

Modeling the Crystal Structure and Ion Exchange Mechanisms of Rare Earth Elements in Zorite

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Objectives

- Synthesize pure Na-zorite for the ion exchange process.
- Exchange yttrium for sodium in zorite channels.
- Model the exchange process and site of exchange.

Introduction

Nanoporous inorganic materials, such as zeolites and zeolitic analogues, have long been known to have excellent ion selectivity. These ion selectivities have been exploited for many industrial applications in areas such as petroleum refinement, agronomy, and water purification. As the need for rare earth elements (REEs) continues to increase, our methods of refinement must also increase in efficiency and ion selectivity. This research is focused on developing a nanoporous material and accompanying technique to accurately and precisely extract different REEs from solution.

Results of Raman Studies

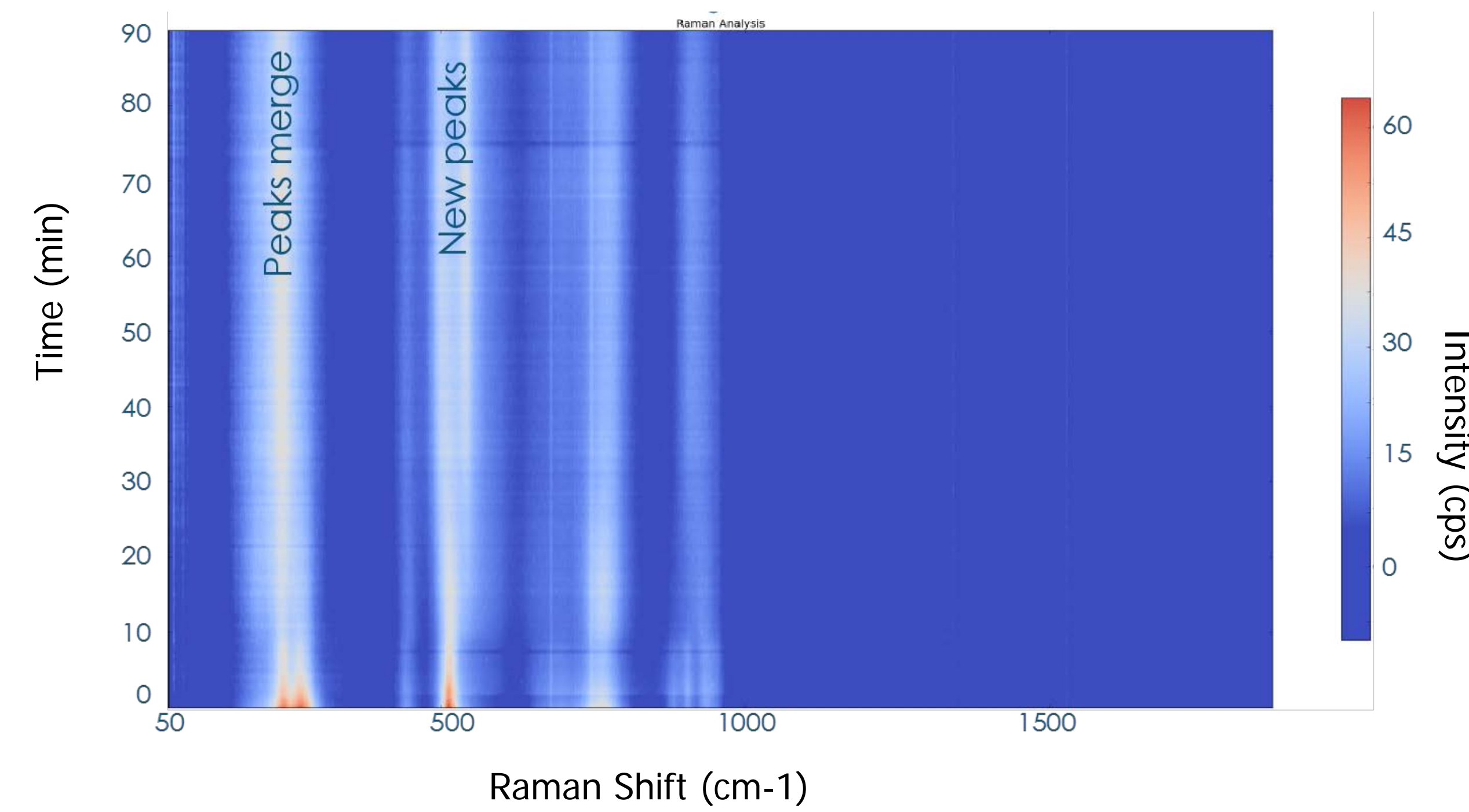


Figure 2. Genesis and consolidation of peaks during ion exchange.

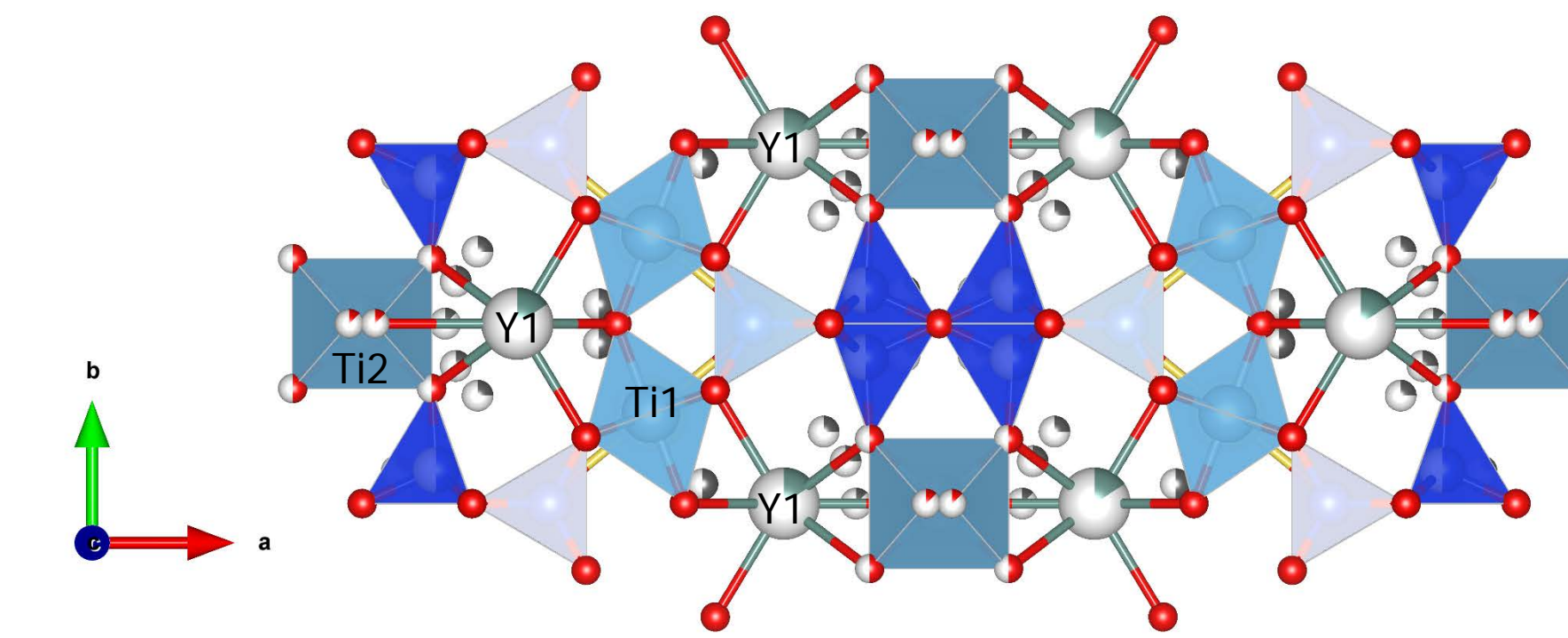


Figure 5. Yttrium exchanged zorite, looking down c-axis.

