Supporting Information

Sustainable From the Start – An Exploration of Green Chemistry Utilizing Second-Year Inorganic Principles

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Contents

Activity 0 – Peering Into the Mist: A murder mystery to build partnerships for the goals.

1.1 Materials

This section lists all components required to construct and run the activity. File names match the uploaded PDFs for consistency.

Print Files (provided as PDFs):

- **Item 1 – Portrait Print-Outs (Single-Sided)**
  Role cards for: Environmental Monitoring Scientist, R&D Specialist (Verdanta Inc.), Industrial Company Executive (Verdanta Inc.), Logistics & Production Manager (Verdanta Inc.), Community Advocate, Government Policy Official.
  Includes supplementary data: station data, environmental limits, etc.
- **Item 2 – Half-Page Print-Outs (Single-Sided)**
  Unique role clues (emails, memos, degradation graphs, toxicity tests, maps of use sites, community complaints, etc.).
- **Item 3 – Verdanta Business Plan (Double-Sided)**
  A fictional strategic plan detailing Prime-X product launch and future expansion.
- **Item 4 – Beaker Print-Out Part 1 (Blue Text)**
  Water samples showing pH values and hidden concentration fields.
- **Item 5 – Beaker Print-Out Part 2 (Red Overlay)**
  Printed red layer enabling hidden-text reveal when used with acetate magnifying glasses.
- **Item 6 – Community Board Files (Single-Sided)**
  Newspaper articles, weather report (including acid-rain warnings), flyers, contextual materials.
- **Item 7 – Town Map (50 × 50 cm)**
  Spatial layout of Elbury showing industrial sites and monitoring stations.
- **Item 8 – Participant Booklet**
  Contains: scenario introduction, systems thinking primer, hotspot analysis primer, guiding questions, and reflection space.

Other Materials:

- Red acetate sheets (3 layers per magnifying glass)
- Cardstock (magnifying glass frames; beaker prints)
- Scissors / craft knives
- Tape, glue, yarn/string (for linking clues on community board)
- Envelopes (one per participant/role)
- Pins/thumbtacks (for the community board)
- Pens/pencils
- Large foam board or equivalent for community-board assembly
- Stapler (for assembling booklets)

1.2 Set-Up and Preparation

1. **Preparation of Role Envelopes:**
   Assemble one envelope per participant. Each envelope includes:
   a. Role card (Item 1)
   b. Role-specific clues (Item 2 and relevant items 3–6)
   c. One beaker print-out (pH depends on role:
      i. pH 4.5 → Environmental Monitoring Scientist
      ii. pH 5.6 → R&D Specialist)
2. **Construction of Magnifying Glasses**
   a. Cut two cardstock frames per magnifying glass.
   b. Cut out the interior window.
   c. Layer three red acetate sheets between cardstock frames.
   d. Glue or tape securely.
   These are placed on or near the community board as a shared investigation tool.
3. **Community Board Assembly**
   Attach the following in a loosely organized "town bulletin board" arrangement:
   a. Newspaper articles
   b. Flyers
   c. Weather report (highlighting acid rain warnings)
   d. Town map
   e. Optional magnifying glasses
   f. Any additional contextual materials
4. **Room Setup**
   a. Arrange participants in groups of 4–6, ensuring coverage of most roles.
   b. Provide each participant with a booklet, writing utensil, and role envelope.
   c. Recommended duration: ~60 minutes (as per symposium constraints).
   d. In the classroom implementation, the activity was run during a single class period with 8 students, using the same physical materials and layout, adapted to a smaller room and group size.

The centralized, shared placement of the community board materials was a deliberate design choice intended to encourage physical movement, cross-group interaction, and the synthesis of distributed evidence across roles.

1.3 Facilitation

1.3.1 Overview:

Participants collaboratively investigate an emerging environmental and public-health crisis in Elbury. The activity was intentionally designed to place participants in a partially ambiguous problem space, mirroring the uncertainty, incomplete information, and competing perspectives characteristic of real-world sustainability challenges. By situating the investigation within a fictional but realistic scenario, participants are able to engage with disagreement, accountability, and ethical trade-offs in a psychologically safe environment without real-world consequences. Each role holds partial information; only by sharing clues can the group identify the root cause.

1.3.2 Facilitator Responsibilities:

- Provide a short introduction using the booklet scenario page.
- Briefly outline systems thinking and hotspot analysis (optional).
- Instruct participants to first examine the community board, then open envelopes.
- Circulate to encourage:
  - Cross-role communication
  - Synthesis of clues
  - Examination of beaker overlays
  - Use of the town map to identify spatial correlations
  - Provide guiding questions (also included in booklet).

1.3.3 Guiding Prompts for Participants:

- "What information does each of you have? Who might be missing key details?"
- "Where do your clues overlap or contradict?"
- "How are the monitoring stations, pH changes, and industrial sites connected?"
- "Which part of the system produces the most harm?" (hotspot identification)

1.3.4 Expected Activity Resolution:

Participants should be able to construct a coherent causal explanation for the environmental event (material transformation + exposure pathway). Responsibility and appropriate prevention strategies are intentionally open to interpretation and negotiation. The following is a common causal chain for this activity:

1. Verdanta's Prime-X primer breaks down into microparticles.
2. Under acid rain, the polymer further transforms into Compound-X.
3. Monitoring stations near Prime-X application sites show elevated concentrations beyond environmental limits.
4. Resulting harm includes respiratory illness and fish/bird deaths.
5. This should lead to a concluding conversation about due diligence, regulatory oversight, and sustainable design.

While there is an identifiable causal chain underlying the scenario, the activity is not designed to yield a single definitive interpretation of responsibility; instead, participants are encouraged to negotiate accountability, trade-offs, and preventative strategies through discussion.

Based on facilitator observation, groups generally reached a coherent explanation of the environmental event, with facilitators acting primarily as sources of clarification rather than directing progress. No systematic tracking of group conclusions was conducted.

1.4 Recommendations for Educators

1.4.1 Suggested Prerequisite or Complementary Lessons:

- Introduction to systems thinking.[1]
- Basics of environmental fate/transformation of chemicals.[2]
- Hotspot analysis in green chemistry.[3]

- Case studies of unintended sustainability failures (6PPD-quinone,[4] PFAS, etc.)

1.4.2 Intended Learning Objectives:

While the activity was originally designed as a narrative sustainability investigation, subsequent iterations have clarified the following intended learning objectives. Activity 0 is designed to help learners:

- Collaborate with others to communicate information and important interconnections within a shared problem space.
- Explore and analyze a sustainability problem using a systems-thinking lens.
- Engage with key ideas related to systems thinking, hotspot analysis, and environmental transformations of pollutants as they arise in the scenario.
- Interpret a complex system and propose a defensible solution to the presented problem.

1.4.3 Scalability & Modifications:

The activity was implemented without modification to physical materials in both symposium and classroom contexts; differences between implementations primarily reflected participant experience and instructional framing rather than changes to activity design. While the intentional use of ambiguity supported productive discussion among symposium participants, undergraduate students benefited from additional scaffolding to clarify task goals and support evidence synthesis, highlighting the need to balance productive uncertainty with appropriate instructional guardrails.

In the classroom implementation, students benefited from additional clarity regarding the goals of the activity. While students were able to identify the environmental root cause and engage in discussion once prompted, they required explicit guidance to articulate what they were meant to determine beyond "solving the mystery." Based on this observation, future classroom implementations would benefit from adding a brief statement to the participant booklet explicitly outlining the intended task (e.g., identifying responsible actors, causes of sustainability failure, and preventative measures), as well as guided discussion prompts to support post-activity reflection.

No modifications to physical materials were required; however, the level of facilitator prompting differed substantially between contexts. Undergraduate students required more structured prompts to engage with distributed evidence and contextual materials, whereas symposium participants were generally self-directed once the activity was underway. These observations suggest that the activity is flexible across instructional settings but benefits from increased scaffolding when used with less experienced learners.

1.5 Insights

The following insights are based on facilitator observations during these implementations and should be interpreted as descriptive rather than as evidence of measured learning gains.

1.5.1 Symposium Implementation:

The activity was implemented during a 60-minute interactive symposium session at the 2025 Canadian Chemistry Conference and Exhibition, with approximately 45 participants. The author served as a circulating facilitator throughout the session, supporting participants, redirecting questions to primary facilitators when needed, and coordinating engagement between participants and invited industry professionals present in the room.

Participants were engaged immediately, though some initial uncertainty was observed as groups oriented themselves to the activity. Unlike typical undergraduate classroom settings, participants demonstrated a high degree of agency and willingness to engage, likely reflecting both self-selection into the symposium and the professional context. Participants readily formed groups, initiated discussion within those groups, and showed no observable skepticism or resistance to the activity format.

Engagement remained consistently high throughout the session. Even groups that appeared less enthusiastic initially continued working with the materials and engaging in discussion. No obvious disengagement was observed, and participants who remained in the room after the activity began stayed actively involved until its conclusion.

Participants primarily engaged first with the materials contained in their role envelopes, using the community board, town map, and magnifying-glass acetate sheets as secondary resources. Use of the acetate overlays required occasional prompting early in the session, but approximately halfway through the activity most groups accessed the community board and shared materials without facilitator intervention. The centralized placement of the poster board and magnifying glasses appeared to encourage physical movement and shared information-seeking. These behaviors reflect the activity's design emphasis on externalizing cognition through shared physical artifacts and spatial exploration, rather than relying solely on individual or role-bound reasoning.

While explicit collaboration between different groups was not observed, groups were situated closely enough that informal cross-pollination of ideas was likely. Within groups, active discussion, debate, and joint problem-solving were observed. Participants discussed possible causes of the environmental event, proposed additional testing and controls, and engaged with questions of responsibility and prevention, even when not using formal sustainability or systems-thinking terminology.

Facilitator intervention was generally limited to clarification rather than direction once groups became established. Groups appeared self-driven and maintained momentum independently, with facilitators acting primarily as informational resources rather than drivers of progress. Although no formal debrief was conducted at the symposium, informal observation suggested that participants broadly recognized the relevance of the sustainability challenge presented.

Several limitations should be noted. The symposium format constrained opportunities for structured reflection and assessment, and only a small number of post-event survey responses were collected. As a result, while participant engagement and perceived value were high, no claims regarding learning gains or long-term impact can be made.

1.5.2 Classroom Implementation (Third-Year Inorganic Chemistry Course):

The activity was implemented with 8 students in a third-year Inorganic II course as an introductory session designed to build community and foreground the sustainability themes of the semester. The full "mystery" component of the activity was used.

Students initially demonstrated hesitation: they were slow to begin speaking with one another, reluctant to explore the contextual materials displayed around the room, and unsure of how to approach the task beyond the surface framing of a "murder mystery." Once conversations began, however, students became more engaged and ultimately enjoyed solving the scenario. Approximately half the class contributed actively to the closing discussion.

A central challenge in the classroom implementation was the need for clearer articulation of task goals, rather than difficulty with the investigative process itself. This observation underscores the importance of pairing narrative, open-ended activities with explicit framing when working with less experienced learners. Students did not understand what they were meant to identify beyond discovering "what happened," and they required prompting to articulate ideas related to sustainability failures, accountability, or systems-level reasoning. They also needed explicit encouragement to use the distributed evidence: for example, several groups ignored the community board until directed to use "everything in the room," and some misinterpreted concentration data in the beaker cards without guidance.

Students successfully identified the environmental root cause, but required intermittent facilitator interventions to connect disparate clues, prioritize relevant evidence, and interpret the data. The instructor noted that this level of prompting is consistent with broader trends in classroom activities, in which students increasingly require structured nudges to explore, discuss, and synthesize information.

Once prompted during the post-activity discussion, students gravitated toward themes of accountability, experimental design, and organizational responsibility. When asked who was responsible for the sustainability lapse, students identified two key actors: the company CEO, who ignored internal warnings, and the production manager, who recognized emerging concerns but did not escalate them. Students correctly recognized acid rain as the environmental factor driving the transformation of Prime-X into harmful compounds.

