

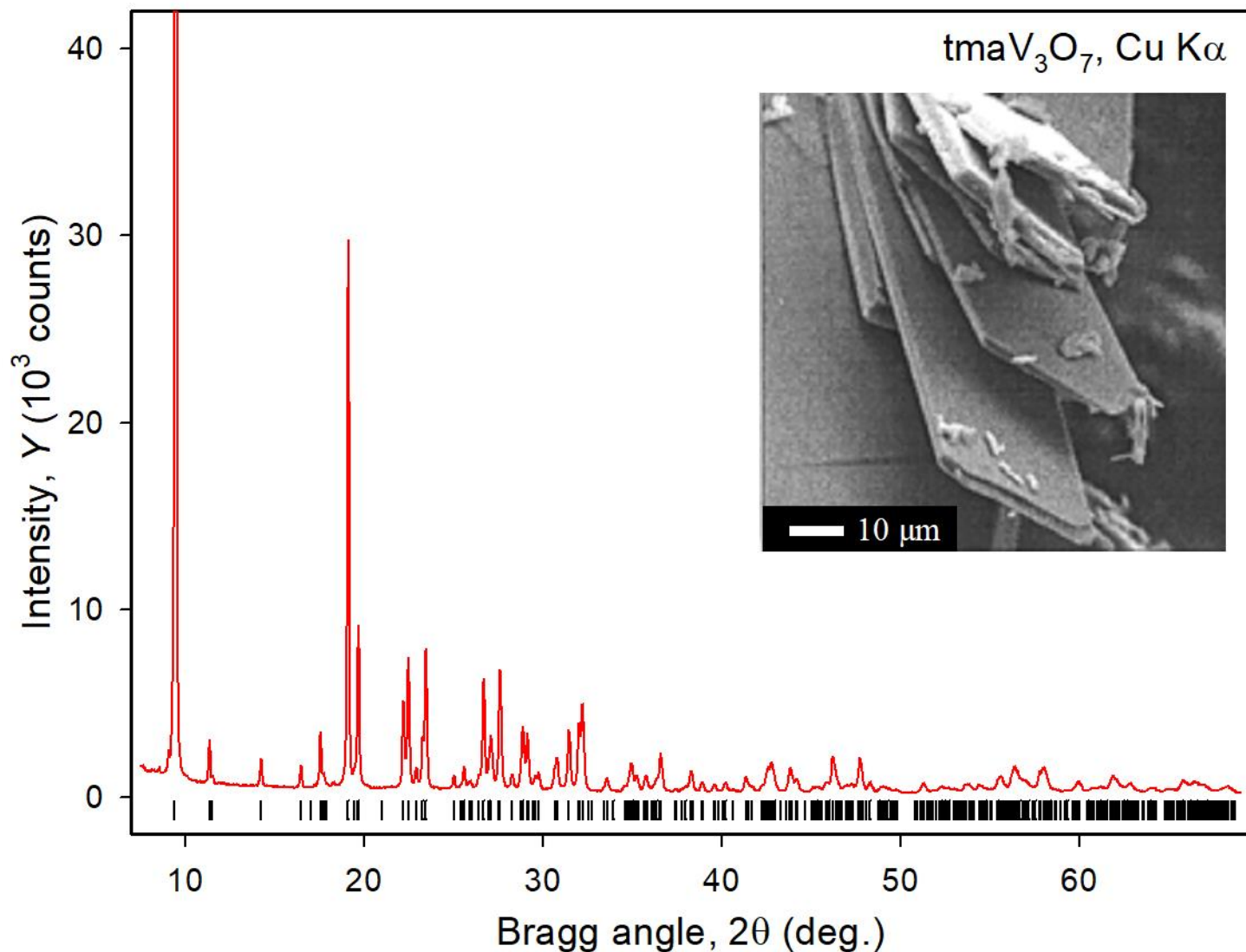
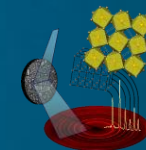


Figure 21.1. Powder diffraction pattern collected from the $tmaV_3O_7$ powder using $Cu\ K\alpha$ radiation on a Scintag XDS2000 diffractometer.

The experiment was carried out in a step scan-mode with a step 0.02° and counting time 60 s per step. The *vertical bars* indicate calculated positions of the $K\alpha_1$ components of all possible Bragg reflections. The inset shows the SEM image of particle morphology in the as-received state.

