Supplemental Information

RCD framing as a diagram or graph distinction

Graphs are often distinguished from diagrams on the basis that they describe quantitative data in two dimensions (Scaife and Rogers, 1996). However, the distinction between graphs and diagrams is not always clearly defined given the inconsistent nature of the term "diagram" and the broad span of representations that may be defined as a diagram. In the case of RCDs, we have made the distinction that organic chemistry frames RCDs as diagrams, while physical chemistry frames RCDs as graphs. This statement is made to highlight the different ways in which a RCD is presented and applied across sub-disciplines; however, the reasons for choosing to distinguish the framing of RCDs by these terms is important to consider.

Before discussing the choice of the words "diagram" and "graph" when discussing the framing of RCDs in organic and physical chemistry, it is important to first recognize that RCDs in both contexts may be classified as "graphical external representations" (Zhang, 1997; Superfine *et al.*, 2009). The dual purpose of comparing thermodynamic energy states and activation energies for the purposes of evaluating the thermodynamics and kinetics of a reaction is a mutual element across organic and physical chemistry curricula. Most importantly, numerical values of energy are associated with molecular configurations that give meaning to the displacement of these states from one another on the diagram, at least in the vertical direction. The idealized nature of the x-axis, and the lack of numerical labels that often accompanies it, qualifies it as a diagram for the purposes of terminology within the chemistry community. However, RCDs are still "graphical" external representations by their numerically comparative and evaluative nature. External representation research has demonstrated that the skills of knowing how to interpret and evaluate certain representations impacts students' translation of knowledge into such representations (Superfine *et al.*, 2009), and so the distinctions made regarding RCDs across organic and physical chemistry are significant from a pedagogical standpoint. The tendency for physical chemistry textbooks to label the x-axis of a RCD according to a defined nuclear distance variable (Levine, 2002; Atkins and de Paula, 2014) brings the RCD, as a representation, to something more comparable to a Lennard-Jones potential in terms of the level of quantitative content present in the diagram.

Based upon these reflections, we believe it is most appropriate to view the representations that involve comparative values in chemistry as existing along a diagram-graph properties spectrum (Fig. S1). The "bounds" which may be considered to define "graphical external representations" includes the inclusion of numerical values for the purposes of comparison and a guiding context. These important distinctions serve to emphasize that (1) many diagrams in chemistry have graphical character and (2) the trends we consider to be graphs in chemistry differ from pure mathematics in that they are always informed by the underlying physical context of the modeling situation. Therefore, when stating that RCDs in a physical chemistry context are framed as "graphs," we are referring to this term in a field-specific manner that takes for granted the inherent physical contexts underlying our graphical trends. We believe that the term "graph" may very well vary depending on the field-specific lens which is used to view the term depending upon the conventions at play and the types of numerical external representations that are relevant. However, the key differences in phrasing across the ACS anchoring concept maps for organic and physical chemistry, as previously discussed, reflect the qualitative role of RCDs in an organic chemistry context and the more quantitative purposes of RCDs in a physical chemistry setting. As such, the differences in how RCDs are utilized in organic and physical chemistry curricula is critical when considering how general chemistry instructors should introduce these representations to properly prepare students for their intended chemistry coursework.