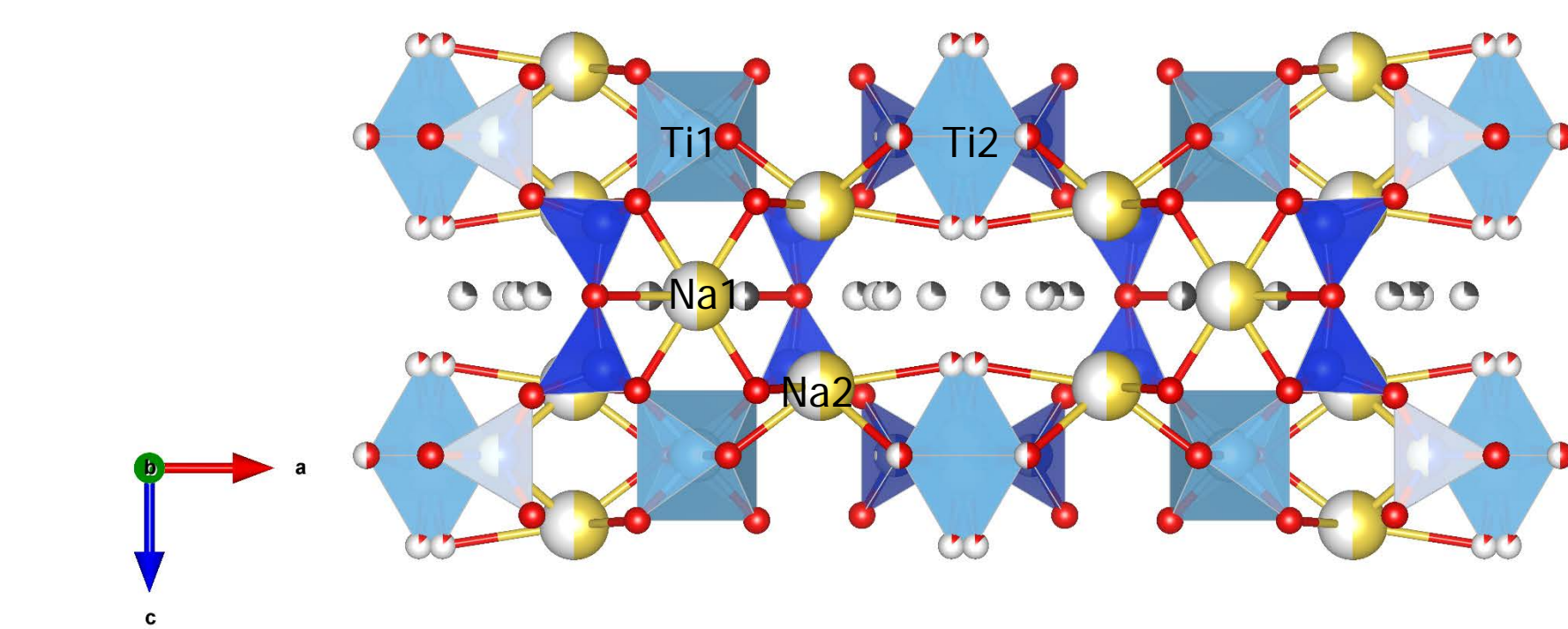


Figure 1. Looking down the b-axis of the Na-zorite structure.

Methods

The sample was packed into an environmental cell (pictured below) and supported by glass wool and polyimide tubing. Several spectra were taken while deionized water was running over the sample, to obtain a spectra for when the sample was wet. Once this was set, 0.1M YCl3 solution was run over the sample for 90 minutes while *in-situ* Raman spectra were collected.

