Betty A. and Donald J. Baumann Family Scholarship Fund Application Form

1. **Name and NetID**

   Saanvi Basak
   sba58449

2. **Chemistry faculty research director**

   Dr. Eric Villa

3. **Proposal title**

   Syntheses and Structural Characterizations of Novel Heavy Metal Heterobimetallic Complexes

4. **Proposal description. Please limit the proposal to about 500 words and include figures as appropriate. Your proposal should briefly outline the overall project and its goal(s). If you have previous results related to your proposed project, concisely summarize those results and describe what you expect to accomplish during the time frame of the scholarship.**

   Proposal is attached below.

5. **Presentation of research results (past and future conferences, publications, seminars, etc.)**

   Past Presentations:

   Basak, S., Payne, A.M., Kuhl, G.M. and Villa, E.M. "Reaction Dynamics of the $Al(OH)_6Mo_6O_{18}^{3-}$ Ion." Poster Presentation, 58th Midwest American Chemical Society Meeting, Omaha, NE, United States, October 13-15 (2024). **Sci-Mix Poster Session. *Awarded Best Undergraduate Poster in Inorganic Chemistry***

   Basak, S., Payne, A.M., Kuhl, G.M., Spriet, M.R. and Villa, E.M. "Aqueous Reactivity of Anderson-type Polyoxometalate Ions – A Comparative ^{17}O-NMR Study." Poster Presentation, 269th American Chemical Society National Meeting, San Diego, CA, United States, March 23-27 (2025).

   Basak, S., Payne, A.M., Kuhl, G.M., Spriet, M.R. and Villa, E.M. "Aqueous Reactivity of Anderson-type Polyoxometalate Ions – A Comparative ^{17}O-NMR Study." Poster Presentation, Creighton University Research Week – St. Albert's Day, Omaha, NE, United States, April 1-2 (2025).

   Basak, S., Payne, A.M., Kuhl, G.M., Spriet, M.R and Villa, E.M. "New Advancements in Antimony Molybdate Polyoxometalate Chemistry." Poster Presentation, 59th Midwest American Chemical Society Meeting, Columbia, MO, United States, October 12-14 (2025).

   Future Presentations:

Basak, S. and Villa, E.M. “Single Crystal Investigations of Heavy Metal Benzenethiosulfonate Complexes.” Poster Presentation, 271st American Chemical Society National Meeting, Atlanta, GA, United States, March 22-26 (2026).

Basak, S. and Villa, E.M. “Single Crystal Investigations of Heavy Metal Benzenethiosulfonate Complexes.” Poster Presentation, Creighton University Research Week – St. Albert’s Day, Omaha, NE, United States (2026).

6. **Post-graduate plans (job market, graduate school, medical school, etc.)**

   I plan to attend graduate school to pursue a Ph.D. in inorganic chemistry in the Fall of 2026.

7. **Number of semesters involved in research, including current semester (summers count as two semesters)**

   9 semesters

8. **Anticipated graduation date**

   May 16th, 2026

Syntheses and Structural Characterizations of Novel Heavy Metal Heterobimetallic Complexes

Heterobimetallic complexes have enriched the fields of catalysis and materials science due to their high specificity and cooperativity to their substrates.[1] With two different metals bonded through a ligand or metal-metal interaction, the electronic behavior of multi-metal compounds incorporating hard and soft metals is poorly understood in comparison to monometallic complexes.[1] To further explore the properties of these mixed-metal compounds, my project involves the synthesis and structural characterization of novel heterobimetallic complexes with the sodium benzenethiosulfonate (NaBTS) ligand to create air-stable catalysts.

Organic thiosulfonates contain two sulfur donor atoms and two oxygen donor atoms, which allows the anion to bond to multiple metals, thus increasing the synthetic ability of the ligand. In particular, I am interested in the NaBTS ligand (Figure 1) due to the simple aromaticity of the anion and the various applications of the ligand in the pharmaceutical and agrochemical industry.[2] By reacting soft transition metals and hard lanthanide metals with this aromatic thiosulfonate ligand, I will examine the inorganic coordination chemistry of heavy metal heterobimetallic complexes to further broaden their catalytic capabilities.

