PROPOSAL OVERVIEW AND OBJECTIVES

Student-centered pedagogies have been developed and demonstrated to improve student learning. For example, in the Process Oriented Guided Inquiry Learning (POGIL) approach, students construct their own knowledge through a learning cycle of exploration, concept invention, and application. Students progress through carefully constructed worksheets in small groups to explore a 'model' (an information rich data display), answer questions that make them think about the model, propose explanations for what they have explored, and then apply those concepts to further problems. As successful as I have found POGIL to be, the assessment strategies I have used are still teacher-centered. Typical programs of high stakes assessments fundamentally undermine my learning goals for students. Rather than focusing on growing as a learner and improving as a scholar, traditional grading incentivizes a grade focus in which students try to maximize the points they can get from any assignment for the minimum of effort, independent of their learning. Poor performance on an assessment is met with the attitude that it is too late to do anything about it, so move on to the next chapter. As I result, I hate grading not because it requires effort, but because students pay no attention to the feedback and do not use the feedback as a learning opportunity. The traditional grading approaches that I have used are a problem because they lead to student frustration, stereotype threat, and attrition from STEM.

A long range goal of my teaching is to help students embrace a life of growth and learning both in the subject matter of Chemistry and in the metacognitive and metaemotional skills they need to succeed beyond the Chemistry classroom. The overall objective for this proposal is to develop a proficiency-based assessment structure for General Chemistry 1 that will be transferrable to other instructors in the General Chemistry program. The *central hypothesis* is that a proficiency-based grading structure – in which questions are aligned to explicit learning objectives, student work is either proficient or not proficient (no partial credit), and students have multiple attempts at each assessment – will better encourage and motivate students to identify their weaknesses and work to improve, leading to better learning outcomes, better attitudes about self and the subject, and a stronger growth mindset. This hypothesis is based on the demonstrated effectiveness of specifications grading and standards-based grading in other General Chemistry courses.[1–4] The *rationale* of this project is that the combination of student-centered pedagogy and student-centered assessment will synergistically improve learning outcomes for students. These course materials will be developed with a team of General Chemistry faculty to maximize the transferability of the materials. Our team is uniquely qualified to successfully execute this project because of our experience implementing POGIL in the large-enrollment General Chemistry classroom. The specific goals for this project are to:

1. **Develop a hierarchical set of student learning objectives aligned to a mastery-based grading scheme.** We will design a set of learning objectives based on Marzano's taxonomy, which provides a structure to specify appropriate learning objectives at multiple levels of conceptual difficulty. The four tiers of achievement – *retrieval*, *comprehension*, *analysis*, and *knowledge utilization* – will be articulated for each learning objective. With this set of learning objectives, we will craft a grading scheme based on a standards-based grading that incorporates the many modes of frequent, low-stakes student work.
2. **Design assessments that implement a mastery-based grading scheme.** For each learning objective and each level of mastery, assignments will be refactored to best align with the stated learning goals. While many materials exist in the form of question banks, rarely are these questions explicitly aligned with learning objectives. This aim will curate materials like quiz questions and build quizzes for each learning unit. Questions will mix computer and human grading to manage the grading load to current levels. In addition, a framework to articulate to students what learning objectives they have mastered and what areas need development will be implemented in the Canvas LMS.
3. **Assess and disseminate the course transformation.** This aim will measure the impact of the transformation on student learning and attitudes. Based on our previous attitudinal data, we will compare the effect of the course on student self-efficacy and engagement, especially measures of student frustration. In addition, we will measure differential impact on students based on demographic factors such as gender. Women tend to underperform men on high-stakes assessments even though they outperform them at low-stakes assessments. We will measure student performance in the transformed course to see if it alleviates this gender bias.

Specific Aim 1 will develop a clear, comprehensive set of learning objectives and an associated grading scheme. *Specific Aim 2* will develop the actual assessment instruments that will assess student learning and communicate to students their progress. Finally, *Specific Aim 3* will measure how effectively the course transformation has achieved each of its goals and share these results with other faculty.

This project is a *creative* and *original* approach to grading reform in the context of large-enrollment courses. The *expected outcomes* of this project will be course materials – learning objectives, learning assessments, and course infrastructure – whose effectiveness has been tested and is ready to be shared. Finally, this work engages a question very timely question in the broader scholarship of teaching and learning for large-enrollment courses – how do we best build student-centered assessments that match student-centered pedagogies with our limited grading resources?

EXPECTED SIGNIFICANCE

This course transformation has the potential to affect many hundreds of Pitt undergraduates each term. If this transformation proves useful, other faculty in the General Chemistry teaching pool can adopt this approach beginning with the materials we will develop and share. The transformation may also inspire other efforts to reform grading policies in other STEM disciplines through the dB-SERC community. Finally, the results of the course transformation will be disseminated in the national POGIL community.

BACKGROUND AND PRELIMINARY RESULTS

Guided inquiry methods [5–9] and Process Oriented Guided Inquiry Learning [8] (POGIL) in specific, effectively bring active learning into the science classroom. Since 2012, Garrett-Roe has implemented POGIL in upper-level Physical Chemistry classes and, since 2018, in large-enrollment General Chemistry classes.[10] As such, the POGIL pedagogy is already well-established. On the other hand, grading reform is a much newer development and a variety of approaches have been adopted. We here introduce the learning taxonomy that guides our proposed grading scheme, and introduce related grading schemes that have been demonstrated to be efficacious.

A hierarchical taxonomy for student learning objectives

We are basing our proficiency-based grading scheme on a learning taxonomy with a hierarchical structure because that hierarchy more clearly articulates which tasks must be completed before progress to higher levels. This taxonomy is, naturally, very similar to Bloom's taxonomy, but we will highlight how this taxonomy helps make good choices for question design.

