Synthesis of $BaXP_2S_6$ and $BaX_2P_2S_8$ Nonlinear Optical Material Crystals (X = Zn, Cd)

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01. INTRODUCTION

Nonlinear Optical Materials have military and civilian applications, namely laser production to upconvert frequencies and produce different intensities.(1)

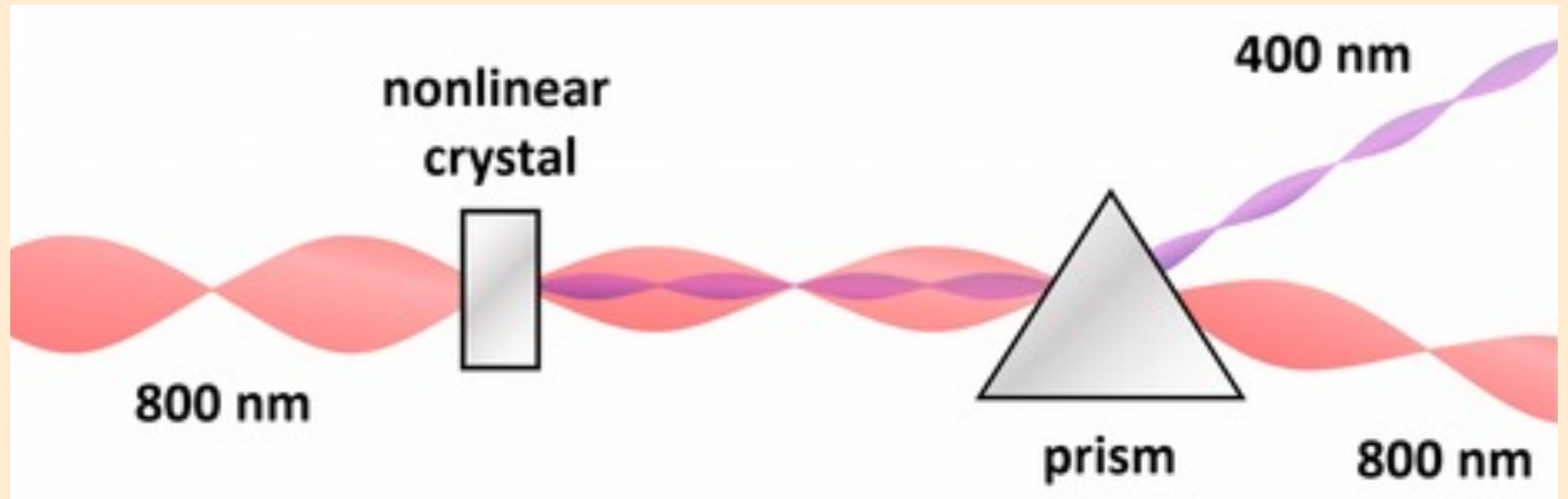

Figure 1 - Diagram of 800 nm of laser beam upconverted to 400 nm after shot through a crystal with nonlinear optical response.(2)

Main focuses of this study:

- Synthesize inorganic NLO crystals with 7 ideal qualities
- NLO applicable in the mid-IR and UV spectrum
- Target compounds were inspired by $Ba_2P_2S_6$ parent compound: $[P_2S_6]$ motifs contribute to high second harmonic generation (SHG) responses(3)

02. HYPOTHESIS

Based on the Jahn-Teller Theory, the disordered arrangement of Zn^{2+} and Cd^{2+} may increase the likelihood of the target compounds to be noncentrosymmetric by influencing $[P_2S_6]$ motif alignments.

03. METHODOLOGY

5 samples made for each target compound (each with different salt flux) in glove box

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Vaccuum & Torch: sealed sample tubes

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Furnace: samples heated to 800°C in 20 hours, kept there for 96 hours, cooled down naturally

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Microscope: made observations (see Figure 5)

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Powder X-Ray Diffraction: Intensity vs. 2-Theta

