

Comparative Analysis of Polyhedral Oligomeric Silsesquioxane (POSS) Using ToF-SIMS

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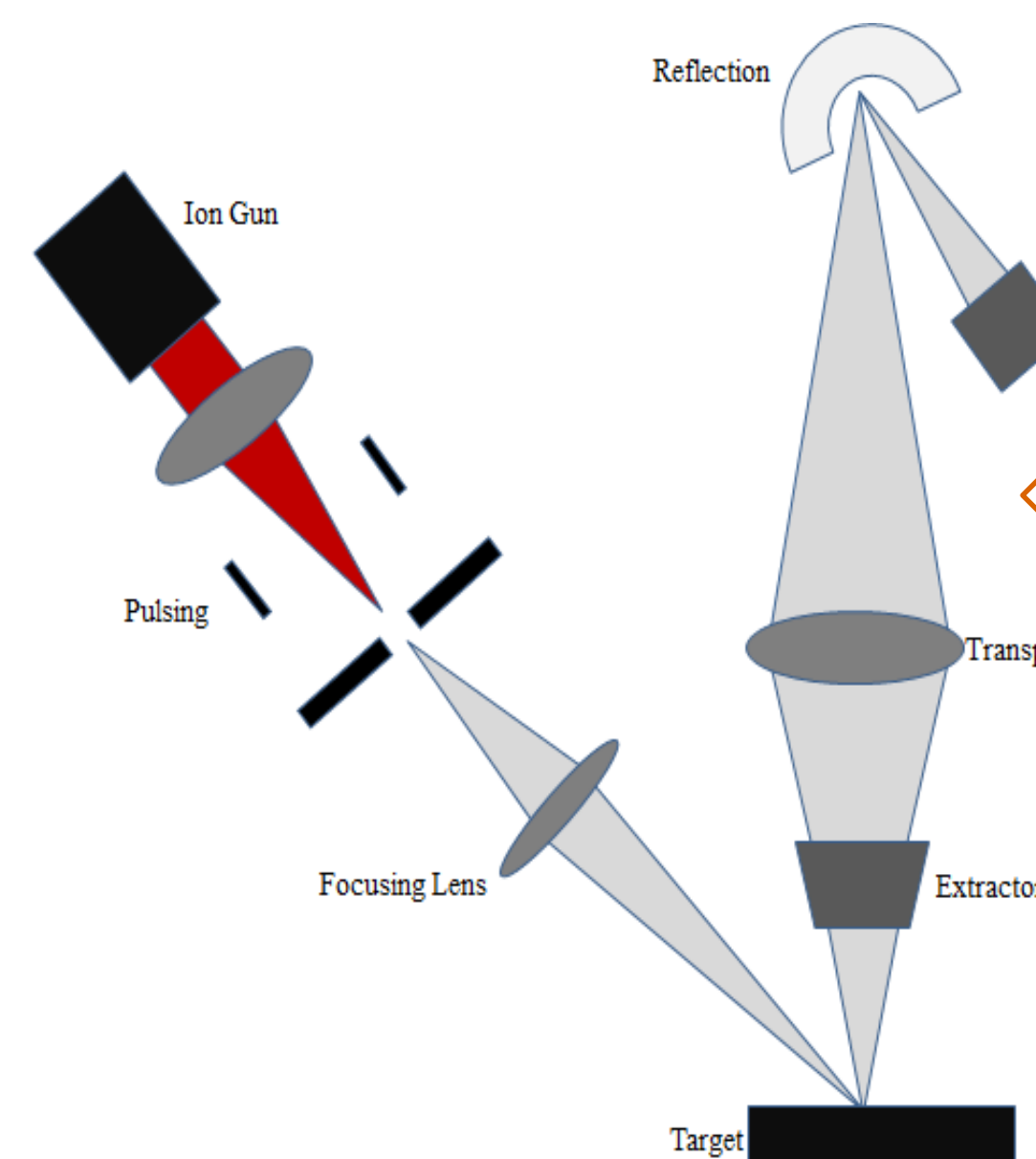
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Introduction

- Polyhedral Oligomeric Silsesquioxane (POSS) is an important type of nanostructured chemical compound;¹
- Applications as an additive, a plastic, and a preceramic;
- Valuable features of POSS including large molecule building block and the intermediate composition between SiO₂ and R₂SiO;^{2,3}
- Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS) is used to study POSS to provide more insight in its molecular structure and functioning group.

