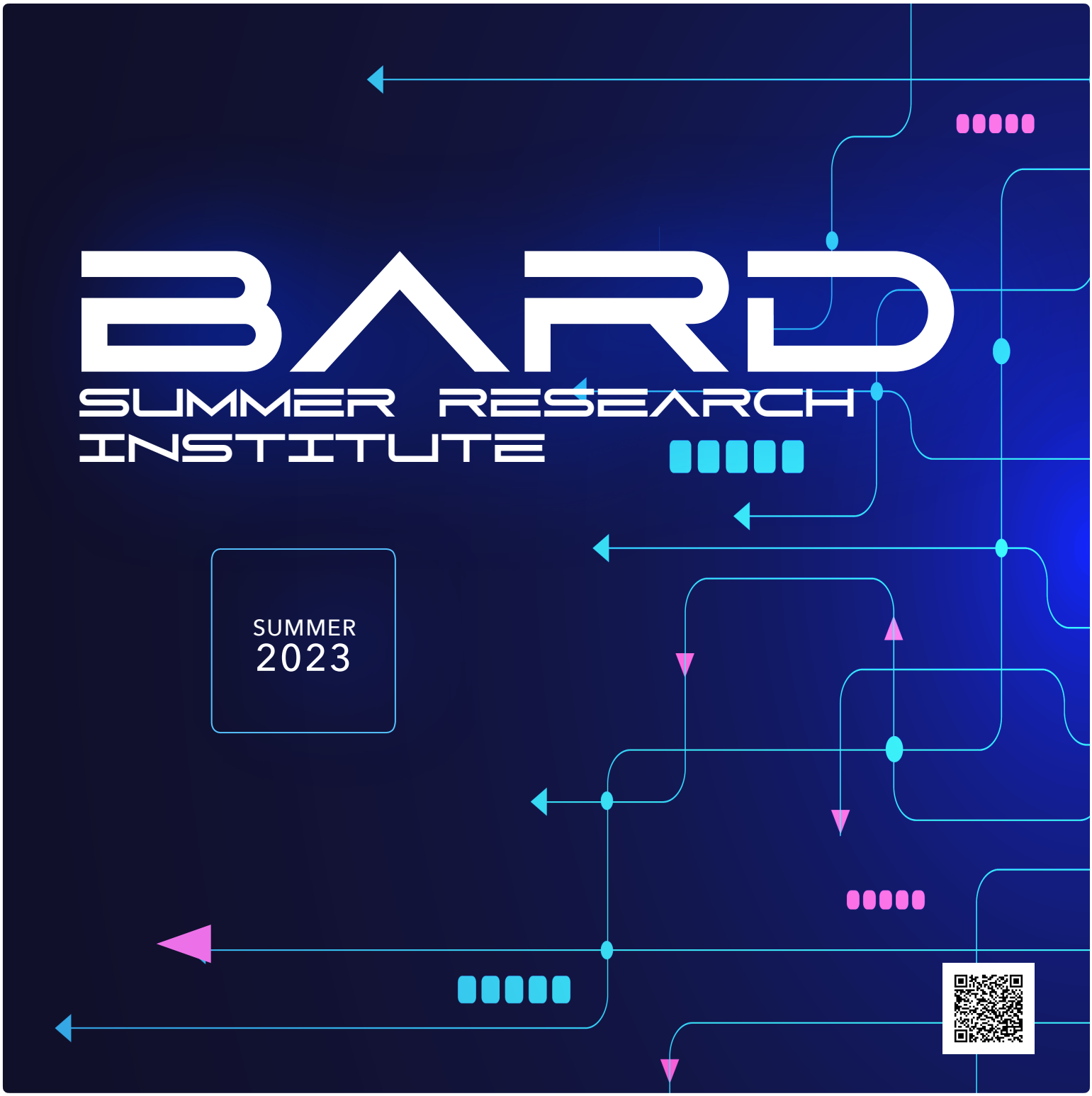
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Shedding light on carbon-nitrogen bond formation: An exploration of the alkene substrate in photocatalytic aziridination

Zachary P. Burmeister, Jay Lee, Ligia A. Monterroza Orellana, and Abena Wirekoh
Advisor: Emily McLaughlin