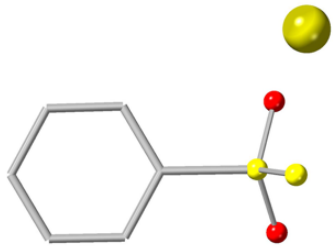

Figure 1. Structure of NaBTS ($Na(S_2O_2C_6H_5)$). The large yellow sphere is the sodium cation, red spheres are oxygen atoms, and yellow spheres are sulfur atoms. The benzene ring is in gray with the hydrogen atoms omitted for clarity.

My research project, started in the Fall of 2025, has three primary goals. Firstly, I will synthesize and structurally characterize inorganic compounds by reacting soft transition metal cations with the NaBTS ligand to illustrate bonding through the sulfur atoms. Secondly, I will synthesize and structurally characterize inorganic compounds by reacting hard lanthanide metal cations with the NaBTS ligand to

illustrate bonding through the oxygen atoms. Finally, I will combine these two synthetic approaches to create novel heterobimetallic complexes with both hard and soft metals. I aim to expand the magnetic and redox-active properties of these mixed-metal compounds,[3] as there is precedence in the Villa group for heterobimetallic complexes using the thiosulfate and 1,10-phenanthroline ligands (Figure 2). After synthesizing the desired complexes, I will characterize the compounds via single crystal X-ray diffraction.

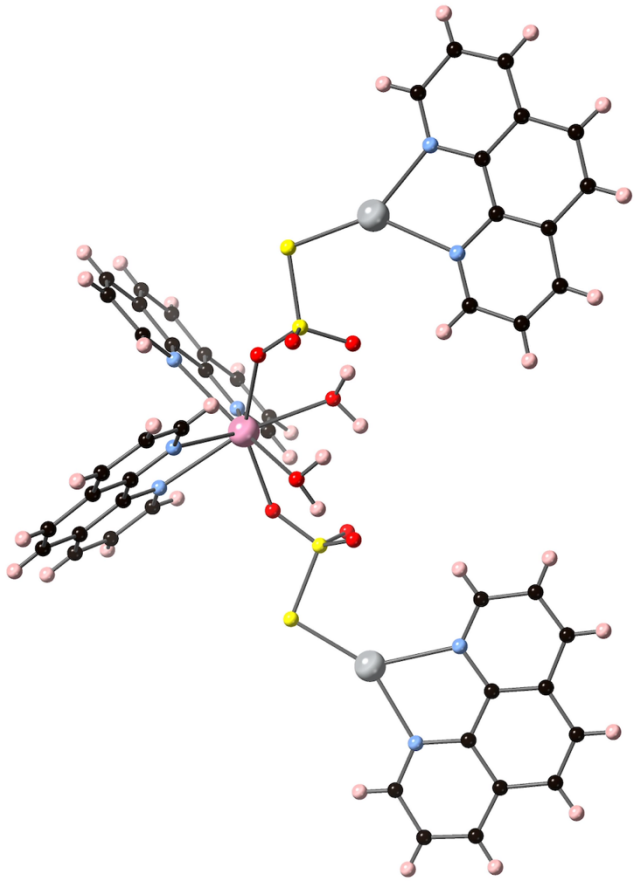

Figure 2. Ball-and-stick model of the $\{[Nd(C_{12}H_8N_2)_2(H_2O)_2(S_2O_3)_2][Ag(C_{12}H_8N_2)_2]OH\} \cdot H_2O$ complex, derived from the single crystal X-ray diffraction data, is shown. Color scheme: silver, gray; carbon, black; hydrogen, pale pink; nitrogen, blue; neodymium, bright pink; oxygen, red; sulfur, yellow. The neodymium cation is bonded through the oxygen donor atoms while the silver cations are bonded through the sulfur donor atoms, demonstrating the versatility of thiosulfate ligands.

I have recently started reacting multiple soft transitions metals, including silver(I), thallium(I), and lead(II), with the NaBTS ligand via a room temperature synthetic method using a 1:1 metal:ligand ratio in ethanol. I am now utilizing other organic solvents in my syntheses to determine which solvents yield the highest quality crystals. Thus far, I have synthesized and characterized a new and exciting thallium(I) benzenethiosulfonate (Tl(BTS)) complex using ethanol (Figure 3). The one crystallographically unique thallium cation in this compound possesses a stereoactive lone pair that is interacting with the benzene ring perpendicularly.