Marzano proposed a hierarchical ordering of four cognitive processes – *retrieval*, *comprehension*, *analysis*, and *knowledge utilization* [11]. The lowest level, retrieval, focuses on the recognition or recall of information. For example, when a student is asked to define a word or provide a synonym, they demonstrate simple declarative level knowledge. The next level, comprehension, includes integrating and symbolizing. The process of integration involves understanding general relationships related to how the information is organized. For example, a student would be able to describe all variables associated with a model and the subsequent relationships between these variables. Symbolizing requires the learner to translate the knowledge into some nonlinguistic or abstract form like a graph or equation. Processes that extend beyond identifying essential and non essential characteristics of a topic fall in the domain of analysis. An analysis task requires the learner to reorganize the information in a way that generates new conclusions. Marzano's Taxonomy proposes five processes associated with the analysis level – matching, classifying, analyzing errors, generalizing, and specifying. Finally, the highest cognitive level, knowledge utilization, includes tasks such as decision making, problem solving, experimenting, and investigating. The key distinction from analysis is the focus of the mental activity on a specific situation rather than the actual knowledge itself. For example, when a student analyzes an error involving a gas law relationship the focus is on the gas law. When the student uses a gas law to make a decision regarding whether or not to transport a container of helium gas, the focus is the situation.

Mastery-based grading

The grading practices of instructors generally fall into two categories – a summative, points-based approach and a formative, mastery based method of evaluation. The three defining characteristics of a mastery based grading system include [12] **1).** listing all the course content learning objectives that are assessed, **2).** awarding the "mastery" of an assignment rather than partial credit, and **3).** allowing multiple opportunities for students to achieve mastery. Specific implementations of these principles are found in standards-based grading [13], specifications grading [14], and mastery-based testing [15]. Mastery grading naturally fits with guided inquiry instruction since both are ways of promoting a growth mindset by treating knowledge and learning as an evolving process [16].

The proposed approach

Based on this literature, we propose to revise the assessment model of CHEM 0110 in a mastery-based approach (fig. 1). Each week, students will complete a learning assessment aligned to specific learning objectives for each cognitive level, *retrieval*, *comprehension*, *analysis*, and *knowledge utilization*. Preliminary learning objectives (Appendix, page 8) and example questions (Appendix, page 12) are provided. Every three weeks students will have another opportunity to repeat earlier assessments (fig. 1).

In some ways, this approach is very similar to the Quiz, Midterm, and Final model that is commonly implemented. Content units are indicated by color. Within each unit, students take two small assessments (12-15 mins, like a quiz) followed by a longer assessment ($4 \times 15 = 60$ min, like a midterm). Because each assessment presents new questions, students are encouraged to participate throughout the course.

		Assessment attempt		
Unit	Week	First	Second	Third
	1 Syllabus and introduction			
1	2 Atomic structure	1.1		
1	3 Moles and nomenclature	1.2		
1	4 Chemical Equations and Solutions	1.3	1.1-2	
2	5 Aqueous reactions	2.1		
2	6 Enthalpy	2.2		
2	7 Calorimetry	2.3	2.1-2, 1.1-3	
3	8 Coulomb's Law and Shell Model	3.1		
3	9 Electron configurations	3.2		
3	10 Spin and Orbitals	3.3	3.1-2, 2.1-3	
4	11 Fundamentals of Bonding	4.1		
4	12 Molecular Shape and MO Theory	4.2		
4	13 Properties of Molecules	4.3	4.1-2, 3.1-3	
5	14 Ideal Gas Law	5.1		
5	15 Intermolecular Forces and Phases			
	Final Exam Period	5.2	5.1	1.1-4.3

Figure 1: The working plan for the assessment schedule. Students have three opportunities to master each learning objective.

On the other hand, there are important differences. Questions are clearly mapped to specific learning objectives. Student work is either proficient or not proficient – partial credit is not awarded, but student answers do not need to be perfect to be marked proficient. The cognitive level is clearly indicated for each question. An informal analysis of exams in earlier terms of CHEM 0110 (Garrett-Roe) indicate most questions are at the *analysis* level (~ 50), and the remainder are evenly split between *retrieval* and *comprehension*; essentially no questions reach the *knowledge utilization* category. On the planned assessments, questions will be evenly split across these levels by design. This will help poorer performing students by providing questions that focus their attention first on the fundamentals (*retrieval* and *comprehension*), then on higher levels (*analysis* and *knowledge utilization*). Higher performing students will also be challenged by *knowledge utilization* questions that ask them to put their understanding to work proposing, deciding, and creating.

Specific aim 1) Develop a hierarchical set of student learning objectives aligned to a mastery-based grading scheme.

Though the object of teaching is for students to learn, the assessments used and the grading scheme applied grading often align with those learning objectives in only an intuitive, unexpressed, or traditional way. Clear-headed assessment of student learning should begin with a clear articulation of the learning objectives that is integrated into all aspects of student work and communication with students. This wholistic approach will help students identify the areas that they have mastered and the areas in which they need to improve.

1.1 Student Learning Objectives

Student learning objectives that span the essential content and the hierarchy of cognitive levels from *retrieval* to *knowledge utilization* will be refined for the General Chemistry 1 course. Preliminary work has identified 11 major learning objectives and expressed the four mastery levels (Appendix, page 8). These objectives will be refined to accommodate consensus among the team of POGIL instructors at Pitt.

1.2 Grading scheme

Task 1: Levels of mastery Four levels of content mastery are *retrieval*, *comprehension*, *analysis*, and *knowledge utilization*. Each level will be worth one point for that learning objective on a Knowledge Assessment. We will examine the feasibility of allowing students to only answer *knowledge utilization* questions in Canvas when they have demonstrated master of two or three of the lower levels.