When guided toward thinking about preventative measures, students proposed additional stress testing, including evaluating product components under a broad range of acid/base conditions and weathering variables (temperature, pH). When asked whether companies should reasonably be expected to anticipate such tests, students hesitated to commit to a definitive judgment but agreed that applying systems thinking early in research and development could help identify overlooked testing needs. Finally, when prompted to consider organizational strategies to prevent future sustainability failures, students suggested implementing a dedicated sustainability officer within companies.

The instructor would run the activity again, with planned modifications to strengthen goal-clarity in the booklet. Proposed additions include explicit statements such as:

"Your task is to identify the person(s) responsible for the lapse in sustainability and the cause of the environmental event."

and guided prompts such as:

"Who is responsible for ensuring green chemistry compliance?"

"How could this company have prevented this issue?"

These additions are intended to support student reasoning, encourage richer discussion, and reinforce connections to sustainability concepts; future implementations could examine their impact more systematically.

1.6 General Reflections

Across both symposium and classroom implementations, *Peering into the Mist* provided a structure for engaging participants in collaborative investigation of a complex sustainability scenario. In both contexts, participants were able to construct coherent explanations of the environmental event when provided with distributed information and opportunities for discussion.

Differences between implementations were primarily associated with participant experience and context rather than with the activity itself. Symposium participants, who self-selected into the session and largely represented graduate students, postdoctoral researchers, and professionals, demonstrated high agency, sustained engagement, and relatively low reliance on facilitator prompting once the activity was underway. In contrast, undergraduate students required clearer articulation of activity goals and more frequent prompts to engage with contextual materials and to connect the investigation to broader sustainability concepts.

These observations highlight the importance of explicit framing and guided reflection when using narrative, game-based activities in classroom settings. While the activity successfully prompted discussion of responsibility, experimental design, and organizational decision-making, such themes did not emerge spontaneously for all participants and benefited from structured prompts.

Several limitations should be acknowledged. Neither implementation included a formal assessment of learning outcomes, and opportunities for structured reflection were constrained, particularly in the symposium setting. As a result, no claims regarding learning gains or long-term impacts can be made. Future implementations could incorporate explicit debrief sessions or reflective assignments to better support concept integration and to evaluate the activity's impact on sustainability reasoning.

Overall, these implementations suggest that *Peering into the Mist* is well suited as an introductory or priming activity for sustainability-focused instruction, particularly when paired with explicit learning goals and post-activity reflection.

Taken together, these implementations suggest that the effectiveness of Peering into the Mist lies not in resolving ambiguity, but in deliberately leveraging it, supported by facilitation strategies calibrated to participant experience, to prompt systems-level reasoning about sustainability challenges.

Activity 1 - Our Role: Exploring individuals' roles in developing sustainable alternatives.

2.1 Materials

Print Files (provided as PDFs):

- **Activity 1 Sustainability Poster (Figure S2),** print file "Activity 1 Poster.pdf".
- **Stakeholder Persona Cards,** print file "Activity 1 Personas.pdf".
- **Undergraduate Laboratory Experiment,** print file "Activity 1 Friedel Craft Acylation Experimental Procedure.pdf".
- **Activity Handout,** print file "Activity 1 handout.pdf".

Other Materials:

- Yellow, pink, and green post-it notes (for categorizing suggestions)
- Pens or markers for post-it notes
- Tape, pins, or adhesive putty (to mount posters, if not using a stand or board)

2.2 Set-Up and Preparation

For this station, the physical set-up is minimal. Display the sustainability poster in the room or mount it on a wall or board. For small classes or workshops, a single poster can be used as a shared discussion artifact; for larger groups (>20 participants), printing one poster per group is recommended to reduce bottlenecks.

1. Prepare one set of stakeholder persona cards per group.
2. Provide each group with 2-3 printed copies of the undergraduate laboratory experiment.
3. Arrange participants into groups of 4–6 prior to beginning the activity.

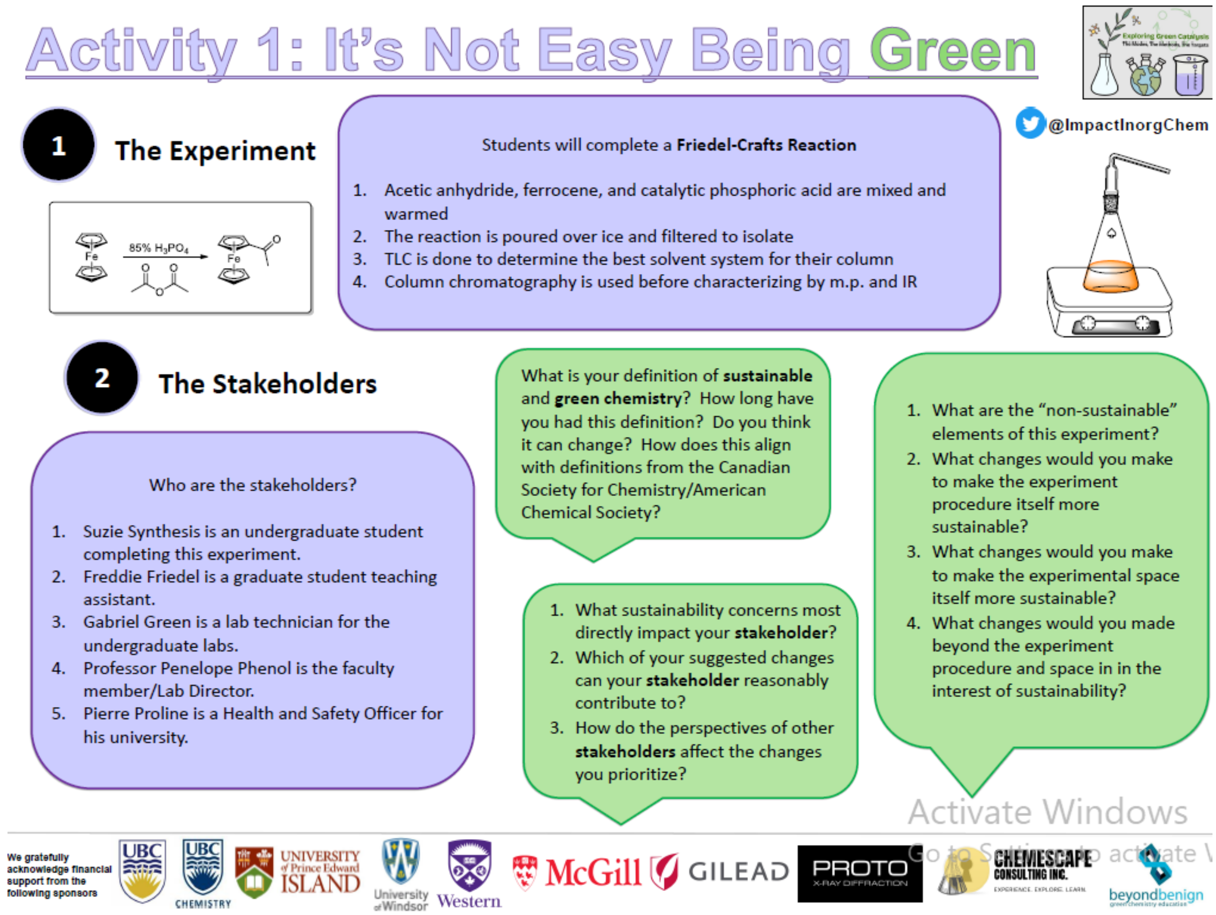

Figure S1. Poster Used for Activity 1: It's Not Easy Being Green. The poster includes activity directions, a visual of the reaction being assessed, and conversation prompts.

2.3 Facilitation

2.3.1 Overview

In this activity, participants collaboratively examine an undergraduate laboratory experiment through the perspectives of different academic and institutional stakeholders. Rather than identifying a single correct redesign, the activity is intended to surface sustainability considerations across experimental procedure, laboratory infrastructure, and broader systems that shape laboratory practice.

Participants work in groups of 4–6, with each individual assuming a stakeholder role (undergraduate student, teaching assistant, laboratory technician, faculty member or laboratory director, or health and safety professional). Groups review the laboratory experiment and discuss sustainability considerations from their assigned perspectives, externalizing ideas using color-coded post-it notes on a shared sustainability poster.

While participants are **not expected to fully understand the underlying inorganic chemistry** of the experiment, a knowledge of the related inorganic chemistry will add additional depth to the activity, providing discipline specific green chemistry recommendations.

2.3.2 Participant Flow:

Participants should be guided through the following general progression:

1. **Group Formation and Role Assignment**
   Participants organize into groups of 4–6. Each participant selects or is assigned a stakeholder role using the persona cards, depending on session constraints. Each group is provided with a copy of the undergraduate laboratory experiment or given electronic access.
2. **Initial Reading and Orientation**
   Groups review the laboratory experiment to gain a general sense of the procedure, materials, and laboratory context. Full technical mastery is not required at this stage.
3. **Definition-Setting Discussion**
   Participants discuss their personal definitions of sustainable and green chemistry, how long they have held these definitions, and whether they think these definitions can change. Groups are encouraged to compare their definitions with those from the Canadian Society for Chemistry and the American Chemical Society.
4. **Sustainability Analysis**
   From their stakeholder perspectives, participants consider:
    a. non-sustainable elements of the experiment,
    b. changes that could make the experimental procedure more sustainable,
    c. changes that could make the experimental space more sustainable,
    d. changes beyond the experiment and space that could support sustainability (e.g., policies, training, infrastructure).
5. **Externalization of Ideas**
   Participants record suggestions on color-coded post-it notes and place them on the sustainability poster:
    a. Yellow: experimental procedure
    b. Pink: experimental space
    c. Green: beyond experimental procedure and space
6. **Reflection and Synthesis**
   Groups reflect on:
    a. which sustainability concerns most directly impact their stakeholder,
    b. which proposed changes their stakeholder could reasonably contribute to,
    c. how differing stakeholder perspectives influence which changes are prioritized.

2.3.3 Facilitator Responsibilities:

Facilitators play an active role in supporting progress and maintaining momentum throughout the activity. Key responsibilities include:

- Providing a brief verbal introduction outlining the purpose of the activity and the role of stakeholder perspectives.
- Encouraging groups to move from reading into discussion within the first 5–10 minutes, even if the experiment is not fully understood.
- Using definition-setting discussions (e.g., CIC/ACS definitions of green chemistry) as an entry point when groups are hesitant to begin talking.
- Encouraging participation from all group members; facilitators may suggest that each participant contribute at least one post-it note, and ideally one note in each category.
- Circulating to monitor pacing and redirect groups that become stalled on narrow technical details toward broader sustainability considerations.
- Prompting participants to consider domains beyond experimental procedure, including laboratory space, institutional practices, and systemic constraints.
- Reinforcing that uncertainty and disagreement are expected and productive components of the activity.

2.3.4 Guiding Prompts for Participants:

Facilitators may use the following prompts to support discussion and maintain forward progress:

- "From your stakeholder's perspective, what aspects of this experiment raise sustainability concerns?"
- "Which parts of the procedure generate the most waste, risk, or resource use?"
- "What changes would be possible within your role, and which would require action from others?"
- "Are there sustainability considerations that go beyond the experiment itself, such as training, policies, or infrastructure?"
- "If you are unsure why something is done a certain way, what assumptions are embedded in that choice?"

These prompts are intended to support discussion rather than direct participants toward specific conclusions.

2.3.5 Use of the Sustainability Poster:

Participants are encouraged to use the sustainability poster as a shared visual space to organize ideas. Color-coded post-it notes are used to distinguish between proposed changes to:

- the experimental procedure,
- the experimental space, and
- broader systems beyond the laboratory.

Facilitators may prompt participants to place notes on the poster as ideas arise, rather than waiting until discussions feel "complete," to help externalize thinking and prevent groups from becoming stalled.

2.4 Recommendations for Educators

Activity 1 would be best incorporated into a second-year or third-year inorganic chemistry course or dry laboratory. The activity could also be incorporated into an upper-year ethics of chemistry class or honours class with the expectation that the answers would be more complex. This activity is best suited early in a course for upper-year students and could be run wherever logical with a second-year or third-year group of students. They may need guidance on how to participate in group discussions if they are more junior students.

See facilitation notes above for ideas to get groups talking if they are shy - this includes asking them to look up the definitions of green chemistry or sustainability from the Canadian Institute of Chemistry and/or the American Chemistry Society.