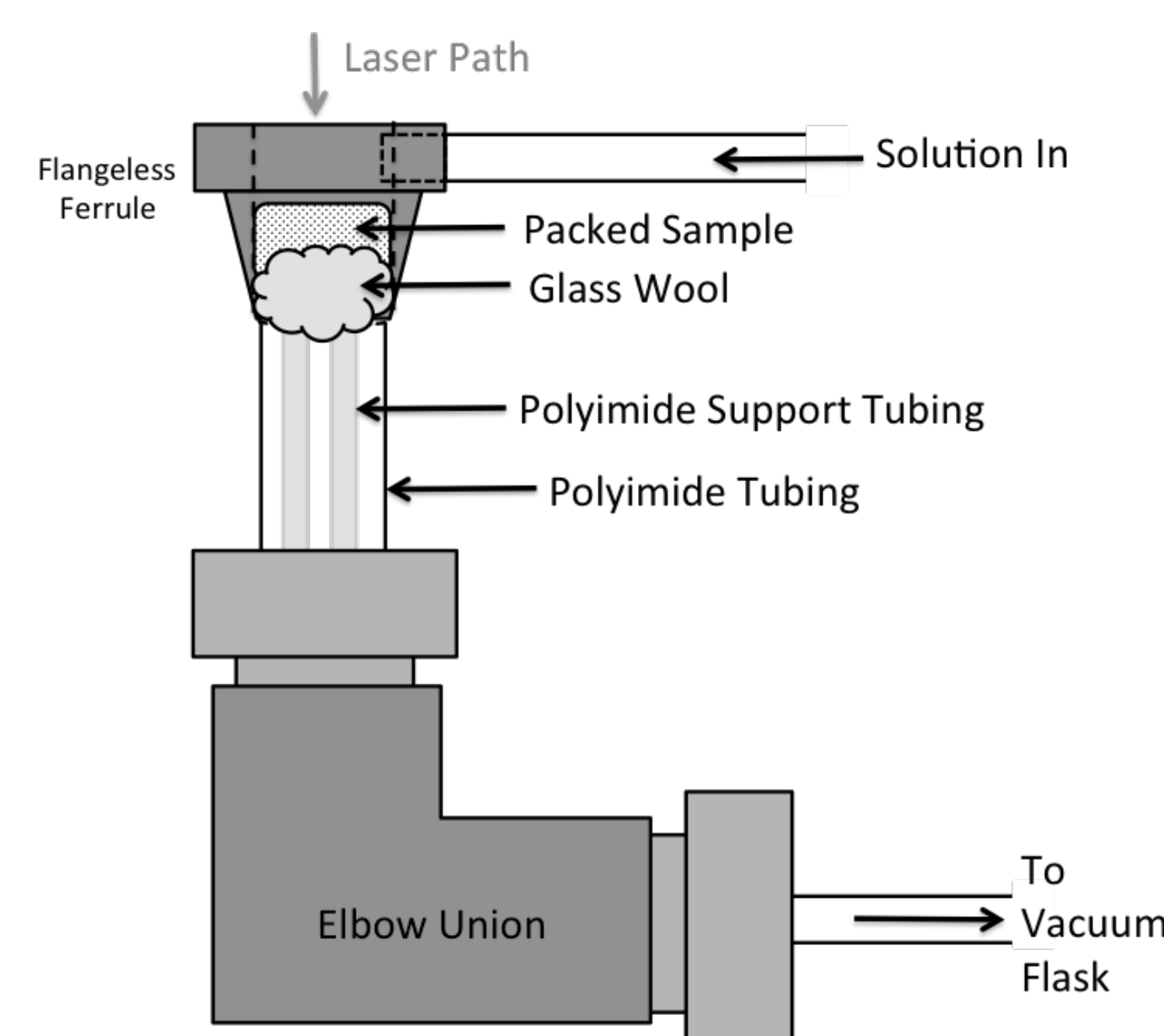


Figure 2. Environmental cell

Discussion

Raman studies indicate that yttrium has at least partially occupied the sodium 2 site. Based on the Raman shifts observed in peaks 545, 520, 870 and 905, it is reasonable to conclude that the change in bond geometry is likely due to the yttrium entering the sodium 2 site. Powder XRD results also suggest a small expansion of the unit cell as a whole, most likely as a consequence of the introduction of the larger yttrium ions. Inductively Coupled Plasma Emission Spectroscopy (ICP-ES) analysis confirms that yttrium is present within the crystal structure at 4.81%.

