# Structure Evolution and Reactivity of the $Sc_{(2-x)}V_xO_{3+\delta}$ ($0 \leq x \leq 2.0$) System

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**Table S1:** List of heating times required in order to synthesize phase-pure samples of $Sc_{2-x}V_xO_3$.

| x | Time Required |
|---|---|
| 0.25 | 12-24 hrs |
| 0.50 | 24-64 hrs |
| 0.75 | 64 hrs |
| 1.00 | 164 hrs |
| 1.25 | N/A |
| 1.50 | N/A |
| 1.75 | 24-64 hours |
| 1.90 | < 12 hrs |

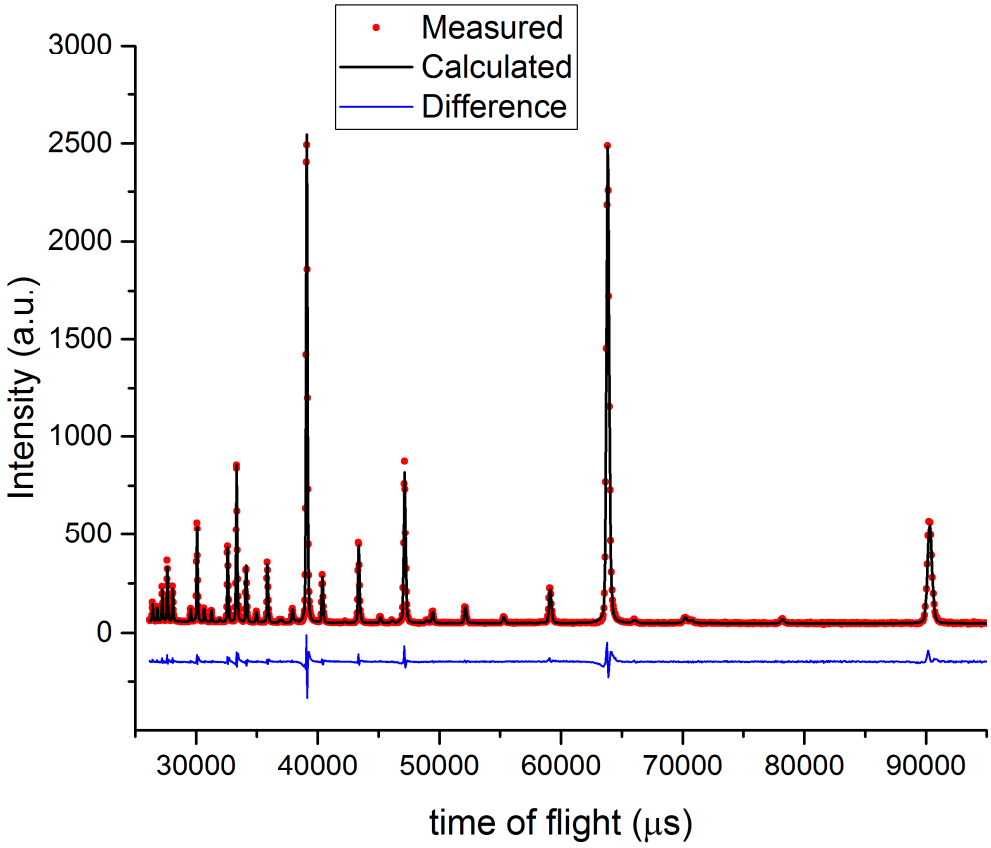


**Figure S1:** Rietveld plot of the time-of-flight neutron powder diffraction data collected at POWGEN (1.066 Å center wavelength) for the refinement of the cubic bixbyite phase $Sc_{1.75}V_{0.25}O_3$. Red symbols = observed data, black line = fit, blue line = difference. All crystallographic information can be found in table 1.