2.4.1 Suggested Prerequisite or Complementary Lessons:

- Friedel-Crafts electrophilic aromatic substitution – mechanism, focusing on the role of the Lewis acid (noting that this reaction can be catalyzed by a Brønsted or Lewis acid).
- Basics of environmental fate/transformation of chemicals.[2]
- Greener Solvent Guide and alternative solvents.[5,6]
- Truncated life cycle analyses, how to determine "problem" areas in a synthesis.[7]
- Creating accessible laboratory spaces.[8,9]

2.4.2 Intended Learning Objectives:

While the activity was originally designed as a narrative sustainability investigation, subsequent iterations have clarified the following intended learning objectives. Activity 0 is designed to help learners:

- Utilize systems thinking to adopt alternative perspectives when exploring green chemistry considerations, challenging one's own definitions of green chemistry and sustainability.
- Apply current green chemistry tools to adapt existing resources to be "greener" through changes to chemistry, infrastructure, policies and mindset.
- Collaborate with an interdisciplinary team in developing sustainable laboratory processes and procedures, considering both chemistry and EDI-AR.

2.4.3 Scalability & Modifications:

Activity 1 was implemented in a symposium setting and is intended to be adaptable across classroom and workshop contexts; however, its effectiveness is sensitive to participant background, facilitation approach, and experiment selection.

The activity can be run in both classroom and conference environments, provided that participants can be organized into groups of approximately 4–6 individuals. In larger sessions, duplicating materials (e.g., posters and experiment handouts) may reduce bottlenecks and support parallel discussion. In smaller classes or workshops, a single shared poster can serve as a focal discussion artifact.

Participant experience level plays a significant role in how the activity unfolds. Groups composed of more junior students or participants with limited prior exposure to laboratory safety or sustainability discussions may require additional facilitation support to initiate discussion and maintain momentum. In these contexts, the activity may take longer than anticipated, particularly if participants spend substantial time reading or attempting to resolve technical details of the experiment.

Similarly, experiment choice influences the pace and depth of discussion. Participants appeared to engage more readily when working with laboratory experiments that were familiar or recognizable, whereas unfamiliar or highly technical procedures may increase cognitive load and contribute to discussion stalls. When selecting experiments for future implementations, instructors may wish to balance authenticity with accessibility, ensuring that sustainability considerations can be identified without requiring specialized content expertise.

Across contexts, facilitator involvement is an important determinant of success. Facilitators may need to actively support pacing, redirect groups away from narrow technical debates, and reinforce the expectation that partial understanding of the chemistry is sufficient for meaningful engagement. These considerations suggest that while the activity is flexible across instructional settings, it benefits from intentional adaptation to participant background and instructional goals.

2.5 Insights

The following insights are based on facilitator observations during implementation and should be interpreted as descriptive rather than as evidence of measured learning gains.

Discussion quality was influenced by group composition and familiarity with laboratory practice. Participants appeared to engage more readily when working with a laboratory experiment that was familiar or recognizable, suggesting that prior exposure to similar procedures may reduce cognitive load and support more sustained discussion.

When participants were permitted to select their stakeholder roles, many chose roles that did not align with their current positions or career stages. This role misalignment appeared to support productive perspective-taking and discussion, as participants articulated concerns and constraints outside of their usual frames of reference. This observation suggests that allowing flexibility in role assignment may support richer conversation in future implementations.

Group dynamics varied substantially depending on participant experience. Groups with prior exposure to laboratory safety, sustainability, or institutional decision-making tended to move more quickly into discussion, whereas groups with less experience required additional prompting to move beyond reading and procedural details. In these cases, discussion often progressed once facilitators redirected attention toward broader sustainability considerations rather than technical optimization.

Overall, participant engagement was supported when facilitators actively reinforced the purpose of the activity and normalized uncertainty in both chemistry content and sustainability decision-making. These observations highlight the importance of facilitation in shaping how participants navigate open-ended sustainability discussions, particularly in mixed-experience groups.

Activity 2 – A Sustainability Puzzle: Leveraging second-year inorganic principles for sustainable catalyst design.

3.1 General Materials

- Symposium Workbook or Classroom Workbook
    - Workbooks contain linked to the Flippity online locks
- Four virtual locks accessed via printed QR codes (e.g., Flippity). Each workbook and puzzle handout contains the QR code link. Facilitators may choose to print additional QR codes. Each lock requires a code derived from puzzle completion to proceed. Access at: https://www.flippity.net/vb.php?k=e/2PACX-1vSe1q9dhjbgWYPM_qXjxBEWR_FnOOjyFT-ZwVw1k1cIsp_9SbivbjdABuxHhXjJ6PXQqz1e62OuV-99
    - Lock #1: Puzzle 1 progression
    - Lock #2: Puzzle 2 progression
    - Lock #3–4: Puzzle 3 progression
- Pens or pencils for participants
- Optional timers or clocks (for time-bounded implementations)

3.2 General Overview

In this activity participants are challenged to combine their first-year inorganic chemistry knowledge and green chemistry considerations to solve a series of three puzzles. Puzzles focus on topics such as ligand design, coordination complexes, complex reactivity (substitution reactions, cross coupling reactions, small molecule activation), inorganic spectroscopy (IR spectroscopy and Tolman's Electronic Parameter), and green chemistry metrics.

Participants work in groups of 2-4, solving the puzzles sequentially. Puzzle answers are entered into an online escape room platform, Flippity,[10] accessible through a QR code. We recommend providing participants with a minimum of 30 minutes to solve all three puzzles. Upon completion participants should have a stronger understanding of the balance between green chemistry applications and coordination complex functionality.

3.3 Puzzle 1– Dissociative Mechanisms

3.3.1 Materials

- Laminated N-heterocyclic carbene (NHC) ligand cards (R = H, OCH_3, F)
    - Circular Velcro stickers (approximately 1cm in diameter).
- Ball and stick phosphine ligand representations (PR_3, where R = CH_3, Ph, ^tBu)
    - Styrofoam balls (3 balls in 3 sizes), toothpicks, hot glue, pink paint, paint brush, wooden bead (interior diameter = 3/8-inch).
- Bead-on-dowel model representing the metal center (Ru) and *trans* metal–ligand bonds
    - wooden dowel (diameter = 3/8-inch, length = 10 in), wooden bead (interior diameter = 3/8-inch), green paint, black sharpie.

- Physical components are used to model relative bond strengths and dissociation tendencies
- Plastic container labelled “Puzzle 1”
- Print-outs of *Activity 2 Puzzle 1 handout.pdf*

3.3.2 Set-Up and Preparation

Phosphine construction:

- Paint all the Styrofoam balls pink using a paintbrush. These will represent the R groups on the phosphine ligand.
- Paint the wooden beads yellow. These will represent the central Phosphorus (P) atom. Let all of these components dry.
    - Tip: prior to selecting the wooden beads, ensure that the beads that you selected will fit on the wooden dowel (this accounts for any possible bead variations)
- Take 3 toothpicks and using hot glue, glue one end of each of the toothpicks together, spacing them evenly to form a trigonal pyramidal shape (like a tripod).
- Apply hot glue around this connection point, and glue on one of the yellow wooden beads, being sure that the toothpicks only go halfway into the bead.
    - This will ensure that the bead can still be used to attach it to the dowel.
- On the free end of each toothpick, hot glue a pink Styrofoam ball to represent the different R groups. Ensure that on one phosphine, all of the Styrofoam balls are the same size.
- Once complete, allow model to completely dry and cool before handling (Figure S2).

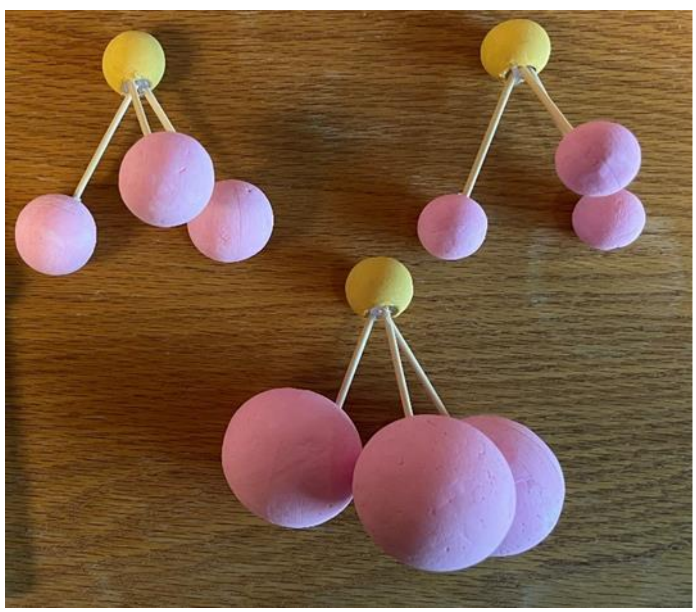

Figure S2. Image of phosphine models showing three different sized phosphines.

NHC ligand construction:

- Print the NHC ligands as provided in NHC_Printout.pdf.
    - Ensure high quality printing for clear visual

- Cut out each ligand around the shape.
- Laminate each of the cut-out ligands using a laminator and appropriate laminating sheets.
    - If you do not have access to a laminator, print out on heavy card-stock paper.
- Once laminated, cut out the laminated shapes again, leaving a small margin to maintain the lamination.
- Attach a Velcro dot (loop side) to the back of each of the laminated ligands (Figure S3).

<u>Construction of metal centre and axial bond lengths:</u>

- Cut the 3/8-inch dowel so that it is approximately 6 inches long.
- If cut, sand down any rough edges present.
- On the dowel, draw three evenly spaced black line horizontally around the shaft. These will represent bond lengths as the NHC donicity changes.
    - Suggested spacing: 1 inch apart.
    - Be sure to ensure lines are neat and parallel for clarity.
- Paint 3/8-inch wooden bead green to represent the Iridium metal centre.
    - Choose beads that slide easily but snugly along the dowel. Be sure to test each one before use.
- Allow the bead to dry. Confirm that it is able to slide to the 3 different lines on the dowel.
- On one end of the dowel, hot glue a 3/8-inch wooden bead.
- Once secured, attach a Velcro dot to the surface (hook side). This will act as the connection point for the NHC ligands.
- The opposite end of the dowel is to remain unmodified to allow for insertion of bead, and for phosphine ligand attaching (Figure S3).

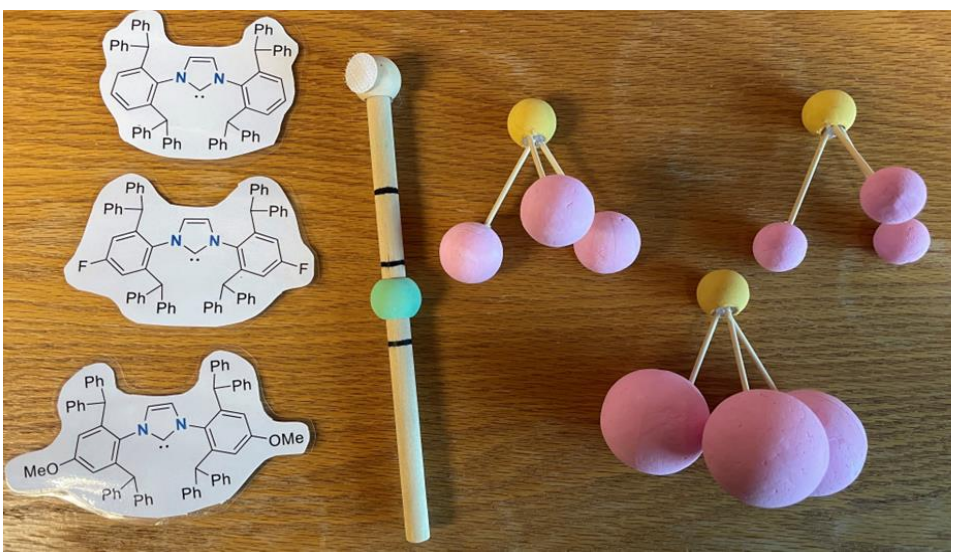

Figure S3. Image of the puzzle contents as seen by participants. NHC ligand with Velcro dot on the back (left), wooden down representing axial ligand-metal bonds with green bead representing the metal (middle), three phosphine ligand models (right).