Carbon-nitrogen (C-N) bonds are ever-present in both natural and unnatural small molecules. Our research group has been interested in developing new synthetic methods to create two C-N bonds, simultaneously, to produce substituted aziridine products. This study uses a visible light-driven process where a metal photocatalyst alongside blue LED light promotes the direct aziridination of substituted alkenes (C=C) using N-aminopyridinium ylides as the nitrogen source. Reports in the literature and previous data collected from our lab have suggested that nitrenes can be generated from both azidoformates and N-aminopyridinium ylides using visible light catalysis and can result in the formation of aziridines in the presence of alkenes. With a focus on identifying the alkene structures which react most effectively with the N-aminopyridinium ylide, under visible light photocatalysis, we designed an experiment to evaluate their relative reactivities. The formation of aziridine products and the percent consumption of the alkene starting materials were monitored over time through proton nuclear magnetic resonance spectroscopy (NMR). From the NMR yield calculations, the alkene electronic and steric effects were evaluated and described in this study.

Measuring Accuracy and Precision of TPP using Structure-For-Motion

Sophie Cherif and Katie Lowney
Advisor: Chris LaFratta

Our research used an ultrafast titanium sapphire laser to micro-fabricate 3D structures in the photoinitiator TPO-L. These structures were then photographed using a scanning electron microscope to reconstruct a 3D file of the structure, and compare the dimensions of the reconstruction to the original file that was used to fabricate it. The goal of this project was to test the accuracy and precision of two photon polymerization.

Measuring Defects in Optical Coatings for Gravitational Wave Detection

Kace Colby, Emma Derrick, Bobby King, and Freddy Coronel
Advisor: Antonios Kontos

The Laser Interferometer Gravitational-Wave Observatory (LIGO) uses a technique known as laser interferometry to detect gravitational-waves produced by astrophysical events such as black hole mergers and binary neutron star systems. These gravitational-wave detectors require optical coatings that produce very little noise from both optical and mechanical losses. Our research focused on developing an improved experimental setup and procedure for characterizing small defects within mirror coatings using scattered light, improving and utilizing image analysis techniques for scattering measurements, measuring total scattering losses from lenses, and despeckling images using a spatial light modulator.

Synthesis of Novel Photoinitiator Incorporating a Radical Quencher for Direct Laser Writing

Anders Dollard and Lucas Rodriguez
Advisors: Chris LaFratta and Matthew Greenberg

Photopolymerization, the underlying process in direct laser writing (DLW), involves a resin composed of a photoinitiator (PI) and monomer. This resin is exposed to light with a wavelength that corresponds to the absorption or fluorescence spectra of the PI. Typically, the light source is either a laser or a UV lamp. Upon exposure, the PI undergoes cleavage, generating reactive species containing free radicals, which initiate the reaction with the monomer present in the resin. The exposure the resin undergoes in DLW generates slight amount of reactive species in a gradient past the focal point - which diffuse out in the resin as consequence. The objective of this study is to develop and characterize a derivative of an existing PI (TPO-L) to minimize this observed diffusion - called the proximity effect (also known as the memory effect), which can negatively impact resolution and structural integrity by the formation of unintended microstructures.

Graphene on a Curved Surface

Nafis Farhan, Miles O'Rourke, and Jacinta Creel
Advisor: Paul Cadden-Zimansky

Our research group studied the properties of graphene. Graphene is a one-atom thick lattice of carbon atoms with special properties such as high thermal and electrical conductivity, high elasticity, and flexibility. In this project we took advantage of its high elasticity by isolating graphene and transferring it onto a curved surface a curved surface, which had not been done before. We worked on making sure this transfer was clean and stable. The curved surface medium was fabricated using direct laser writing. Future goals include designing a circuit and taking transport measurements of our shaped graphene.

Synthesis and Characterization of Luminescent Platinum(IV) Compounds

Zander Grier, Ava Maki, Angelina Mannino, Everest Oppenheimer, Matthew Greenberg, and Craig M. Anderson

This material is supported by the National Science Foundation under CHE-1665435 (Craig M Anderson, P.1)

Platinum complexes are celebrated for their catalytic and photophysical properties. Specifically, they're known for their long excited state lifetimes and high quantum yields. Our project focuses on the luminescence of platinum (IV) compounds which are generally understudied compared to the set of well-studied platinum(II) compounds. A series of different chelate and pincer ligands were synthesized and reacted with our tetramethyl platinum dimer to produce six-coordinate platinum (IV) compounds. Our products were characterized mainly by proton NMR spectroscopy. Additionally, some of their photophysical properties were measured, including emission spectra and quantum yields.