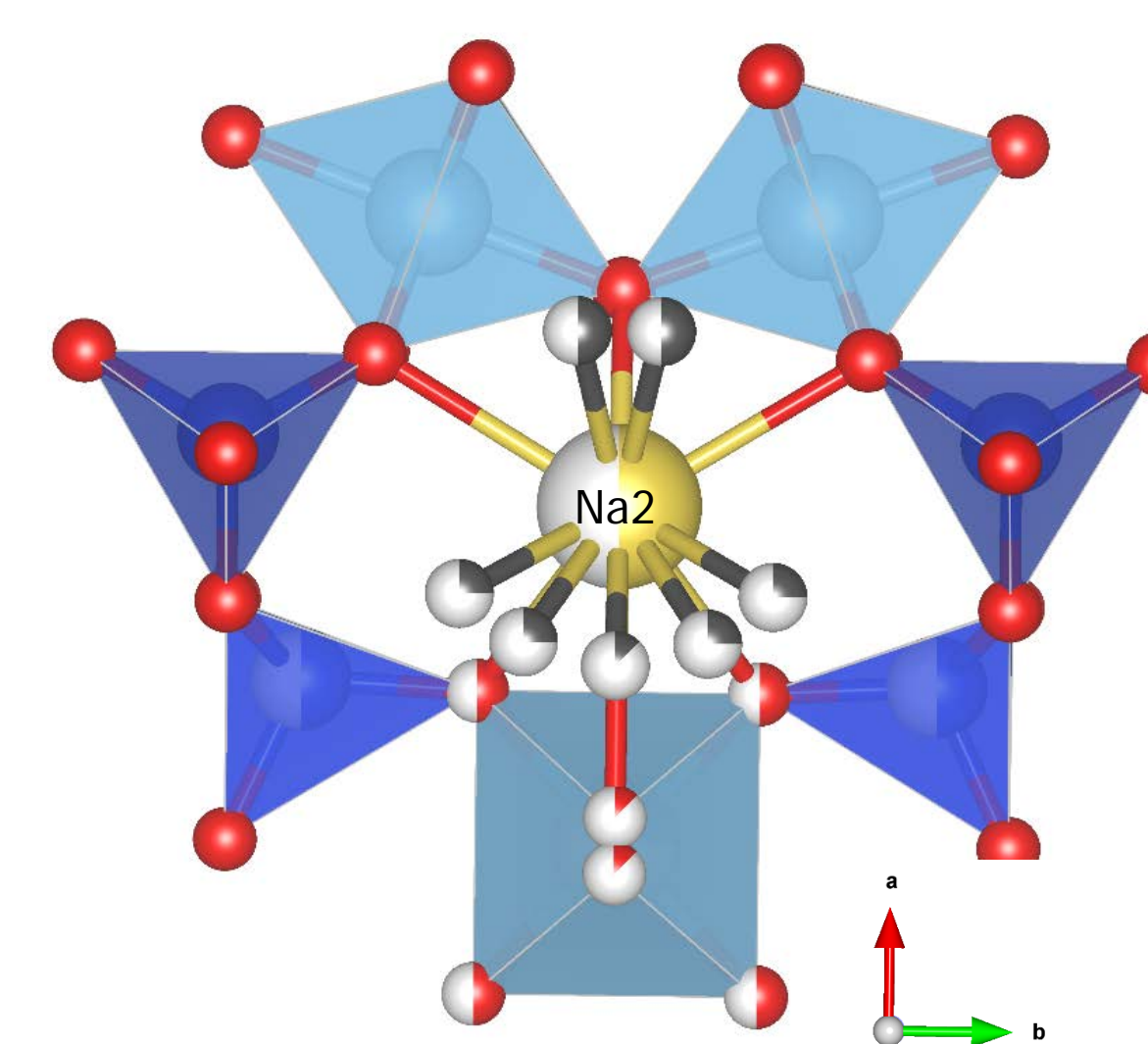


Figure 4. Looking down the c-axis of zorite into the sodium 2 site.

