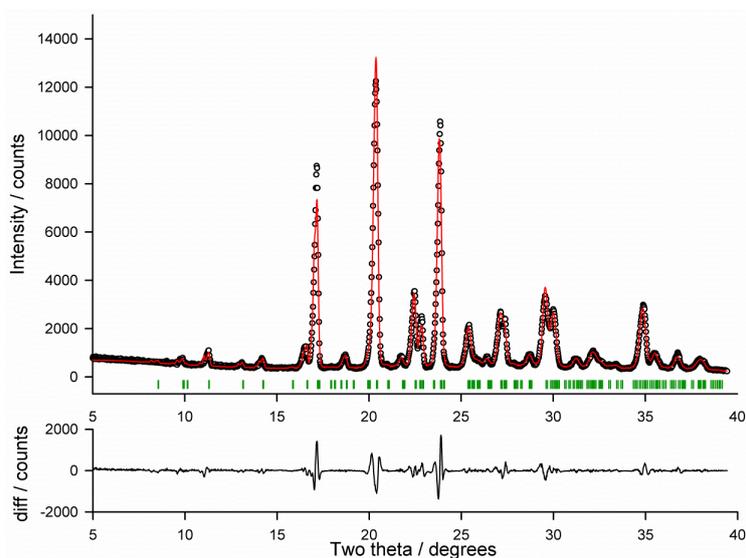


## Supporting Information

**Figure S1.** Le Bail fit ( $R_{wp} = 9.98\%$ ) between the reflection PXRD data of **1** with a model consisting of the cell parameters derived from the single crystal structure ( $a = 9.5670$ ,  $b = 20.5293$ ,  $c = 17.6775$  Å). Black dots indicate raw data, while the red line indicates the calculated model. Tick marks (green) are the  $2\theta$  positions for the  $hkl$  reflections. The difference pattern is shown at the bottom.



**Figure S2.** Le Bail fit ( $R_{wp} = 16.24\%$ ) between the reflection PXRD data of **3b** with a model consisting of the cell parameters derived from the single crystal structure ( $a = 16.0291$ ,  $b = 7.5748$ ,  $c = 11.5224$  Å). Black dots indicate raw data, while the red line indicates the calculated model. Tick marks (green) are the  $2\theta$  positions for the  $hkl$  reflections. The difference pattern is shown at the bottom.