An Automated Approach to Nanocrystal Structure Solution and Refinement Using the Real-Space Atomic Pair Distribution Function

Farman Hossain Sayem and Nadia Mehjabin
Advisor: Matthew Greenberg

This research aims to automate the process of nanocrystal structure solution and refinement from X-ray atomic Pair Distribution Function measurements (PDF). Traditional phase analysis using XRD in reciprocal space is complicated by the broad peak shapes for nanocrystalline materials. A comprehensive algorithm has been developed to retrieve CIF data from the Materials Project online structural database, calculate real space PDFs from these structures, and refine them to best fit experimental data. The algorithm is implemented in Python, utilizing Pymatgen and DiffPy-CMI libraries for atomic structure manipulation and PDF calculations. Initial sorting of candidate structures by their Pearson correlation coefficients with the experimental data was found to be a highly efficient method for identifying the correct nanocrystal structure.

Visualizing Quantum Logic Gates in a 2-Qubit Entangled State

Yasher Khan
Advisor: Paul Cadden-Zimansky

In computing, a bit is the most basic unit of information, denoted in 1s and 0s. In Quantum Mechanics, a "quantum bit", or Qubit, is the smallest unit of information, keeping track of quantum states. A Bloch Sphere is able to provide a one-to-one mapping of qubit states to points in 3D space. When dealing with multiple qubits, we use a separable torus to visualize properties of the qubits, such as the entanglement. Understanding how states with multiple qubits work is essential to understanding many important concepts in Quantum Mechanics. We aimed to improve upon current visualization bases by implementing quantum logic gates into a 2-Qubit separable torus, and observing how the statepoint changed according to each gate. We created algorithms that would reparameterize a 2-Qubit system from a pre-existing ($\alpha,\beta,\gamma,\delta$) parameterization into ($r,\theta1,\theta2$) parameters, which the gates would then act on. This would then allow us to visualize the impacts of quantum logic on qubits, which can have various applications in quantum computing. We found that the two separate parameterizations of the qubit system create certain complications in the implementation of the logic gates, and we aim to improve upon this in the future.

Machine Learning for Emotional Text to Speech Modeling

Josef Lazar
Advisor: Rose Sloan

In this research project we attempted to make a text to speech model that can read any inputted text in a selected emotional tone. We started by downloading the MSP-Podcast corpus which contained excerpts from podcasts, along with metadata of the excerpts, such as the transcript, the gender of the speaker, and the emotion of their tone. We then used openSMILE to extract audio features from the audio files in the corpus. To make models that predict the emotion of an inputted audio file, we trained machine learning algorithms, including logistic regression, SVMs, random forests, and feedforward neural networks, on the data we extracted from the MSP-Podcast corpus. To increase performance we added features that we got from examining the audio feature transcripts using LIWC, which classifies sentiments behind words. These models were used to assign emotion labels to audio files in the LibriTTS corpus. Once the labels were assigned, the last step was to use the Merlin toolkit to train a text to speech models on audio files of particular emotions, producing models that speak in the emotional tone they were trained on.

A Semi-Automatic Process for Discovering NP-Complete Knots

Husna Manalai
Advisor: Bob McGrail

This poster presents a semi-automatic process for producing non trivial quandle colorings for three dimensional knots. Researchers first need to discover a system of equations which they generate from a labeled and oriented visual representation of the knot. The equations and a quandle are then fed to a declarative program that searches for a non trivial coloring by that quandle.If such a coloring exists researchers then produce an image of that knot together with this coloring.

The Attractiveness of Face Cues does not Modulate the Gaze Cuing Effect

Hominy McMahon, Clara Retzloff, Alua Samat and Calum Tinker
Advisor: Tom Hutcheon

The direction in which someone is looking (gaze direction) represents an important signal in our social environment. The gaze cueing effect refers to the finding that participants are faster to respond to a stimulus preceded by a face gazing towards the stimulus location compared to when a stimulus is preceded by a face gazing away from the stimulus location. Importantly, this effect is found even when the gaze direction is not informative of the upcoming stimulus location, suggesting the operation of a fast, reflexive process that draws attention. However, accumulating evidence suggests that this gaze cuing effect is modulated by additional contextual features including characteristics of the participant, the stimulus, and the task. In the current set of experiments, we sought to test whether the attractiveness of the face cue is one such factor that would modulate the size of the gaze cuing effect. Across three experiments in which the stimulus set, task, and stimulus onset asynchrony were manipulated, we found no evidence that attractiveness impacts the gaze cuing effect. We interpret these findings to mean that perceived attractiveness is not a contextual feature that modulates the impact of gaze on spatial attention.