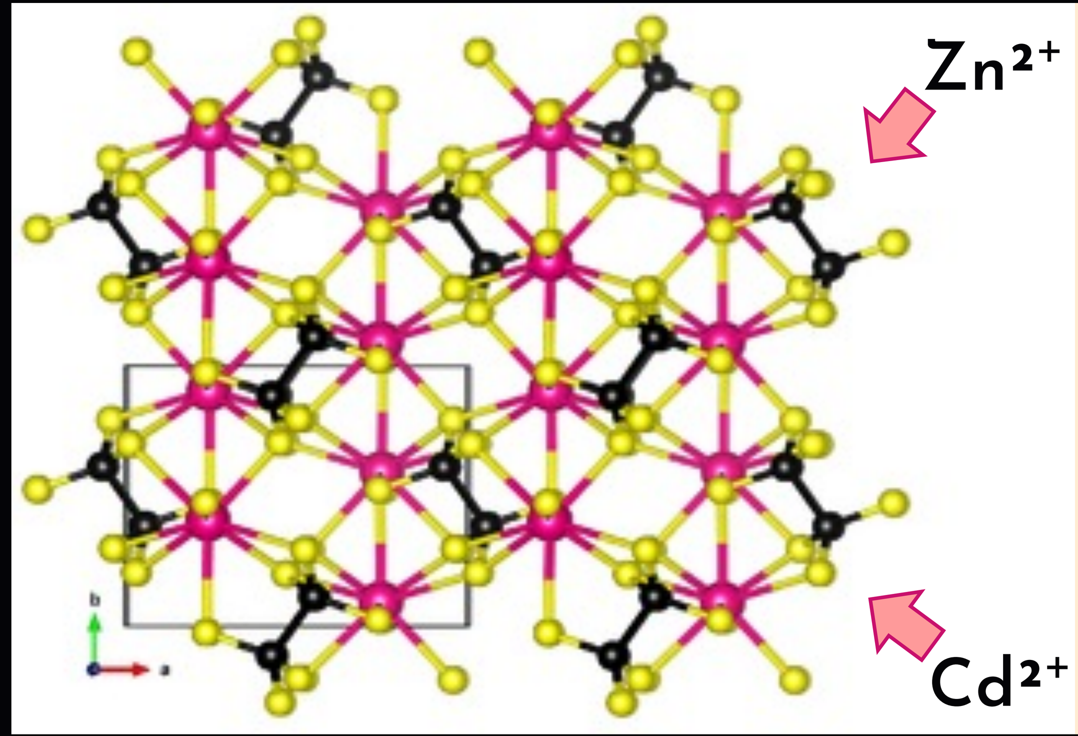

Figure 2 - Model of parent compound $Ba_2P_2S_6$ is shown. Arrows indicate the goal of adding Zn^{2+} or Cd^{2+} into the system.