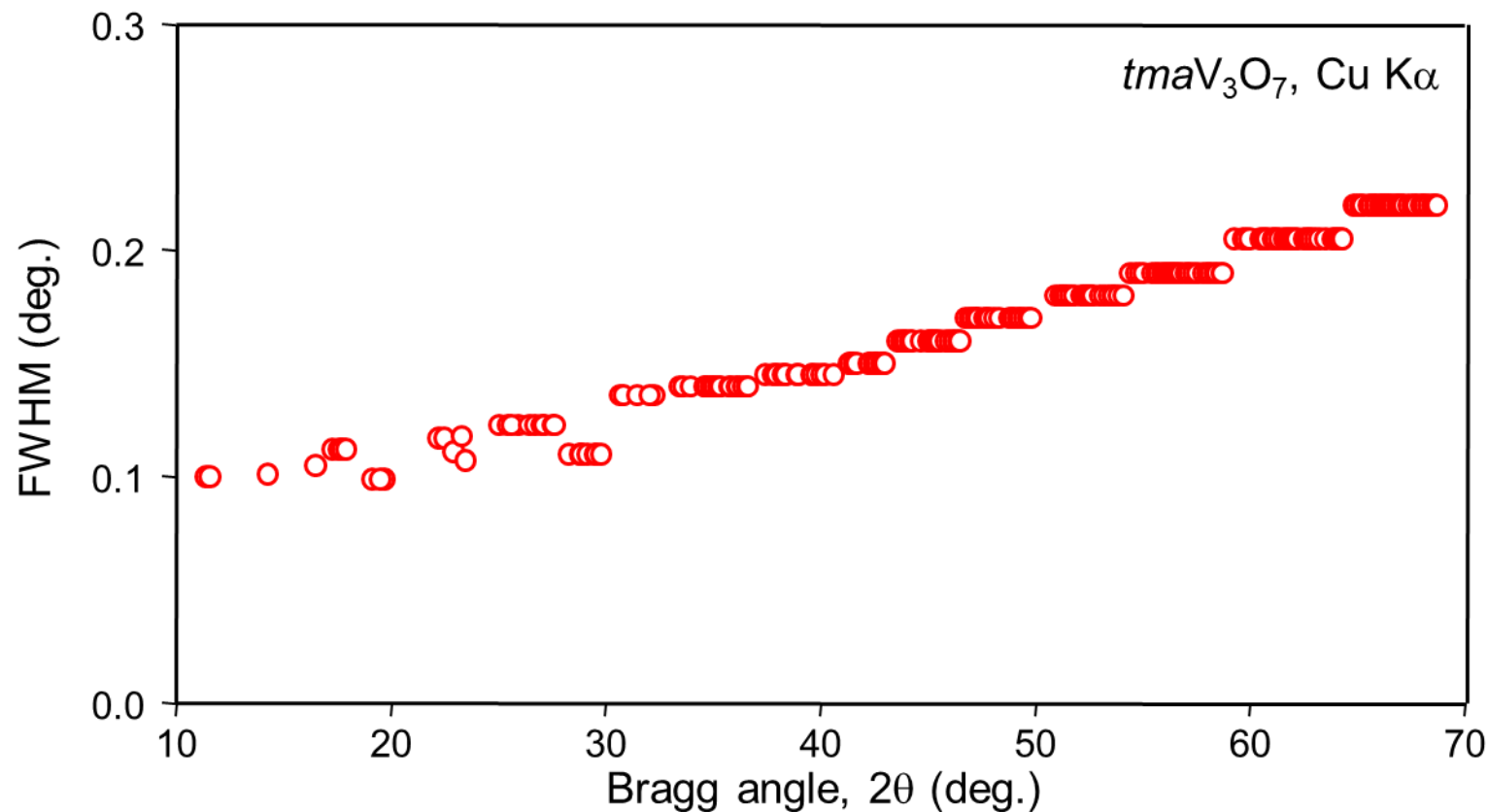
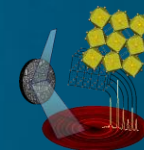


Figure 21.2. Full width at half maximum as a function of Bragg angle observed (below $2\theta = 35^\circ$) and linearly interpolated (above $2\theta = 35^\circ$) in the powder diffraction pattern of $tmaV_3O_7$ shown in Figure 21.1.