- *Retrieval* questions test simple recognition, recall, or execution of knowledge. For example, multiple choice, sorting, and multiple selection questions without significant distractors are at the *retrieval* level. These questions likely can be computer graded.
- *Comprehension* questions test for the integration and symbolic representation of knowledge. Multiple choice, sorting, and multiple selection questions in the presence of significant distractors that express common misconceptions are at the *comprehension* level and can be computer graded. Additional questions such as explaining and drawing will likely require human graders.
- *Analysis* questions test the ability to generate new conclusions. Many free-response calculations fall into this category. Free response numerical result questions can be computer graded. Additional proficiency in the presence of minor errors can be noted by students uploading their work and human graders regrading the response.
- *Knowledge Utilization* questions ask students to extend beyond *analysis* and put their knowledge to work for their own goals. *Knowledge Utilization* questions involve steps of deciding, choosing, proposing. We anticipate that human grading will be required for all of these student responses.

Examples of questions at each of these levels are provided (Appendix, page 12).

Task 2: Map Progress to Points We anticipate that the existing scheme for translating course points to letter grade will suffice for the course transformation. We can project how performance on the assessments will affect students' grades using typical values for performance in the other categories. Typical students will accumulate 90% of homework, 90% of discussion, 85% percent lab, and 70% on the ACS exam. The expected base score would then be 43%. To pass the course with a C, a target of many biology students, students would need to score 54% on the assessments, which translates to an average of 2.16 on all assessments, *i.e.*, slightly better than to achieving proficiency in all *retrieval* and *comprehension* areas. To score an A, a student would need to score 3.6 on all assessments, which corresponds to achieving proficiency in all *retrieval*, *comprehension*, and *analysis* areas as well as $\sim$ 60% of *knowledge utilization* questions.

	percent of grade
Knowledge Assessments	**55**
Lab	15
Homework	15
Discussion board	10
In-class participation	*
ACS Final exam	5
Extra credit	*

Table 1: The revised point structure will be quite similar to the existing point distribution.

Specific aim 2) Design assessments that implement a mastery-based grading scheme.

2.1 Evaluate, revise, and write assessments

Task 1: Grow a taxonomically organized question bank Existing assessments will first be sorted by their learning outcome (subject area and cognitive level). We have a library of $\sim$ 200 questions that been designed in accordance with this grading scheme for human grading (Shepherd) and $\sim$ 200 unsorted questions that have been implemented in Canvas for automatic grading (Garrett-Roe). The pool of unsorted questions will be evaluated, grouped according to their learning level, and revised as necessary. Additional questions will be written to fill any identified gaps. We aim to develop question banks of $\sim$ 6 questions per learning objective (264 questions total).

Task 2: Assemble assessments All assessments will be drafted for the term based on the item banks developed in (*Task 1*). Each assessment will contain one question, drawn from the item banks, at each cognitive level. Item banks of 6 questions will provide a reasonable likelihood that students will see new questions on each attempt.

percent	Grade
93–99	A
90–92	A-
87–89	B+
83–86	B
80–82	B-
77–79	C+
73–76	C
70–72	C-
67–69	D+
63–66	D
60–62	D-
0–59	F

Table 2: We anticipate that the scoring structure will remain unchanged.

2.2 Implement integration canvas

The grade book infrastructure will be developed to calculate grades according to the grading scheme and to efficiently communicate to students their current learning progress. Potential approaches to be explored are quizzes with multiple attempts, multiple assignments with grade pooling, alignment with the

Learning Objectives feature, and Mastery Paths in content Modules. We will select, from these options, the approach that offers the clearest implementation from the instructor perspective and the clearest communication to the student. Appropriate syllabus text will be developed and shared.

2.3 Deploy the course transformation

In Fall 2021, the transformed course will be implemented in the class of Garrett-Roe. Other POGIL instructors will evaluate whether or not to adopt the transformation in 2021.

Specific aim 3) Assess and disseminate the course transformation.

3.1 Assess Student Learning

Task 1: Course content We will compare student performance on assessment items to 2018-2021 data.

Task 2: ACS General Chemistry 1 Paired Question exam. These exams were purchased in 2018 and are available in the Department. We will compare to both national norms exam data and, perhaps more importantly, to the scores from POGIL sections in 2018 and 2019.

Task 3: Follow on performance We will request support from dB-SERC to track students going into General Chemistry 2.

Task 4: Student learning self-assessment Student perception of learning gains will be assessed through an instrument developed through `salgsite.org`, which provides easy implementation and analysis of the questionnaires. The question areas relevant to course learning will include **1.)** how do in-class activities support learning, **2.)** how does assessment structure support learning.

Task 5: Demographic effects We will compare student performance sorted by demographic category and compare against prior years. Gender performance gaps have been identified in STEM classrooms at Pitt and suggested to be present in our Chemistry program. We will identify the magnitude of the gender performance gap in our previous General Chemistry classes 2018–2021 and compare this with student performance after the course transformation.

3.2 Assess Student Attitudes

We will reimplement the assessment strategy used in the 2018-2019 terms that measured several axes of student attitudes. We will also capture data from concurrent POGIL and traditional lecture courses, as available. Instructors will be encouraged to offer students extra credit or some reward for participation.

Task 1: Questionnaires We will use questionnaires, which can be implemented in Qualtrix, for example, to assess student attitudes. We will ask positively and negatively coded questions to measure several axes of student attitudes. We expect dimensions to increase (self-efficacy, chemistry identity), decrease (anxiety), and not to change (engagement).

Task 2: Focus groups In addition to these quantitative surveys, qualitative data will be obtained in focus group sessions. The sessions will elicit feedback on the effectiveness of the assessment approach in the course. Sessions will be voluntary and occur at three points in the semester.

Engagement "I feel engaged during class time." "I do not feel engaged during class time." "I feel engaged when I am working on my homework or out of class assignments." "I do not feel engaged when I am working on my homework or out of class assignments."

Self-efficacy "When I face a hard problem, I feel like I can solve it," "I get frustrated easily when I face a challenging problem."

