Non-Lead Broad Spectrum Absorbing Metal Halide Compounds: Synthetic Exploration

Chester Lao

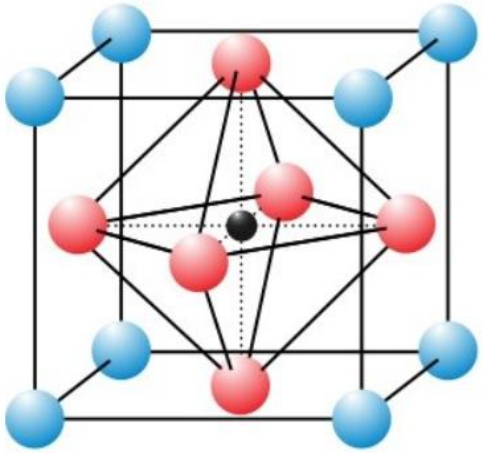
PI: Dr. Andrea Goforth

Mentor: Katherine Weinfurter

Context

Silicon-Based (most popular)	Perovskite-Based (ABX_3)
Expensive	Spin coating solution (cheap)
Large energy consumption	High efficiency, no extensive heating

[1]



[2]

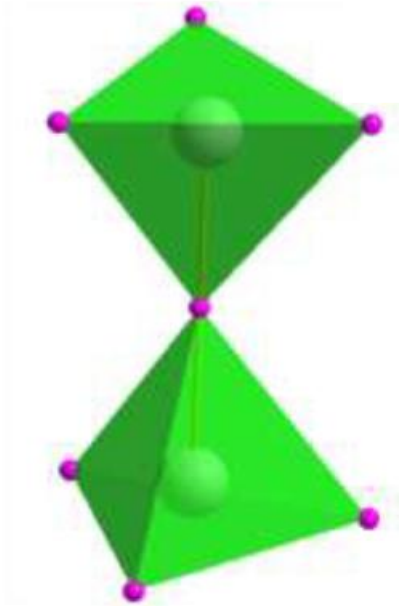
Most popular perovskites contain lead

But what if we didn’t have to use it?

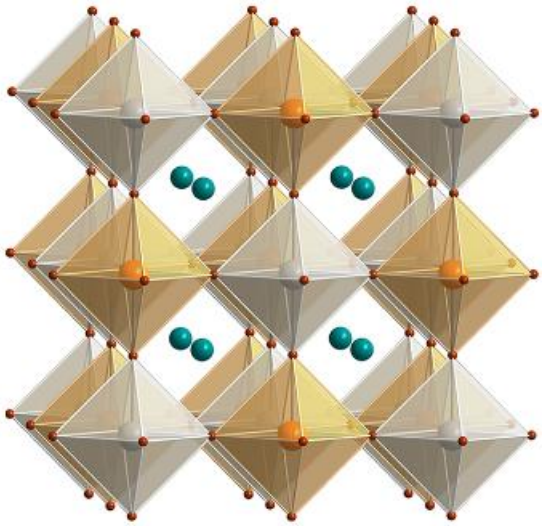
Motivation

- Three main methods used
- Replicating established methods from prior papers

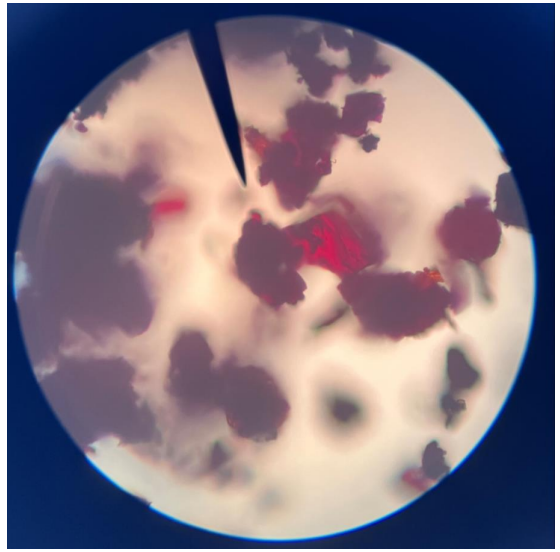
Silver/Bismuth Halide Framework



Silver-Bismuth Double Perovskite

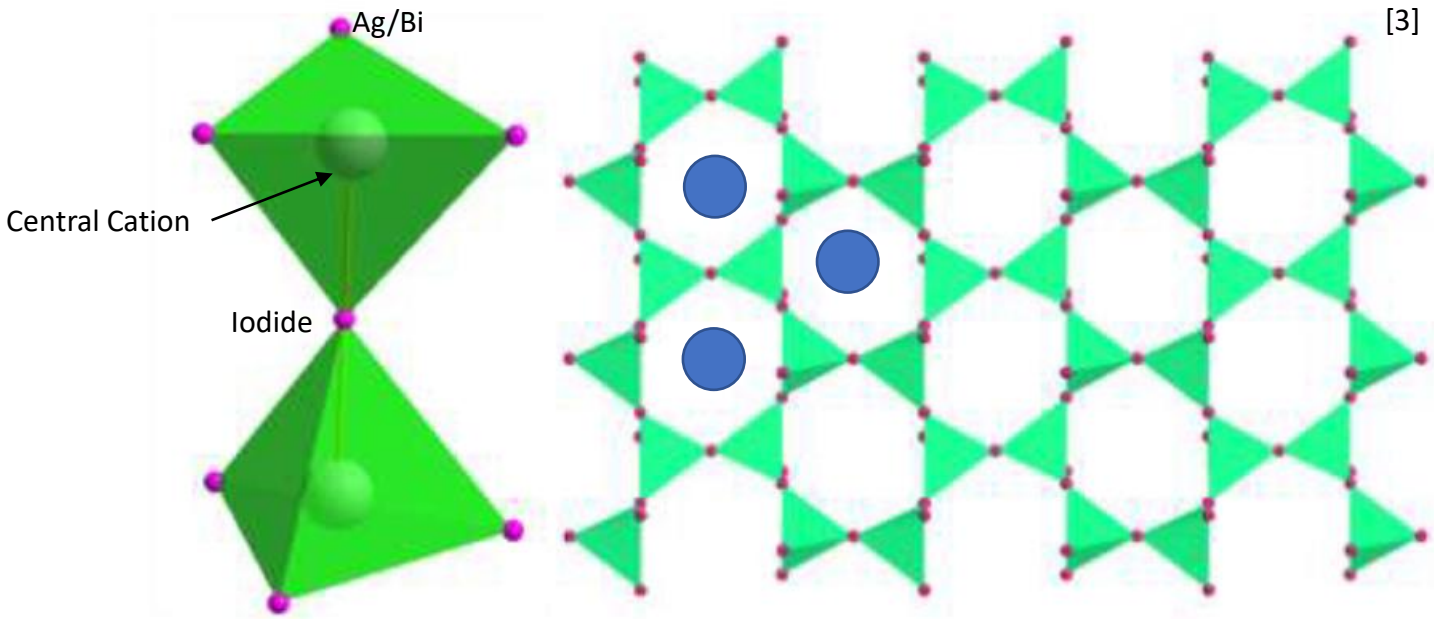


Cation Templated Bismuth Halide



Bismuth-Silver Halide Framework

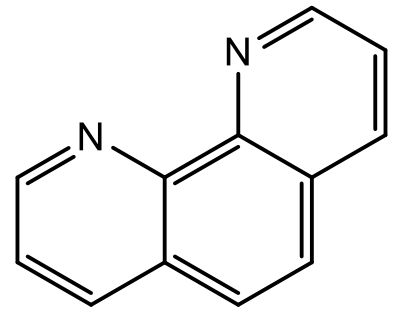
- Silver iodide surrounding coordination compound similar to perovskite structure

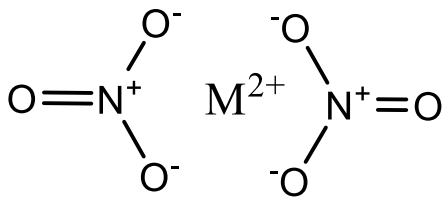


[3]

H.-G. Yao, L.-J. Deng, P.-X. Wu, J.-X. Li, and X.-C. Zhang, “SYNTHESIS, CRYSTAL STRUCTURE AND PROPERTY OF A NEW TRIDYMITE-TYPE IODOARGENTATE,” vol. 4, p. 6, 2014.