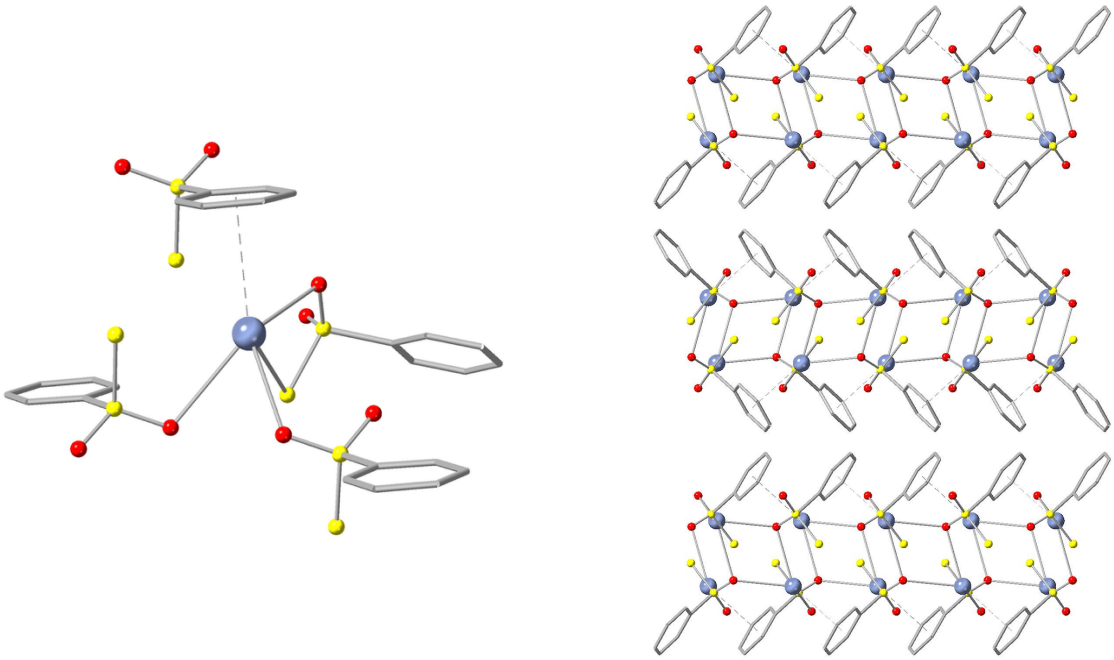

Figure 3. Ball-and-stick model of the Tl(BTS) ($Tl(C_6H_5O_2S_2)$) complex, acquired from the crystallography data, is shown (left). The thallium cation is in pastel blue, oxygen atoms are in red, and sulfur atoms are in yellow. The benzene rings are in gray with the hydrogen atoms omitted for clarity. The two-dimensional extended structure of the same complex is also shown (right).

During the timeframe of the scholarship, I plan to continue tuning my synthetic methods and create novel inorganic complexes with soft metals preferentially bonded to the sulfur donor atoms on the NaBTS ligand. Then, I will create new lanthanide complexes to exploit the remaining oxygen donor atoms on the

NaBTS ligand. Ultimately, I intend to synthesize and structurally characterize the desired heterobimetallic complexes. Overall, these investigations involving the synthesis of mixed-metal compounds will enhance their multifunctional catalytic abilities and expand the fundamental understanding of heterobimetallic catalysts in inorganic coordination chemistry.

References

1. Chaudhary, A.; Singh, A.; Kamboj, R. Heterobimetallic Complexes as Promising Catalysts. *Chem. Sci. Rev. Lett.* **2016**, *5* (17), 170–192. https://chesci.com/wp-content/uploads/2017/01/V5i17_17_CS20204612.pdf
2. Mampuys, P.; McElroy, C.; Clark, J.; Orru, V.; Maes, B. Thiosulfonates as Emerging Reactants: Synthesis and Applications. *Adv. Synth. Catal.* **2020**, *362*, 3–64. DOI: 10.1002/adsc.201900864
3. Mondal, A.; Tang, J.; Layfield, R. Masked Divalent Reactivity of Heterobimetallic Lanthanide Isocarbonyl Complexes. *Angew. Chem. Int. Ed.* **2025**, *64*, e202420207. DOI: 10.1002/anie.202420207