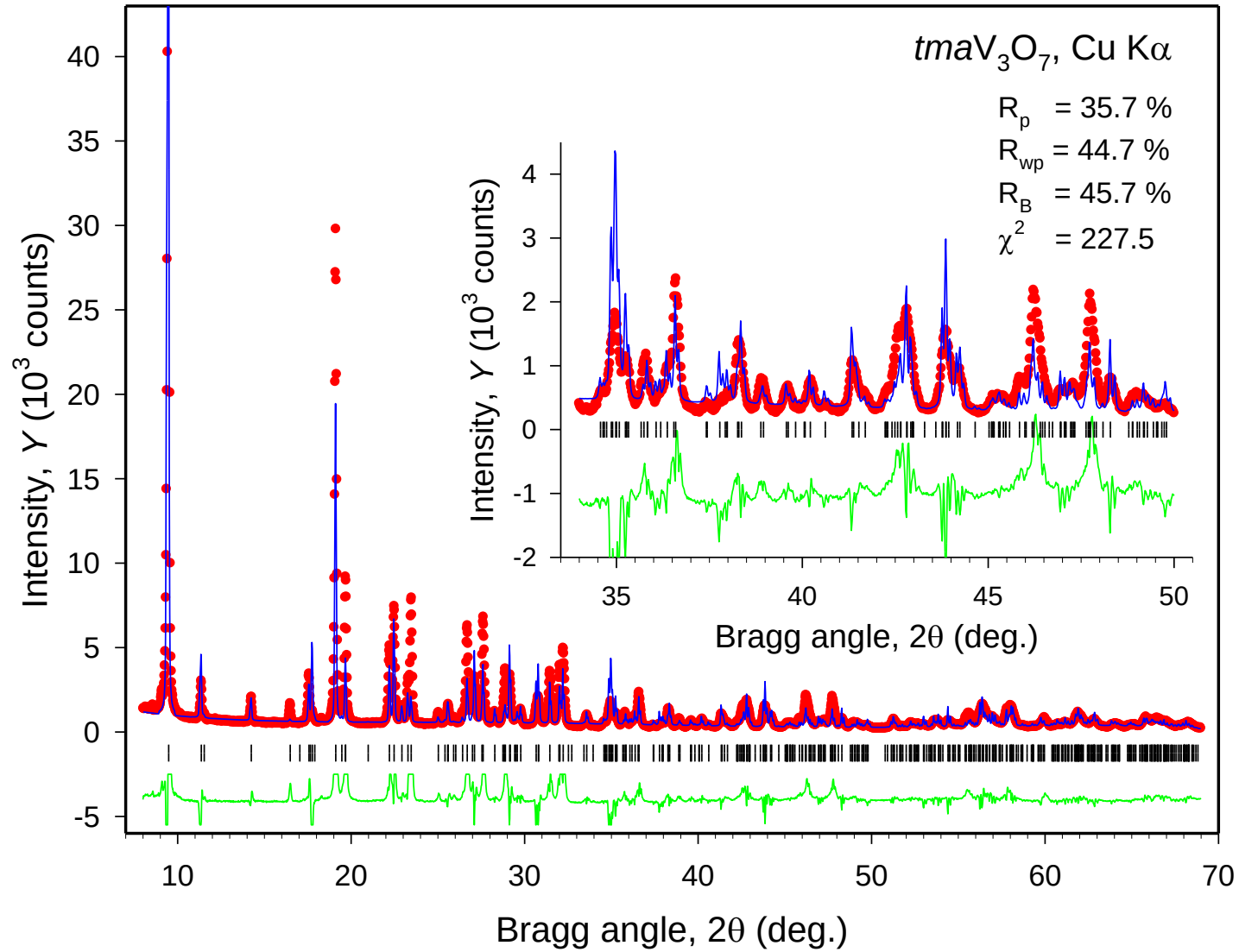
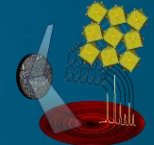


Figure 21.3. The observed and calculated powder diffraction patterns of *tmaV₃O₇* after the initial Rietveld least-squares refinement, where only the scale factor and shifted-Chebyshev polynomial background were refined.