3.3.3 Facilitation

3.3.3.1 Participant Flow:

Participants should be guided through the activity in the general order described below.

- Review the Workbook PDF, focusing on:
    - NHC and phosphine ligands, steric and electronic effects, dissociative substitution mechanisms
- Rank NHC ligands by electron donicity using the provided information.
    - More electron-donating ligands form stronger (shorter) bonds with the metal.
- Rank phosphine ligands by steric bulk.
    - Larger cone angles increase the rate of dissociation by destabilizing the metal-ligand bond.
- Assemble the physical puzzle:
    - The dowel represents the axis between NHC–Metal–Phosphine. Attach the NHC ligand (via Velcro) on one end. Slide the green bead (Ir-metal) to the correct position based on NHC donicity — more donating ligands mean the metal should sit closer to the NHC end. Place the phosphine (pink bead) on the unmodified end. Use the ranking and model to determine how ligand choice influences the dissociative rate (Figure S4).
- Enter the final conclusion/code into Flippity to complete the digital puzzle.

Figure S4. Photograph of Puzzle 1 as seen by participants at the beginning of the activity (left). Assembled puzzle with example solution (right).

3.3.3.2 Facilitator Responsibilities:

Facilitators play an active role in supporting progress and maintaining momentum throughout the activity. Key responsibilities include the following:

- Before the Activity, ensure that all materials are set up and available:
    - Physical models (dowels, beads, laminated NHC ligands, Velcro attachments), Workbook PDF (with background on phosphines, NHCs, steric/electronic effects, and dissociative substitution), Digital platform (e.g., Flippity) with the puzzle/code input
    - Review key concepts in the workbook to help guide discussion if needed.
- During activity:
    - Welcome students and briefly explain the goal: To determine how different ligands affect the reaction rate by modeling their influence on bond lengths and substitution mechanisms.
    - Let students explore the workbook and begin ranking the ligands (NHCs and phosphines).
    - Monitor progress but only intervene minimally, unless they are clearly stuck or heading in the wrong direction.
    - Guide students through assembling the physical puzzle, modeling the effect of ligand properties on bond strength and placement.

3.3.3.3 Puzzle Answers:

- The expected ranking of NHC from most to least electron donating:
    - 2 >3 >1 or iPrOMe > iPr > iPrF
- The expected ranking from smallest to largest steric bulk of phosphines:
    - C < A < B or PMe_3 < PPh_3 < $PtBu_3$
- Flippity puzzle:
    - Question: provide the ligand combination that would result in the fastest phosphine dissociation (corresponding phosphine number, then the NHC number) then the slowest (corresponding phosphine number, then the NHC number).
    - Answer: 2231

3.3.3.4 Intended Learning Objectives:

Puzzle 1 is designed to help learners:

- Explain how steric and electronic properties affect relative ligand-metal bond strength through the Trans-Effect.
- Rationalize donicity and steric trends utilizing inorganic spectroscopic data.
- Predict relative reaction rates of ligand dissociation pathways.

3.4 Puzzle 2 - Considerations in Experimental Design for Suzuki-Miyaura Cross-Coupling

3.4.1 Materials

- Laminated green chemistry design tables representing (Print file *Activity 2 Puzzle 2 Tables.pdf*):
    - Metals (e.g., Fe, Ni, Pd, Cu)
    - Ligands
    - Solvents
    - Additives
    - Reaction Conditions

Note: Tiles are color-coded to indicate compatibility across reaction pathways. Sustainability indicators (e.g., number of green leaves) are printed on relevant tiles.

- Plastic sheet protector
- Black dry-erase pen
- Plastic document folder labelled "Puzzle 2"
- Print-outs of *Activity 2 Puzzle 2 handout.pdf*

3.4.2 Set-Up and Preparation

- Print *Activity 2 Puzzle 2 Tables.pdf* in colour.
- Insert both tables into the plastic sheet protector. The table showcasing the leaves and metal colours should be hidden underneath of the other table.
- Place the tables, dry-erase pen, and activity handout into the plastic document folder.

3.4.3 Facilitation

3.4.3.1 Participants Flow:

- Review the Workbook PDF
- Using the dry erase marker, circle the catalytic components that you believe will lead to the greenest synthesis (Figure S5).
    - Note, only common-coloured components can be used together.
- Reveal table two (containing the green leaves). Count the number of green leaves associated with your proposed system.
    - If your system contains any reagent or condition tiles with an exclamation mark, an alternative reagent must be selected
- If you believe your answer is correct based on the number of leaves ("greenness" of the system) then enter the final code into Flippity to complete the digital puzzle.
    - If your code is incorrect, return to table 2 and select an alternative catalytic system.

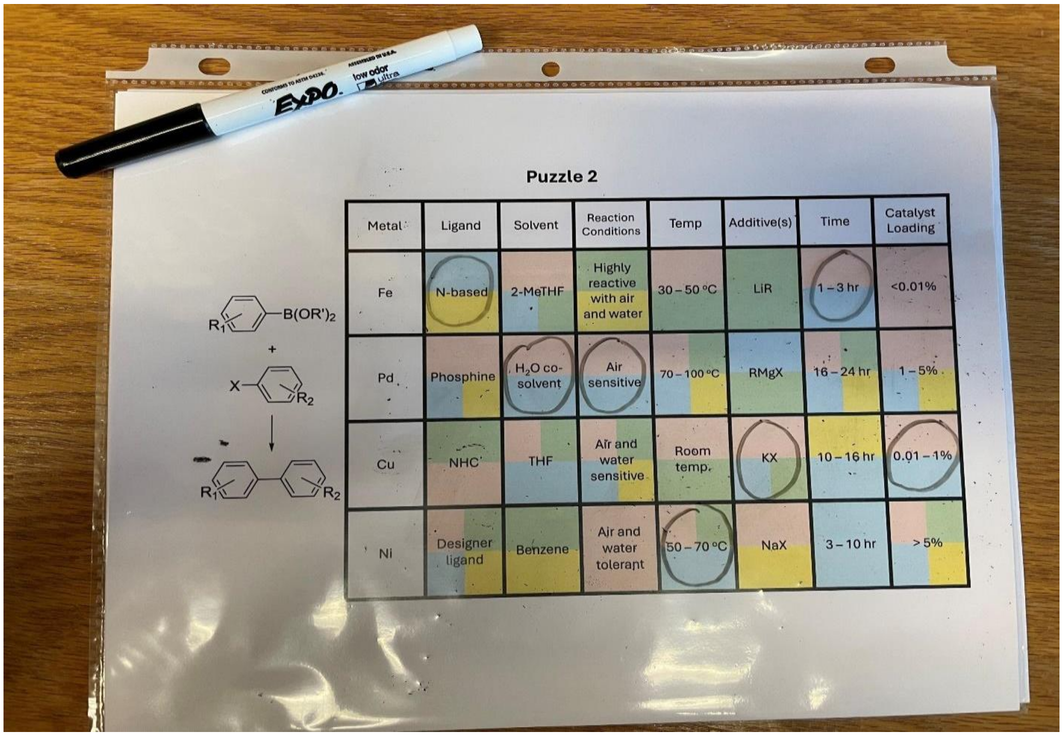

Figure S5. Photograph of Puzzle 2 revealing the first catalytic system table 1. An example selection of components has been selected. The common colour connecting the components is blue.

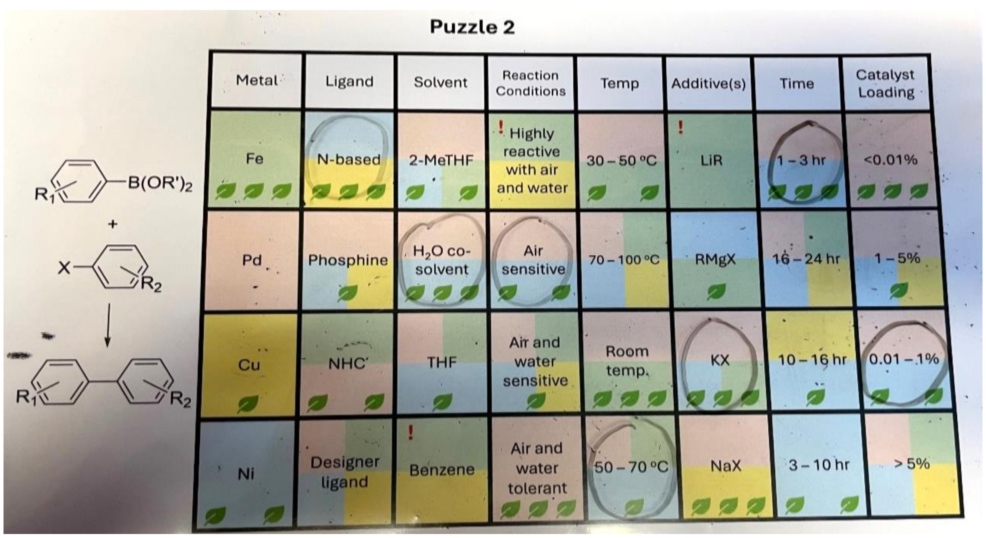

Figure S6. Photograph of Puzzle 2 revealing the second catalytic system table 2 featuring the green leaves. The previous components selected remain circles. Nickel (blue) is the only metal compatible with the proposed system. The total number of leaves is 19, leading to the combination Ni19.

3.4.3.2 Facilitator Responsibilities:

- Before the Activity: Ensure that all materials are set up and available:

- Both tables should be stored inside of the plastic protector. The table showcasing the green leaves should be hidden under the other table. Any markings should be erased from the plastic sleeve.
  - Review key concepts in the workbook to help guide discussion if needed.
- During activity:
  - Welcome students and briefly explain the goal: To determine the combination of metal, ligand, additive(s), and reaction conditions that will lead to the greenest catalytic system to perform a Suzuki-Miyaura cross coupling reaction.
  - When appropriate, remind participants that catalytic components must have a common colour to be combine with one another. For example, if the ligand is purple, the corresponding solvent conditions must also be coloured purple.
  - Remind participants that the second table is only to be revealed once a combination is first proposed. Circling the selected catalyst criteria on the sheet protector using the dry erase marker allows for easy comparisons between tables.

3.4.3.3 Puzzle Answers:

While Fe, Ni, and Cu are greener than Pd, the ability to utilize palladium under ambient conditions, in aqueous media at low catalysts loadings leads to its overall higher "greenness". Greenest system combinations for each metal: Fe14, Pd20 (Correct answer, Figure S7), Cu10, Ni19.

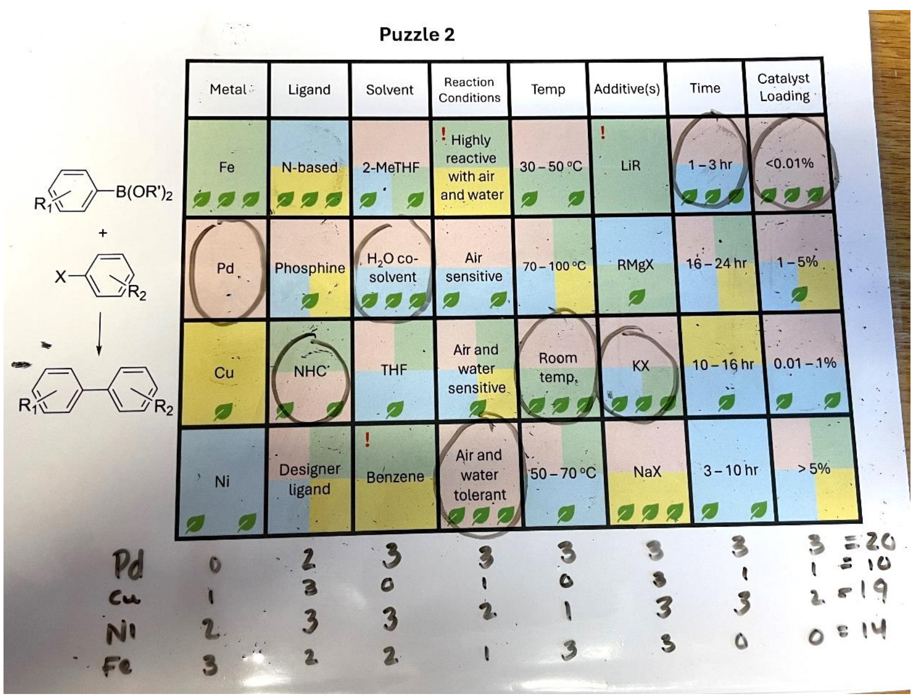

Figure S7. Photograph of Puzzle 2 showcasing the correct puzzle answer (Pd20). Total greenness scores for each metal are highlighted at the bottom of the table.