Major peaks during exchange process

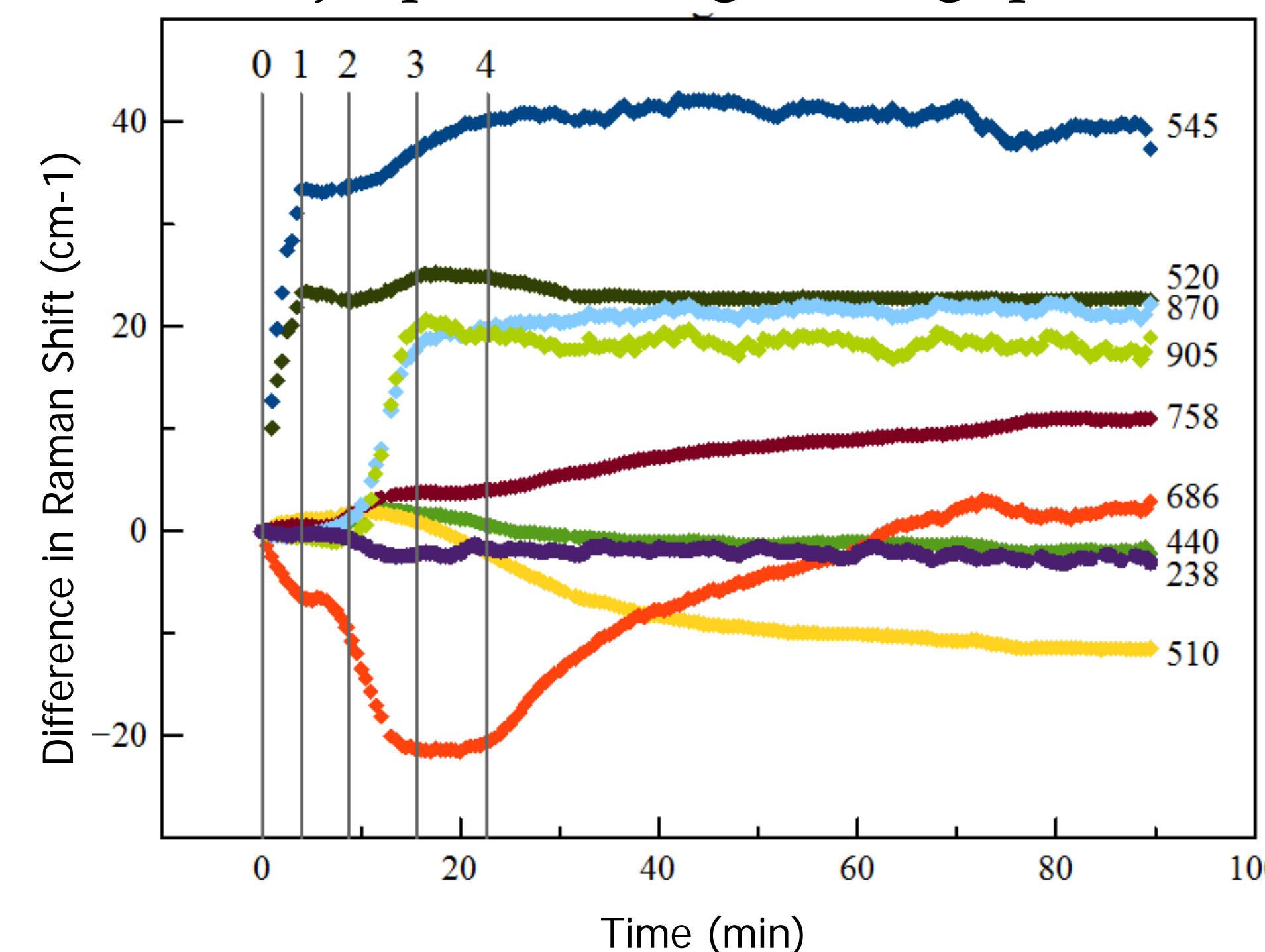