Identity "I am a science kind of person." "I am a biology kind of person." "I am a chemistry kind of person." "I am a physics kind of person."

Anxiety "I felt relaxed completing assessments (quizzes and exams)." "Taking the assessments (quizzes and exams) was stressful." "I feel confident about my next assessment (quiz or exam)." "I am worried about my performance on my next assessment (quiz or exam)."

Figure 2: Examples of positively and negatively coded survey questions to assess different dimensions of student affect.

3.3 Disseminate to Other Chemistry Faculty

At the beginning and end of the term of work, the POGIL Chemistry faculty (Madison, Meyer, Garrett-Roe) will meet to review the plan for the transformation and provide input into the project design. When approximately half of the course assessment material has been revised, the POGIL faculty will, as a team, review the status of the project. Feedback will be incorporated. At the end of the project, Madison and Meyer will be able to choose if they will also adopt the class transformation at this point or if Garrett-Roe will run a year as a pilot program. During the summer term, the transformation will be presented to other faculty in the General Chemistry program.

APPENDICES

List of Appendices

References

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Budget and Budget Justification

APPENDIX: EXAMPLE STUDENT LEARNING OBJECTIVES

This appendix provides examples of student learning objectives that are organized according to Marzano's taxonomy. These learning objectives are a preliminary set that will be extended and revised to match the Pitt General Chemistry curriculum.

Marzano's Learning Taxonomy:

1) *Retrieval* (perform a procedure, produce information on demand, determine if information is accurate, inaccurate or unknown)

2) *Comprehension* (construct symbolic representation of information, identify basic structure of information)

3) *Analysis* (Specifying, Generalizing, Error Analysis, Classify, Matching)

4) *Knowledge Utilization* (Investigate, Experiment, Problem Solve, Decision Making)

Unit 1: Atoms, Molecules, and Compounds

1.1 Atoms

1) Identify the number of protons, neutrons, and electrons in an atom or ion based on the mass number, atomic number, and the overall charge

2) Draw a model or appropriate symbol to accurately represent a particular element, ion, or isotope

3) Convert quantities representing mass, numbers of atoms, or moles of an element

4) Decide the most appropriate way to express the amount of matter based on how the information will be used

1.2 Compounds

1) Identify whether a compound is ionic or molecular based on the type of elements that make up their composition

2) Draw an appropriate microscopic representation depicting both the chemical composition and phase (solid, liquid, gas)

3) Specify the name and symbolic notation representing an ionic or molecular binary compound using an appropriate microscopic or symbolic model

4) Decide what type of microscopic composition should be selected based on a desired observation or application of the material.

1.3 Solutions

1) Identify whether a compound is soluble or not based on the solubility rules

2) Represent a solution both qualitatively through an appropriate microscopic representation and quantitatively in terms of molarity

3) Identify all species present at any point upon the addition of a series of aqueous ions to the same beaker and their concentration in terms of molarity

4) Describe an appropriate procedure to make a solution based on available materials and intended use

Unit 2: Fundamentals of Chemical Reactions and Heats of Reaction

2.1 Reactions

1) Identify appropriate molar quantities based on chemical formulas and reaction equations

2) Represent a balanced chemical reaction symbolically and draw an appropriate microscopic representation illustrating the effect of a limiting reactant

3) Calculate specific quantities representing mass, numbers of atoms, or moles for a chemical reaction

4) Propose the most likely scenario that would generate a particular observation resulting from a chemical reaction

2.2 Bond Energy

1) Define what is meant by enthalpy of atom combination and the terms exothermic and endothermic in terms bond making or breaking processes

2) Draw a reaction energy diagram based on energies of atom combination data and describe how it relates overall energy of reaction

3) Analyze and compare individual molecular bond energies and overall reaction energies based on bond order, bond length or enthalpies atom combination

4) Select the best compound for a reaction based on an assessment of the amount of energy absorbed or released.

2.3 TBD

Unit 3: Origins of Properties in Quantum Mechanics

3.1 Shell Model

1) Identify the key terms of Coulomb's law and describe how it is used to assess the amount of attraction or repulsion between two particles

2) Describe the relationship between potential energy, ionization energy, core charge, and distance. Use these concepts to create an appropriate shell model representation of an atom

3) Analyze and compare properties of elements in terms of their ionization energy based on core charge and number of shells

4) Decide what element best fits the properties described based on experimental data provided and justification according to Coulomb’s Law

3.2 Electronic Configuration

1) Define what each specific quantum number is used to represent about an electron in an atom

2) Describe the experimental evidence justifying each of the four quantum numbers and the general region of space an electron would most likely be found (or not) based on this information

3) Appropriately represent and analyze features of the electron configuration or photoelectron spectra of any element

4) Select the best element for an application based on the energy and configuration of its electrons

3.3 TBD

Unit 4: Nature of Chemical Bonding

4.1 Molecular Bonding

1) Define what is meant by electronegativity and how it relates to ionization energies or AVEE trends.

2) Illustrate how to determine the partial charge for one particular atom type in a molecule

3) For a given skeletal structure, draw the "best" Lewis structure based on formal charges and describe any resonance effects on properties such as bond length and bond strength.

4) Propose a particular arrangement of elements that would most likely form a molecule

4.2 Molecular Structure

1) List the different molecular geometries and identify corresponding bond angles & hybridization

2) Describe valence bond theory and why hybrid orbitals are defined for atoms in a molecule

3) Assign molecular geometries, number of pi and sigma bonds, and assess the overall magnitude and direction molecular dipole moments

4) Select the best molecule for an application based on its 3D structure and polarity

4.3 MO Theory & Valence Bond Theory

1) Identify the types of hybrid and unhybridized orbitals associated with a type of bond and bond angle

2) Characterize the region of space electrons occupy in molecules based on either molecular orbital theory or valence bond theory

3) Compare the properties of molecules (e.g., spin, bond order, pi & sigma bonds) using an appropriate bonding theory

4) TBD

Unit 5: Intermolecular interactions

5.1 Ideal Gases

TBD

5.2 Molecular Forces

1) Define and list different types of intermolecular forces that exist between molecules

2) Draw a graph and describe differences in the system due to changes in temperature and intermolecular forces and clearly describe the types of bonds broken

3) Analyze and compare properties of molecules based on the types of intermolecular forces present

4) Select the best molecule for a desired property or application based on intermolecular forces

APPENDIX: EXAMPLE ASSESSMENTS ALIGNED TO LEARNING OBJECTIVES

This appendix provides examples of student assessment questions that are organized according to Marzano's taxonomy and the preliminary learning objectives for the course.