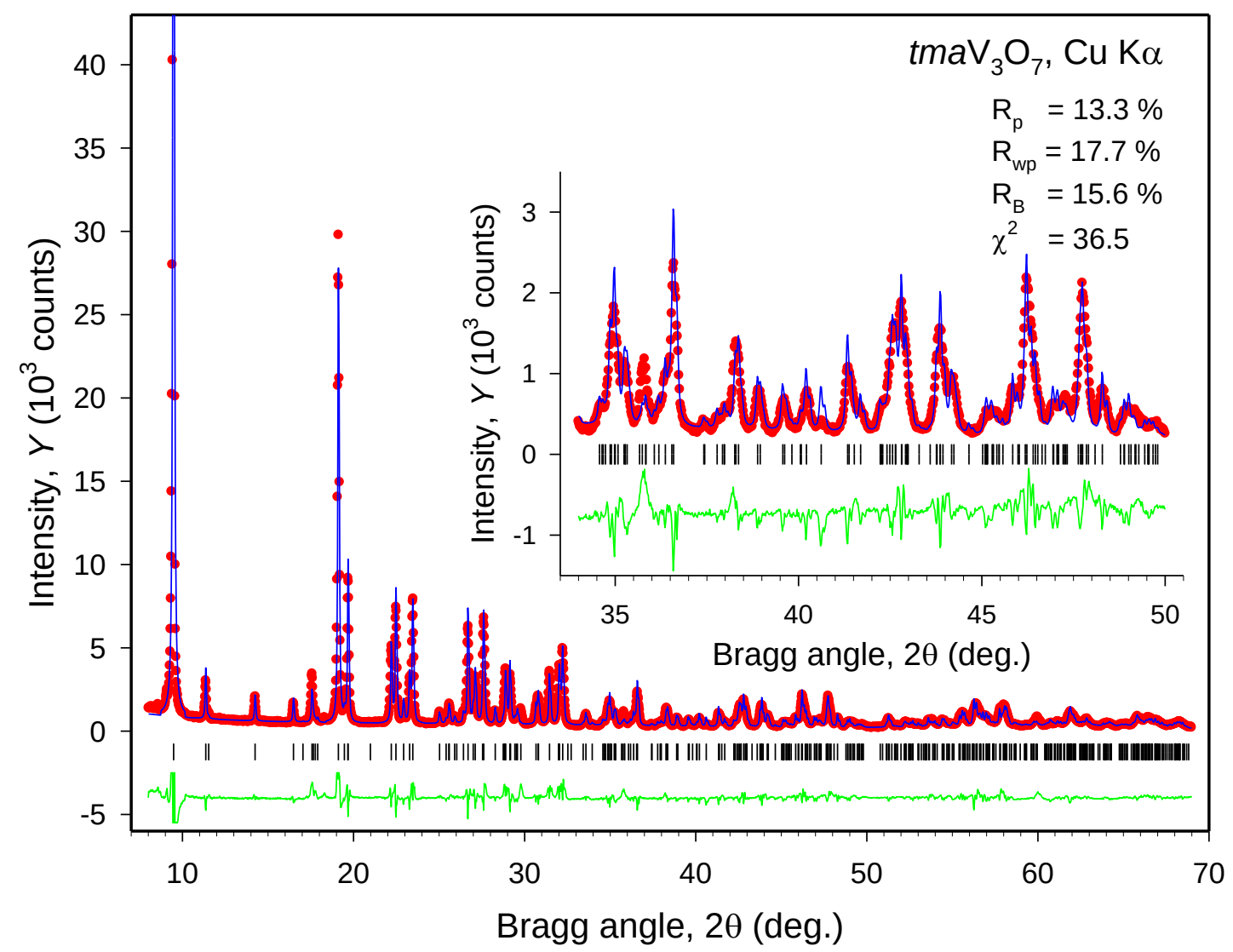
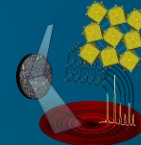


Figure 21.4. The observed and calculated powder diffraction patterns of *tmaV₃O₇* after all non-hydrogen atoms have been placed.

