

Impact of Atom Removal and DFM-Based Filtering on Highest Difference Peak in LTA and STW Zeolites

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September 5, 2024

Abstract

This report investigates the impact of filtering on the Highest Difference Peak (HDP) when one atom is removed from the structure. The study focuses on LTA and STW zeolite samples and assesses how the HDP behaves relative to target completeness. We compared data with and without atom removal, analyzing changes in the structure with filtering. The findings suggest that filtering reduces the HDP when an atom is removed, implying a potential degradation in data quality as filtering progresses.

Introduction

The goal of this analysis was to study how filtering diffraction data affects the Highest Difference Peak (HDP) when one atom is removed from the structure. By observing how the HDP changes as a function of target completeness, we can evaluate the effectiveness of filtering. Our analysis focused on LTA and STW zeolite samples, using SHELXL maps to visualize the structural changes before and after filtering, and comparing results with one atom removed.

Methodology

The following steps outline the methodology used for the analysis:

- Samples: LTA zeolite (various thicknesses) and STW zeolite were used in this study.
- Data: For each sample, the diffraction data was filtered at different target completeness levels.
- Atom Removal: One atom was removed from the structure to analyze the effect of filtering on the HDP.
- SHELXL Maps: Structural maps were generated before and after filtering for both LTA and STW zeolite samples.
- HDP Calculation: The Highest Difference Peak was calculated at each level of target completeness, both with and without atom removal.

Results

LTA Zeolite - Thickness 1

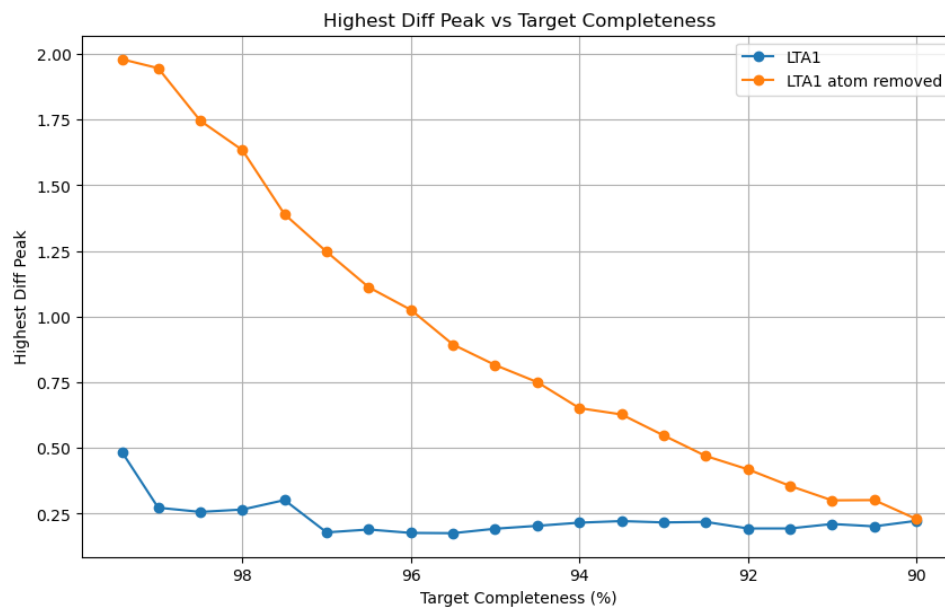


Figure 1: Highest Difference Peak vs Target Completeness for LTA Zeolite (Thickness 1) with 1 atom removed.