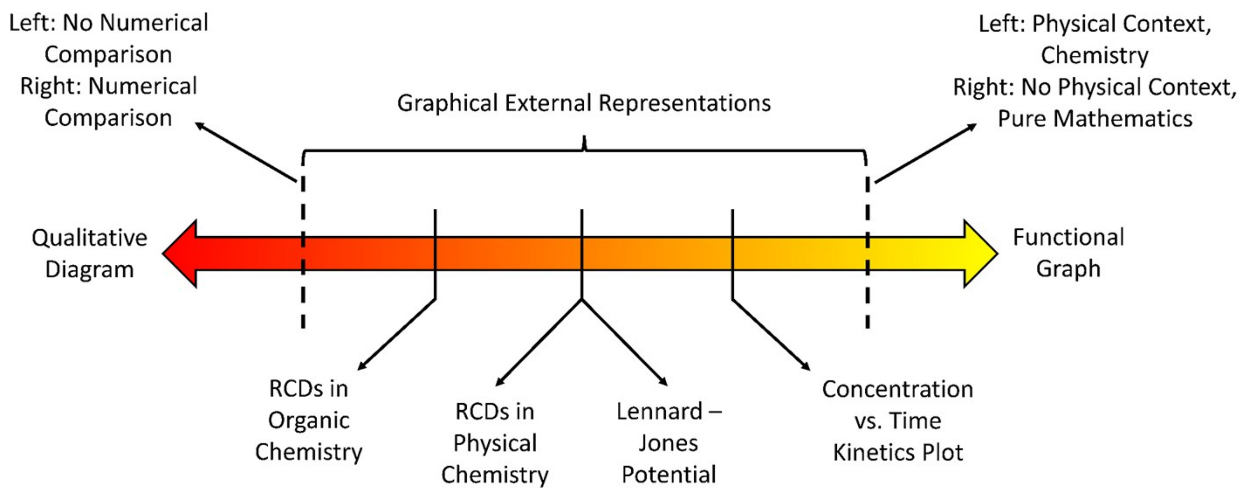

Fig. S1 Summary of the diagram-graph property "spectrum" discussed that is used to distinguish the role of RCDs in organic and physical chemistry settings.

Full codebook

Table S1 The codebook implemented in this study with emergent definitions and examples

Code	Definition	Participant Quote Examples
	Graphical Reasoning Codes	
Graphical Read-out	A statement comparing points, regions, or trends of (the) RCD(s) based on the read-out surface features from the diagram (i.e. no inferences made regarding related parameters, metrics, or physical processes)	P: *"I think so. I think so. It would just commonly register. My brain is, Nope, this is incline, this is decline. I would just leave it like that. I wouldn't say it's anything else."*
Value-Thinking, Coordinate	A statement associating the PE of a point with a numerical x-axis value/variable (such as time or coordinate) OR the difference/interval between two x-axis values OR the association of PE with any specified area underneath the RCD.	P: *"Yeah, so at, they're [referring to two Points] at different reaction coordinates, so they're at different times."* P: *"Um, it looks like Region 2, has like a wider like range in like reaction coordinate. Um, those would be, I guess key differences*

		that I've noticed."
Value-Thinking, Slope/Derivative	A statement associating the slope or derivative of a point with the change OR lack of change of specified parameters (such as rate or stability).	P: *"Like, um, like the distance on the x-axis of the reaction coordinate axes to go from where the slope is zero at the start and where the slope is zero at the end is, like that distance is greater for reaction 3 then Reaction 2."*
Location-Thinking, States	A statement associating the region(s) of (a) RCD(s) or the PE of (a) point(s) with (a) physical state(s) or physical process(es) (such as reaction, products, molecular collisions, catalysis etc.).	P: *"As I mentioned before, like I think of it starting at the reactants and then ending at the products. So I'd say that, uh, Point 1, I guess that's what I'll call it. Uh, Point 1 would be say the potential energy where in this case, cause chemistry, chemical energy of the reactants is Point 1."*
Location-Thinking, Trend	A statement associating the region of a RCD or PE of a point as an energy/value along the RCD trend, while making no associations with (a) physical state(s) or physical process(es).	P: *"Um, because we're, as the reaction proceeds, the energy is like what's being measured. So we can't like change the amount of energy that is either required or is being produced."*
Graphical Forms, Shape	A statement that associates the shape of the RCD trend or relative shapes of RCD(s)/graphical trends with the change OR lack of change of specified parameters (such as rate or stability).	P: *"But, given that 7 is leveling out, I can tell that that's, I guess more stable, like it's going to stay like that."*
Graphical Forms, Slope/Derivative	A statement that associates the slope or derivative of the RCD trend or the relative slopes or derivatives of RCD(s)/graphical trends with the change OR lack of change of specified parameters (such as rate or stability).	P: *"Um, I think it's faster because it has a sharper peak and these lines at the end, like right here and right here are longer and it achieves this incline at a faster pace than this incline."*