Marzano's Learning Taxonomy:

1) *Retrieval* (perform a procedure, produce information on demand, determine if information is accurate, inaccurate or unknown)

2) *Comprehension* (construct symbolic representation of information, identify basic structure of information)

3) *Analysis* (Specifying, Generalizing, Error Analysis, Classify, Matching)

4) *Knowledge Utilization* (Investigate, Experiment, Problem Solve, Decision Making)

1.2 Compounds

1) *Retrieval Level*

Learning Objective: Identify whether a compound is ionic or molecular based on the type of elements that make up their composition

Assessment question: Give an example of two elements that could form an ionic compound and two elements that would not.

2) *Comprehension Level*

Learning Objective: Draw an appropriate microscopic representation depicting both the chemical composition and phase (solid, liquid, gas)

Assessment question: Draw an appropriate molecular-level (microscopic) representation depicting each of the following.

(a) $CoO(s)$
(b) $CO(s)$

3) *Analysis Level*

Learning Objective: Specify the name and symbolic notation representing an ionic or molecular binary compound using an appropriate microscopic or symbolic model

Assessment question: For each of the following identify either the correct name or the correct formula based on the information given:

a) V_2O_5
b) Cl_2O_4
c) calcium nitrate

4) *Knowledge Utilization Level*

Learning Objective: Decide what type of microscopic composition should be selected based on a desired observation or application of the material.

Assessment question: You are given a set of three unique **binary** compounds each of which contains exactly a total of 4 atoms per unit. Within this set, you determine that exactly two of the three compounds contain chlorine, only one contains sodium, and only one is molecular. Propose a possible formula for each of the three different compounds comprising this set.

2.2 Bond Energy

1) *Retrieval Level*

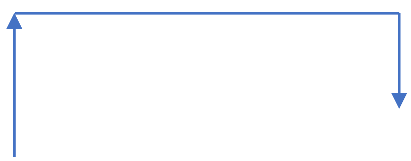
Learning Objective: Define what is meant by enthalpy of atom combination and the terms exothermic and endothermic in terms bond making or breaking processes

Assessment question: $\Delta H^{\circ}_{ac} = -2184.76$ kJ/mol for SO_4^{2-} (aq). Define what this quantity represents.

2) *Comprehension Level*

Learning Objective: Draw a reaction energy diagram based on energies of atom combination data and describe how it relates overall energy of reaction

Assessment question: Below is an example energy diagram for a chemical reaction. What specific factors on a molecular level affect the quantities represented by the arrows in the diagram? Is the overall reaction endothermic or exothermic?



3) *Analysis Level*

Learning Objective: Analyze and compare individual molecular bond energies and overall reaction energies based on bond order, bond length or enthalpies atom combination

Assessment question: Iodine reacts with the halogens to form a wide variety of compounds. Two reactions are shown below.

$$I_2\,(g) + Cl_2\,(g) \rightarrow 2\,ICl\,(g)$$
$$I_2\,(g) + Br_2\,(g) \rightarrow 2\,IBr\,(g)$$

a) Which do you expect to have a stronger bond Cl_2 or Br_2? Explain.

b) Explain why the overall change in enthalpy of reaction for both reactions is approximately the same magnitude.

4) *Knowledge Utilization Level*

Learning Objective: Select the best compound for a reaction based on an assessment of the amount of energy absorbed or released.

Assessment question: The N-N bond lengths in the following compounds are N_2, 110 pm; HNNH, 125 pm; and H_2NNH_2, 146 pm. Which molecule would you select if you needed a source of N atoms using the least amount of energy. Explain.

TRICIA D. SHEPHERD

Curriculum Vitae

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Education

2002	Ph.D. Physical Chemistry, Georgia Institute of Technology Advisor: Dr. Rigoberto Hernandez Thesis: *Models of Chemical Processes: Activated Dynamics across Stochastic Potentials*
1995	M.S. Analytical Chemistry, University of Idaho Advisor: Dr. Chein M. Wai Thesis: *The Removal of* ^{137}*Cs from Acidic Nuclear Waste*
1994	B.S. Professional Chemistry, University of Idaho

Employment History

2020-2021	Adjunct Professor *Tuskegee University,* Tuskegee, AL *Courses Taught*: Physical Chemistry I & II, Experimental Physical Chemistry I & II
2019-2020	Visiting Associate Professor *Franklin & Marshall College,* Lancaster, PA *Courses Taught*: General Chemistry I, Structure & Bonding
2018-2019	Teaching Fellow *Moravian College,* Bethlehem, PA *Courses Taught*: Physical Chemistry I, Physical Chemistry II, General Chemistry
2014-2018	Professor of Chemistry & Department Chair *St. Edward's University,* Austin, TX *Courses Taught*: General Chemistry, Analytical Chemistry, Quantum Mechanics and Spectroscopy, Thermodynamics and Kinetics, Molecular Modeling, Capstone w/embedded Ecuador study abroad
2013-2014	Professor of Chemistry/Physics *Westminster College,* Salt Lake City, UT *Courses Taught*: Principles of Chemistry I & II, Physical Chemistry I & II, Principles of Physics I & II, Scientific Computing, Molecular Modeling
2007-2013	Associate Professor of Chemistry/Physics *Westminster College,* Salt Lake City, UT
2002-2007	Assistant Professor of Chemistry/Physics *Westminster College,* Salt Lake City, UT
1996-1997	Visiting Instructor *Georgia Southern University*, Statesboro, GA *Courses Taught*: Introduction to Chemistry, Organic & Biochemistry, and Principles of Chemistry I & II

Research Experience

Fall 2010 — Sabbatical at the University of Utah, Salt Lake City, with Valeria Molinero
Course grained Molecular Dynamics simulations were used to investigate the structure of water at various interfaces including a vacuum, hexagonal ice, a hydrophobic substrate like methane, and in the presence of clathrate hydrates, solid water cages that contain small, hydrophobic guest molecules.