3.4.3.4 Intended Learning Objectives:

Puzzle 2 is designed to help learners:

- Leverage knowledge on hard-soft acid base theory, coordination geometry, and solubility to pair metals with compatible ligand designs and reaction conditions.
- Utilize knowledge on common cross-coupling mechanisms (Suzuki-Miyaura, Kumada, Negishi) and metal reactivity (oxidative addition, transmetalation, reductive elimination) to select complementary additives.
- Balance green chemistry alternatives (solvents, energy input, chemical safety) with catalyst function to determine a feasible catalyst design.
- Discuss the barriers in applying sustainable alternatives while maintaining chemical functionality.

3.5 Puzzle 3 – Green Catalyst Design for N_2O Reduction

3.5.1 Materials

- Puzzle board representing the framework for catalyst-selection pathways as a maze
  - Maze layout is used to indicate relative sustainability and reactivity outcomes.
  - Wooden boards (the boards used were wooden puzzle boards from Michaels, with the inside square being 7 x 7 inches in dimension, with rounded edges).
  - Thumb tack.
  - White and Black permanent markers.
  - Wooden Frame.
  - Self-adhesive laminating sheets (optional).
  - Super glue
- Colored ligand tiles corresponding to ligand options provided in synthesis notes
  - White foam core boards
  - X-Acto knife
  - Orange, Yellow, Green, Blue, and Black paint (plus paintbrushes)
- Wooden pegs or markers representing metal choices
  - Wooden pegs
  - Clear tape
- Plastic document folder labelled "Puzzle 3"
- Print-outs of "*Activity 2 Puzzle 3 handout.pdf"*
- Print-out of *"Puzzle 3 Template.pdf"*
- Print-out of *"Puzzle 3 Board Labels.pdf"*

3.5.2 Set-Up and Preparation

<u>Constructing the Foam Puzzle Pieces</u>

1) With the printouts of the template (*Puzzle 3 Template.pdf*), cut out each rounded square out and cut along the red lines to have templates for each corner piece (A to D) and a template for each square middle piece (A to D). You will only need one template for each

corner piece, but the pieces all appear on each page of the template. You can discard the extra sets of corner pieces or keep them as spares.

2) With a pencil, trace the outline of each corner piece twice onto the foam core board, and use the X-Acto knife to cut out each piece. One piece will be used for the base of the maze, and one piece will have the maze pattern cut out to create the path.
3) For each puzzle piece, use the knife to lightly trace along both sides of each thick black line on the template, then cut out the blacked-out areas, discarding the cut-out pieces.
4) Using superglue, glue the pieces onto the second corner piece, making sure to line up each cut-out piece with the template. Repeat for each corner (A to D).
5) Once dry, paint all of the indented areas black and each raised piece on the surface of the puzzle piece with the corresponding colour: A is yellow, B is blue, C is green, and D is orange. Once dry, use the permanent marker to distinguish which piece is which by writing the letter on the corner of the piece.
6) Repeat steps 2 - 4 for each square middle piece (A to D), using the square pieces you cut out as the templates instead of the corner pieces. In the end, for one puzzle you will need one of each corner piece (A to D) and one of each square middle piece (A to D). Figure S8 shows how the pieces should look after glueing together the maze but before paint is applied. Figure S9 shows how the center pieces should look after being fully assembled and painted.

Figure S8. Photograph of the center puzzle pieces after the maze pattern has been cut out of the top piece and glued onto the bottom piece.

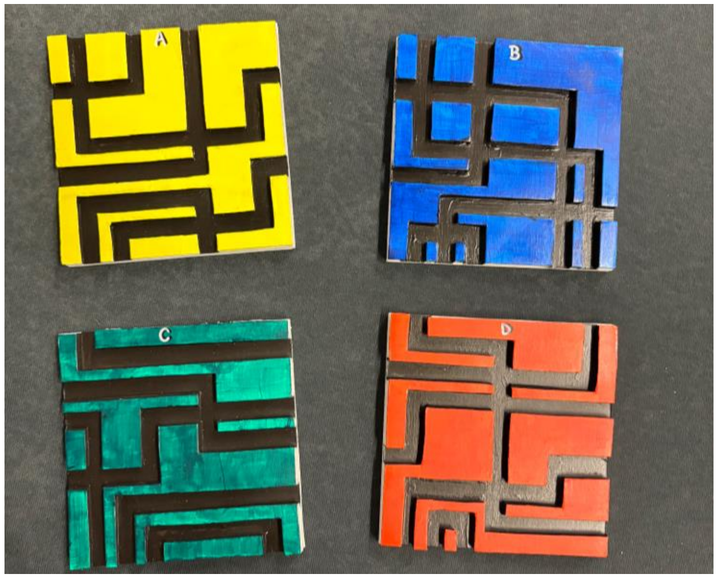

Figure S9. Photograph of the center puzzle pieces after they have been fully painted.

Setting up the Puzzle Board

7) To create the outline in the puzzle board, put one foam corner piece into a corner and trace around the edges. Repeat this for each corner and then you should have a full outline of each corner piece with a square in the middle (see Figure S10). The writing in the board should be as follows:
    - In the top left corner, write a number 1 and add "Strongest Donor"
    - In the top right corner, write a number 2
    - In the bottom left corner, write a number 3
    - In the bottom right corner, write a number 4 and add "Weakest Donor"
8) Assemble the board with each corner piece in its correct position, then mark four holes on each side that line up with the entrances and exits of the maze on the left- and right-hand sides of the board (see Figure S11 below for a diagram). Drill a shallow hole in each of the marked spots. You want this hole to be wide enough to fit the peg inside.
9) Print out the document with the board labels (*Puzzle 3 Board Labels.pdf*). For the title ("Green Catalyst Design for N_2O Reduction"), you can cut it out and glue it at the top of the board. An optional step is to glue it onto some foam core, cut out the label and then paste it onto the board if you want it to stick out more.
10) For the labels for the wooden pegs (the smaller of the two sets of element labels), cut those out and glue each one to a wooden peg. An optional step to reinforce the peg labels is to take a small strip of clear tape and wrap it around the peg plus label.
11) For the larger of the two sets of element labels, cut those out then glue them above the holes on the left-hand side of the board, the order corresponding to Figure S10 below.
12) Finally, for the outcomes on the right-hand side of the board, an optional step to reinforce the labels is to cut each of the rounded rectangles out (following along the red lines) and then laminate each piece. An alternative is to just sandwich each cut out between two pieces

of clear tape to serve as a makeshift lamination. The slips should all be cut out once laminated.

13) To attach the slips to the puzzle board, flat thumb tacks will be used to pierce through the black dot printed on the slips. They will be attached on the reverse side of the board so that they can be swung out and in for easy storage. See Figure S10 below for the order in which they should be attached and see Figure S12 for a diagram showing how the outcome slips should be attached at the back of the board and should be able to swing back behind the board.

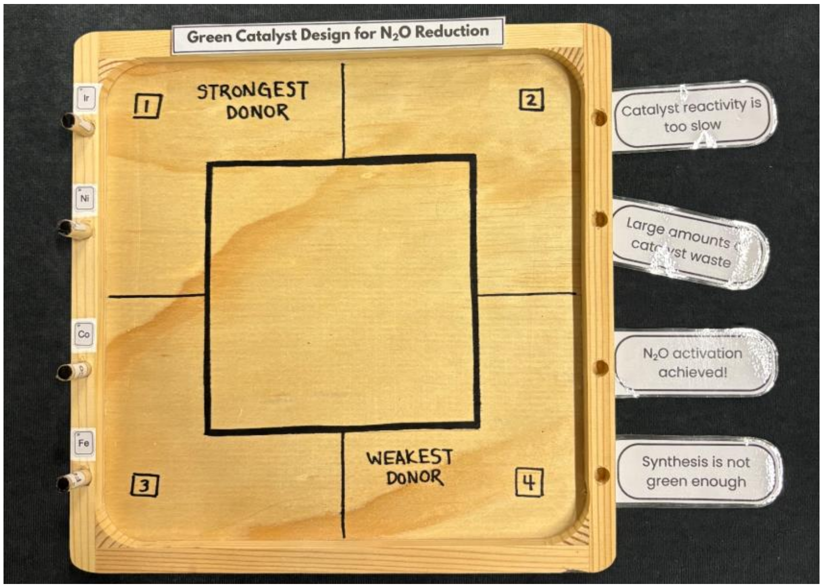

Figure S10. Photograph of the puzzle board fully set up.

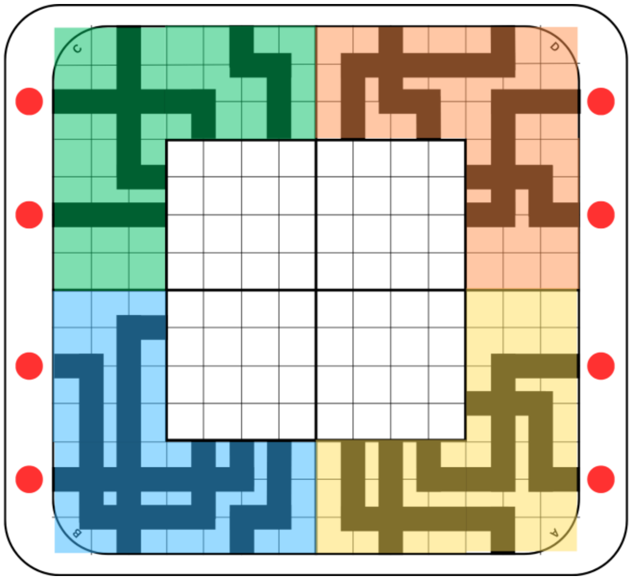

Figure S11. Diagram of where the holes should be drilled on the left and right sides of the board, marked with red circles.

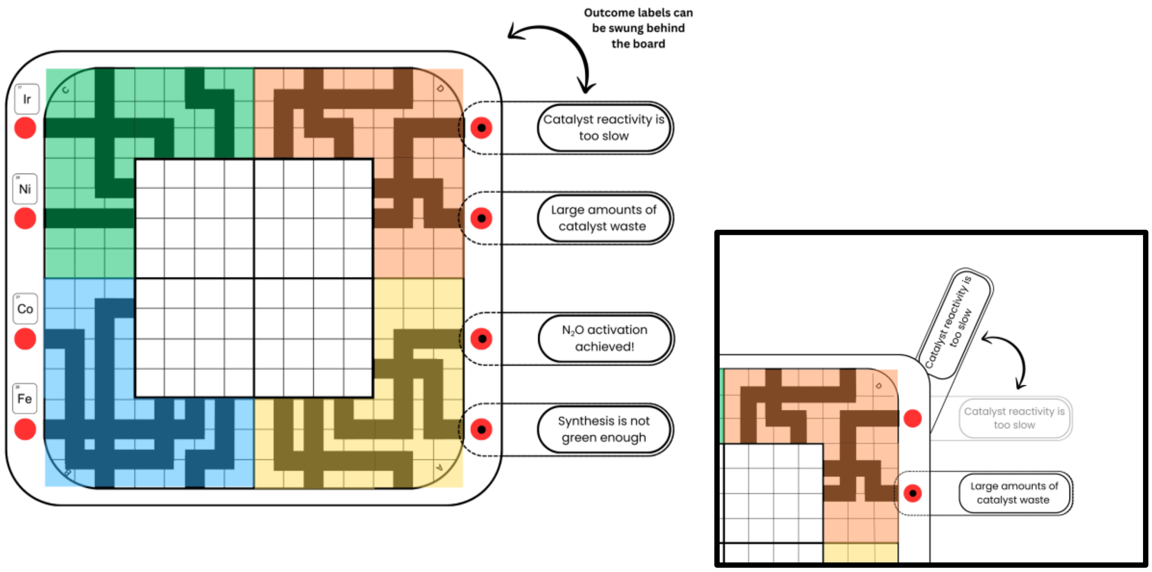

Figure S12. Diagram of the board after metal element labels have been included on the left side of the board and outcome labels have been added on the right side of the board, attached at the back (left picture). A zoomed in illustration to show how the outcome labels can be swung behind the board for storage (right picture).

