Electronic Supplementary Material (ESI) for Chemistry Education Research and Practice.

Appendix A

Definition of Analytical Categories and selected examples

Toulmin's Model of Argumentation
Definitions adapted from Toulmin (1958).

Argument Component	Description
Claim	A conclusion whose merit must be established. This is a statement that you are asking others to accept.
Data	The facts one appeals to as a foundation for the claim. These are the facts used to support and provide reasoning for the claim.
Warrant	A statement bridging the claim and data, thus legitimizing the claim by showing the data to be relevant.
Backing	Generalizations that refer to basic assumptions that are used to establish the trustworthiness of the argument. Backings provide additional support to the warrant.
Qualifier	Indicates the strength conferred by the warrant and may limit how universal the claim is.
Rebuttal	Challenges made to the claim, data, or warrant. The rebuttal indicates circumstances in which the general authority of the warrant must be set aside. These statements recognize the restrictions that may legitimately be applied to the claim.

Appendix B

Definition of Analytical Categories and selected examples
Representational Levels- Symbolic, Sub-Microscopic, and Macroscopic Coding Definitions

Symbolic Level Codes

Sub-code	Description	
Mathematical	Claim, evidence, or reasoning related to the validity of a mathematical expression under a particular set of conditions	
	Related to how quantities will change with respect to one another according to a particular mathematical representation (relates to qualitative interpretation of a mathematical expression)	
	Related to the sign or value of a quantity NOTE: more general claims about macroscopic quantities such as enthalpy can be coded as macroscopic	
	Known equations when appealed to as evidence	Algorithmic – explanation appeals to procedure of obtaining a mathematical result
		Qualitative - student interprets what the mathematical expression means
Graphical or Numerical Data	Prediction of shape of graph, slope of line, etc.	
	Appeal to graph feature or numerical trend observed in data	
Physical Model	Appeal to features of physical model or drawing	
Model of Composition and Structure	Appeal to information from balanced equation	
	Appeal to information from chemical formula	
Definitions and Rules	Fundamental description of concept	

Sub-Microscopic Level Codes

Sub-code	Description
Atomic/Molecular	Claim, evidence or reasoning related to molecular structure
	Includes discussion of presence or absence of bonds and molecular geometry
	References to properties of atoms when not referring to sub-atomic particles
Multi-particle	Claim, evidence or reasoning related to motion or spacing of particles or nature of interaction between multiple particles
	Includes references to electrical interactions between two or more particles
	Excludes discussion of electrical interactions within atoms or molecules
Definitions and Rules	Fundamental description of concept

Macroscopic Level Codes

Sub-code	Description
Macro-Concrete	Claim, evidence, or reasoning related to measurable physical properties of system including mass, temperature, pressure, volume
	Concrete in this context is used to refer to properties that can in some way be experienced or measured directly
Macro-Abstract	Claims about properties of the system which are not directly measurable including enthalpy, entropy, Gibbs energy, work, heat capacity, or heat. **NOTE**: Appeals to T, V, etc. when used as variables in a mathematical expression in explaining how one quantity would vary with respect to another would not be considered "macroscopic"; they would be considered symbolic
Macroscopic Observation	Relates to experience of phenomena or observation
Definitions and Rules	Fundamental description of concept

Appendix C

Inquiry Oriented Discursive Moves Coding Definitions.
Definitions adapted from Marrongelle & Rasmussen (2008).

Revoicing. Revoicing is defined as reuttering or saying again (this could be verbal, symbolic, or gestural) – of someone else's utterances.

Revoicing Category	Description	Example
Repeating	Teacher repeats a student's utterance using (essentially) the same words or a portion thereof.	S: As the reaction occurs the piston moves up because there is an increase in moles. T: my volume is gonna go up because our moles is going up
Rephrasing	Teachers states a student's utterance in a new or different way	S: dS, dV, and dU are exact differentials. T: all of these variables are state functions.
Expanding	Teacher adds information to a student's utterance	S: Volume is a state function because you can use the final volume and the initial volume. T: So my change in volume doesn't depend on the path I use to get there, just what it is.
Reporting	Teacher attributes an idea, claim, or argument to a specific student.	T: So when the weight's removed, like Mary said, it's gonna expand till I can restore equilibrium.

Questioning. We used questioning codes in cases when there was an expectation that students actually respond or take action (as opposed to rhetorical questions).

Questioning Category	Description	Example
Evaluating	The intention is to check for understanding against what the teacher sees as an expected response.	T: What does dH equal at constant pressure? S: dH = dU + PdV
Clarifying	Purpose of the request is to seek clarification of detail what a student is saying. a. Request for clarification is directed to the speaker b. Request for clarification is direction to someone other than the speaker	T: We're going to have reactions that have a negative entropy change. The substances won't, and for it to be spontaneous what has to be true? S: It's positive? T: What's positive? S: The entropy? T: The entropy of what? S: Of the reaction? Of the substance?
Explaining	Intention is for student(s) to share ideas however tentative. (Could be in question or request form.) a. Requests to explain your/group's thinking b. Requests to explain or comment on another student's/ group's thinking	T: Ok, so what are some first impressions? You don't have to be right. Just kind of what are your first impressions about what's going on here. S1: Well, we said that because there is constant motion for, it must be a positive for it to move S2: we said that things are always moving, things always move from order to disorder.
Justifying	Requests to provide warrants or backing for a some conclusion	T: Why are all entropies positive? S: Because you can't go lower than zero degrees Kelvin, and at zero degrees there's no movement so the entropy's zero.

***Telling*.** Telling is an important, but often underemphasized, part of a teachers' repertoire

Telling Category	Description	Example
Initiating	a. Describing or presenting a *new* concept, representation, procedure, solution method, etc. b. Telling students what problem they are to work on next. Involves some contextualization of task. c. Reminding students of conclusions from a previous problem.	T: So in our first model we have our system here, our piston/cylinder thing that we've been analyzing as we go through. We've made one change now, we have indicated the surroundings because when we look at energy exchange, we're looking at the exchange between the system and the surroundings.
Facilitating students' progress	a. Providing information that students need, for a task that students are in the midst of working on. b. Reminding students of a conclusion or a way to think about a problem for which there has already been some agreement or public voicing.	T: So I should clarify that, we're not talking about the entropy of a reaction, we're talking about the entropy of a substance.
Responding to students	a. Answering a direct student question. b. Evaluating a student utterance, can add additional reasoning	S: You can substitute in nRT/V for P because we are working with ideal gas. T: That correct.
Summarizing	This discursive move summarizes ideas, highlights particular mathematics of importance, and/or points to next steps related to the summary.	T: So when we look at heats of formation, you have to do it from the elements. And so when you look at the table in the back of your book that gives you all of those heats of formation, they calculated what the heat of reaction for this, and then we can just add all of those reactions together.

***Managing*.** Teachers, like a general manager at most any company, typically engage in actions that organize their workers in both structural and affective ways.

Managing Category	Description	Example
Arranging	Classroom management of physical space or arrangement of work space or work tasks.	T: Let's look at the focus question for T2. You guys have got a minute to come up with an answer in your small group.
Directing	Mathematical management that directs students to carry out a particular mathematical action.	T: Take the total differential for H = H(T,P)
Motivating	Provides encouragement or motivation for students	T: That's a really good question.
Checking	Check on current status of student progress	T: Does this make sense? Yes, no, maybe?