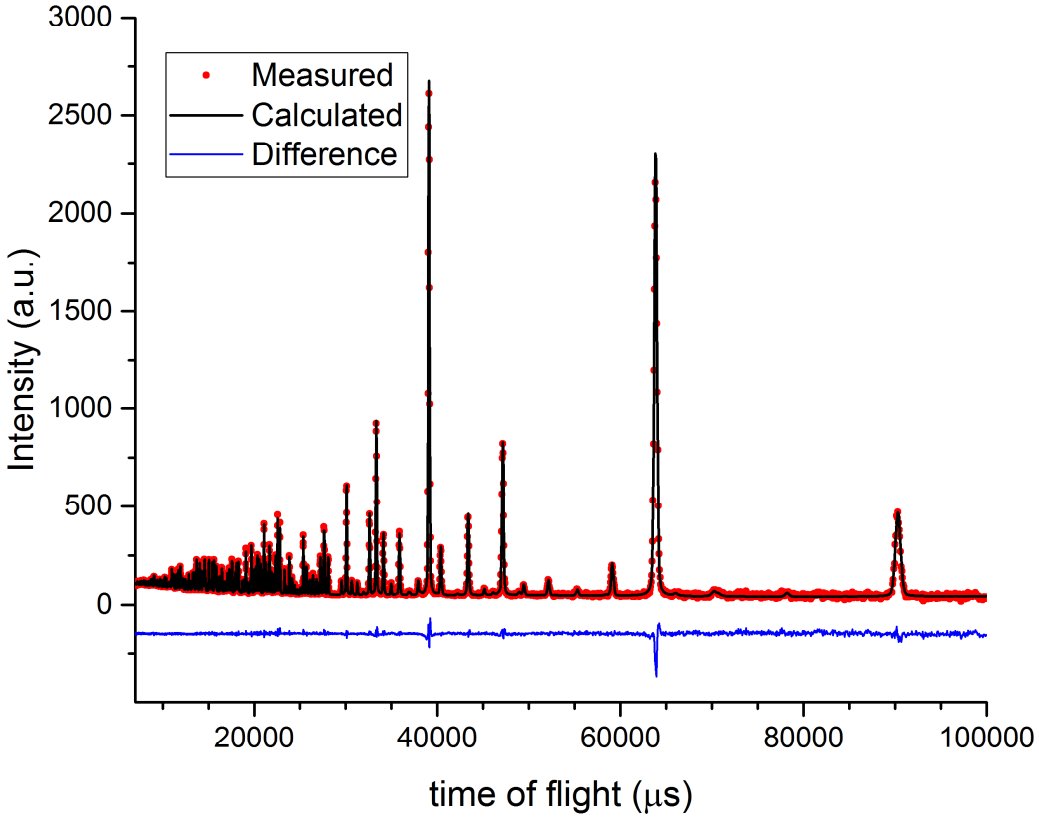


**Figure S2:** Rietveld plot of the time-of-flight neutron powder diffraction data collected at POWGEN (2.665 Å center wavelength) for the refinement of the cubic bixbyite phase $Sc_{1.75}V_{0.25}O_3$. Red symbols = observed data, black line = fit, blue line = difference. All crystallographic information can be found in table 1.