Summer 2003 — Visiting Research Associate at the University of Kansas, Lawrence, with Ward Thompson
Investigated vibrational relaxation of a diatomic solute in a solvent confined within nanoscale frameworks using molecular dynamics simulations

1998-2002 — Doctoral Research Assistant
Georgia Institute of Technology, Atlanta, GA
A stochastic equation of motion (Langevin Type) with a time-dependent potential of mean force was used to model chemical reactions or dynamical events in complex environments. Various extensions of this stochastic potential model were developed in order to investigate underdamped activated dynamics and diffusion over mulitiple potential barriers.

1994-1995 — Undergraduate/Graduate Research Assistant
University of Idaho, Moscow, ID
Copper ferrocyanide was immobilized on a chelating resin for selective removal of cesium from neutral to acidic solutions. Radioactive ^{137}Cs was used as a tracer for this study. Analytical measurements were made using a gamma spectrometer, flame atomic absorption spectrometer, FTIR spectrometer, and UV-Vis spectrophotometer.

Other Activities

2019 — Project Mentor – IntroCS POGIL Project (NSF DUE 1626765)
Meet biweekly with new IntroCS POGIL instructors to provide feedback and advice regarding the initial implementation of POGIL in and introductory CS course

2017-present — POGIL Workshop Facilitator Trainer
Training potential POGIL workshop facilitators

2008-present — POGIL Workshop Facilitator
Facilitated workshop sessions including: Introduction to POGIL, Writing POGIL Activities, Assessing POGIL Activities, Classroom Facilitation, Scholarship of Teaching and Learning

2009-2014 — K-12 Workshop Instructor
Developed a workshop exploring the molecular basis for water and fat solubility using molecular modeling software (Spartan by Wavefunction, Inc.). This workshop is offered every summer as part of a 3-day science and math camp for 8th grade girls and a Diversity Summer Camp hosted at Westminster College.

2009-2012 — Regional Coordinator for POGIL Project
Organized and facilitated POGIL workshops for Southwest/Rocky Mountain Region (NM, CO, UT, WY, CA, NV, AZ, HI). Events hosted at Westminster College, MiraCosta College, and University of Redlands

2008-2014 — Faculty Advisor for Mastering Chemistry (Pearson)
Sharing best practices and tips for successfully integrating the online homework system Mastering Chemistry into the General Chemistry curriculum. Lead advanced training sessions at Mastering Chemistry workshops hosted at BYU and Salt Lake Community College

2002-2014 CWCS Theoretical and Computational Chemistry Workshop Instructor
This one-week NSF-CCLI sponsored workshop is designed for faculty from 2- and 4-year colleges and universities across the U.S. It provides a background and modern perspective on theoretical and computational chemistry along with methods to introduce these topics into the undergraduate curriculum.

2001-2002 Education Research (STEP) Fellow
Georgia Institute of Technology & *North Springs High School*, Atlanta, GA
Participated in summer training workshops on inquiry-based learning pedagogy, classroom management, effective teaching skills, and appropriate uses of educational technologies. Classroom and one-on-one instruction at the high school; Designed and implemented classroom websites.

Awards and Honors

2017-2018	Lucian Professor
2016	Inaugural POGIL Early Achievement Award
2013	The Myriad Excellence in Learning Leadership Award
2001-2002	NSF-sponsored Student Teacher Enhancement Partnership (STEP) Fellowship
1997	Dean's Professional Development Fellowship, Georgia Institute of Technology
1994	NSF-Idaho EPSCoR Research Experience for Undergraduates (REU) program
1994	Honors Certificate from the University of Idaho Honors Program

Publications (**Undergraduate*)