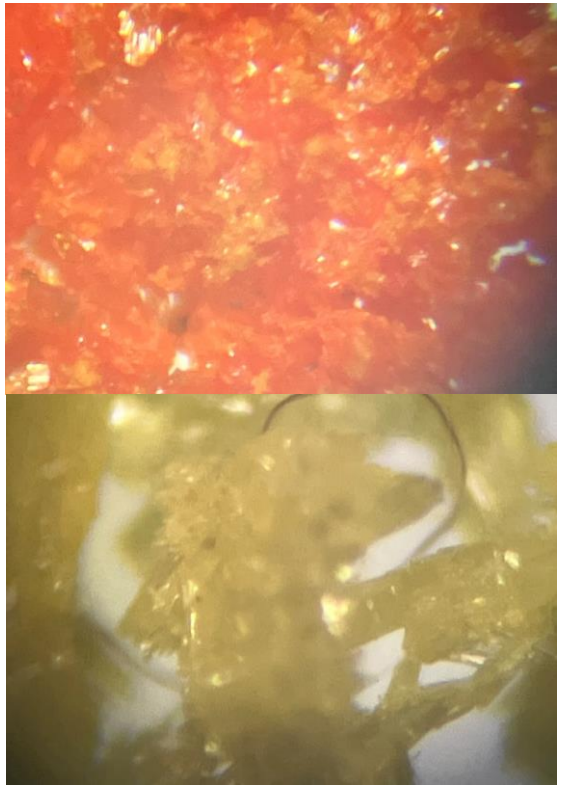
Bismuth-Silver Halide: Procedure





1. Ag_2I_4/BiI_3+DMF

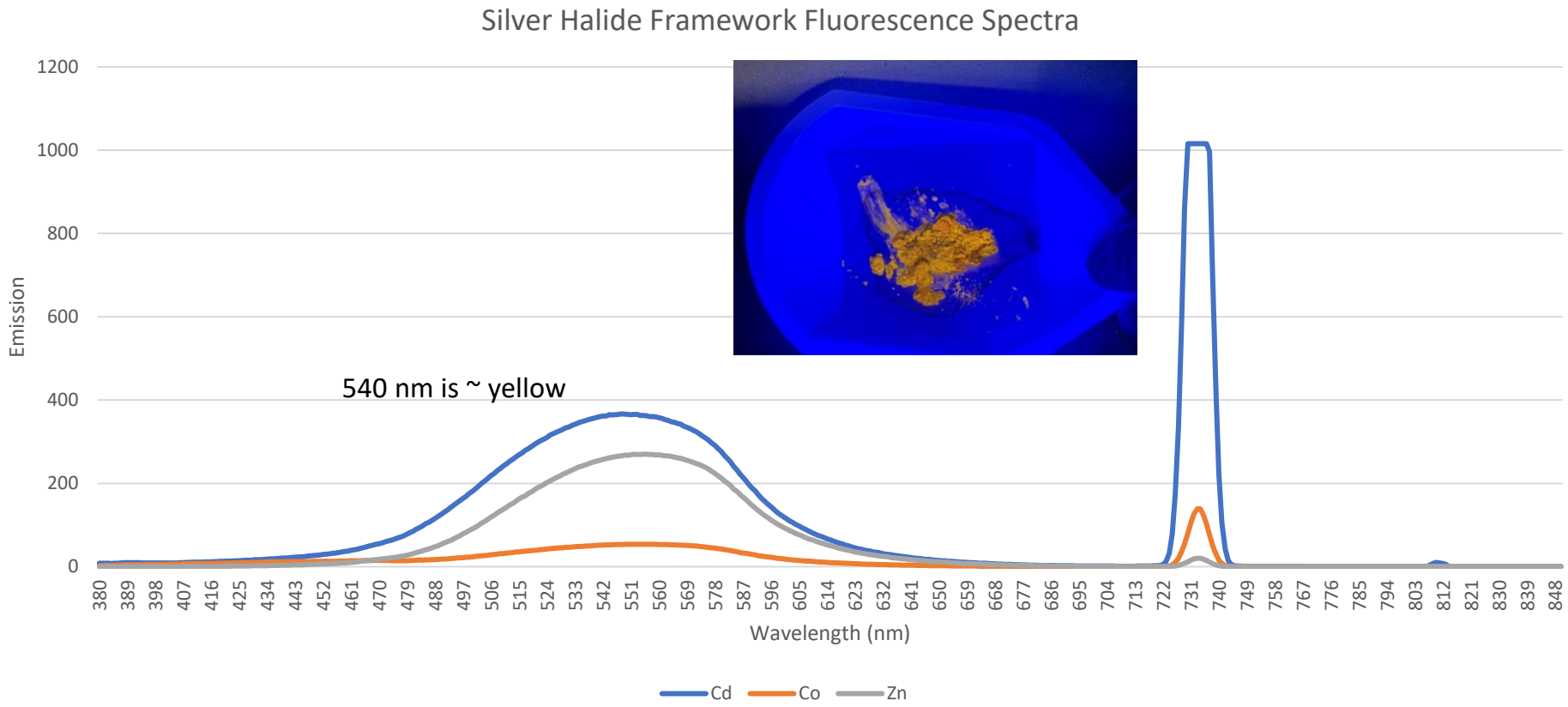
2. ~6 days wait



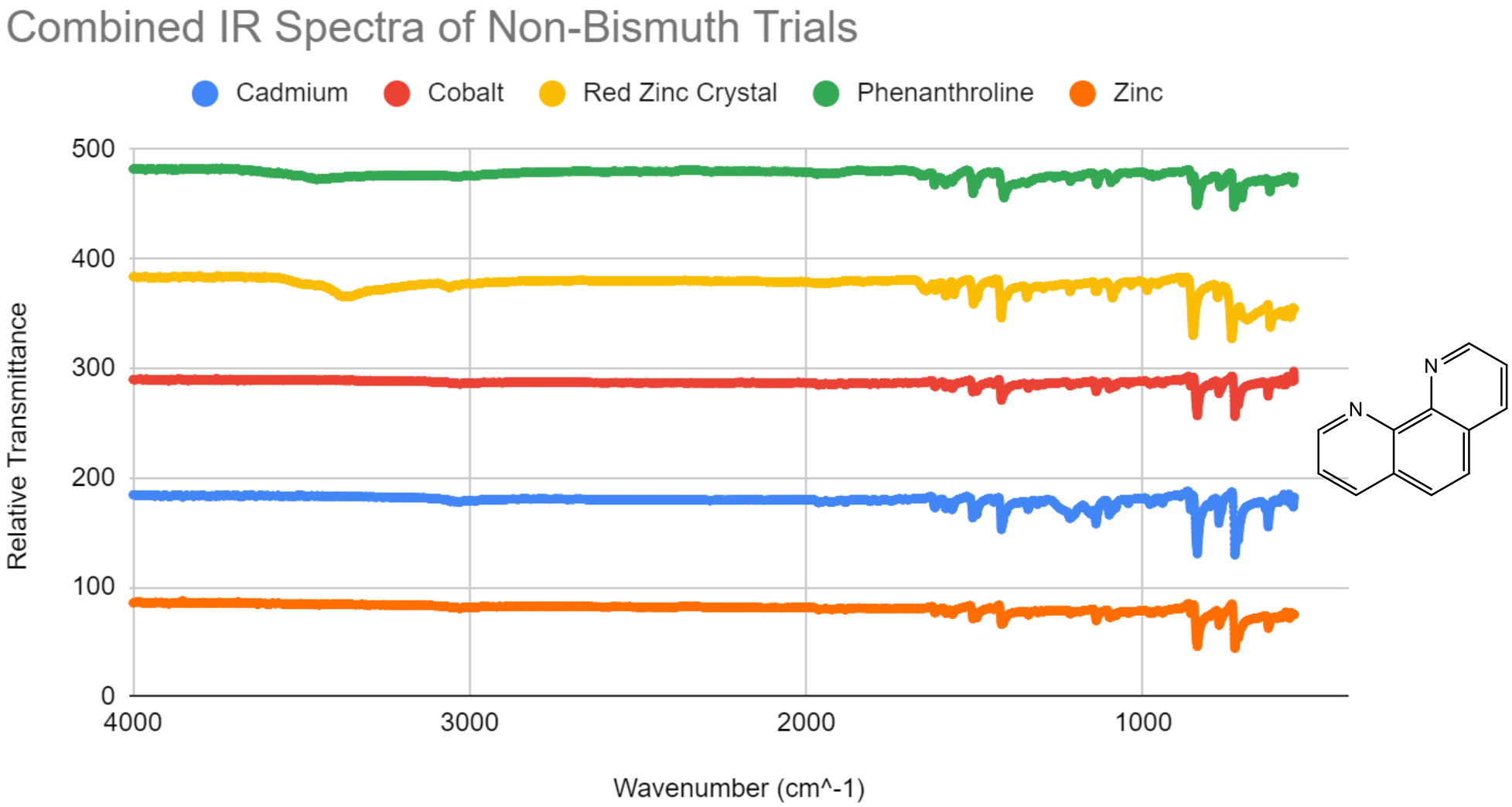
Substitutions, 5 variants:

1. $Zn \leftrightarrow Cd \leftrightarrow Co$
2. ethylaminediamine ↔1,10-phenanthroline
3. $Ag_2I_4 \leftrightarrow BiI_3$

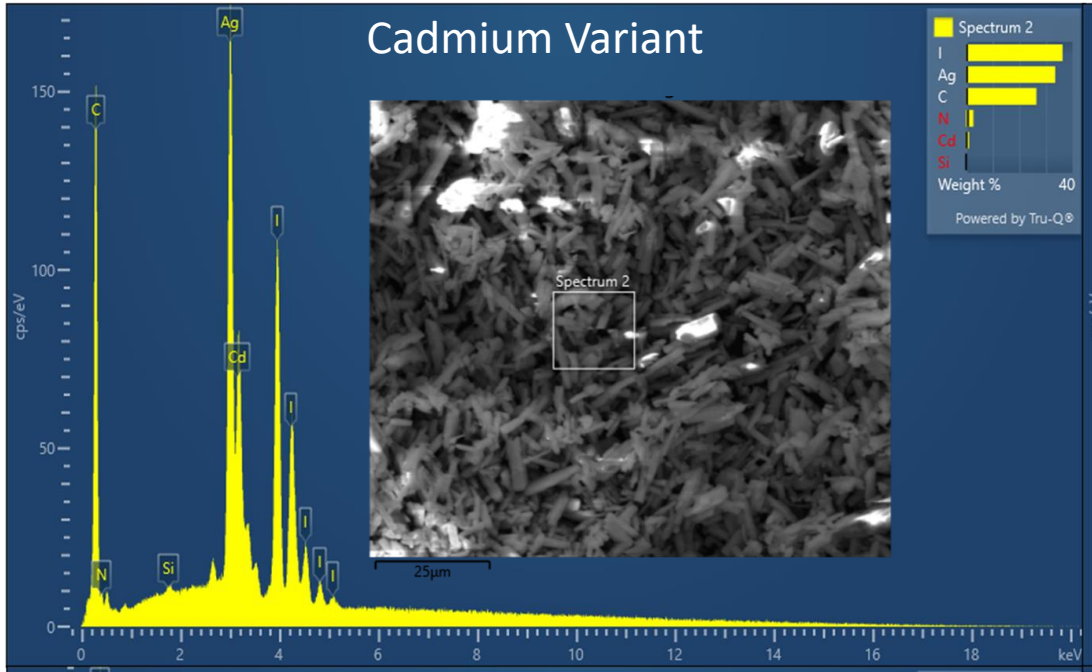
Silver Halide: Fluorescence

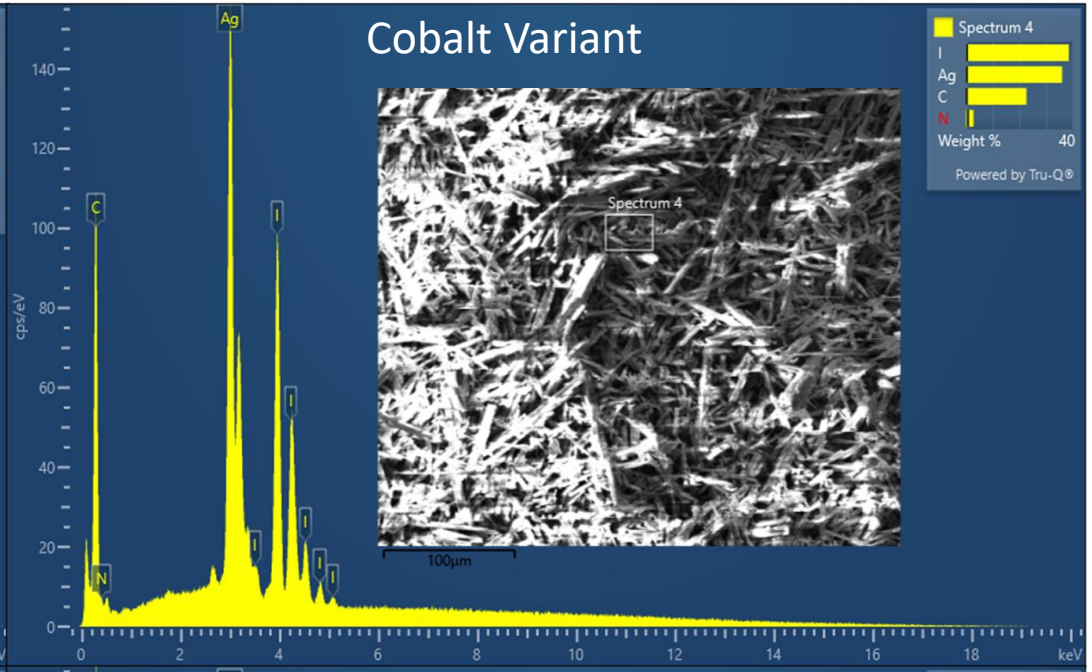


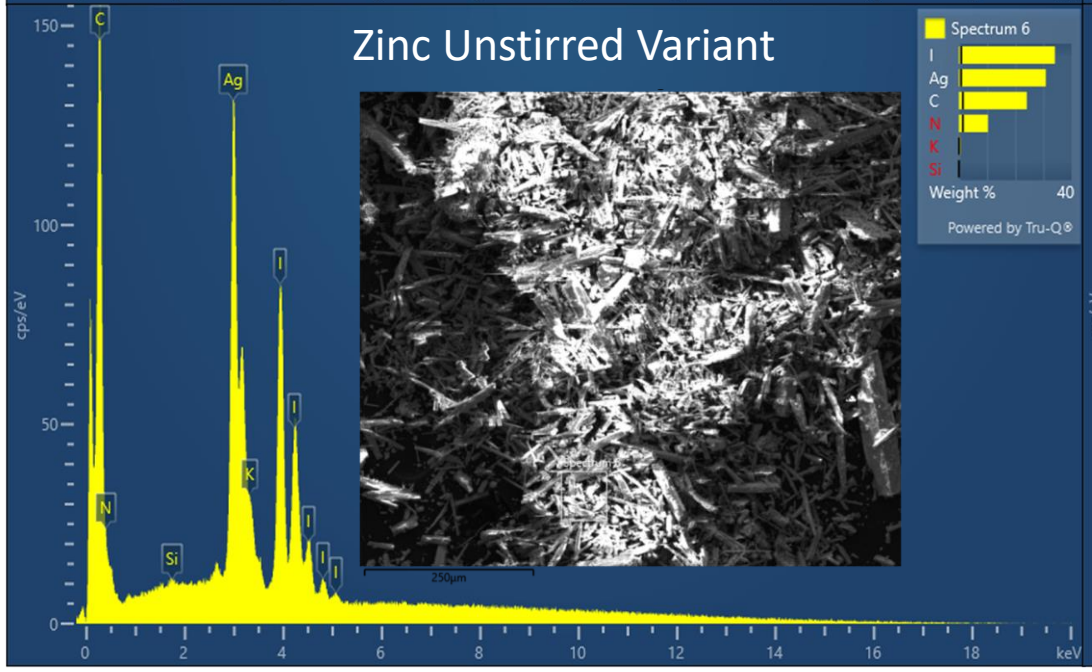
Silver Halide: IR Data

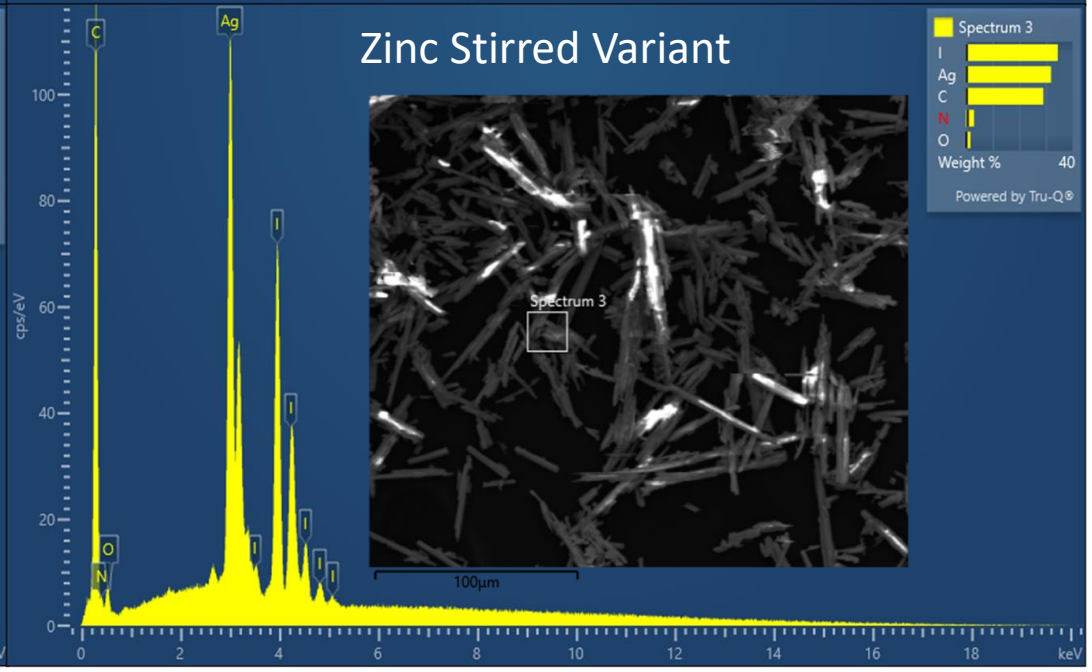