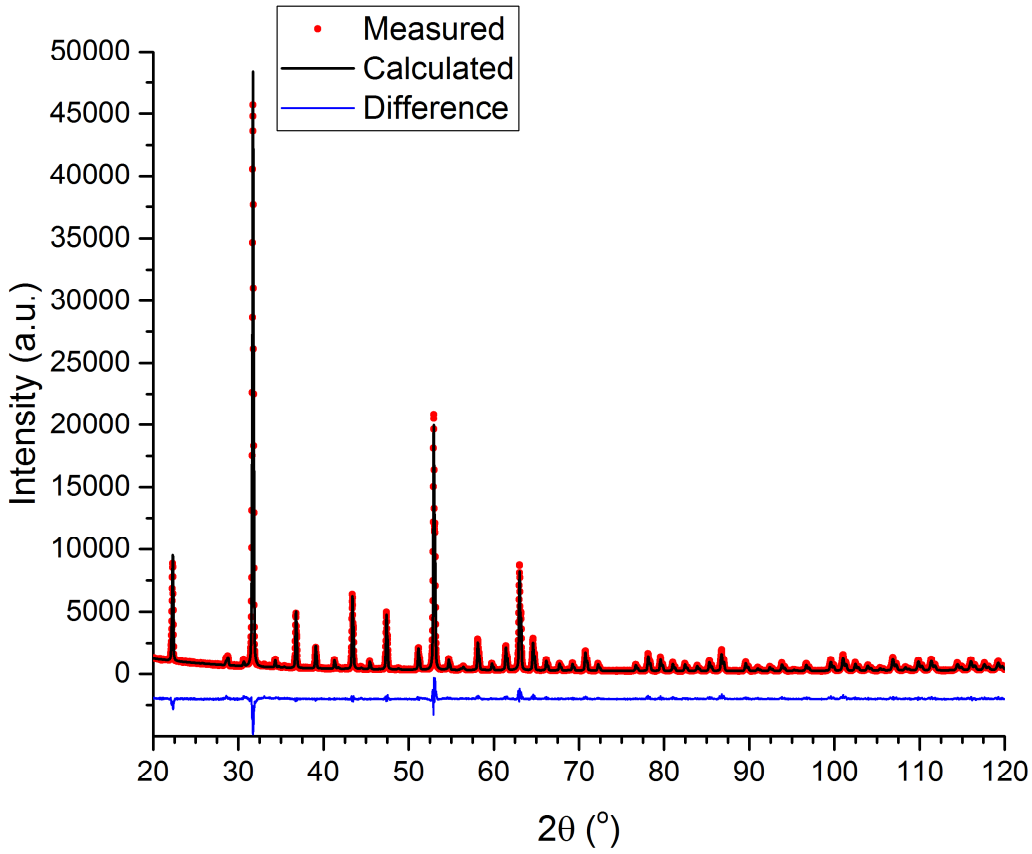


**Figure S3:** Rietveld plot of the powder X-ray diffraction data for the refinement of the cubic bixbyite phase $Sc_{1.75}V_{0.25}O_3$. Red symbols = observed data, black line = fit, blue line = difference. All crystallographic information can be found in table 1.