Assembling the Puzzle:

14) Each of the pegs should be set-up in their corresponding holes on the left side of the puzzle board.
15) Each puzzle set up should contain four corner puzzle pieces with four square center pieces.
16) Each puzzle should also contain a print-out of the instructions to complete the puzzle (*Puzzle 3 Handout.pdf*).
17) For ease of transportation and storage, all the pieces (puzzle board, four corner pieces, four center pieces, instructions print-out) can be stored in a plastic envelope labelled Puzzle 3.

Setting Up the Puzzle:

18) To make the puzzle ready to be used, take the materials out of the envelope. Ensure that the pegs for each metal are in the corresponding holes on the left side. Twist the tabs for each outcome out so that they are visible on the right side.
19) Place each square center piece off to the side and each corner piece off to the side in a separate pile.
20) Place the copy of the instructions near the puzzle set up for reference. See Figure S13 below for reference on how to set up the puzzle for participants.

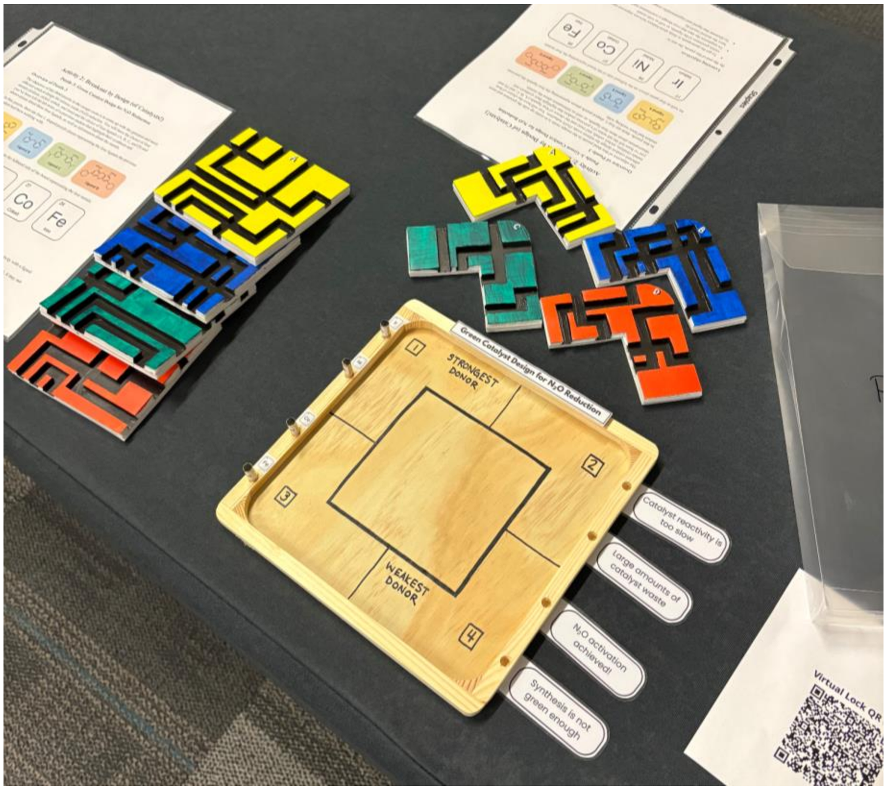

Figure S13. Photograph of Puzzle 3 set-up as seen by participants.

3.5.3 Facilitation

3.3.3.1 Participant Flow:

Participants should be guided through the activity in the general order described below.

- Review the Workbook PDF, focusing on:
    - Pincer ligand design, synthetic pathways, and green metrics.
- Rank pincer ligands by electron donicity using the provided information.[11]
    - More electron-donating ligands increase the back bonding occurring between the metal and a *trans*-carbonyl ligand, in the corresponding carbonyl complex, resulting in a lower wavenumber for the carbonyl stretching frequency in the IR spectra.
- Rank pincer ligands by the greenest synthesis, balancing with complex reactivity.[12–23]
    - Participants should consider the number of synthetic steps, the greenness of reagents, as well as the reactivity notes for each complex.
- Assemble the physical puzzle:
    - Participants must first build the outside of the puzzle using the corner pieces. Each corner piece (number and colour) represents one of the four pincer ligands. The pieces are place in order of ligand donicity.
    - Select the greenest and most effective ligand for the centre of the puzzle. The puzzle piece should be orientated upwards (showcased by a number in the corner of the puzzle piece).

- Utilize the pegs representing each metal system to move through the map. Note the available movements described below.
- Enter the final conclusion/code into Flippity to complete the digital puzzle.

3.5.3.2 Facilitator Responsibilities:

Facilitators play an active role in supporting progress and maintaining momentum throughout the activity. Key responsibilities include the following:

- Before the Activity:
  - To make the puzzle ready to be used, take the materials out of the envelope. Ensure that the pegs for each metal are in the corresponding holes on the left side. Twist the tabs for each outcome out so that they are visible on the right side.
  - Place each square center piece off to the side and each corner piece off to the side in a separate pile.
  - Place the copy of the instructions near the puzzle set up for reference.

- During the Activity:
  - As participants come to start this puzzle, the facilitator should welcome them and explain the goal of this puzzle.
  - The facilitators should be standing nearby as the participants follow the instructions to complete the puzzle to help with clarifications and give hints when necessary.
  - Let the students explore the workbook and supplemental information given at their leisure.

3.5.3.3 Guiding Prompts for Participants:

Facilitators may use the following prompts to support discussion and maintain forward progress:

- For the first part of the puzzle, get the participants to think of the Tolman electronic parameters to determine which ligand is the strongest donor. The CO stretching frequencies are provided for each ligand,[1] noting that smaller wavenumber corresponds to a longer C≡O bond, a result of increasing the donicity of the pincer ligand.
- For the second part of the puzzle, prompt the participants to think about what aspects of synthesis and catalyst design would make it greener (i.e., number of synthetic steps, greenness of the metal, if the catalyst can be reused or if the reaction is stoichiometric).

3.5.3.4 Puzzle Answers:

- For part one, where participants rank the ligands based on how strong of a donor they are, the answer is (from strongest to weakest): *C, B, D, A*

- When the participants are inputting their answer in virtual lock #3, it should be formatted as: **CBDA**

- For part two, where participants choose one ligand and one metal to use in their catalyst design, the answers should be: *Ligand B and Iridium* (Figure S14).
  - When the participants are inputting their answer in virtual lock #4, it should be formatted as: **Iridium, B**
  - Ligand A synthesis is not green enough, ligand C and its corresponding metal complex decompose over time due to its high reactivity, and ligand D has very slow overall reaction times. Ligand B is the best balance of green synthetic components (see synthesis), metal reactivity, and complex stability.
  - Iridium is the only metal that will do N_2O reduction.[2–4] Nickel does E-H activation via 1,2-addition mechanisms.[5,6] Cobalt has been shown to perform C-H activation[7] and CO_2 reduction reactions.[8] Iron has been shown to perform 2+2 cycloadditions and formal enyne metathesis.[9,10]

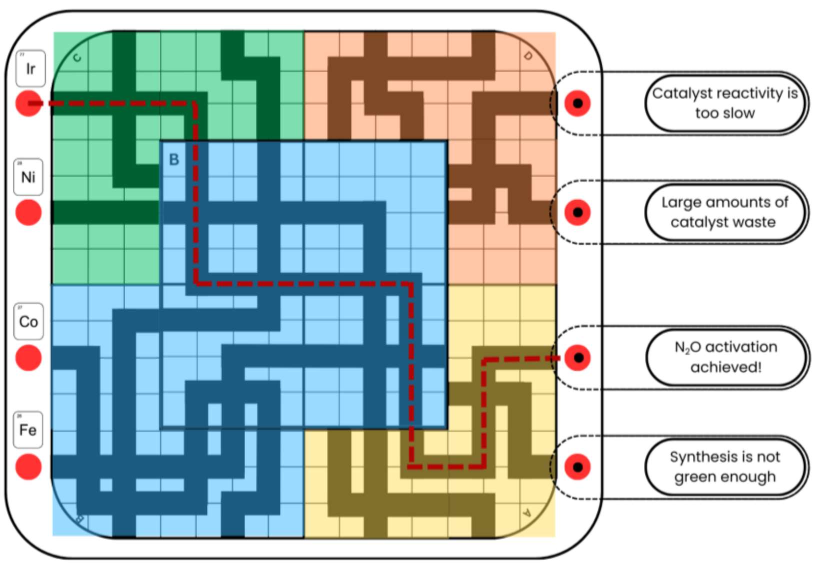

Figure S14. Diagram of the correct puzzle layout and path (red dotted line) for puzzle 3.

3.5.3.5 Intended Learning Objectives:

Puzzle 3 is designed to help learners:

- Apply knowledge of the Tolman Electronic Parameter and the effects of electron-withdrawing and electron-donating functional groups to rank relative ligand donicity.
- Exemplify the differences in complex reactivity between alternating metal and ligand selections.
- Emphasize the cyclical process of alternating ligand design, metal combination, and green chemistry considerations in catalyst development.

3.5 Recommendations for Educators

Activity 2 was readily integrated from a conference setting into a classroom setting. The puzzle content knowledge is appropriate for second-year inorganic students, studying coordination complexes, ligand design, inorganic spectroscopy, and preliminary green chemistry as an end of year activity – working to reinforce student knowledge. Alternatively, the puzzles can be readily applied to upper year inorganic courses as a tool to teach green chemistry in an inorganic context, or as a review tool for the above topics. While the puzzles tackle specific reactivity of species, cross coupling or N_2O reduction, they can be readily solved without a deep understanding of the chemistry content. Students will best benefit from the puzzles if they have prerequisite knowledge on the concepts described above as well as an introductory understanding of green chemistry.

Assigning a grade to active learning tools such as escape rooms is difficult. Time limits on the puzzles may be introduced to spur competition-based learning; however, we do not recommend grading based on student speed to complete the puzzles. Rather, we recommend pairing the puzzles with lecture material and later a later assignment, self-assessment, or exam. Examples lecture notes for a third-year inorganic audience are provided *"Green Chemistry Lecture.pdf"*. Research is currently underway exploring the educational benefits of green chemistry interventions such as this on student understanding in second and third year inorganic chemistry classrooms.

3.5.1 Suggested Prerequisite or Complementary Lessons:

- Ligand design, donicity, cone angle, *Trans* Effect, back bonding, Tolman Electronic Parameter.[24–27]
- Truncated life cycle analyses, how to determine "problem" areas in a synthesis.[7]
- Considerations in green catalytic design.[28]
- Suzuki-Miyaura cross coupling reactions.[29–37]

3.5.2 Scalability & Modifications:

Activity 2 can be readily scaled to accommodate large audiences, limited mainly by the layout of the room. In a classroom or workshop setting we strongly recommend providing participants with tables at which to work. This set-up allows participants to better view and engage with the puzzle materials while creating an environment for easy communication between team members. We recommend that group sizes not increase above 4 members to allow for all members to engage with the puzzle materials. Similarly, we recommend providing groups with two copies of printed materials where applicable. This allows more than one team member to read key information required to solve the puzzles.

Puzzles can be easily stored in small Tupperware or plastic folders. We recommend keeping all puzzle materials stored together and with their accordingly puzzle for ease of implementation. We also recommend that facilitators print an answer key for themselves, this avoids any confusion for new facilitators. Applied with larger audiences, we recommend each facilitator have a copy of the answers as well as a brief description of why the answer is correct. These puzzles can be readily integrated into the Battle Box set-up previously described by Clapson *et al.*[38]

3.6 Insights

The following insights are based on facilitator observations during implementation and should be interpreted as descriptive rather than as evidence of measured learning gains.