1. D. J. Schmucker, S. R. Dunbar, T. D. Shepherd, M. A. Bertucci "$n\rightarrow\pi^*$ interactions in n-acyl homeserine lactone derivatives and their effects on hydrolysis rates" *J. Phys. Chem. C,* **2019** *123,* 6088.
2. R. Cole, T. D. Shepherd "Making Sense of Mathematical Relationships in Physical Chemistry" **2019** ACS Symposium Series, *1316*, 173.
3. A. Kumar, A. H. Nguyen, R. Okumu*, T. D. Shepherd, V. Molinero "Could Mesophases Play a Role in the Nucleation and Polymorph Selection of Zeolites?" *J. Am. Chem. Soc.,* **2018***, 140,* 16071.
4. A. H. Nguyen, M. A. Koc*, T. D. Shepherd, V. Molinero "Structure of the Ice-Clathrate Interface" *J. Phys. Chem. C,* **2015** *119,* 4104.
5. R. C. Fortenberry, A.R. McDonald, T. D. Shepherd, M. Kennedy, C. D. Sherrill "PSI4Education: Computational Chemistry Labs Using Free Software" **2015** ACS Symposium Series, *1193*, 85.
6. H. Hu, T. D. Shepherd "Teaching CS 1 with POGIL Activities and Roles" *Proceedings of the 45th ACM Technical Symposium on Computer Science Education*. Atlanta, GA March **2014**
7. T. D. Shepherd and A. Grushow "Quantum Chemistry & Spectroscopy: A Guided Inquiry" John Wiley & Sons, Inc. **2013**
8. H. Hu, T. D. Shepherd "Using POGIL to help students learn to program" *ACM Transactions on Computing Education*, **2013**, *Vol. 13*, No. 3, Article 13
9. T. D. Shepherd, M. A. Koc*, V. Molinero "The Quasi-Liquid Layer of Ice under Conditions of Methane Clathrate Formation" *J. Phys. Chem. C,* **2012**, *116,* 12172.
10. T. D. Shepherd "Book & Media Reviews: Mastering Chemistry" *J. Chem. Ed.* **2009**, *86*, 694.
11. J. A. Gomez, A. K. Tucker*, T. D. Shepherd, and W. H. Thompson "Conformational Free Energies of 1,2-Dichloroethane in Nanoconfined Methanol" *J. Phys. Chem. B* **2005**, *109*, 17479.
12. J. M. Moix, T. D. Shepherd, and R. Hernandez "A phenomenological model for surface diffusion: diffusive dynamics across incoherent stochastic potentials" *J. Phys. Chem. B* **2004**, *108*, 19476.
13. S. Li, T. D. Shepherd, and W. H. Thompson "Simulations of the vibrational relaxation of a model diatomic molecule in a nanoconfined polar solvent" *J. Phys. Chem. A* **2004**, *108*, 7347.
14. T. D. Shepherd and R. Hernandez "An optimized mean-first-passage time approach for obtaining rates in activated processes" *J. Chem. Phys*. **2002**, *117*, 9227.
15. T. D. Shepherd and R. Hernandez "Activated dynamics across aperiodic stochastic potentials" *J. Phys. Chem. B* **2002**, *106*, 8176.
16. T. D. Shepherd and R. Hernandez "Chemical reaction dynamics with stochastic potentials below the high-friction limit" *J. Chem. Phys*. **2001**, *115*, 2430.
17. T. D. Clarke and C. M. Wai "Selective removal of cesium from acid solutions with immobilized copper ferrocyanide" *Anal. Chem.*, **1998**, *70*, 3708-3711.

Posters and Presentations

1. Educause Learning Initiative (ELI) Annual Meeting, New Orleans, LA, *Sometimes all it takes is some tables and chairs: Reports from Steelcase Active Learning Center Grant,* Invited Presentation (January 2018)

2. Steelcase Education Active Learning Symposium, Grand Rapids, MI, *Research Story: St. Edward's University,* Invited Presentation (November 2017)
3. National ACS meeting, San Francisco, CA, *Implementing POGIL at a Minority-Serving Institution,* Presentation (April 2017)
4. SWRM ACS regional meeting, Galveston TX, *Using POGIL to teach chemistry majors to program in the context of applications involving data analysis and simulation,* Presentation (November 2016)
5. 43rd Annual NOBCChE Conference, Raleigh NC, POGIL: The fundamentals, Presentation & Workshop (November 2016)
6. AACU 2016 Transforming Undergraduate STEM Education: Implications for 21st-Century Society, Boston MA, *Creating a More Inclusive and Engaging STEM Classroom*, Workshop *(*November 2016)
7. 47th SIGCSE Technical Symposium, Memphis TN, *Facilitating POGIL Activities to Support All Students*, Workshop *(*March 2016)
8. 13th National POGIL meeting, St. Louis, MO, *Reflections on the impact of institutional context on POGIL implementation,* Poster (June 2015)
9. National ACS meeting, Denver, CO, *Rethinking homework – the impact of content, format & process on physical chemistry learning outcomes,* Presentation (March 2015)
10. SWRM ACS meeting, Fort Worth, TX, *Effectiveness of online student-centered assessment to evaluate content and process learning outcomes,* Presentation (November 2014)
11. SERMACS ACS regional meeting, Atlanta, GA, *Using Marzano's Taxonomy to assess and improve learning outcomes,* Presentation (November 2013)
12. SERMACS ACS regional meeting, Atlanta, GA, *Characterization of a stripe liquid crystal phase in simple binary water solutions,* Presentation (November 2013)
13. 11th National POGIL meeting, St. Louis, MO, *Development of Learning Cycle activities for an introductory programming course,* Poster (June 2013)
14. 22th Biennial Conference on Chemical Education, University Park, PA, *Incorporating computational chemistry in undergraduate research and education.* Presentation (July 2012)
15. 10th National POGIL meeting, St. Louis, MO, *Using student authored POGIL activities as assessment,* Poster (June 2012)
16. Invited Talk, Canadian Chemistry Conference, Calgary, AB, *From atoms to nanoparticles – the development and implementation of Process Oriented Guided Inquiry Learning (POGIL) in physical chemistry* (May 2012)
17. National ACS meeting, Anaheim, CA, *Revisiting POGIL methodology in the teaching of quantum mechanics,* Presentation (March 2011)
18. Mastering Chemistry Leadership Conference, New Orleans, LA, *Advanced Authoring Tools* (March 2011)
19. 8th National POGIL meeting, St. Louis, MO, *Using student authored POGIL activities as assessment,* Poster (May 2010)
20. Invited Talk, Utah State University, Logan UT, *Using POGIL throughout the chemistry curriculum* (April 2010)
21. Invited Talk, Utah Valley University, Orem UT, *Molecular Dynamics Simulations of Nucleic Acid Systems* (April 2010)
22. National ACS meeting, San Francisco, CA, *Incorporating computational chemistry in undergraduate research and education,* Presentation (March 2010)
23. Invited Talk, Brigham Young University, Provo UT, *Incorporating computational chemistry in undergraduate education* (October 2009)
24. 7th National POGIL meeting, St. Paul, MN, *Student reflections on learning in a POGIL classroom,* Poster (May 2009)
25. National ACS meeting, Salt Lake City, Utah, *Exposing students to the successes and challenges of molecular modeling and simulation,* Presentation (March 2009)
26. National ACS meeting, Salt Lake City, Utah, *Integrating the use of technology to enhance the implementation of POGIL,* Presentation (March 2009)
27. 20th Biennial Conference on Chemical Education, Bloomington, IN, *Emphasizing the P in POGIL!* Presentation (July 2008)
28. 20th Biennial Conference on Chemical Education, Bloomington, IN, *Illustrating the statistical bridge between the*

microscopic and macroscopic worlds with MD simulations. Presentation (July 2008)