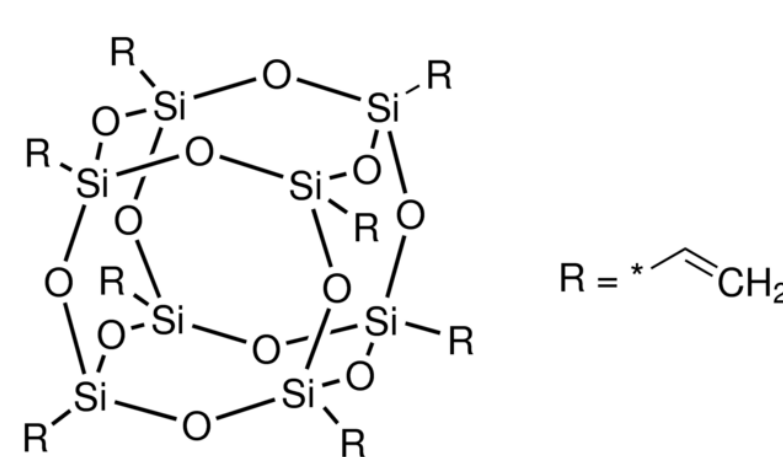
Experimental Design



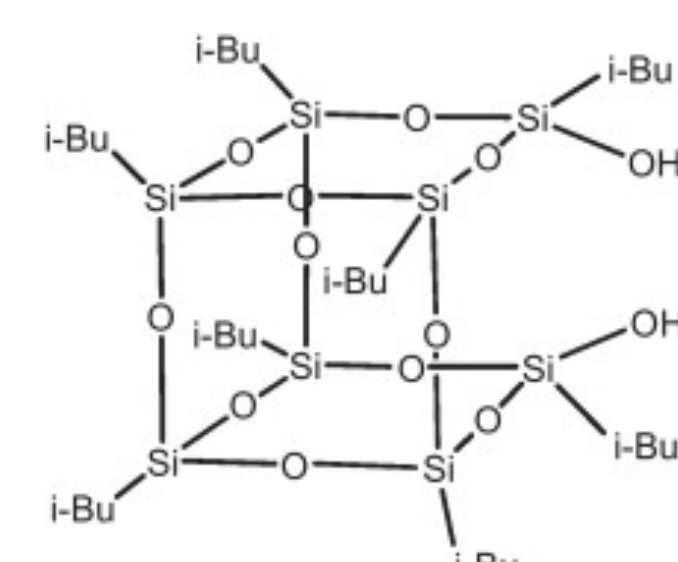
Time-of-flight secondary ion mass spectrometer (ToF-SIMS)
- Interface/surface technique
- Bismuth liquid metal ion beam
- Monitors positive and negative emitted ions