LTA Zeolite - Thickness 4

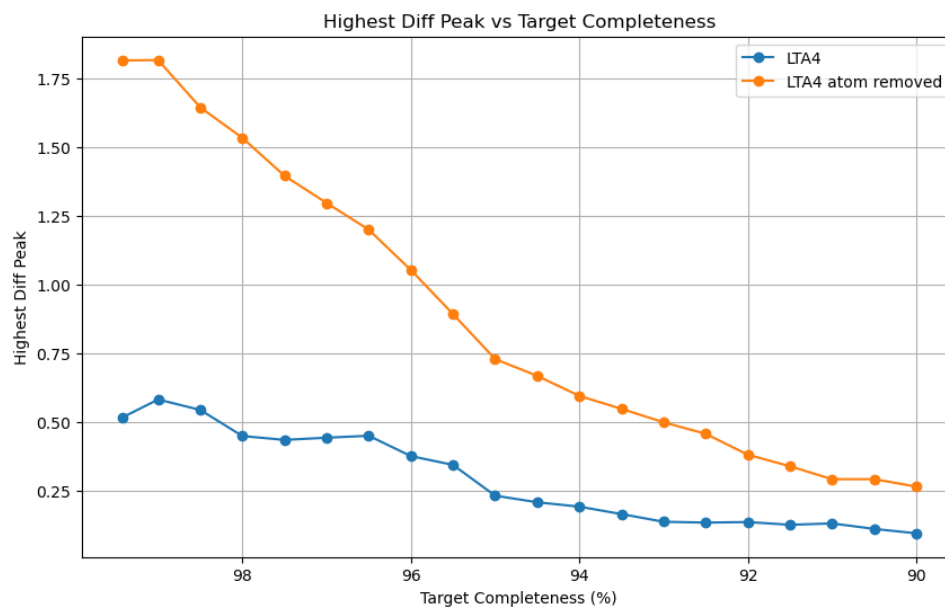


Figure 2: Highest Difference Peak vs Target Completeness for LTA Zeolite (Thickness 4) with 1 atom removed.

SHELXL Maps for LTA Zeolite

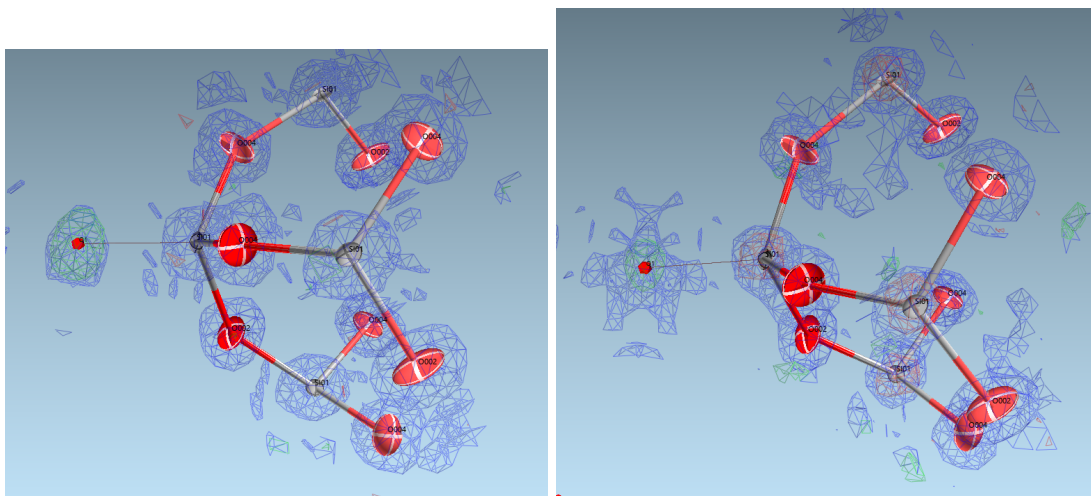


Figure 3: SHELXL Maps for LTA Zeolite (Thickness 1) - Before (left) and after (right) filtering with 1 atom removed.

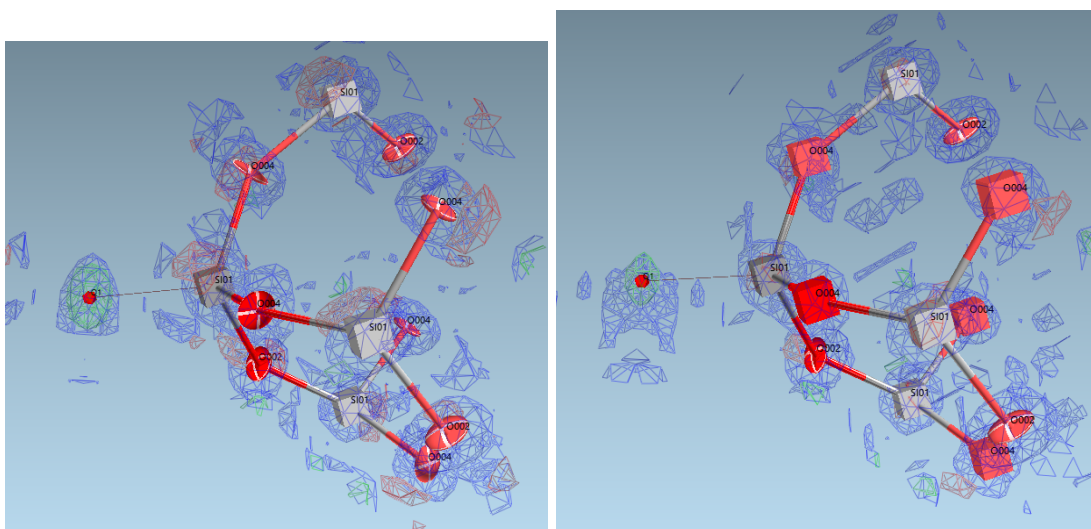


Figure 4: SHELXL Maps for LTA Zeolite (Thickness 4) - Before (left) and after (right) filtering with 1 atom removed.