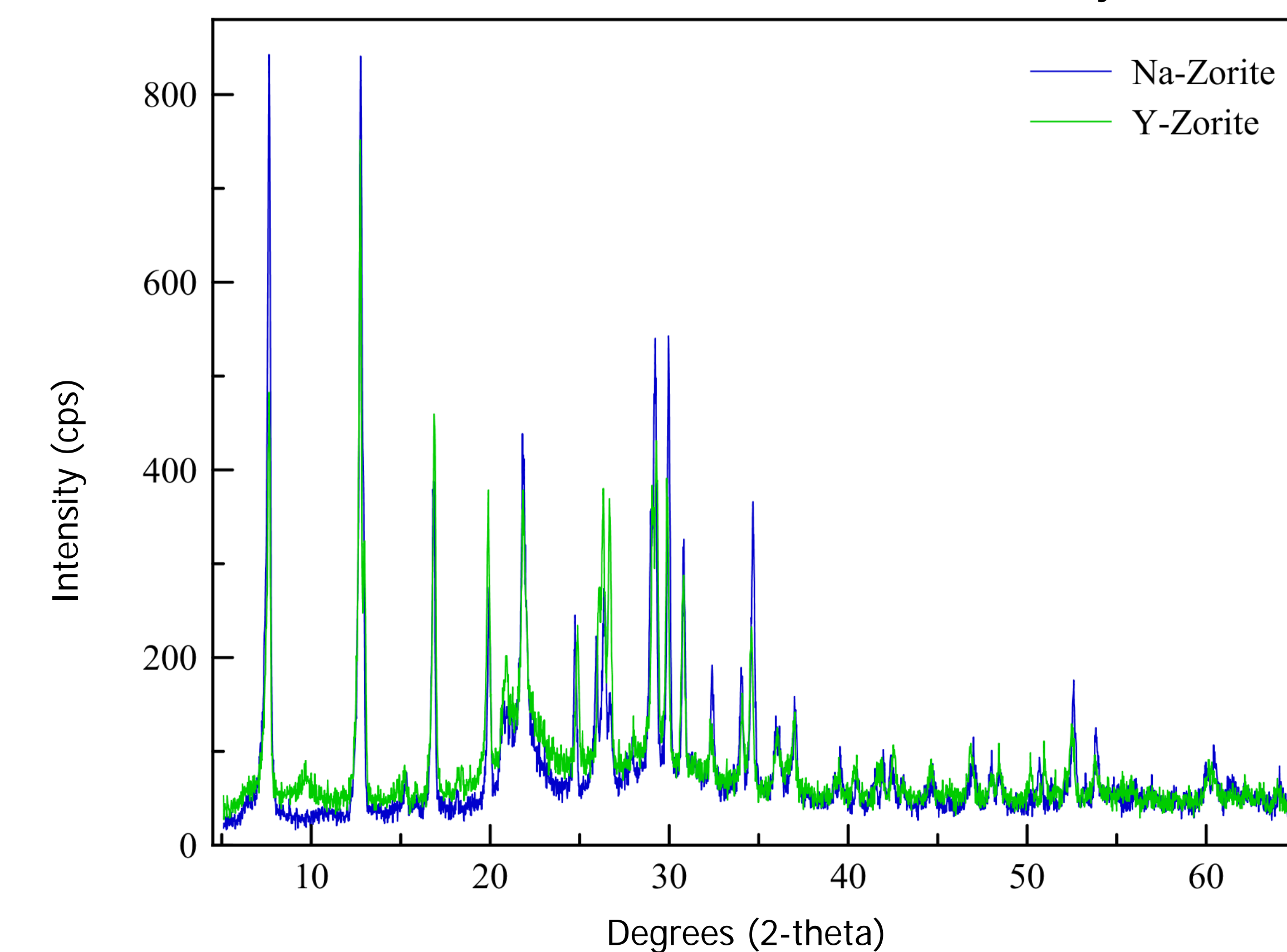