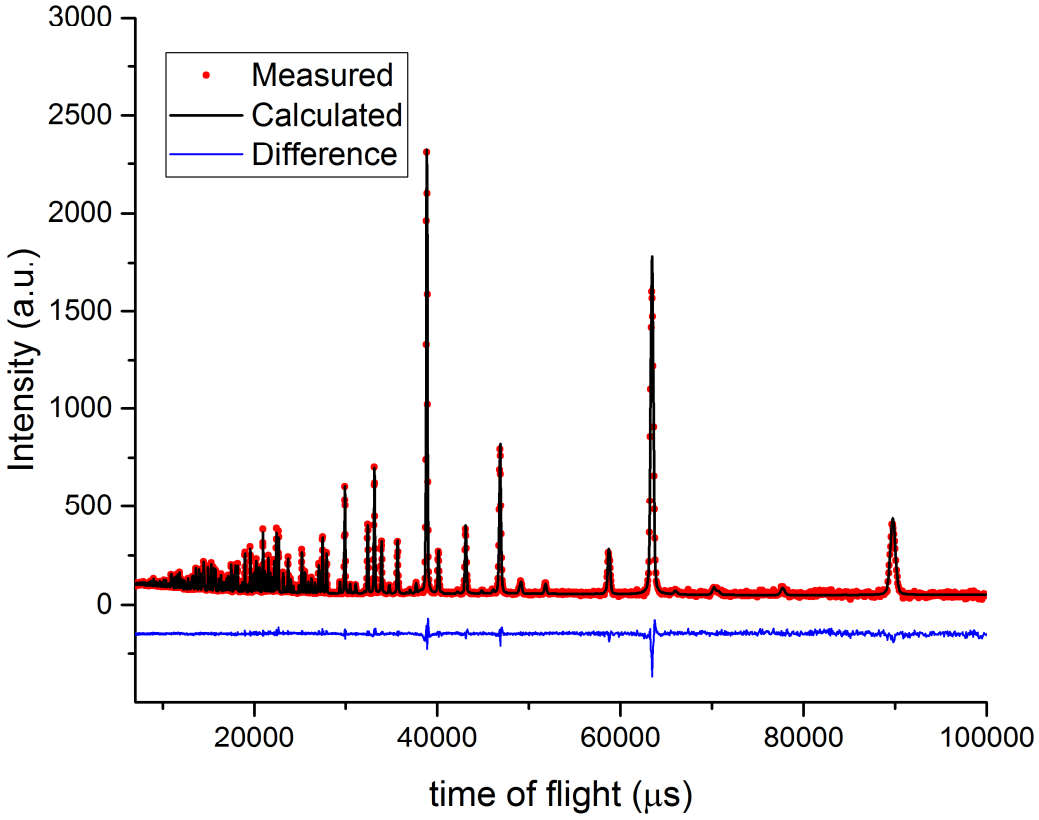


**Figure S4:** Rietveld plot of the time-of-flight neutron powder diffraction data collected at POWGEN (1.066 Å center wavelength) for the refinement of the cubic bixbyite phase $Sc_{1.50}V_{0.50}O_3$. Red symbols = observed data, black line = fit, blue line = difference. All crystallographic information can be found in table 1.

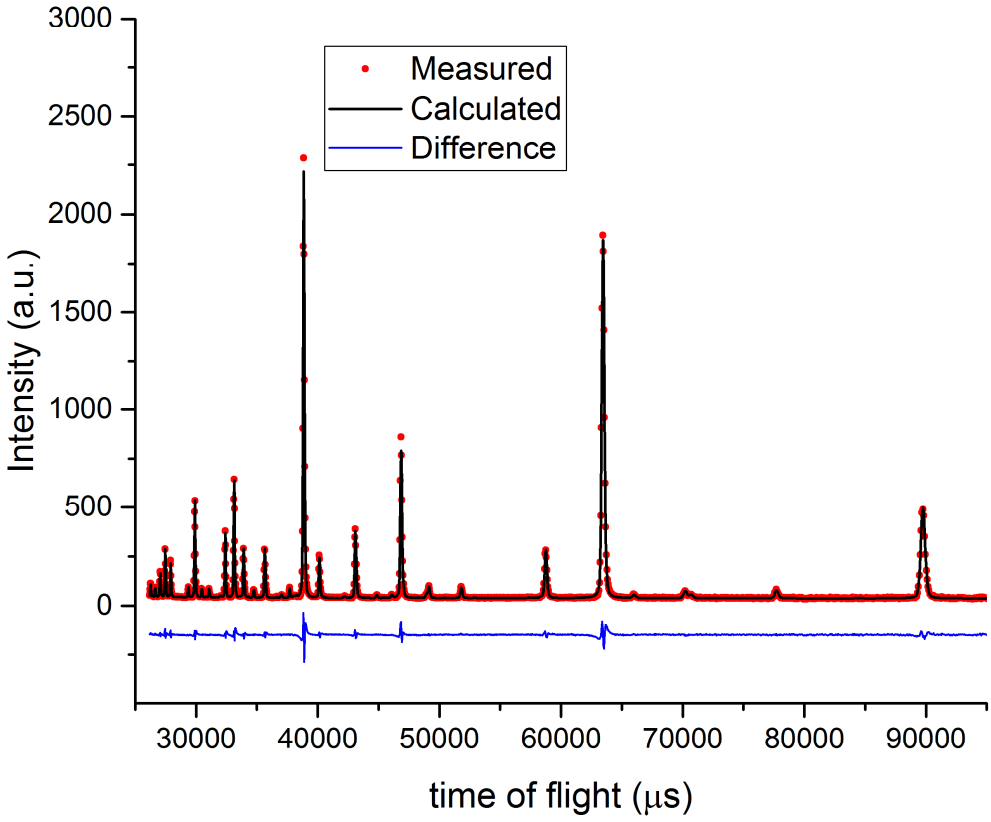


**Figure S5:** Rietveld plot of the time-of-flight neutron powder diffraction data collected at POWGEN (2.665 Å center wavelength) for the refinement of the cubic bixbyite phase $Sc_{1.50}V_{0.50}O_3$. Red symbols = observed data, black line = fit, blue line = difference. All crystallographic information can be found in table 1.