STW Zeolite - Thickness 1

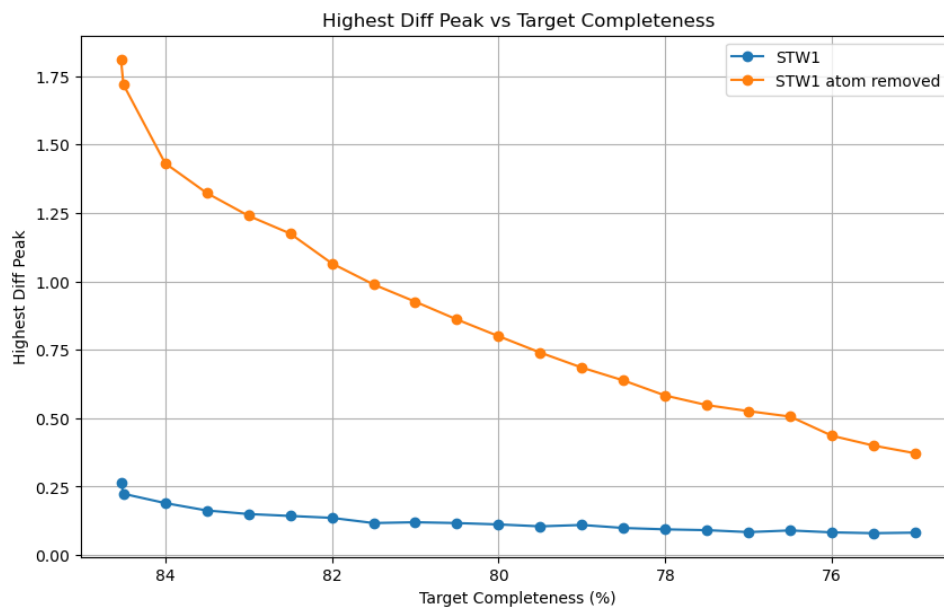


Figure 5: Highest Difference Peak vs Target Completeness for STW Zeolite (Thickness 1) with 1 atom removed.

STW Zeolite - Thickness 4

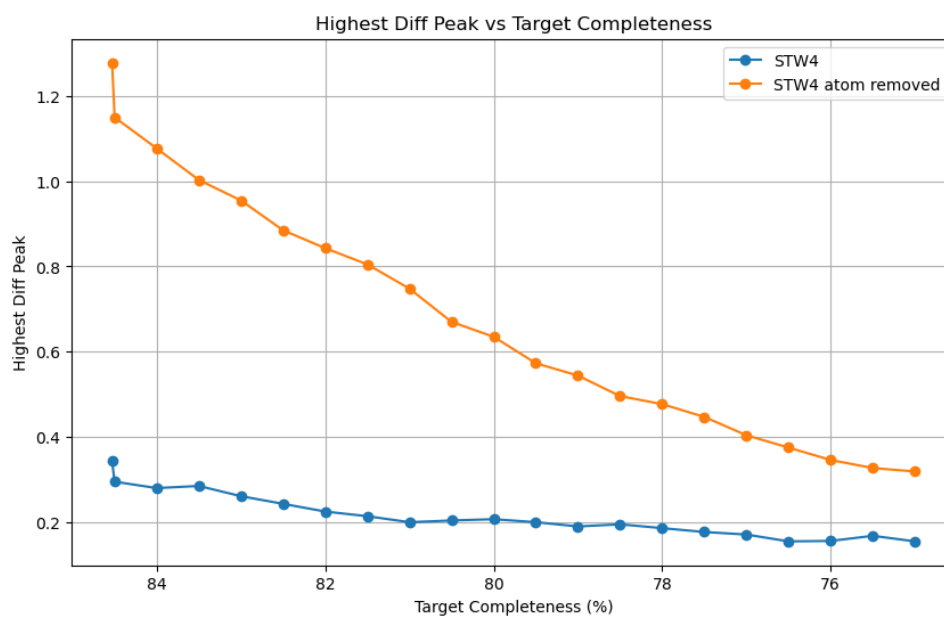


Figure 6: Highest Difference Peak vs Target Completeness for STW Zeolite (Thickness 4) with 1 atom removed.

