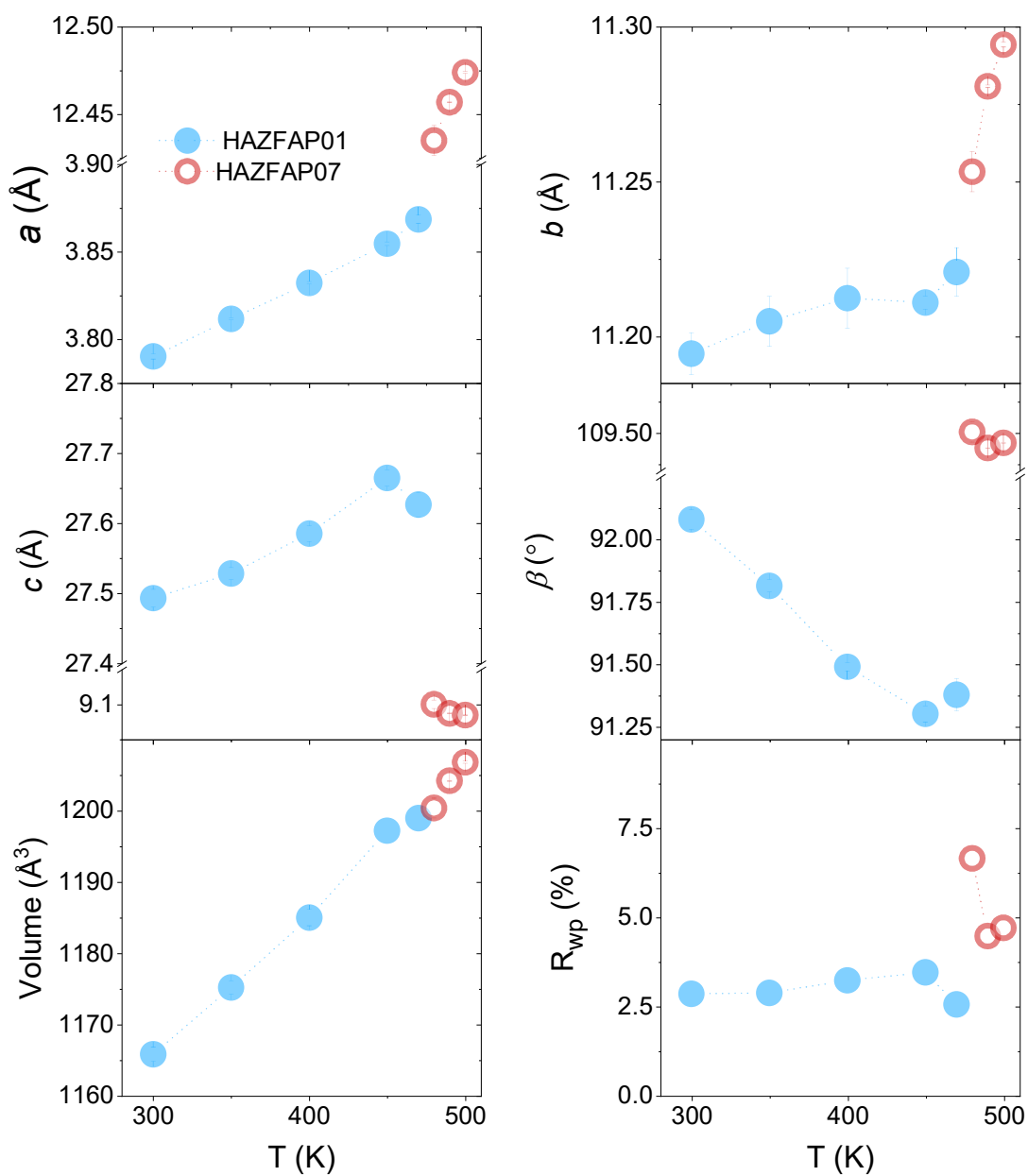


Figure S2. Refined lattice parameters and R_{wp} of the combined refinement.

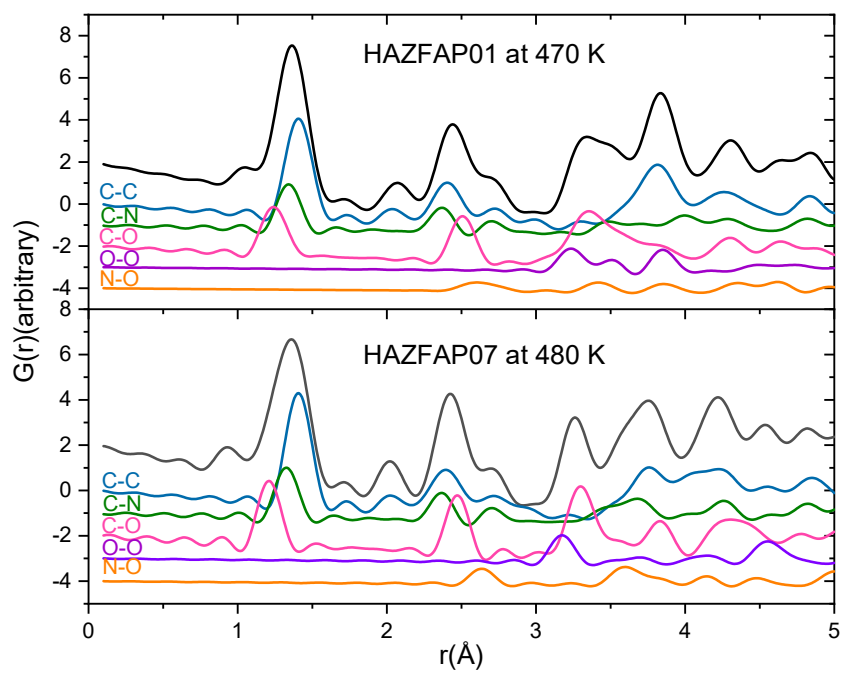


Figure 3. Simulated XPDF of BIPY:SQA models refined against PDF and Bragg data with C-C, C-N, C-O, O-O and N-O partials indicated at 470 K and 480 K.