Silver Halide: PFIB Imaging/EDX

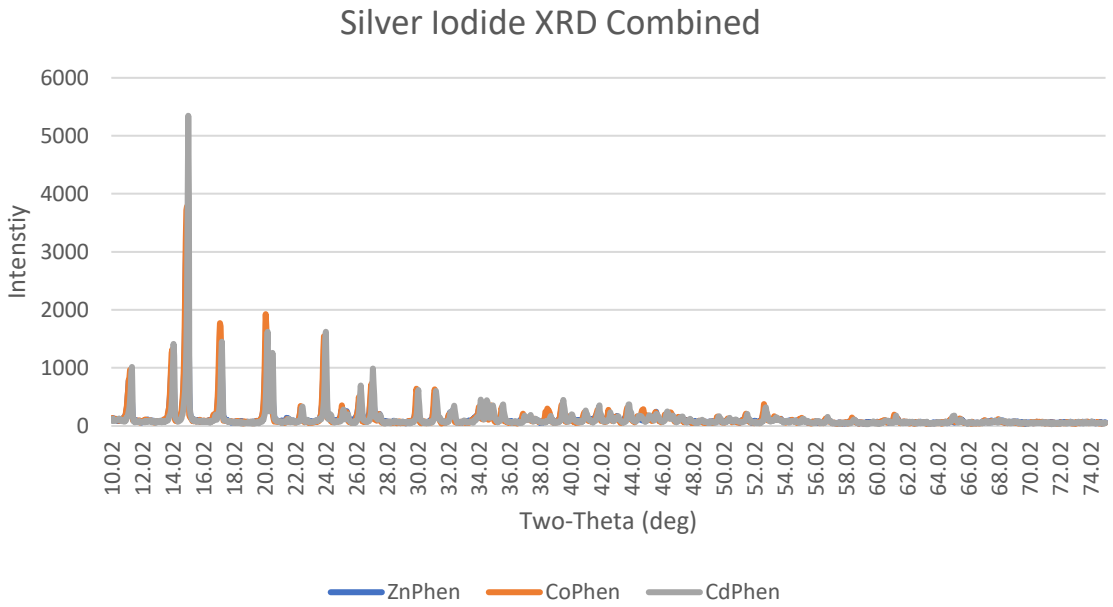


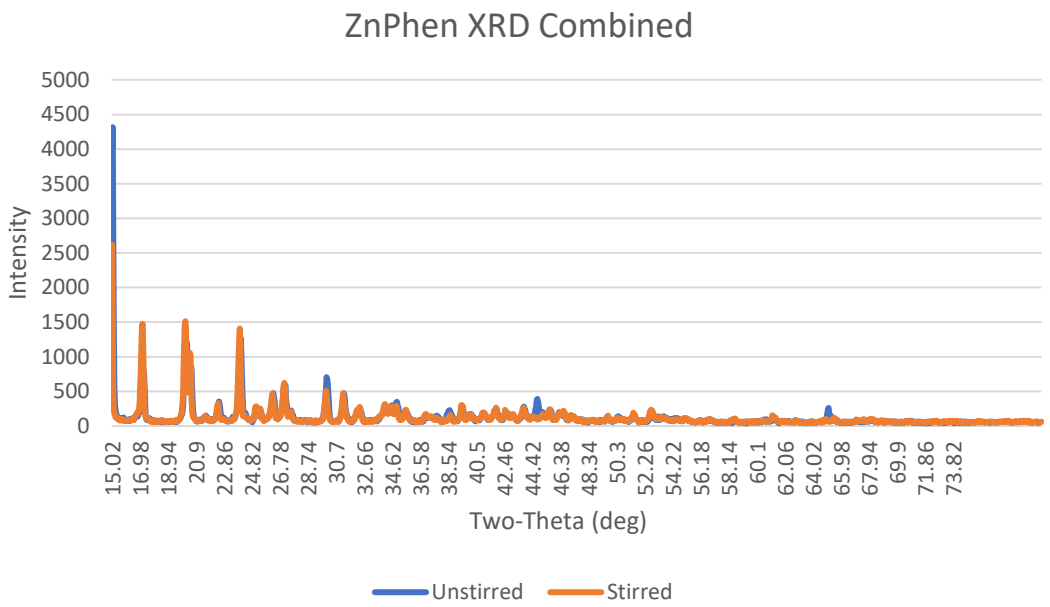






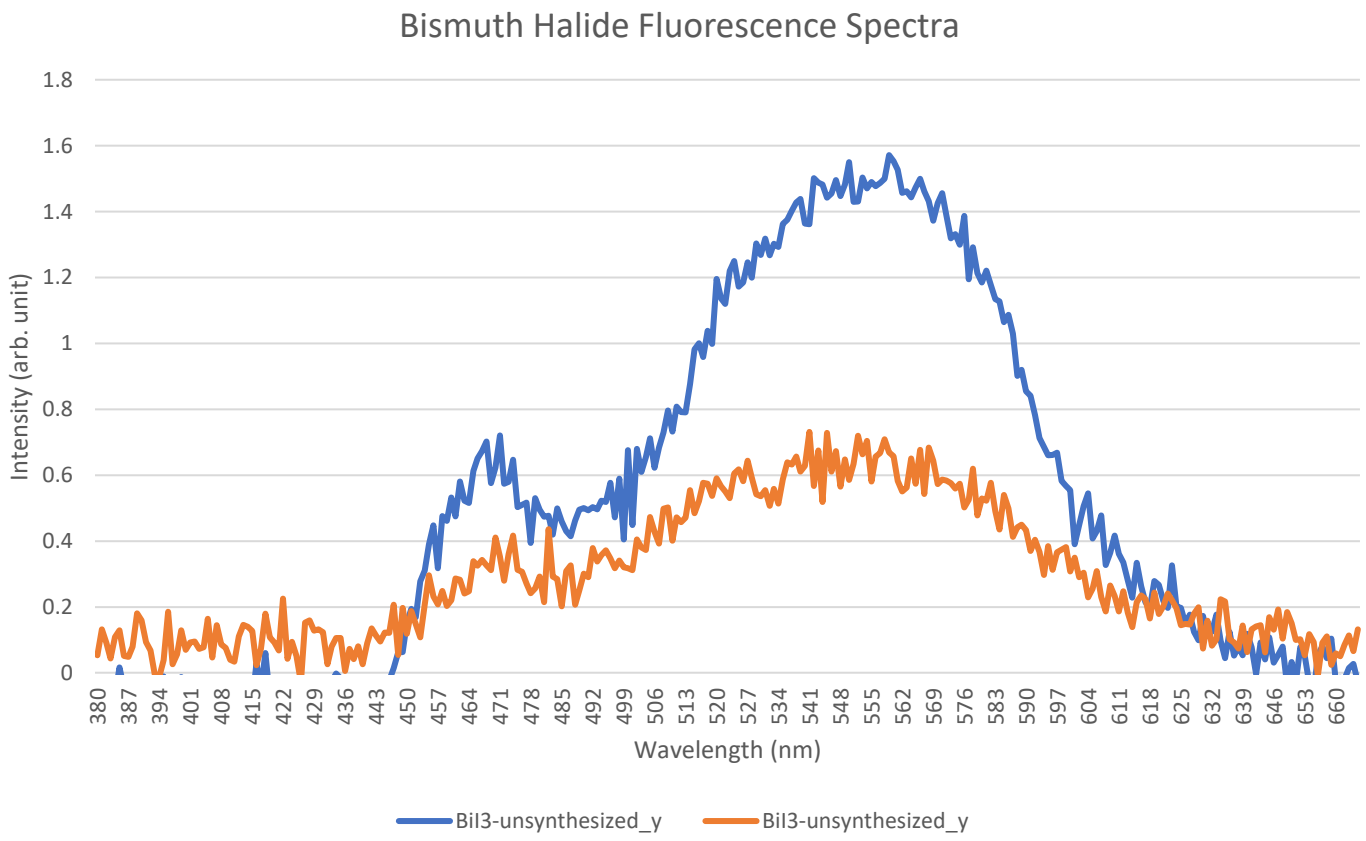
Silver Halide: XRD Powder Diffraction





Regardless of substitution, all variants that used AgI had similar XRD powder diffraction patterns