Figure 3.
 • Major changes observed from marker 0 to marker 1 for peaks 545 and 520.
 • Major changes observed from marker 2 to marker 3 for peaks 870 and 905.

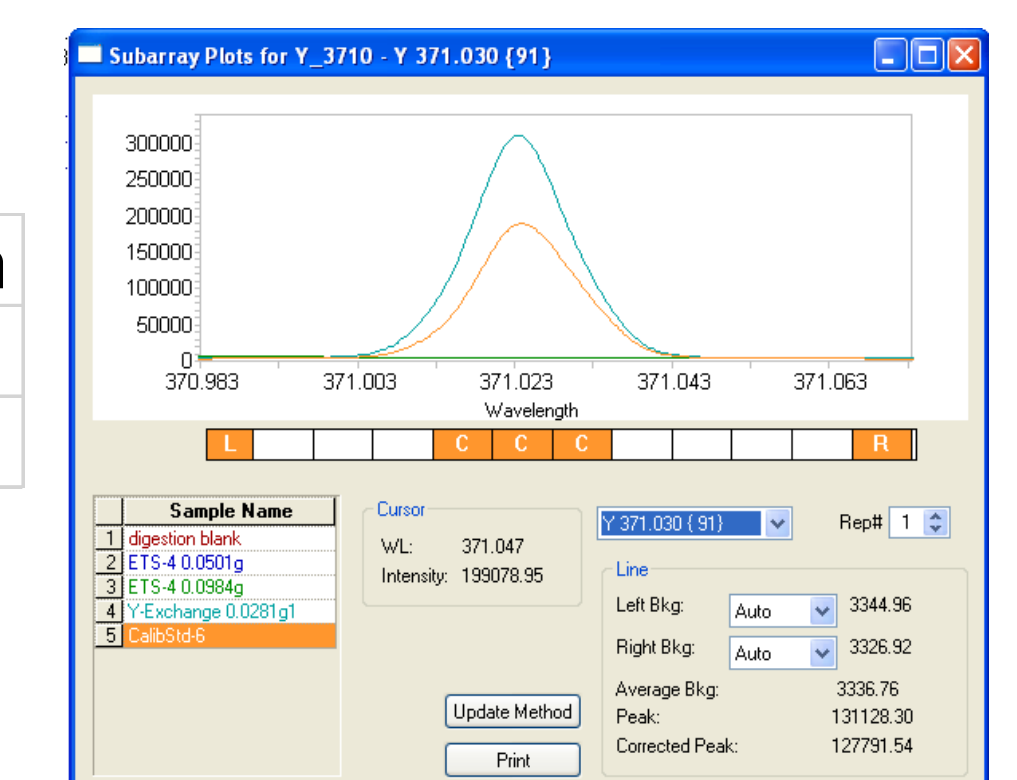
Na and Y Zorite PXRD Overlay



Unit Cell Parameters	a (Å)	b (Å)	c (Å)	Cell Volume
Na-Zorite	23.2356258	7.2073188	6.9630035	1166.070262 Å ³
Y-Zorite	23.3040213	7.1744376	6.9865963	1168.111718 Å ³

ICP-ES Analysis

Sample ID	Wt g	Vol ml	Yttrium ug/ml	Yttrium ug/g	Yttrium %
Y-Exchange	0.0281	100	13.51	48078.29181	4.81



Acknowledgments

Acknowledgments are made to the American Chemical Society Petroleum Research Fund and NSF Kentucky EPSCOR. The contributions of Dr. Jennifer Cole are also greatly appreciated.

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