SHELXL Maps for STW Zeolite

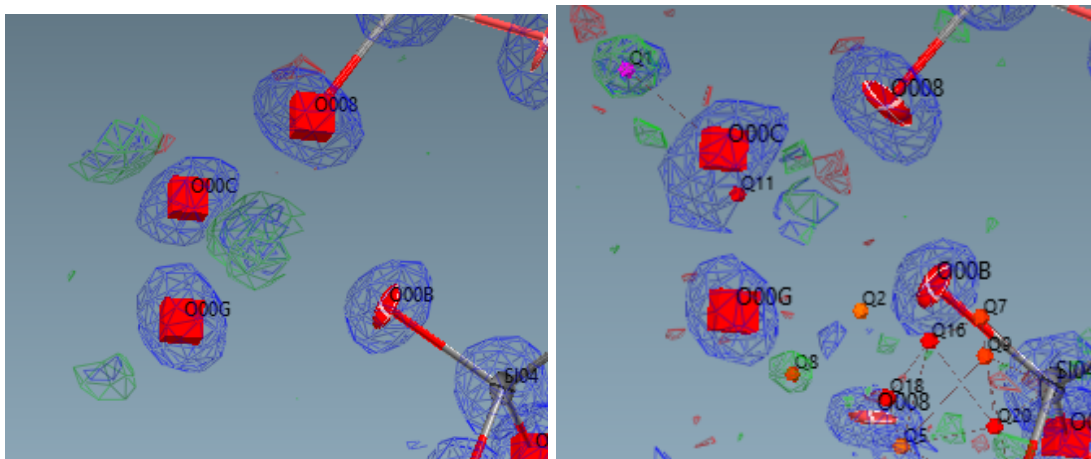


Figure 7: SHELXL Maps for STW Zeolite (Thickness 1) - Before (left) and after (right) filtering with 1 atom removed.

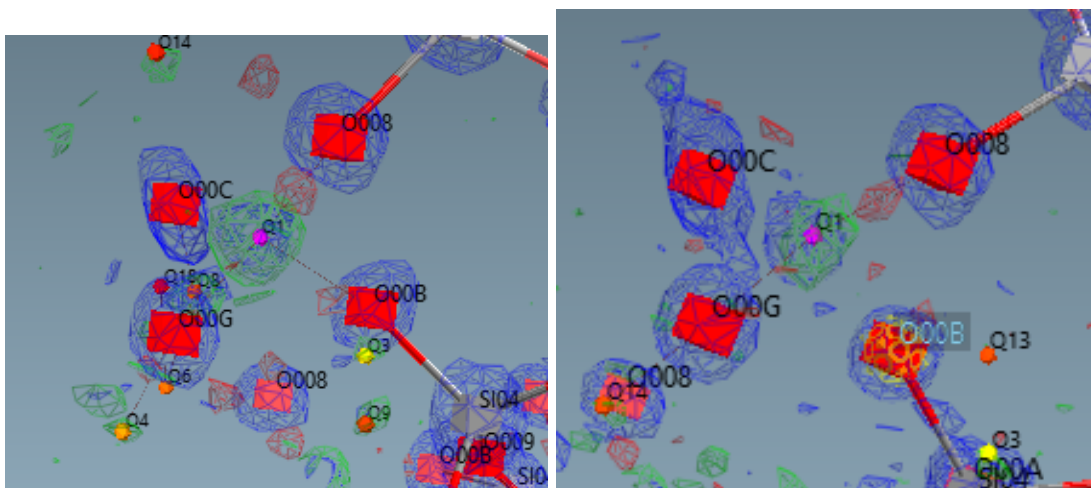


Figure 8: SHELXL Maps for STW Zeolite (Thickness 4) - Before (left) and after (right) filtering with 1 atom removed.

Conclusion

The results indicate that filtering does not improve data quality when an atom is removed, as shown by the decreasing Highest Difference Peak with increased filtering. The SHELXL maps further illustrate this point, with noticeable differences between filtered and unfiltered data. The analysis reveals that atom removal significantly affects the results, suggesting that the Highest Difference Peak is not a reliable metric for evaluating data quality improvement through filtering under these conditions.