3.6.1 Symposium Applications

Participants were eager to engage with the puzzle materials. Several attendees had previously engaged with an educational escape room or a commercial escape room. Group sizes ranged from 1-6 individuals. We found that group sizes over 4 required a second set of puzzles to allow all participants to engage with the material. Despite the size, the larger group displayed the best understanding of inorganic content knowledge and readily engaged in discussion. As is true for many escape room activities, all participant groups required 2+ hints in order to solve all three puzzles. Many of these hints focused on how the puzzle functions, rather than the educational content of the puzzle. For example, with Puzzle 3, participants needed a reminder that the metal pegs are only able to change direction in the puzzle one they have hit a wall. Overall, the activity was well received, noted by the interest of participants and the positive commentary following the symposium.

3.6.2 Classroom Applications

Two green chemistry activities were implemented into a third-year inorganic chemistry classroom (Inorganic II). The course is focused on exploring green chemistry, symmetry and spectroscopy, main group element reactivity, and cross coupling reactions. Inorganic I is the prerequisite course. Students are expected to understand coordination chemistry, ligand design principles, IR spectroscopy, and substitution mechanisms.

Green Chemistry was introduced at the beginning of the semester. The activity and lecture flow was as follows:

- Activity 0 – Peering into the Mist: applied as a community building activity to allow students to become more familiar with each other. The activity helped to foster a sustainable chemistry mindset by having students engage with ideas such as *systems thinking*.
- Green Chemistry Lecture: the lecture provided students with an overview of system thinking, two-eyed seeing, life cycle analysis, green chemistry metrics, and emerging trends in sustainable inorganic chemistry.
- Self-Assessment: gauging student understanding of green chemistry following the lecture.
- Activity 2 – A Sustainability Puzzle: implemented as a material summary and review tool to drive deeper learning in green inorganic chemistry.
- Assignment: probing student understanding of green chemistry following the activity.

A total of 8 students, in two groups, performed Activity 2. Students had 40-minutes to complete all of the puzzles. A brief 10-minute introduction to the puzzles, learning objectives, and key content was provided at the beginning of the activity. A truncated workbook was provided to students compared to symposium attendees. The content therein provided less background knowledge on the principles explored in Inorganic I, challenging students' previous knowledge. Similarly, the clues provided for each puzzle were in a format more akin to a classical escape room rather than lecture notes. For example, knowledge was shared as "lab notes" and internal emails rather than a fully described document. We chose to share information for the puzzles in this manner to reduce procedural dependence and deepen critical thinking.

Surprisingly, compared to symposium attendees, the Inorganic students were hesitant to engage with the puzzle materials. Students were similarly reluctant to engage in conversation while solving the puzzles, mainly relying on the knowledge of top performing students. The instructor needed to prompt students to open the puzzle materials and utilize the tactile components. Students struggled with both content recall and how to use the Flippity escape room lock program to enter their puzzle answers.

The gamified educational style of the activity was new to all students. Similarly, few students had engaged with a commercial escape room. We question if the novel format resulted in lower student engagement, stemming from a lack of understanding for the flow of the activity. Similarly, we considered if more background content knowledge should be provided to students, like symposium attendees, as the instructor had to guide students in puzzle solution. However, the utilization of more prescriptive procedures would reduce the utility of the activity as a mechanism to probe student understanding of prerequisite content and its alignment with green chemistry. We encourage educators to provide clear learning outcomes for the activity before implementing into the classroom. For example, is the activity meant to act as a review tool, and introduction to green chemistry, or simply a method to build communities of practice. Depending on the learning outcomes, either the truncated student workbook, or the symposium workbook may be implemented. We similarly recommend having an example puzzle introduced in an earlier lecture. Solving the sample puzzle together may help student become more familiar with how to solve educational escape room puzzles.

Activity 3 - Keywords: A waste and hazard reduction puzzle

4.1 Materials

- **Foam boards**: Two foam boards (90 cm × 60 cm each), used to fabricate question tiles and answer tiles.
- **Colour dot stickers**: Used to colour-code answer tiles by team; two dot stickers were applied per answer tile.
- **Printer and printer paper**: Used to print questions, answers, and reference materials.
- **Coloured copy paper**: Used to create letter cut-outs for the answer tiles.
- **Adhesive (e.g., glue or tape)**: Used to affix printed questions, printed answers, and letter cut-outs to foam board tiles.
- **Box cutter or scissors**: Used to cut foam board tiles and interior openings.
- (Optional) **Coloured markers**, used to assist with material organization during setup.
- Printed copies of the Symposium Workbook (or the relevant Activity 4 pages), which participants consulted to identify correct answers during gameplay.
- Print-out of *"Activity 3 – Question and Answer Print-Out.pdf"*
- Copy of *"Activity 3 – Answer Key and Letter Coding.pdf"*

4.2 Set-Up and Preparation

Advance Preparation:

All foam board cutting and tile assembly were completed in advance of the session. No cutting or fabrication was performed on-site. This included preparation of all question tiles, answer tiles, and printed materials.

Tile Fabrication:

Foam boards (90 cm × 60 cm) were cut to create the components required for question tiles and answer tiles (Figure S15).

Each question tile was assembled from two foam board pieces:

- One backing piece (12.5 cm × 12.5 cm), left uncut.
- One border piece (12.5 cm × 12.5 cm) with a centered 10.0 cm × 10.0 cm square cut-out, creating a recessed well.

The border piece was aligned and glued onto the backing piece to form a framed question tile. Printed question text was then affixed within the recessed well.

Each answer tile consisted of a single foam board square (10.0 cm × 10.0 cm) with content on both faces. On one face, a printed answer was affixed. On the reverse face, a coloured paper letter cut-out was glued to the tile, and two, coloured dot stickers were applied to indicate team membership.

This fabrication scheme yields one complete question–answer pairing per letter used in the final keyword or phrase.

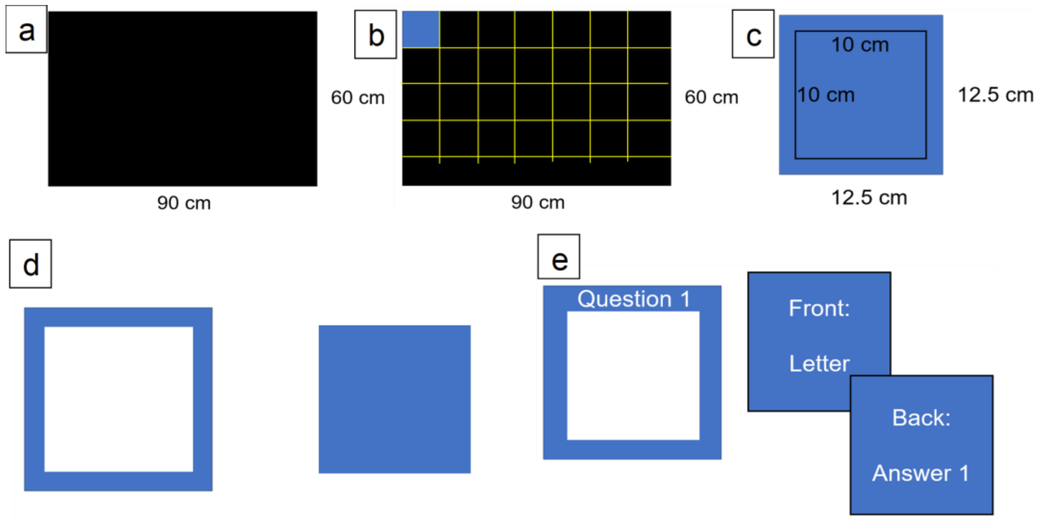

Figure S15. Activity setup - use foam board to create question and answer tiles. Measurements for border tiles and answer tiles included in a-c, question/answer setup in d, e.

Table Layout and Initial Game State:

Gameplay was conducted at two tables, with two teams assigned to each table. Teams were seated facing one another across the table. Prior to gameplay, **question tiles were laid out in fixed order** in a single row in front of each team, oriented so that the text was readable by that team (Figure S16). Each team's row contained its full set of question tiles. All **answer tiles for both teams at a table** were placed together in a mixed pile at the center of the table, with the answer side facing upward at the start of play.

Figure S16 illustrates the progression of gameplay:

- **Figure S16a** shows tiles in use during active play.
  Figure S16b shows the initial setup, with question tiles arranged by team and all corresponding answer tiles mixed centrally.
  Figure S16c shows the completed state, with each answer tile placed into its corresponding question tile to reveal the final keyword or phrase.

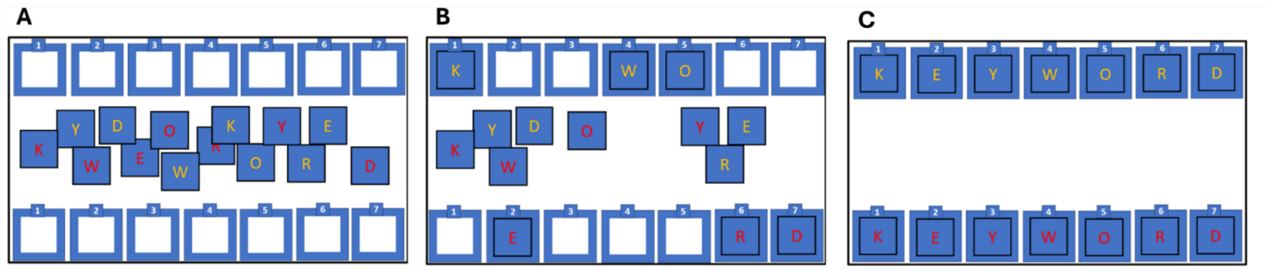

Figure S16. Game setup and gameplay. A. Initial set-up of the tiles. B. Diagram of the tiles during gameplay. C. Diagram of the final keyword answers. Team 1 has yellow letter tiles; Team 2 has red letter tiles.

Question Order and Scaffolding:

Question tiles were arranged in a fixed sequence. This ordering was intentional, allowing participants to use information gained from earlier questions to support reasoning on later, more challenging questions. As answer tiles were correctly matched and placed into question tiles, the revealed letters provided additional scaffolding for solving subsequent questions.

Group Organization and Materials Distribution:

Participants were divided into **four teams**, with **one printed Symposium Workbook provided per team**. Two teams competed at each table, working in parallel. Teams collaborated internally to match answer tiles to their question tiles and assemble the final keyword or phrase (Table S1).

- The total number of questions per team varied by keyword length (11–12 questions per team). Question sets were duplicated across tables as needed to support parallel play. All questions, answers, and corresponding letters can be found in *"Activity 3 – Answer Key and Letter Coding.pdf"*.

Table S1: Example keyword phrases used at CSC 2025

Team	Number of Tiles	Keyword	Notes
1	12	"Go for greener"	Green dots
2	11	"Greener chem"	Blue dots
3	12	"Cool catalyst"	Yellow dots
4	11	"Hinder hazard"	One letter given, red dots

4.3 Facilitation

Activity 3 was facilitated as a structured, collaborative puzzle designed to reinforce green chemistry concepts through guided retrieval and application. At the start of the activity, facilitators provided a brief overview of the objective and gameplay mechanics. This introduction was intentionally concise (typically less than two minutes) to minimize disruption and allow participants to engage quickly with the materials.

Participants were informed that questions could be answered using information provided in the Symposium Workbook and that some questions might admit multiple plausible answers. Facilitators emphasized that teams should use the structure of the puzzle, including fixed question order, revealed letters, and colour coding, as scaffolding to support reasoning when multiple answers appeared possible.

During gameplay, facilitators circulated between tables to monitor progress and maintain pacing. Facilitation focused on clarification and redirection rather than confirmation of correctness. When teams expressed uncertainty or disagreement, facilitators posed guiding questions or redirected participants to relevant sections of the workbook rather than confirming or denying specific answers. The activity design allowed facilitators to suggest that teams temporarily set aside more challenging questions and return to them after solving earlier items, using revealed letters to support inference on remaining tiles.

As the activity progressed, teams placed correctly matched answer tiles into the corresponding question tiles, gradually revealing their keyword or phrase (Figure S17). This process provided immediate mechanical feedback on correctness while also supporting completion of later questions. Once teams completed their puzzle, facilitators acknowledged completion and transitioned participants to the next activity.