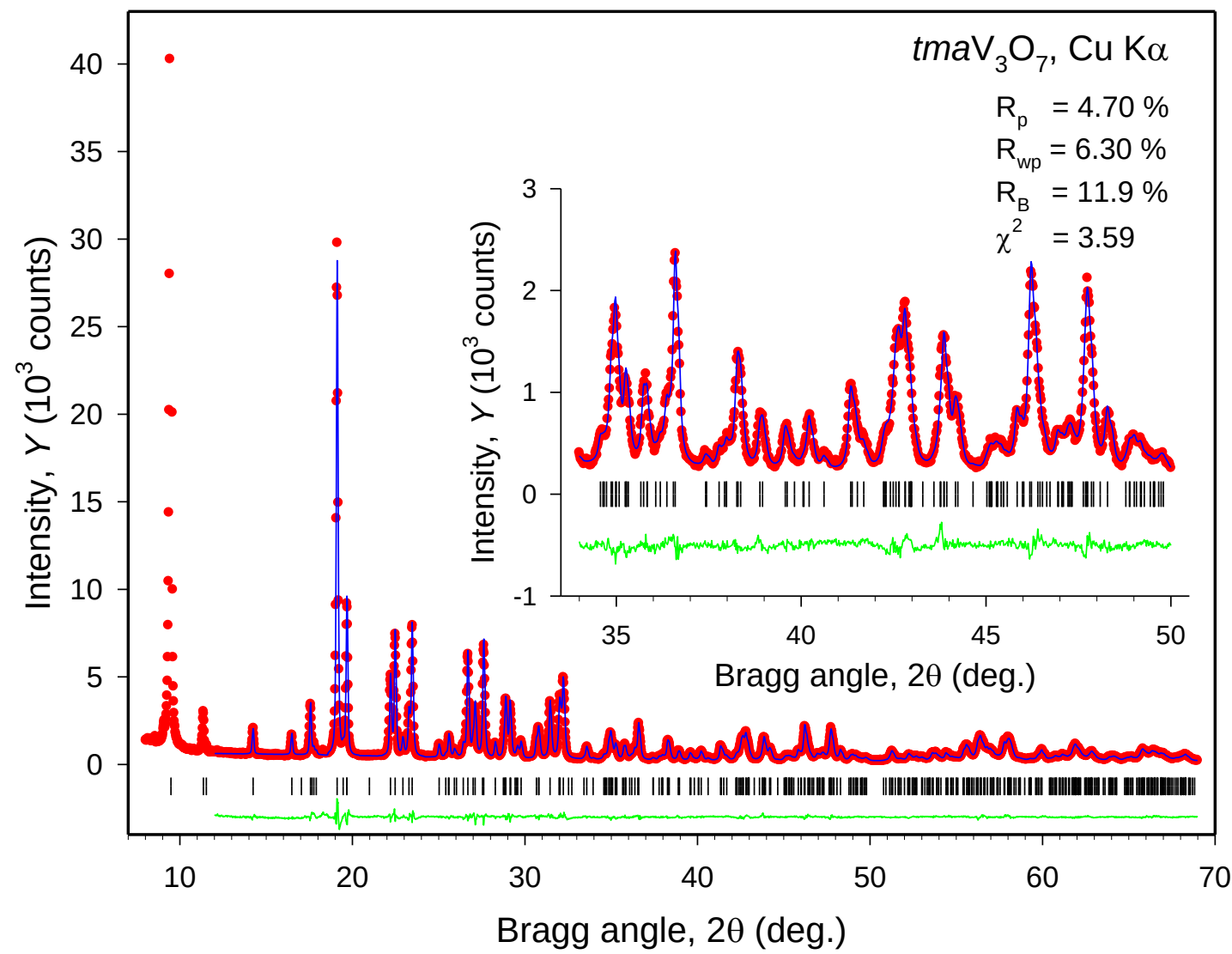
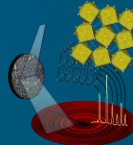


Figure 21.5. The final Rietveld plot of $tmaV_3O_7$ data. The low Bragg angle range ($2\theta < 12^\circ$) was excluded from the refinement because it contains the strongest peak, which is an order of magnitude more intense than the others and is heavily affected by experimental errors, potentially distorting the refinement.