POSS Structures Analyzed

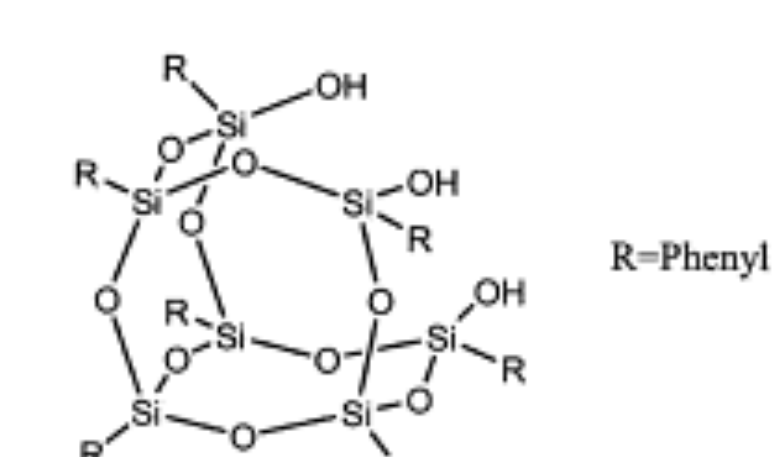
Sample 1: Octaviynil



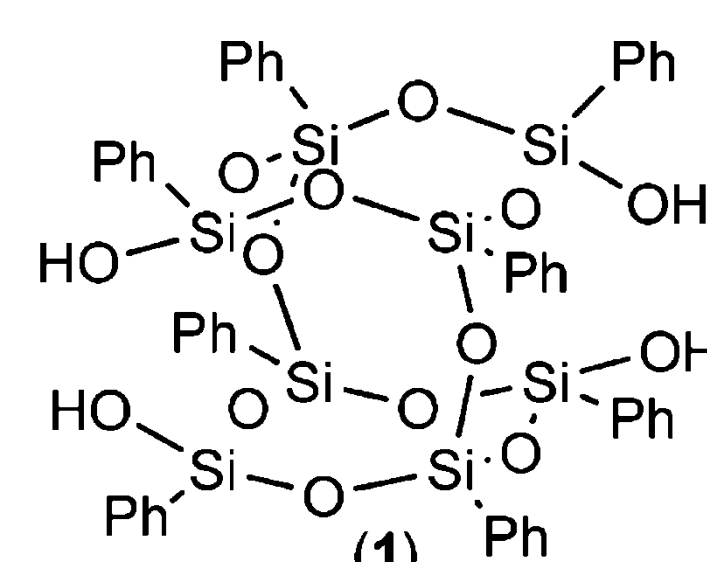
Sample 2: Trisilanol



Sample 3: Disilanol



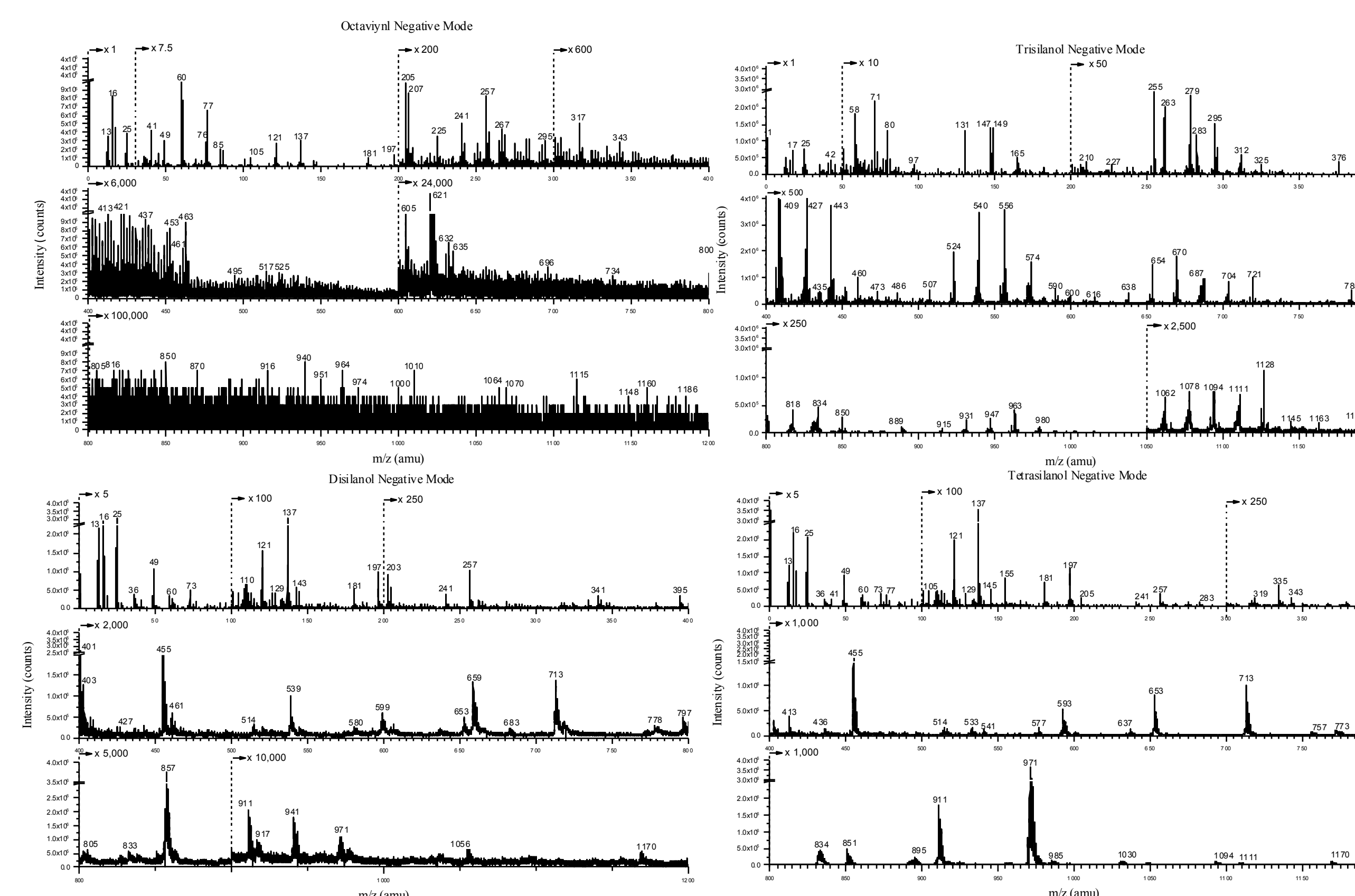
Sample 4: Tetrasilanol



Results