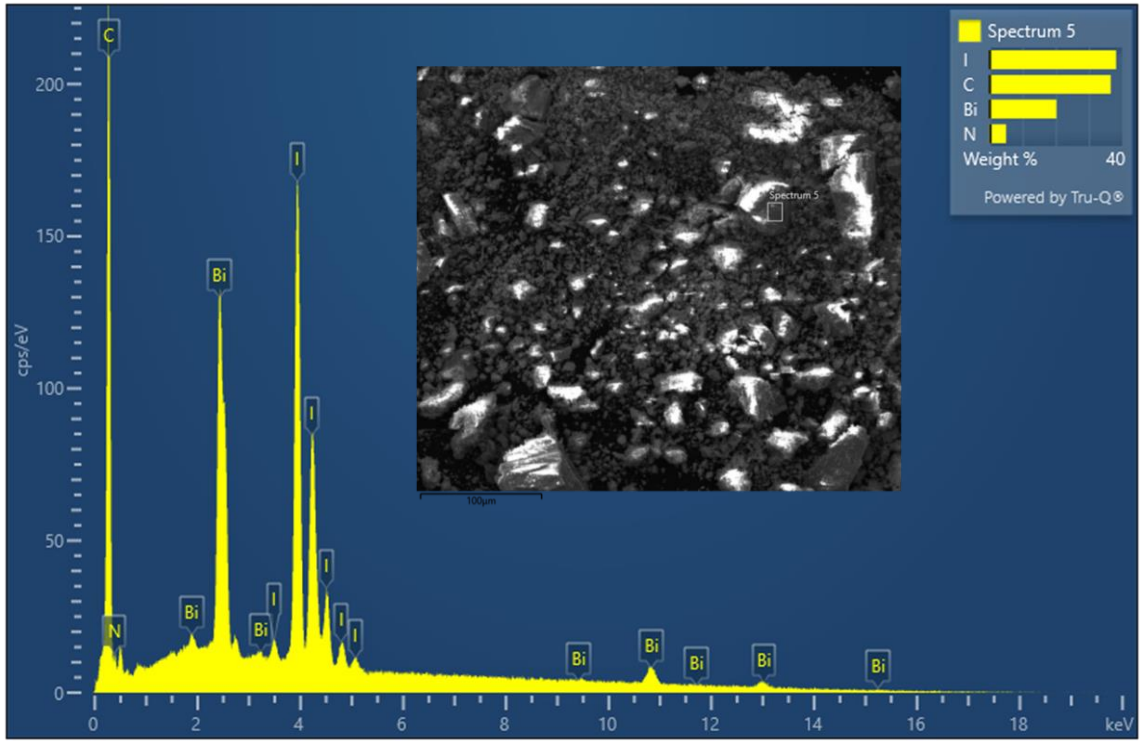
Bismuth Halide: Fluorescence



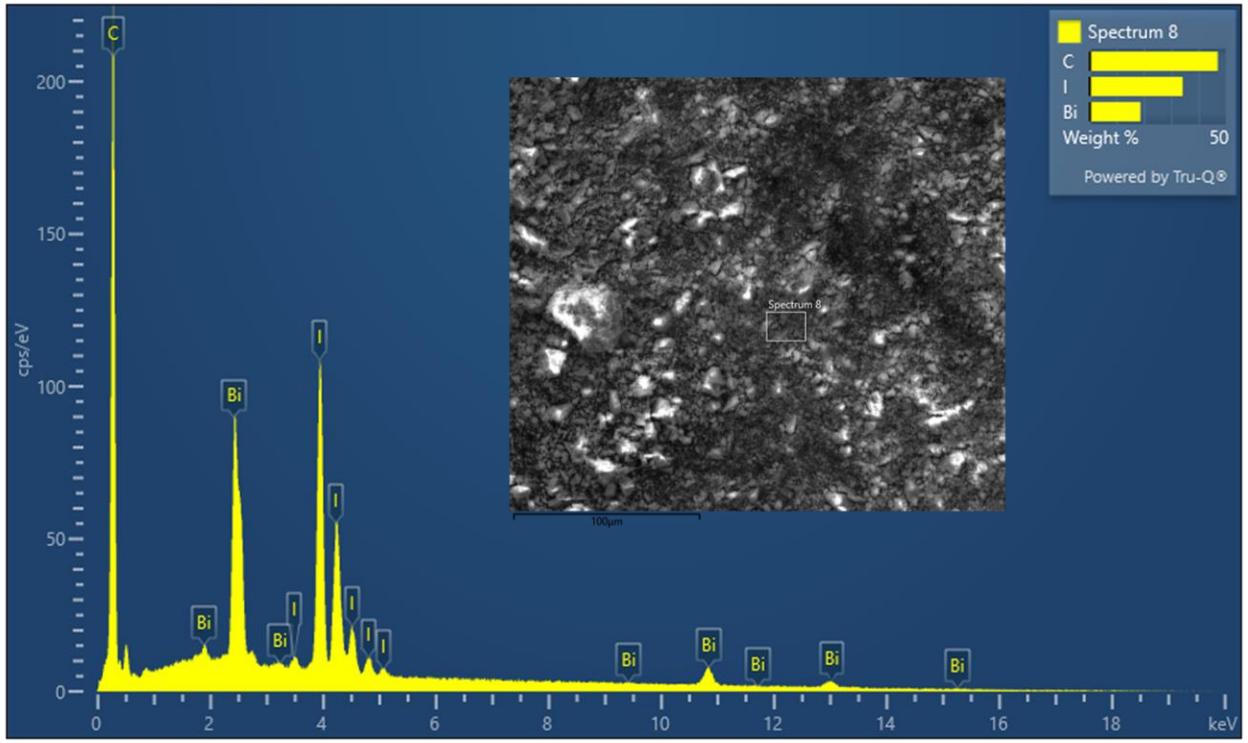
Peak at ~560-570 nm (around orange)