Grappling with the Molecular Spectrum of the Cloud Tops of Venus

Lauren Mendoza
Advisor: Clara Sousa-Silva

Despite being the planet Earth's neighbor and the third brightest object in its sky, the molecular composition of Venus's atmosphere is largely a mystery since data concerning Venus is limited. This summer, we focused on unveiling the molecular composition of Venus's cloud tops by analyzing the infrared spectrum from wavenumbers 1115 cm-1 to 1123cm-1 produced by the TEXES spectrograph located on Hawaii's Mauna Kea mountain, a range that has not been studied prior.

Cisplatin Binding Destabilizes DNA-RNA Hybrid and Inhibits RNA Function

Fuadar Omi
Advisor: Swapan Jain

DNA-RNA Hybrids are structures formed through the hybridization of a single stranded DNA molecule with a single stranded RNA molecule, where the DNA and RNA form base pairs with each other. In this project, we prepared a DNA-RNA hybrid and binded it to cis-diamminedichloroplatinum(II) or Cisplatin, and investigated the changes in the hybrid structure caused by the well known chemotherapy drug. A 20 base pair hybrid complex was prepared by mixing single stranded DNA with RNA, followed by heat annealing and freezing. The hybrid was used to perform UV-Vis melting studies. Radiolabeling was done by running three kinase reactions with DNA, RNA, and a 10/60 ladder, followed by incubation at 37 °C and storage at -20 °C. A separate hybrid was prepared by combining radiolabeled RNA with the unlabeled DNA and analyzed using PAGE (Polyacrylamide Gel Electrophoresis) following binding to Cisplatin.

Finding Spectra with RASCALL

Nicola Paparella
Advisor: Clara Sousa-Silva

RASCALL is a powerful tool which allows us to analyse and explore with relative ease. Its purpose revolves around being able to extrapolate the structure of planet Venus while going around the fundamental problems which lay behind such task such as the impossibility of obtaining a sample from Venus' atmosphere and the high amount of computational resources which would otherwise be spent in attempting to simulate Venus' atmosphere.

RASCALL gets around this problems by using functional groups. Functional groups can be seen as particular and recognizable fragments of molecules. Since these fragments are recognizable and are present in multiple molecules, these constitute the formation of a family of molecules whose members are gathered together by sharing the same functional group. The reason behind the recognizability of each functional group is due to the intensity that it emits when stimulated by electromagnetic radiation which corresponds to a particular wavenumber.

Thus, through a computational analysis, RASCALL makes it its aim to figure out the molecular composition of Venus by allowing its user to identify good candidates which may fall within a certain wavenumber and intensity emitted.

This process, however, can still be extremely time consuming. Thus, the program that I have written (fg_mol_explorer_reversed.py) has the task of
1. Simplifying the process of analysis of a molecule by making RASCALL's interface more user-friendly.
2. Constructing a filter which excludes certain functional groups from a certain wavenumber interval which is decided by the user.
3. Returning to the user the family of molecules which have the functional groups in common with the unfiltered molecules

As a result of these implementations, RASCALL becomes more efficient and easier to use and it allows for a better visualization of the possible candidate molecules.

In conclusion, the possibility of analyzing physical phenomena from a computational perspective is certainly a great opportunity which will hopefully stimulate the cooperation of multiple individuals coming from multiple academic backgrounds on a particular problem. To make this kind of cooperation possible it would be imperative to make the interfaces with which all users communicate information as much efficient and user-friendly as possible.