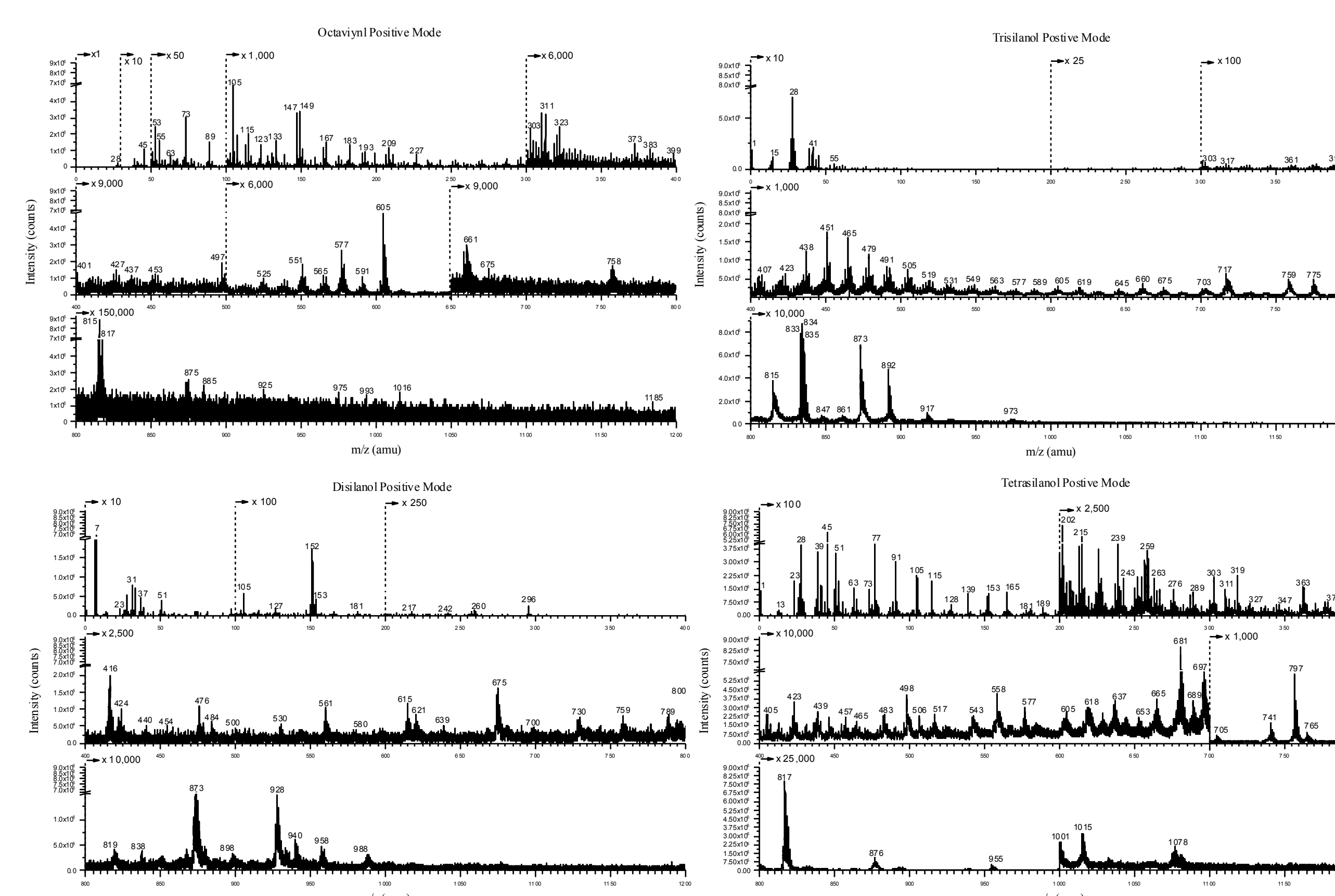
SIMS Negative Spectral Comparison

These plots display the a comparison of four different samples run in the negative mode, these samples show different molecular fragment ions, indicating distinct molecular structure.