Kinematic Heuristic	Statements that frame (a) RCD(s) as a kinematic path as made evident by… framing the transition state as a hill/bump/etc. that must be overcome for a reaction to proceed. OR statements associating potential energy of an RCD with kinetic energy without reference to the underlying mechanism of (a) RCD(s). OR statements associating the length of a path along the RCD trend or when comparing the lengths of RCD paths along trends with specified kinematic parameters (such as time or distance).	P: *"So if I'm saying it's the amount of potential energy that's being released, then I guess I could say that the reaction would proceed quicker because there's just not as much work that's being done per se. Um. So the reaction would go faster. But then also if I'm saying it's the amount of potential energy that is needed for the reaction to get from reactants to products, then the less potential energy needed, the faster it's also going to proceed because there's a smaller bump that the reaction has to overcome."* P: *"I would say that this one you're walking 10 miles in 10 minutes and this one you're walking one mile in one minute. So like you're going the same speed across, it's just taking you less time. Like cause this path is shorter. So like you're going one, you're going one mile a minute here and you're still going one mile per minute here. It's just taking me longer to get there cause you're taking a longer path."*

X-Axis Interpretation Codes

X-Axis as Progress	A statement indicating that the x-axis of the RCD or the horizontal span of the RCD is associated with the "progress" of a reaction OR any provided justification for why the x-axis of the RCD is associated with the "progress."	P: *"I guess I interpret the reaction coordinate as how the reaction has progressed."*
X-Axis as Reaction Coordinate	A statement indicating that the x-axis of the RCD or the horizontal span of the	P: *"There's not, there's no numbers down here. Just it's just*

	RCD is simply the "reaction coordinate" of a reaction OR any provided justification for why the x-axis of the RCD is associated with the "reaction coordinate."	*this reaction coordinate, but I just know that getting higher and then getting lower."*
X-Axis as Time	A statement indicating explicitly or implicitly that the x-axis of the RCD or the horizontal span of the RCD is associated with "time" OR any provided justification for why the x-axis of the RCD is "time."	P: *"Um, like I mean, the potential energy isn't increasing like all over a really, really short period of time, like it's not spontaneous, I guess, like the potential energy increase. Instead, it's happening over time."*
X-Axis as Not Time	A statement that explicitly indicates that the x-axis or the horizontal span of the RCD does not encode for the time or duration of the reaction OR any provided justification for why the x-axis of the RCD is not associated with "time."	P: *"Well, I guess maybe slowing down's not the right term to use in this sense because our X axis is not time."*
X-Axis as Uncertain	Any statement that indicates a participants' uncertainty regarding the x-axis of a RCD.	P: *"Well, it's labeled reaction coordinate, which confuses me a little bit cause I'm not quite sure what that means honestly. Um. I don't know."*
X-Axis as Molecular Distance	A statement that indicates that the x-axis is associated with the distance between or position of reacting molecules OR any provided justification for why the x-axis of the RCD must be associated with the distance between or position of molecules in a reaction.	P: *"I think it [the x-axis] more corresponds to like the positioning of the molecules, but like that happens, like at a certain like time. So like indirectly it's also related to time."*

Outcome Codes for Kinetic and Thermodynamic Reasoning

Productive, Kinetics	Instances in which a participant reasons about the rate of a chemical reaction or relative rates of a set of chemical reactions in a manner that is physically consistent, in both the interpretation of	I: *"I see. Do you feel the catalyst affects anything else about the reaction?"* P: *"Um, I'd say just based on the*