04. RESULTS

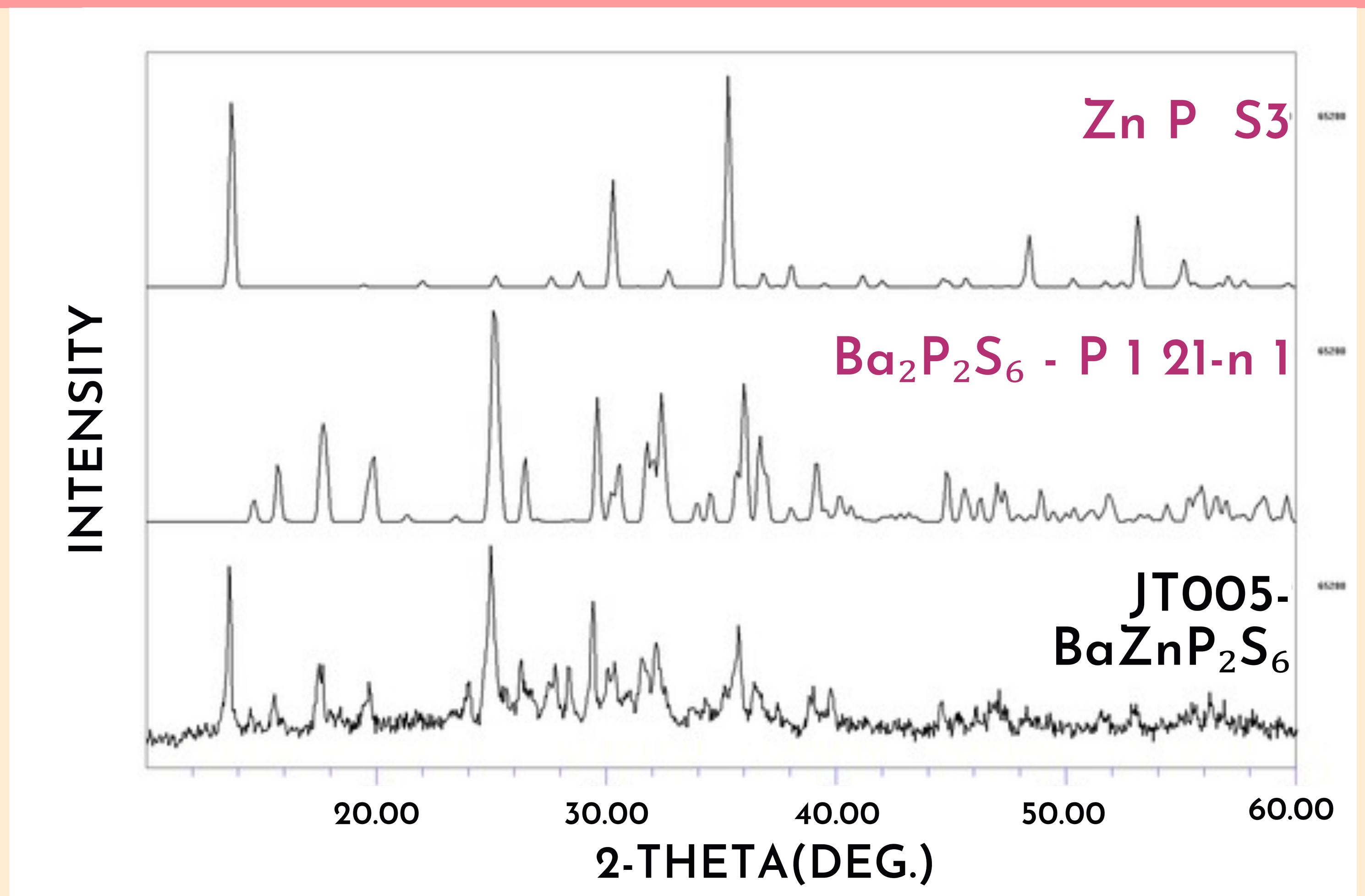

Figure 3 - Comparison of a previously published X-ray diffraction data(4) of $ZnPS_3$ versus experimental results of $BaZnP_2S_6$ (utilized I_2 as transport agents.)