Bismuth Halide: PFIB Imaging/EDX

Bismuth Synthesized

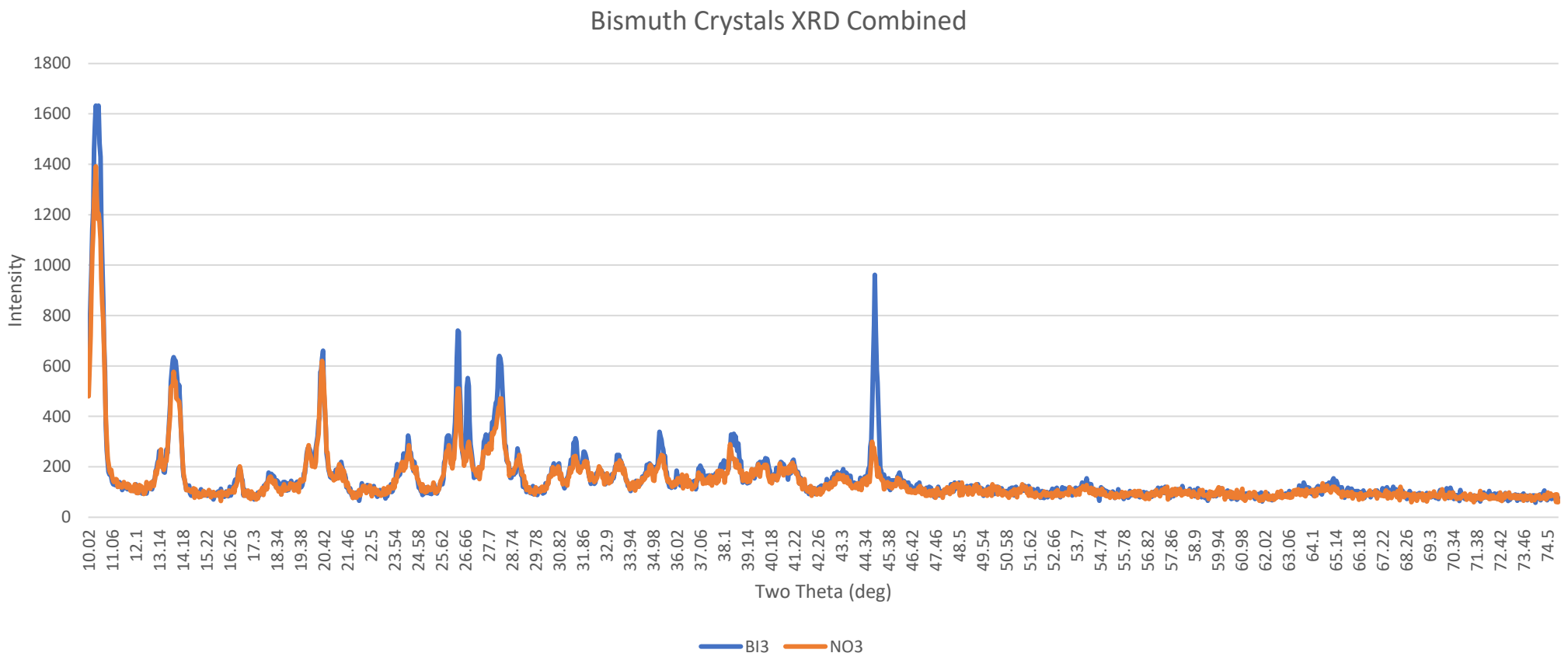


Bismuth Unsynthesized



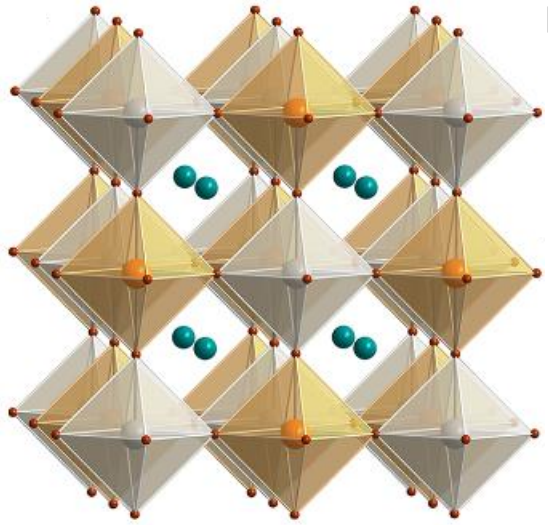
- Zinc not strongly present
- EDX analysis very similar

Bismuth Halide: XRD



Unsynthesized and synthesized compounds created similar structures
Computer unable to generate peaks

Silver Bismuth Double Perovskite



[4]

Double Perovskite: Procedure

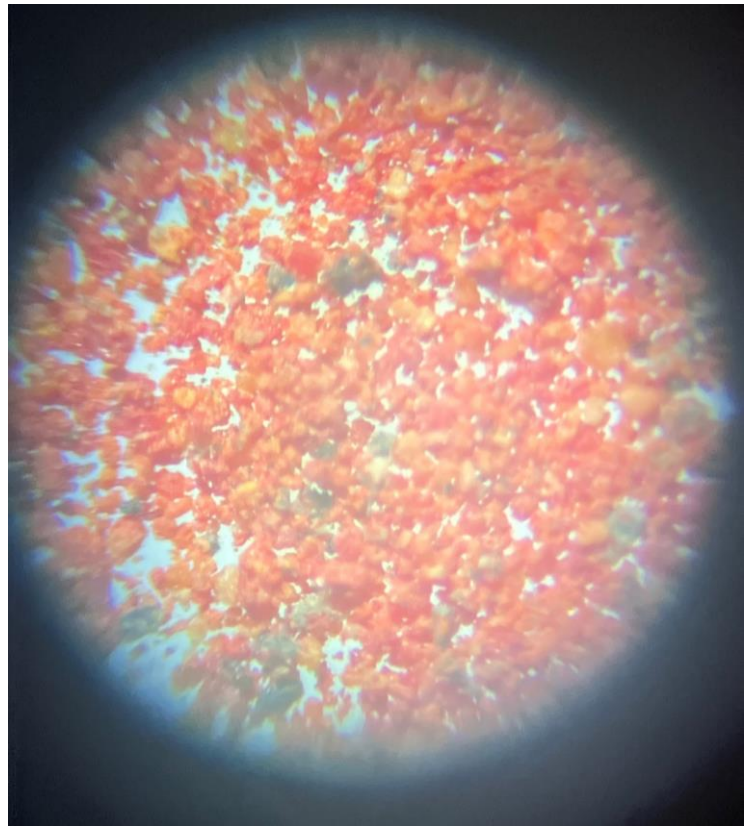
$CsCl\ (0.002\ mol)$

$BiI_3 (0.001\ mol)$

$AgCl\ (0.001\ mol)$

1. 10 mL 9M HCl 2. Heated to 110 C

3. Cooled to 35 C at 0.1 C/min

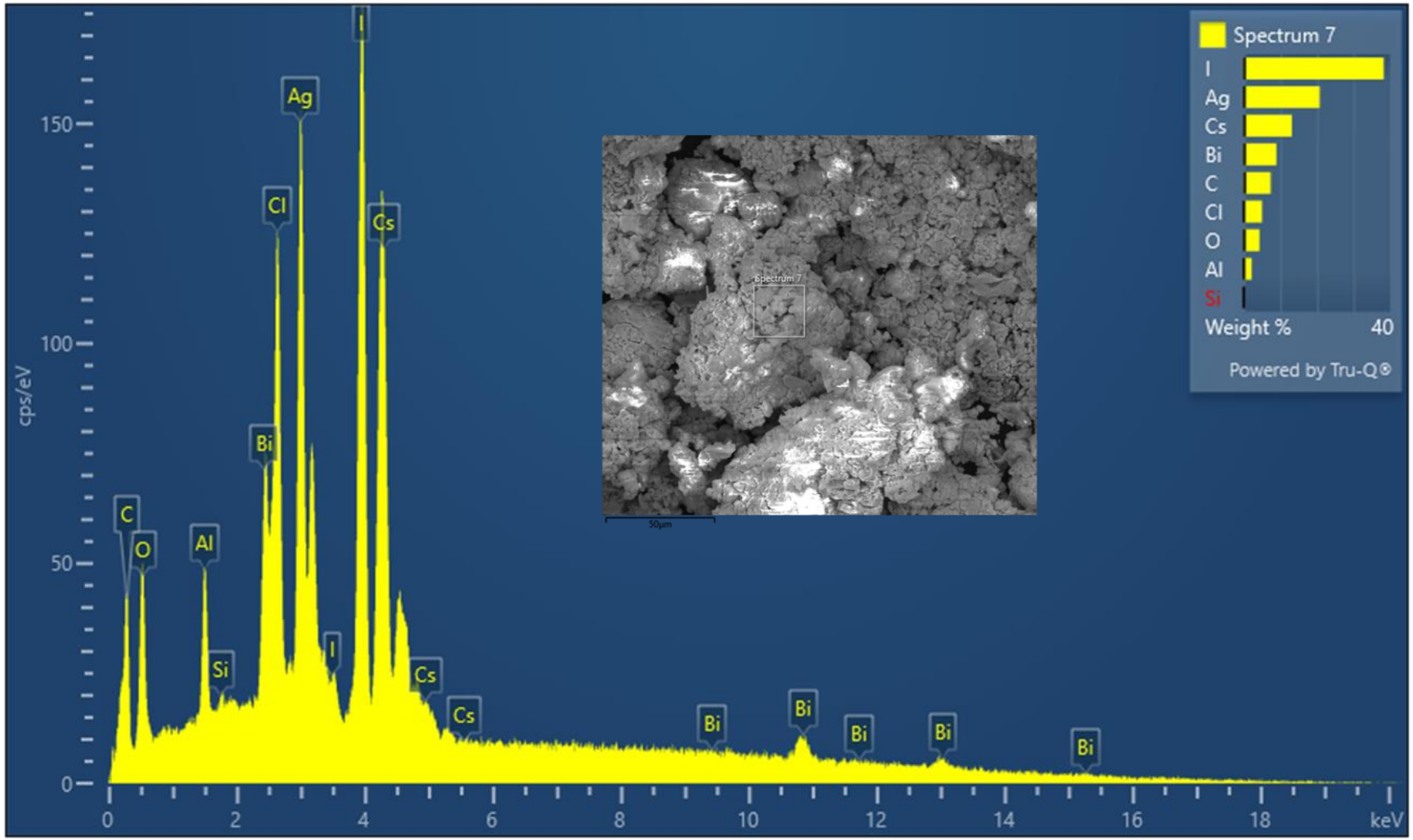


Substitutions:

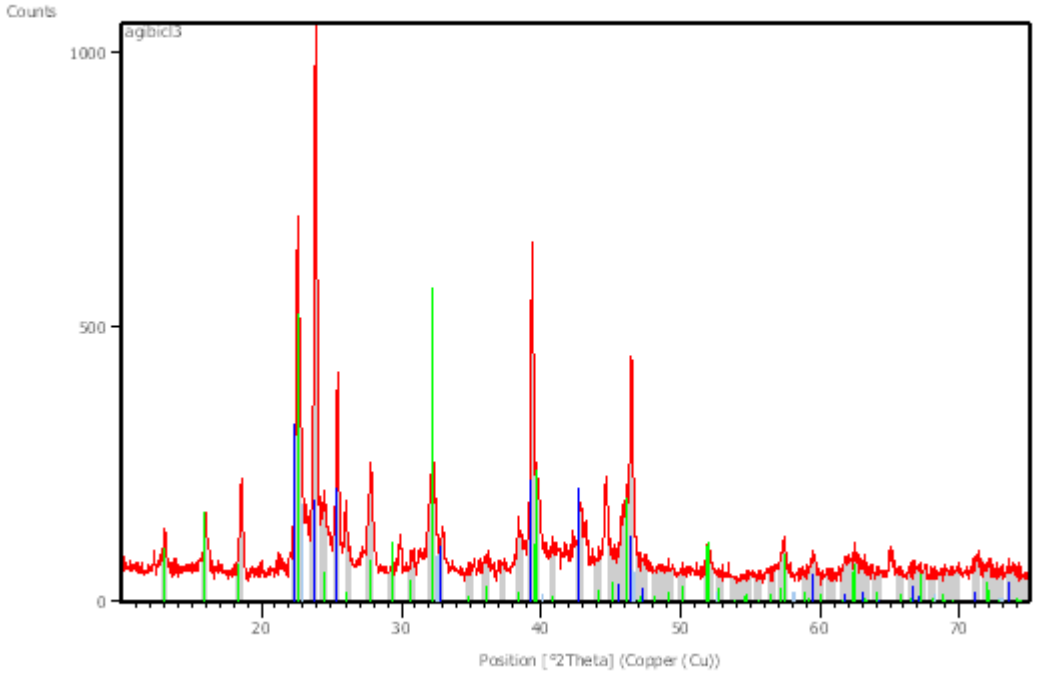
- CsBr for CsCl
- $BiBr_3$ for BiI_3
- $AgBr$ for $AgCl$

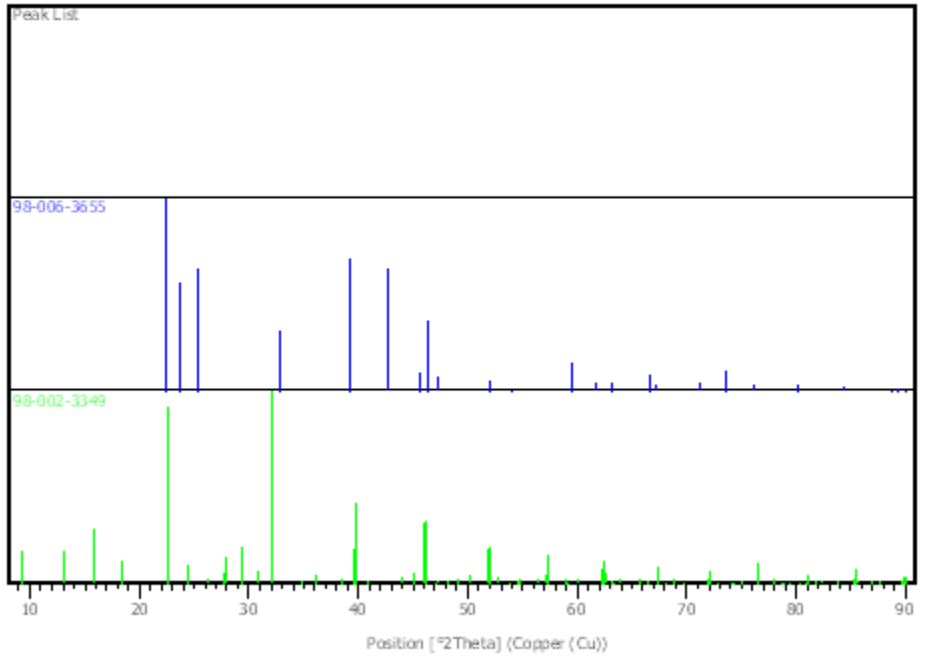
*IR and Fluorescence Spectra did not contain any significant data

Double Perovskite: PFIB/EDX



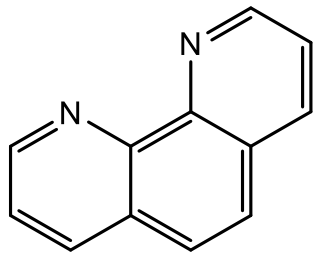
Double Perovskite XRD Data

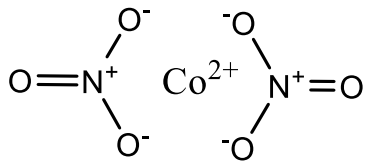




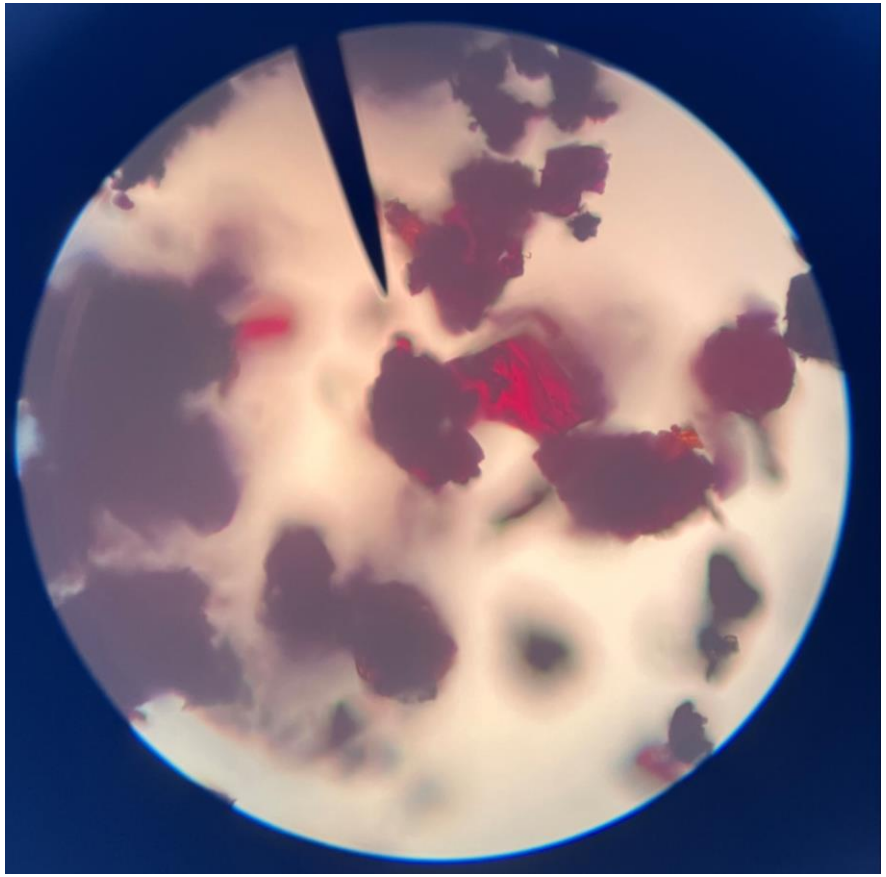
Pattern List				
Reference Code	Score	Compound Name	Scale Factor	Chem
98-006-3655	51	Iodargyrite	0.308	Ag1I1
98-002-3349	46	Tricesium Nonachloride	0.541	Bi2C19Cs3