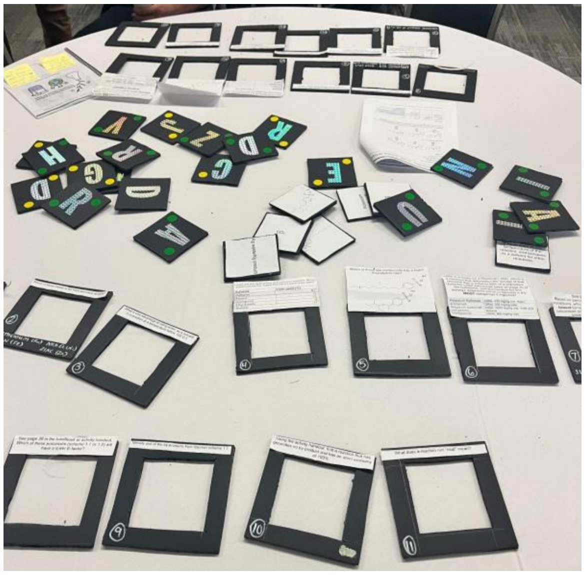

Figure S17. Game setup and gameplay at CSC 2025.

4.3.1 Guiding Prompts for Participants:

Numerous prompts could be provided for each question associated with gameplay. Some general prompts may include:

- What do the coloured dots on the tiles suggest? (several participants initially ignored the coloured dots, which hint towards which tiles belong to which keyword)
- What information in the workbook may help you to answer this question?

4.4 Recommendations for Educators

Activity 3 is well suited for instructional contexts that explicitly address green chemistry principles and metrics. The activity functions most effectively as a **knowledge-consolidation and retrieval exercise**, rather than as an introductory or exploratory intervention. It is particularly appropriate for learners who have already been exposed to foundational green chemistry concepts through lectures, readings, or prior activities.

4.4.1 Suggested Prerequisite or Complementary Lessons:

- Green chemistry basics.[39–44]
- Introduction to systems thinking.[1,45]
- Basics of environmental fate/transformation of chemicals.[2,46]
- Hotspot analysis in green chemistry.[3]
- Green metrical analysis.[5,7,47–50]
- Case studies of unintended sustainability failures (6PPD-quinone,[4] PFAS, etc.)

4.4.2 Intended Learning Objectives:

Activity 3 is designed to help learners:

- Expose participants to metrics relevant to chemical safety – such as LD50, solvent flash points, and safety data sheets.
- Expose participants to questions and metrics that pertain to reaction efficiency – such as atom economy, turnover number, and turnover frequency.
- Expose participants to questions and metrics that pertain to waste reduction – such as E-factor and atom economy.

4.4.3 Scalability & Modifications:

Based on observation during the symposium implementation, the physical size of the printed questions relative to the recessed well of the question tiles occasionally resulted in partially adhered question sheets. In some cases, this led to minor handling challenges during play. Future iterations may benefit from resizing question text, enlarging the recessed well, or integrating questions directly onto the foam board to improve durability and ease of use.

The activity was facilitated in a deliberately low-key manner, with limited emphasis placed on explicit "learning moments" or formal reflection. While informal discussion occasionally occurred within teams during play, no structured debrief or reflective discussion was conducted as part of the symposium schedule. In practice, Activity 3 functioned primarily as a lightweight, interactive transition between sessions rather than as a focal point for extended conceptual discussion.

4.4.3.1 Classroom Integration:

In classroom settings, Activity 3 may be implemented as a short, low-stakes group activity or as a station-based exercise within a larger active-learning session. Groups of **1-4 students per team** are recommended to maintain accessibility to shared materials and to avoid crowding around the tiles. When implemented at scale, multiple tables may be used in parallel, allowing teams to work head-to-head on identical question sets.

The activity may also be adapted to test or reinforce content from specific instructional units. For example, different tables may be assigned question sets aligned with different course topics, allowing instructors to tailor the activity to learning goals within a broader curriculum.

Educators are encouraged to provide **one reference workbook or equivalent resource per team**, containing the information required to answer the questions. The activity is not designed to assess recall in isolation; rather, it emphasizes locating, interpreting, and applying information under mild structural constraints.

Question Design and Customization:

The activity is highly customizable. Questions may be adapted to align with specific course content, learning outcomes, or textbook resources. While multiple answers may be conceptually valid for some questions, the puzzle structure requires that only one answer fits correctly based on the combined constraints of letter placement and colour coding. When adapting the activity, instructors should ensure that:

- each question has a single unambiguous solution within the context of the puzzle,
- answer tiles collectively support reconstruction of the intended keyword or phrase, and
- question difficulty progresses in a way that allows earlier answers to scaffold reasoning on later questions.

When working with cohorts that have varied levels of prior exposure to green chemistry, instructors may wish to include a small number of questions grounded in more general chemistry concepts (e.g., solvent properties, polarity, elemental abundance) that can be interpreted within a green chemistry context. This may support broader participation while maintaining alignment with sustainability-focused learning goals. Educators may also choose to duplicate question sets across teams rather than creating entirely unique question banks, particularly when running the activity in parallel.

<u>Timing and Pacing:</u>

In practice, individual questions typically require **approximately 1–2 minutes** to resolve. Groups are often able to work on multiple questions simultaneously, resulting in variable completion times depending on group size and familiarity with the material. The activity may be completed within a short class segment or used as a timed challenge, depending on instructional goals.

Some instructors may choose to record completion times or observe pacing patterns as a **formative indicator** of relative comfort with specific topics. Such observations should be interpreted cautiously and used to inform subsequent instruction rather than as a summative assessment.

<u>Facilitation and Reflection:</u>

Activity 3 benefits from **light-touch facilitation**. Instructors should circulate to support pacing and redirect students to reference materials when needed, while avoiding confirmation of correctness. The activity design naturally supports inference and self-correction through revealed letters and colour cues. If deeper conceptual integration is desired, instructors may follow the activity with a brief discussion or reflective prompt connecting the solved keywords or questions back to broader green chemistry principles, metrics, or trade-offs. However, such reflection is optional, and the activity may also function effectively as a low-pressure interactive transition or review exercise within a longer session.

4.5 Insights

Activity 3 was implemented in a conference setting alongside three other interactive activities. Gameplay was arranged such that two teams worked at each table, with up to four teams participating simultaneously across multiple tables. Teams typically consisted of 1–4 participants; larger groups tended to experience crowding around the tiles, which occasionally limited individual engagement.

Informal observation suggested that the activity prompted discussion among participants, particularly when multiple answer tiles appeared plausible for a given question. In these cases, teams often discussed why certain answers were conceptually reasonable but ultimately incompatible with the constraints of the puzzle. This dynamic appeared to support peer-to-peer explanation and, in some instances, served as an effective icebreaker for participants who had not previously worked together.

The activity progressed more smoothly for participants with prior familiarity with green chemistry concepts, while participants less confident in the material required more time and relied more heavily on the reference workbook and collaborative discussion. Differences in completion time appeared to reflect variation in background knowledge rather than disengagement.

These insights are based on informal facilitator observation during the symposium implementation and are intended to describe observed patterns of engagement rather than to indicate measured learning outcomes.

Activity 4 - Research in Action: A discussion on current green chemistry research

5.1 Materials

For the round-table discussions, participants were provided with worksheets developed for the 2024 CSC symposium. These materials were made available as physical handouts. Print outs can be found in the supporting information of reference [12].

- *Research Worksheet – Inorganic Chemistry (pdf)*
- *Research Worksheet – Materials Chemistry (pdf)*
- *Education Worksheet (pdf)*

Potential panel speakers submitted presentation abstracts through the CSC 2025 abstract submission portal. Three speakers were selected based on the breadth of topic in green chemistry relating to catalysis as well as presenter education level, seeking to have a blend of students and early career faculty. Once selected speakers were asked to provide short biographies to be shared before their presentation. Facilitators prepared guiding questions to support panel discussion.

5.2 Set-Up and Preparation

Activity 4 was structured around a sequence of short research-focused flash talks followed by a panel-style discussion and an intended transition into round-table conversations. Visiting speakers were invited to prepare **10-minute flash talks** aligned with their abstract submissions and the overall symposium theme. Speakers were informed of expectations in advance, including presentation length and thematic scope.

Flash Talk Speakers:

As articulated in the symposium design, invited speakers were selected to highlight current research directions in green and sustainable chemistry, with an emphasis on early-career researchers and trainees. Speakers represented a range of career stages and research focuses aligned with the themes of the symposium.

Speakers included:

- **Dr. Zhen Dai** (Assistant Professor, McGill University)
    - Organocatalytic peptide coacervates as green microreactors for aldol additions in water.
- **Nelson Rutajoga** (PhD Candidate, University of Ottawa)
    - Diagnostic hydrogen generation method for evaluating remediation capabilities of novel TiO2-based catalysts under visible light

- **Dr. Gillian Thomas** (Assistant Professor, University of Leeds)
    - Expedited reaction optimization: Where transfer learning meets high-throughput experimentation.

Each speaker delivered a 10-minute flash talk introducing their research, followed by participation in a 30-minute facilitated panel discussion.

Worksheets were made available to participants during this portion of the symposium to support reflection and informal discussion. Participants could self-select which worksheet, if any, they wished to engage with based on their interests.

5.3 Facilitation

Activity 4 was divided into two parts. Part 1, speaker flash talks and panel discussion, was hosted from 8:30 – 9:30am during the symposium. Flash talks were delivered sequentially by invited speakers and were followed by a facilitated panel discussion conducted from the front of the room. Facilitator responsibilities during this activity included:

- Introducing speakers and managing time to ensure adherence to the 10-minute format
- Moderating the panel discussion and audience question period
- Preparing and posing initial questions to prompt discussion where needed

Part 2, round table discussions, was hosted from 11:00 – 11:40am during the symposium. Between parts 1 and 2 of activity 4, participants were able to asynchronously engage with Activities 1-3. The round-table component of the activity was designed to allow participants to continue discussion on green chemistry and education using the provided worksheets. Facilitators circulated between groups (2-8 participants) as needed to encourage participation and address questions. Worksheets were intended to function as a guide for discussion and as a resource that participants could retain after the symposium.

5.3.1 Activity Focus and Intended Outcomes:

Activity 4 was designed to foreground **current research in green and sustainable chemistry** while supporting community-building and professional engagement across career stages. By highlighting research perspectives from early-career researchers and trainees, the activity aimed to:

- Expose participants to contemporary research directions in green chemistry and catalysis
- Provide visibility for emerging researchers within the community
- Create space for dialogue between speakers and symposium participants

Unlike earlier activities in the symposium, Activity 4 emphasized exposure and discussion rather than structured problem-solving or task completion.

5.4 Recommendations for Educators

The format used in Activity 4 is well suited for highlighting current research and fostering community connections in both conference and classroom contexts. Flash talks paired with panel discussion can be readily adapted for use with graduate students, senior undergraduates, or mixed audiences by adjusting speaker selection and discussion prompts.

When deeper participant interaction is desired, educators may consider allocating dedicated time for worksheet-supported discussion earlier in a session or embedding speakers within small-group discussions. Worksheets of this style may also function effectively as take-home reflection tools rather than in-session activities, depending on context and time constraints.

5.4.1 Notes on Adaptability:

Activity 4 is flexible with respect to speaker composition and disciplinary focus. Visiting speakers may be drawn from academia, industry, or other sectors, and the activity can be adapted for in-person or virtual delivery. The core structure—short talks followed by facilitated discussion—allows the activity to scale across different group sizes and settings.

5.5 Insights

Based on facilitator observation, the flash talks and panel discussion generated audience engagement and questions, indicating interest in the research topics presented. The worksheets served primarily as optional resources during this portion of the symposium and were available for participants who wished to continue reflecting on the themes discussed after the session concluded.

As this activity took place near the end of the symposium, opportunities for extended round-table discussion were limited by time and participant scheduling constraints. No formal assessment of participant engagement with the worksheets or learning outcomes was conducted. These observations are descriptive and are not intended to imply measured learning gains.

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