29. Regional ACS meeting, Park City, Utah, *Using computational studies to promote interdisciplinary learning,* Presentation (June 2008)
30. American Conference on Theoretical Chemistry, Champion, Pennsylvania, *Chemical reaction dynamics with stochastic potentials,* Poster (July 2002)
31. 9th Georgia Conference on College and University Teaching, Atlanta, Georgia, *The Georgia Tech Student and Teacher Enhancement Partnership (STEP) Program*, Presentation (February 2002)
32. Emory University International Conference: Nanobiology, Atlanta, Georgia, *Chemical reaction dynamics with stochastic potentials below the high-friction limit*, Poster (October 2001)
33. Gordon Research Conference: Chemistry & Physics of Liquids, Plymouth, New Hampshire, *Chemical reaction dynamics with stochastic potentials*, Poster, (August 2001)
34. Gordon Research Conference: Chemical Physics Summer School (Analytical Approaches to Rate Processes and Time-Resolved Spectroscopy in Condensed Phases), Bristol, Rhode Island, *Stochastic dynamics in the presence of a fluctuating barrier*, Poster (June 2000)

External Funding

Steelcase Active Learning Center Grant (2016-2018), $60,000

Welch Foundation Departmental Grant (2016-2019), $105,000

National Science Foundation – Major Research Instrumentation (2016-2019), $225,000
"*Addition of High Performance Computers for the **M**olecular **E**ducation and **R**esearch **C**onsortium in **U**ndergraduate computational chemist**RY (MERCURY)***" Award Number: CHE-1662030.

National Science Foundation – Improving Undergraduate STEM Education (2015-2020), $1,608,224
"*SEU Living Learning Community/Active Learning (LLCAL) Project* Award Number: 1525490.

National Science Foundation – Major Research Instrumentation (2012-2015), $200,000
"*Acquisition of a High Performance Computer for the **M**olecular **E**ducation and **R**esearch **C**onsortium in **U**ndergraduate computational chemist**RY (MERCURY)***" Award Number: CHE-1229354.

National Science Foundation – Major Research Instrumentation (2008-2011), $229,000
"*Acquisition of a High Performance Computer for the **M**olecular **E**ducation and **R**esearch **C**onsortium in **U**ndergraduate computational chemist**RY (MERCURY)***" Award Number: CHE-0849677.

National Science Foundation – Major Research Instrumentation (2005-2008), $100,000
"*Acquisition of a Linux Cluster for the **M**olecular **E**ducation and **R**esearch **C**onsortium in **U**ndergraduate computational chemist**RY (MERCURY)***" Award Number: CHE-0521063.

Other Professional Activities

Supervision of 40+ undergraduate students including three McNair Scholars, eighteen female students, three African-American and four Hispanic. Student work has been presented locally, regionally, and nationally (NCUR, National American Chemical Society meetings, and the MERCURY conference in computational chemistry). Four former female undergraduate research students have received a PhD at Georgia Institute of Technology (physical chemistry), University of Notre Dame (physical chemistry), University of Utah (analytical chemistry), and Dartmouth (Biomedical Engineering). Two female (one African American) and three male research students are currently working toward a PhD at U.C. Santa Cruz (Physical Chemistry), University of Minnesota (Physical Chemistry), U.C. Berkley (Physical Chemistry), University of Utah (Material Science) and Boston University (Bioinformatics).

Advisory Board member, NSF IUSE Grant: IntroCS POGIL in Introductory Computer Science
Consultant, AAC&U Teaching to Increase Diversity and Equity in STEM (TIDES)
AAC&U/PKAL Summer Leadership Institute for STEM Faculty, Crestone, CO, 2015
Panelist, NSF Chemical Theory, Models and Computational Methods
Referee for National Science Foundation and ACS Petroleum Research Fund
Reviewer Journal of Chemical Education

Weber State program review (2013)
Review abstract submissions for NCUR (National Conference on Undergraduate Research)
External Promotion Review for chemistry faculty at University of Minnesota, Morris (2009) and Georgia Southern University (2011), Wheaton College (2013), Hamilton College (2014)
Invited symposium for the ACS National meeting, "*Computational Chemistry Investigations for Undergraduates*" San Francisco (September 10-14, 2006). Symposium co-organized by T. D. Shepherd and Daniela Kohen.

Committees and Service

2016-2018	NSCI Strategic Planning Committee
2015-2017	NSCI Travel Committee
Spring 2015	Curriculum Models Group for General Education Reform Committee (GERC)
2004-2014	Instituted and organized summer undergraduate research meetings
2012-2014	Undergraduate research committee
2011-2013	Westminster Teagle working group
2010-2013	Faculty Senate (2012-2013 Chair)
2010-2012	A&S Travel Committee
2007-2011	Web Content Committee
2006-2010	Meldrum Science Center Building Shepherd
2008-2010	Chair of Teaching and Learning Resources Committee
2007-2009	Facilitator for LE workshop on Leadership, Collaboration and Teamwork
2007-2009	Undergraduate Research Faculty Group
2005-2007	Liberal Education Committee
2006-2007	Academic computing Task Force
2006-2007	President's Advisory Council
2005-2006	Arts and Science Curriculum Committee
2003-2005	Teaching and Learning Resources Committee

Professional Memberships

2002-present	Council of Undergraduate Research
2002-present	American Chemical Society