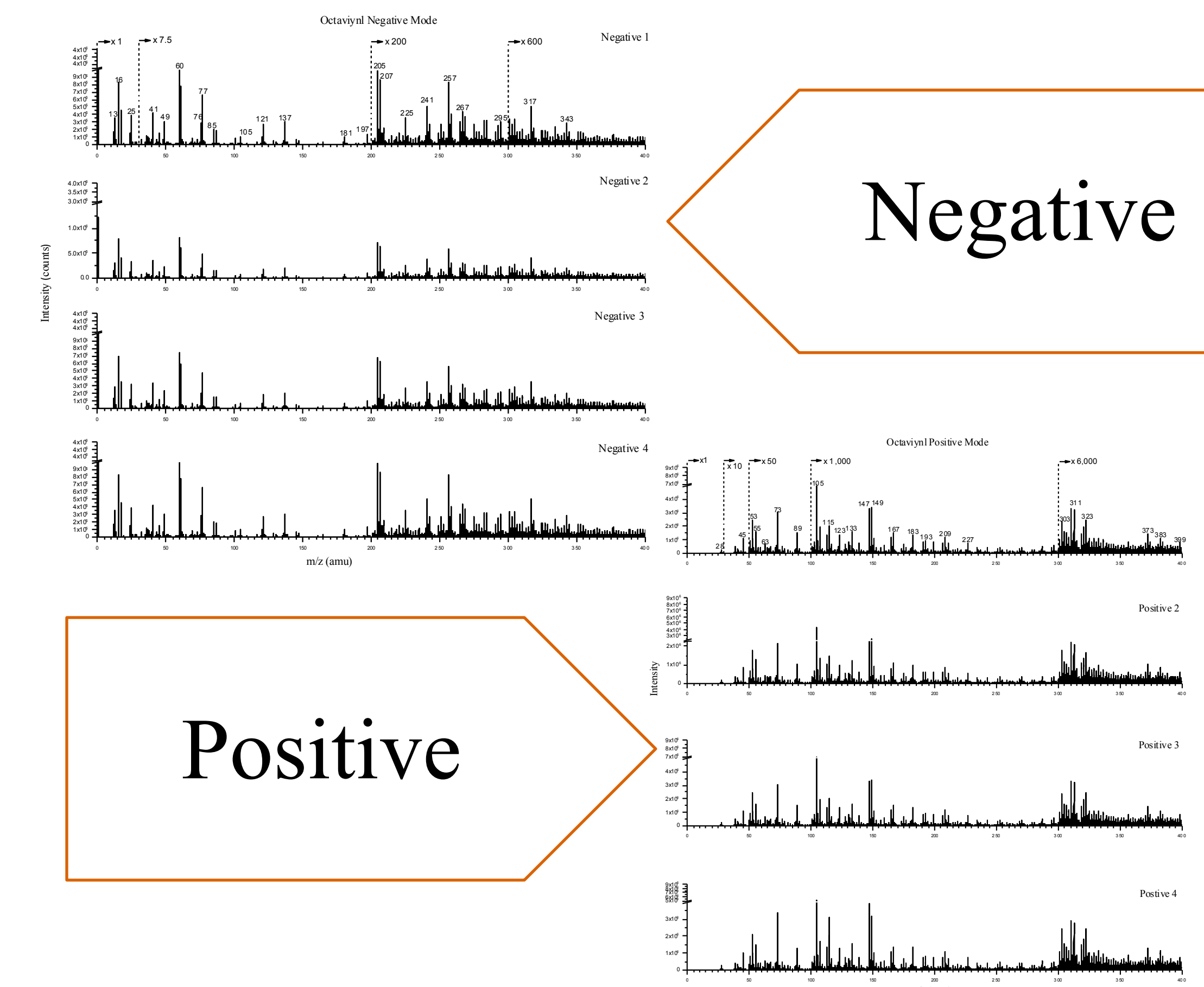
SIMS Positive Spectral Comparison

These plots display the a comparison of four different samples run in the positive mode, these samples also show different molecular ions, in agreement with the negative spectral analysis.



Spectral Reproducibility

The SIMS analysis has shown good reproducibility as illustrated below.



Negative

Positive

Discussion

- Four POSS powder samples with different Si-O bond and functioning groups were analyzed.
- Both positive ion and negative ion spectral plots were analyzed to obtain a more thorough understanding of characteristic peaks of the POSS samples.
- Peaks were then identified by searching for compounds masses and the intensity of these peaks reconfirmed the existence of that compound in the examined sample.
- Our results show that each POSS sample had unique molecular fragments indicative of its structure and building block.
- Our initial SIMS analysis demonstrates that useful structural information can be gained using SIMS.

Acknowledgments

Rachel Komorek, Abhi Karkamkar, James De Yoreo, LaVon Conlin, Zihua Zhu, and the ToF-SIMS research team at PNNL.

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Contact

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References

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