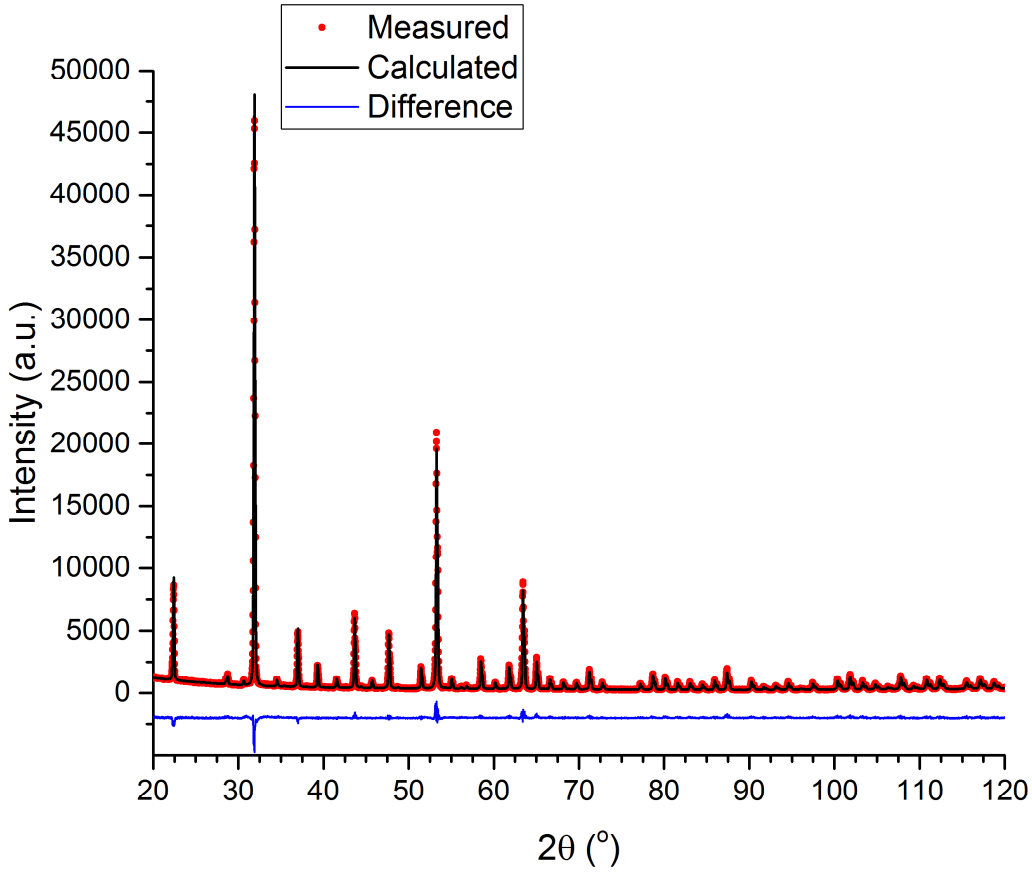


**Figure S6:** Rietveld plot of the powder X-ray diffraction data for the refinement of the cubic bixbyite phase $Sc_{1.50}V_{0.50}O_3$. Red symbols = observed data, black line = fit, blue line = difference. All crystallographic information can be found in table 1.