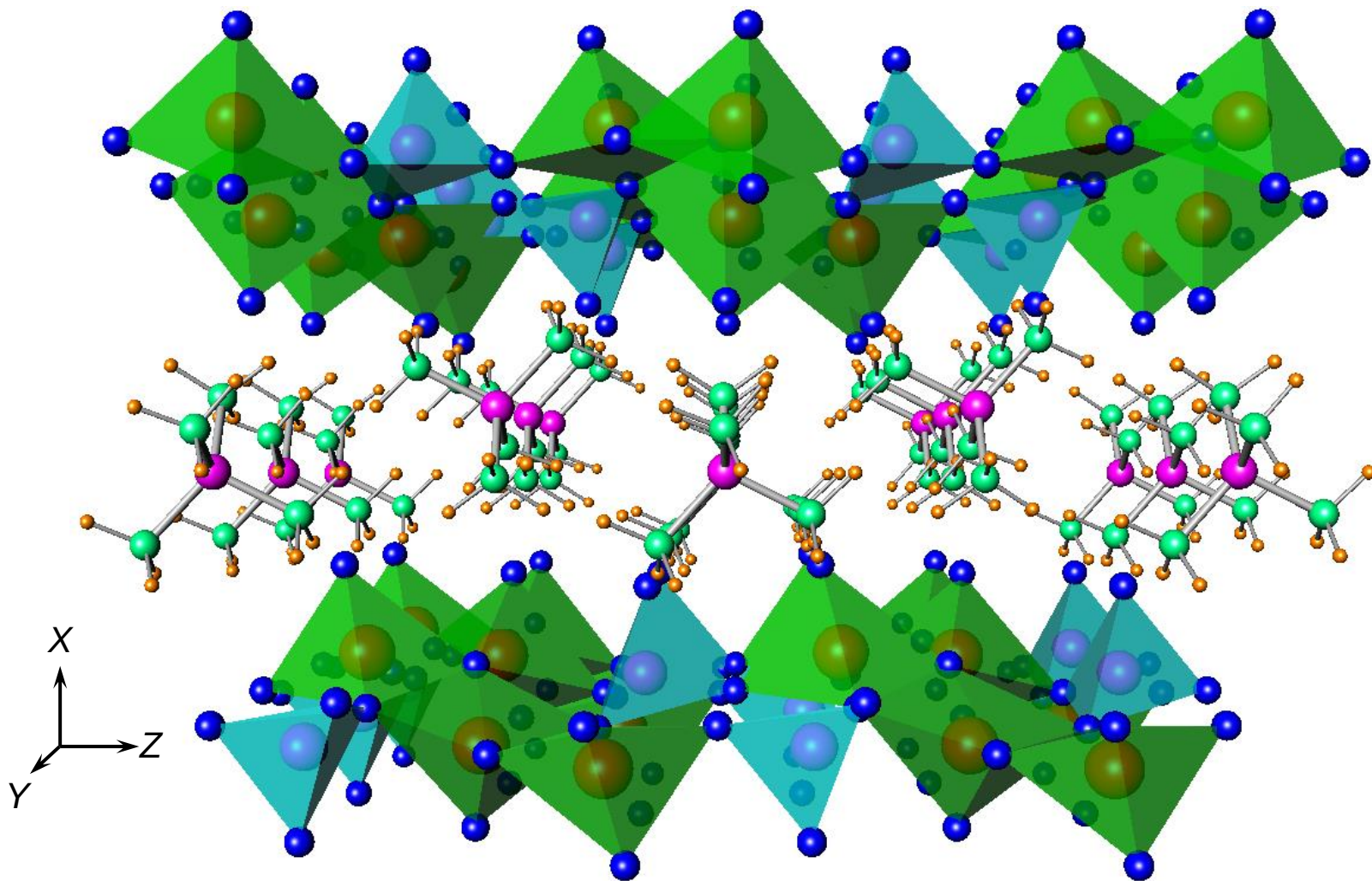
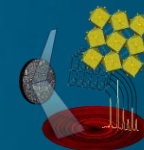


Figure 21.6. The final model of the $tmaV_3O_7$ crystal structure highlighting the layered vanadium oxide framework and the intercalated *tma* ions.

The V1 and V3 atoms (*red spheres*) are located within the *green* $[VO_5]$ square pyramids, the V2 atoms (*purple*) are positioned inside the *blue* $[VO_4]$ tetrahedra, the O atoms are shown in *blue*, N atoms in *magenta*, C atoms in *light green*, and H atoms as *small orange spheres*. The H atoms positions were computed assuming the sp^3 hybridization of carbon and trans-configurations of methyl groups