Cation Templated Bismuth Halide



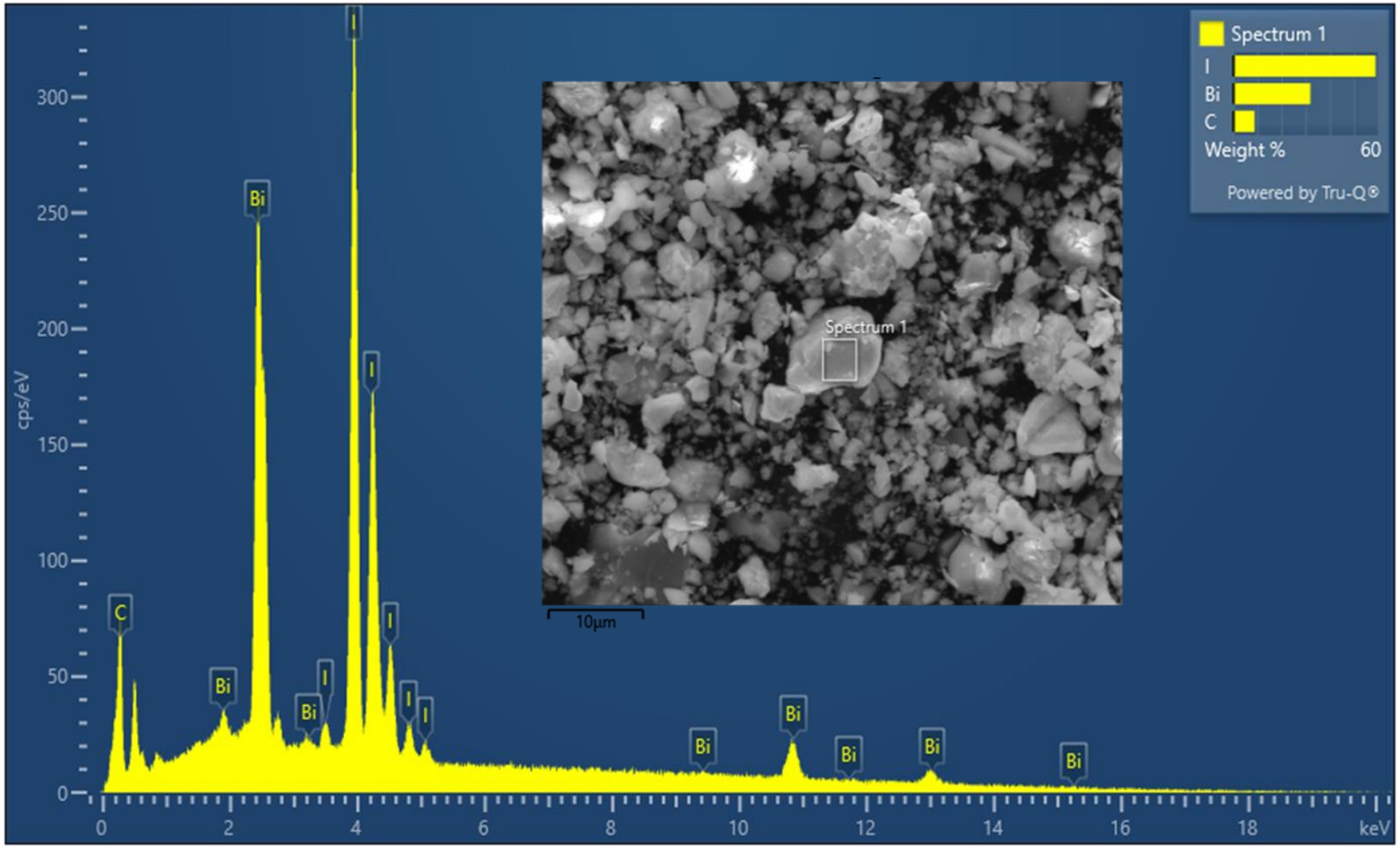


1. BiI_3+EtOH 2. 160 C by 0.1 C/min
3. 160 C for 3 Days
4. 70 C for 6 hrs 5. Cooled to 35 C at 0.1 C/min

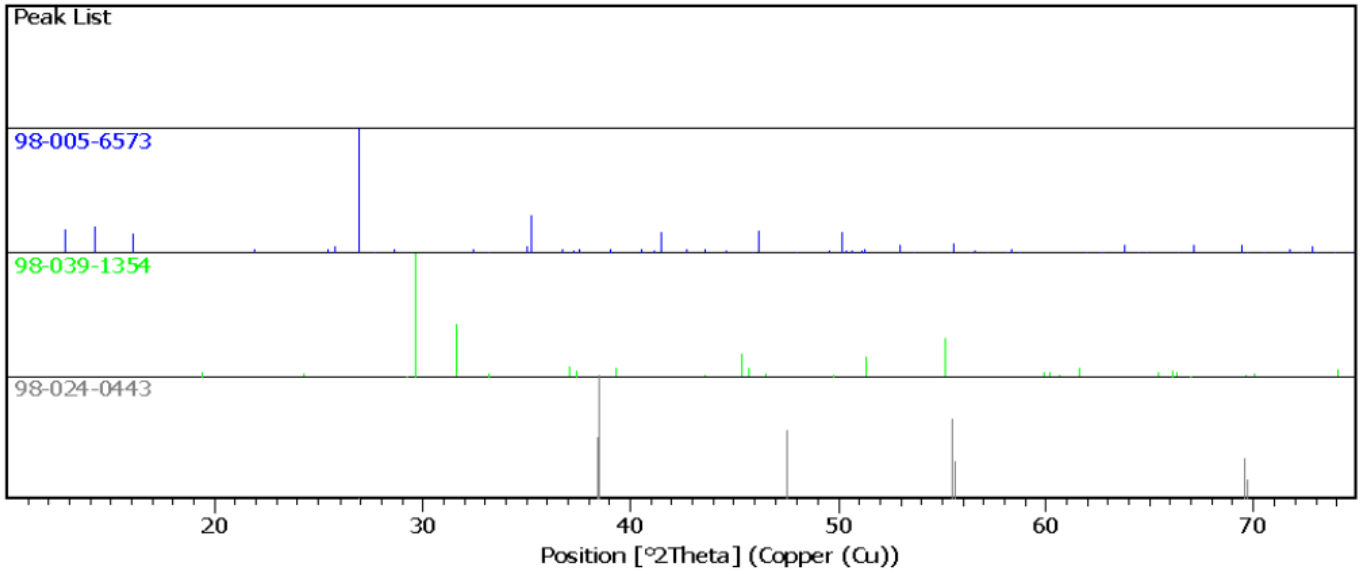


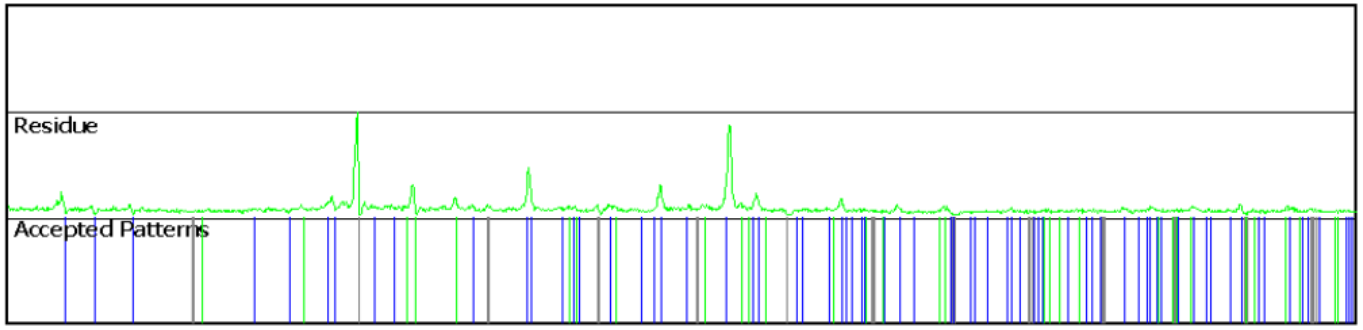
*IR Spectra and Fluorescence did not have any significant data

Cation Templated Bismuth Halide PFIB/EDX



Cation Templated Bismuth Halide XRD





No.	Visible	Ref. Code	Compound Name	Chemical Formula	Score	SemiQuant [%]
1	TRUE	98-005-6573	Bismuth Iodide	Bi1 I3	36	17
2	TRUE	98-039-1354	Bismuth Oxide Iodide	Bi1 I1 O1	25	6
3	TRUE	98-024-0443	Calcium Catena-silicate	Ca1 O3 Si1	23	77

Conclusion/Future Direction

- Crystals synthesized!
- No significant amounts of central cations
  - Adding more central cation for future trials
- “Hair crystals” from filtrate
- Different substitutions
- UV Vis
- Single Crystal Diffraction

Acknowledgements

- The Author's participation in this project was supported by the National Science Foundation's *Application of Microscopy and Microanalysis in Multidisciplinary Research* REU program at Portland State University (Grant # 1851851)

References

[1] ChristofferRiemer, “As solar firmengebaude.jpg.” https://commons.wikimedia.org/, Oct 2009. [Online]. Available: https://commons.wikimedia.org/wiki/File:As_solar_firmengebaude.jpg. [Accessed Aug. 10, 2022].

[2] Korjus, “Perovskite ABO3.jpg.” https://commons.wikimedia.org, May 2011. [Online[. Available: https://commons.wikimedia.org/wiki/File:Perovskite_ABO3.jpg. [Accessed Aug. 10, 2022]

[3] H.-G. Yao, L.-J. Deng, P.-X. Wu, J.-X. Li, and X.-C. Zhang, “SYNTHESIS, CRYSTAL STRUCTURE AND PROPERTY OF A NEW TRIDYMITE-TYPE IODOARGENTATE,” vol. 4, p. 6, 2014.

[4] A. H. Slavney, T. Hu, A. M. Lindenberg, and H. I. Karunadasa, “A Bismuth-Halide Double Perovskite with Long Carrier Recombination Lifetime for Photovoltaic Applications,” ACS Publications, Feb. 10, 2016. http://pubs.acs.org/doi/full/10.1021/jacs.5b13294 (accessed Jul. 12, 2022).

Thank You For Listening!

Questions?