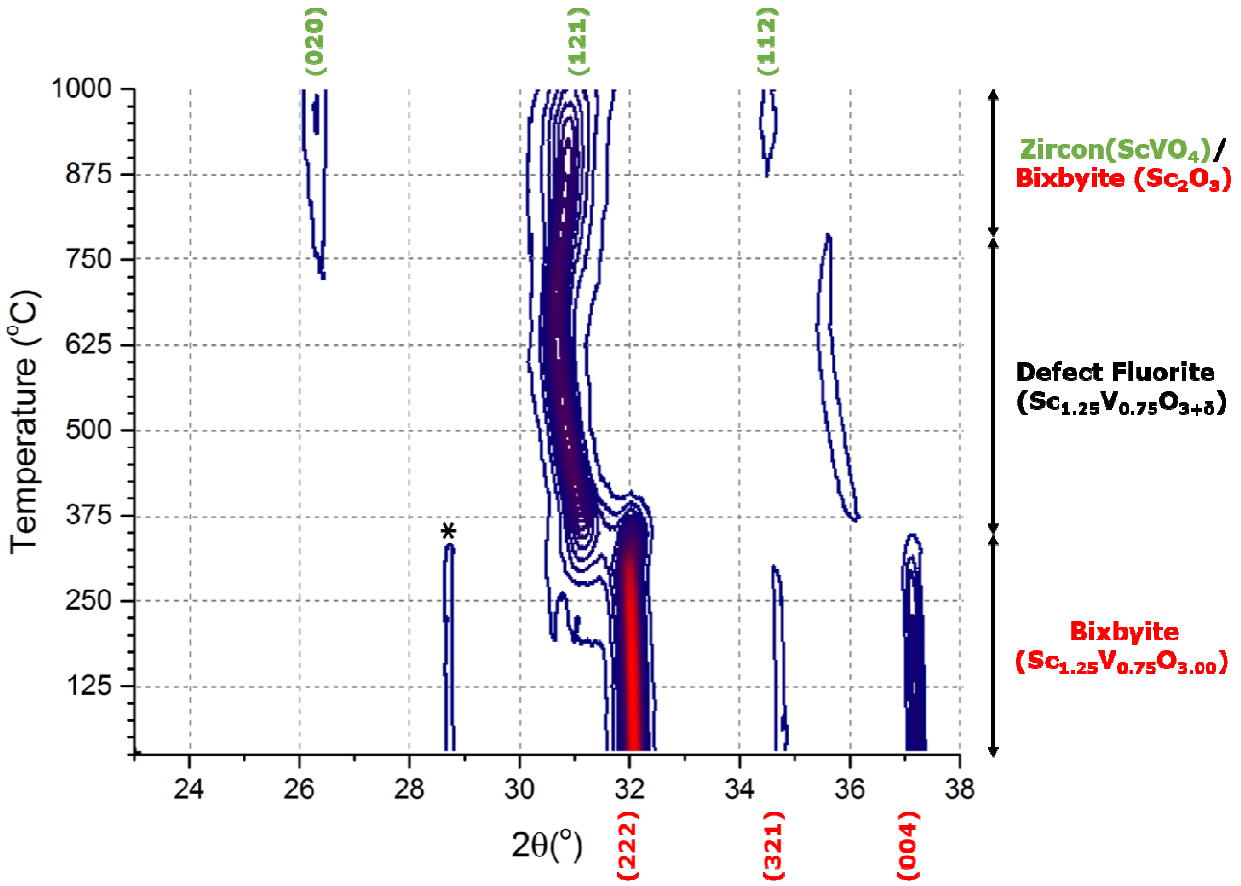


**Figure S7:** Contour plot of high temperature powder X-ray *in-situ* diffraction data showing the oxidation pathway of the bixbyite $Sc_{1.25}V_{0.25}O_{3.00}$ phase. The intermediate and final product phases are indicated with the respective temperature ranges on the right. Miller indices for the diffraction peaks are indicated at the bottom and top of the figures. Intensities are shown as constant increments from blue to red. The peak with an asterix over it belongs to the $Sc_2Si_2O_7$ impurity.