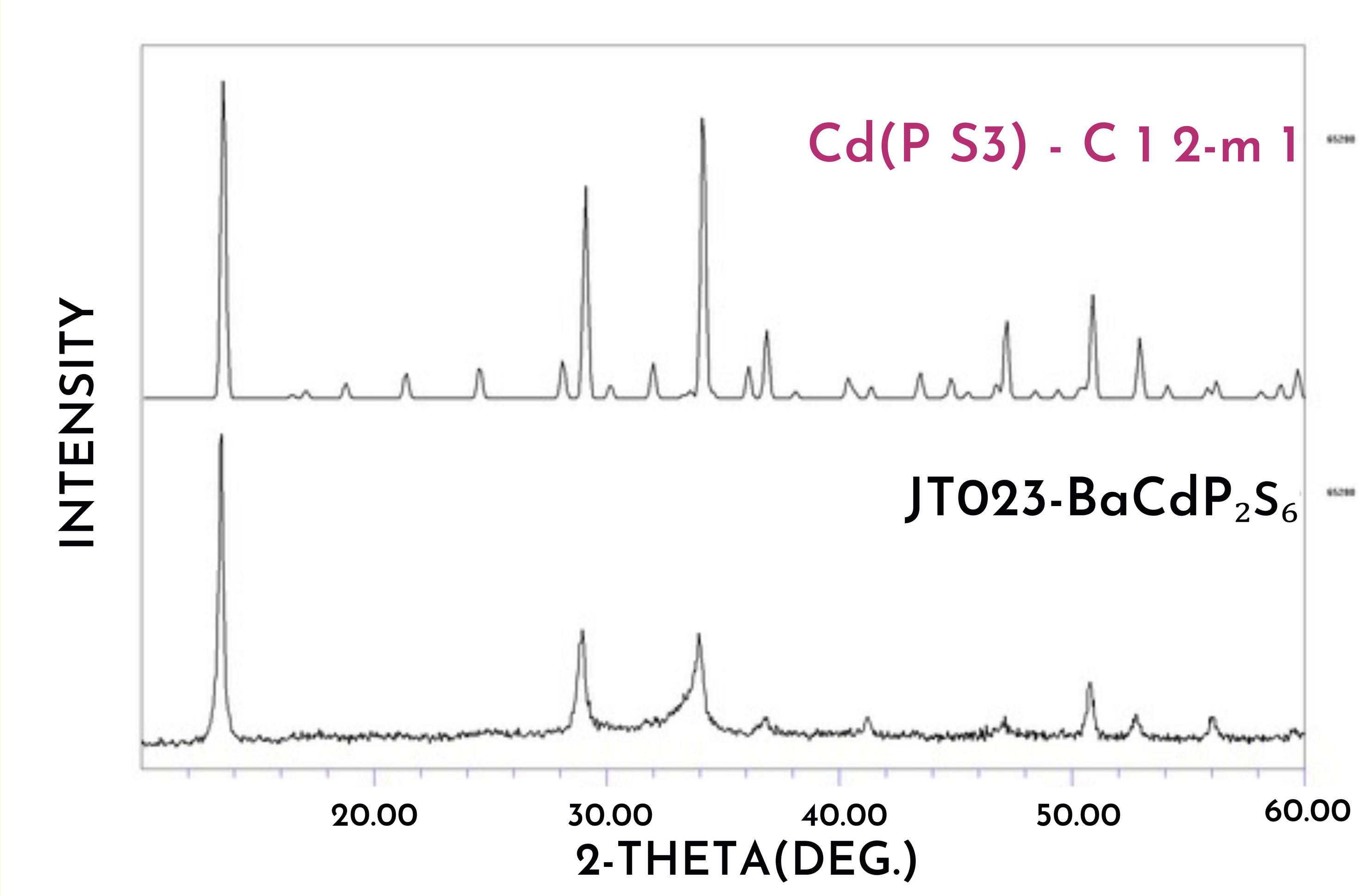

Figure 4 - Comparison of a previously published data(5) for the X-ray diffraction of $CdPS_3$ versus results attempted synthesis of solid state $BaCdP_2S_6$.

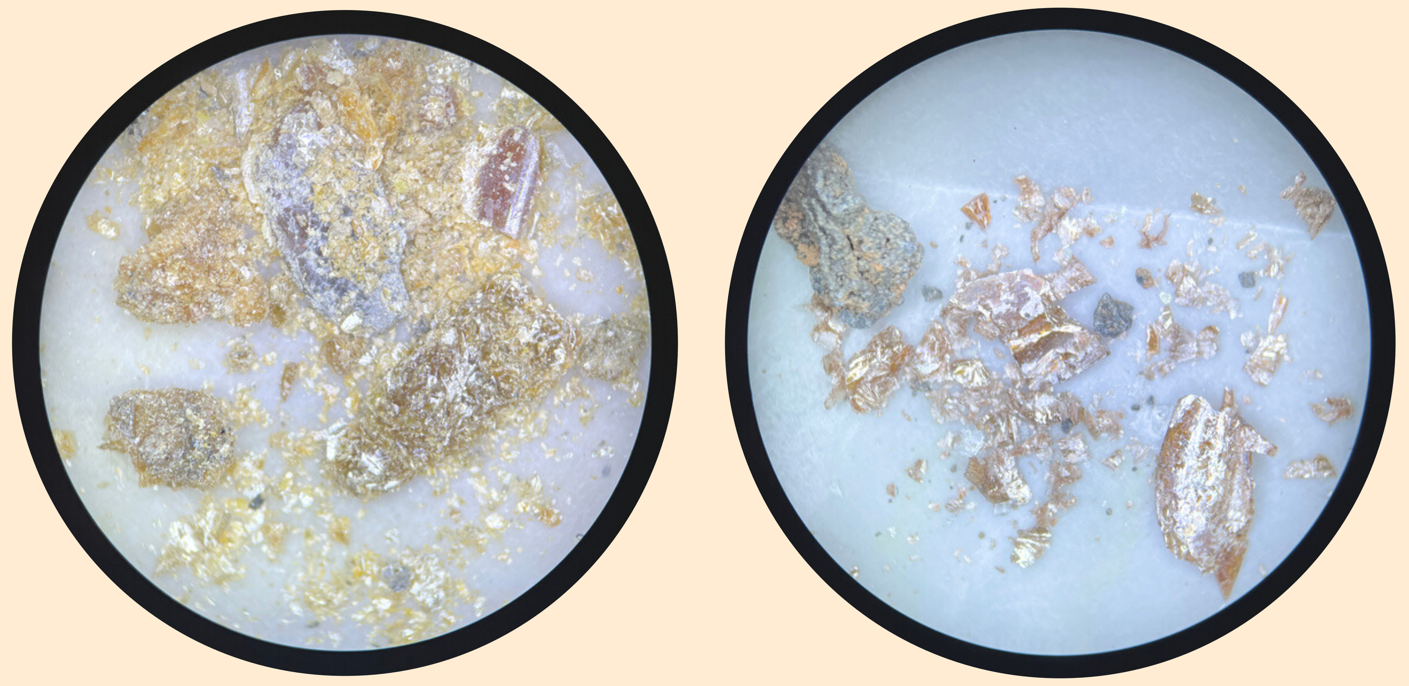

Figure 5 - Optical microscope view of $BaCd_2P_2S_8$ (JT#030) & solid state $BaCdP_2S_6$ (JT#023).

05. CONCLUSIONS & FUTURE

Figures 3-4 reveal target compounds were not achieved

- Experimental peaks matched those of known compounds: $ZnPS_3$ and $CdPS_3$
- Mixed cations were not involved in the system
- Explore different combinations of salt fluxes
- Substitute X for other metals (Pb^{2+}, Sn^{2+}, etc.)

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If successful, carry out theoretical calculations (investigate electronic structure of crystals)

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Investigate SHG coefficient to see if it mostly originates from $[P_2S_6]$ motifs

06. REFERENCES

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07. ACKNOWLEDGEMENTS

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