Inhibition of DHFR enzyme by Ruthenium Metal Complexes

Sage Saccomanno and Luke Collins
Advisor: Swapan Jain

An important target in cancer has been the folic acid pathway in which the enzyme dihydrofolate reductase (DHFR) catalyzes the reduction of dihydrofolate to tetrahydrofolate using NADPH, which is an essential cofactor for the biosynthesis of purines, thymidylate, and several amino acids. Our project focuses on the binding affinity of ruthenium complexes with DHFR enzyme. Our project revolved around the following question: What is the binding strength and enzymatic effect of phenformin and metformin compounds on DHFR enzyme. The in vitro binding affinity of Ru79 and Ru-Cymene was investigated using DHFR enzyme activity assay. Despite some difficulties and delays, we were able to come up with valid conclusions in regards to DHFR DNA and Ruthenium complexes, in particular Ru79. Our methods included seed cultures, plasmid extraction, restriction digestion, isoamyl:phenol:chloroform purification, transcription, incubation with metal complexes, translation, analysis with a DHFR activity assay along with gel electrophoresis. We concluded that there is serious potential of phenformin and metformin based drugs to better hinder the enzymatic activity of the DHFR enzyme and to eventually become successful anti-cancer drugs. Future work will revolve around more studies with the additional ruthenium metal complexes that we were not able to get to this summer, from the Anderson laboratory, along with replicating these studies to further confirm our results.

The Curve Graph of the 5-Punctured Sphere

Darrion Thornburgh
Advisors: Dan Margalit and Wade Bloomquist

The arc graph A(S) (and curve graph C(S)) of a surface S is the graph where vertices are homotopy classes of arcs or curves, respectively, and the edges indicate disjointedness between them. It was proven by Hensel, Przytycki, and Webb in 2015 that A(S) and C(S) are at worst 7-hyperbolic and 17-hyperbolic, respectively. We introduce lower bounds for the hyperbolicity constants of A(S) and C(S), and we prove the curve graph of the 5-punctured sphere is not 1-hyperbolic.

Analysis of NuSTAR X-ray Observations of Galactic Center Filament F.0173-0.413

Vera Topcik and Chloe Dufeu
Advisor: Shuo Zhang

At the center of our galaxy there is a lot of activity happening, including a supermassive black hole: Sagittarius A*, massive stellar clusters, and a molecular cloud. Among these objects are threads of light known as filaments. Galactic center filaments were first discovered through radio observations by Farhad Yusef-Zadeh in 1984. They have only been observed in either the radio and x-ray energy bands, and only a handful have been observed in both. This summer, we analyzed data from NuSTAR x-ray telescope observation of the filament F.0173-0.413, as well as did a joint spectral analysis of the NuSTAR data combined with Chandra telescope data. The results show that our filament, which was uniquely linear and observed in both energy bands, fit the optically thin thermal model, assuming collisionally ionized plasma.

Synthesis, Structure, and Photophysical Properties of Platinum Compounds with Thiophene-Derived Cyclohexyl Diimine Ligands

Kris M. Tulloch, Lily Clough, Matthew W. Greenberg, Michelle E. Reynoso, Juliette L. Knapp, Farman H. Sayem, Daphne D. Bartkus, Ryan Lum, Christopher N. LaFratta, Joseph M. Tanski, Craig M. Anderson*

Chemistry Department, Bard College, Annandale-on-Hudson, NY 12504 canderso@bard.edu. (JMT, Vassar College, Poughkeepsie, NY)

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Platinum(II) and platinum(IV) compounds were prepared by the stereoselective and regioselective reaction of thiophene-derived cyclohexyl diimine C^N^N-ligands with [Pt2Me4(μ-SMe2)2]. Newly synthesized ligands were characterized by NMR spectroscopy and elemental analysis, and Pt(II)/Pt(IV) compounds were characterized by NMR spectroscopy, elemental analysis, high resolution mass spectrometry, and single crystal X-ray diffraction. UV-vis absorbance and photoluminescence measurements were performed on newly synthesized complexes, as well as structurally related Pt(II)/Pt(IV) compounds with benzene-derived cyclohexyl diimine ligands. DFT and TD-DFT calculations were performed, and results compared to the observed spectroscopic properties of the newly synthesized complexes. X-ray total scattering measurements and real space pair distribution function analysis were performed on the synthesized complexes to examine the local and intermediate range atomic structure of the emissive solid states.1

1. ACS Omega, 2023, 8, 38587.

Avoiding Triples in the Card game Spot It!

Minshi Yang and Oliver Vanderploeg
Advisor: Lauren Rose

Spot It! is a card game where each card has 8 symbols and shares exactly one symbol with every other card. A standard Spot It! deck can be viewed as a projective plane of order 7. We created Spot It! decks for projective planes of order $n \leq 16$. The goal of this project was to study sets of cards where each symbol appears at most twice. We will present results, work in progress, and open problems.