	the RCD(s) and answer, with the RCD(s) under discussion.	*graphs, no. Um, but it could react-, it could, um, affect like the reaction speed or like how the rate, reaction rate, like how long it takes for the reaction to progress, potentially make it the rate greater, increase."*
Unproductive, Kinetics	Instances in which a participant reasons about the rate of a chemical reaction relative rates of a set of chemical reactions in a manner that is physically inconsistent, in both interpretation of the RCD(s) and answer, with the RCD(s) under discussion.	P: *"Um, I think Reaction 2 would be the fastest reaction, although it has the same potential energy as Reaction 1. It does have that steeper slope near the top portion of the graph. So that makes me think it has a faster reaction rate."*
Neutral, Kinetics	Instances in which a participant reasons about the rate of a chemical reaction or relative rates of a set of chemical reactions… in an arbitrary manner that is neither consistent nor inconsistent with the RCD(s) under discussion OR in a manner in which the interpretation of the RCD or answer is physically inconsistent with the RCD(s) under discussion but the other (interpretation or answer) is physically consistent with the RCD(s) under discussion.	P: *"Because as I said before, like let's say again, arbitrary number, uh here to here is a difference of 2000, and let's say here to here is a difference of 1700, so if I put in 2000 it takes however long this is to reach a product. If I put in 1700 it takes however long this is to put in the product. The differing amount of energy shouldn't change the rate of reaction. But if I put in say 2000 for this, this reaction would occur faster with more energy because it only needs 1700, does that make sense?"*
Productive, Thermodynamics	Instances in which a participant reasons about the enthalpy of a chemical reaction or relative enthalpies of a set of chemical reactions in a manner that is physically consistent, in both interpretation of the RCD(s) and answer, with the RCD(s) under discussion.	P: *"… you have your reactants, and then once they react, they're at a higher energy level, and then like it goes down to a lower energy, I can't remember what it's called, but yeah, like it goes like this, and then say net energy was that, so if like net energy was that it'd be exothermic or something."*

Unproductive, Thermodynamics	Instances in which a participant reasons about the enthalpy of a chemical reaction or relative enthalpies of a set of chemical reactions in a manner that is physically inconsistent, in both interpretation of the RCD(s) and answer, with the RCD(s) under discussion.	*Not observed in an interview
Neutral, Thermodynamics	Instances in which a participant reasons about the enthalpy of a chemical reaction or relative enthalpies of a set of chemical reactions… in an arbitrary manner that is neither consistent nor inconsistent with the RCD(s) under discussion OR in a manner in which the interpretation of the RCD or answer is physically inconsistent with the RCD(s) under discussion but the other (interpretation or answer) is physically consistent with the RCD(s) under discussion.	P: *"If the products have less energy than your reactants, then it is, um, then your reaction is endothermic because it requires more energy in the beginning than at the end. And if your products have more energy than you react incentives exothermic because it, um, it has more energy towards the end compared to the beginning."*

Additional Figures and Tables

Table S2 Mapping of interview numbers in Table 3 to corresponding participant pseudonyms

Interview Number	Gender	Pseudonym
1	Male	Leonard
2	Male	Jesse
3	Female	Alyson
4	Male	Paul
5	Female	Christy
6	Male	Mark
7	Female	Susanne
8	Male	David
9	Female	Jessica
10	Male	Haley
11	Male	Wayne
12	Female	Hayden
13	Female	Willa
14	Female	Mandy

15	Female	Megan
16	Male	Billy

Table S3 Interview mapping of graphical reasoning codes that resulted in kinetics outcome codes

	Interview Number Designator															
Code	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
LT-S	Grey	Blue	Grey	Grey	Grey	Yellow	Blue	Grey	Grey	Grey	Green	Grey	Yellow	Grey	Grey	Green
GF-S	Grey	Blue	Red	Grey	Red	Grey	Red	Grey	Grey	Grey	Grey	Grey	Purple		Grey	Grey
VT-C	Red	Blue	Purple	Red	Red	Red	Red	Grey	Red	Grey	Red	Red	Red	Purple	Red	
GF-SD	Red	Grey	Purple	Grey		Grey	Red	Grey	Purple	Purple		Grey	Red			Red
KH	Grey	Blue	Blue		Green		Grey	Purple		Purple				Blue		
VT-SD	Red			Red		Grey			Red		Grey				Red	
LT-T	Grey	Blue	Grey		Grey									Grey		

Kinetics Outcome Code Color Key

Green	Red	Blue	Purple	Yellow	Grey
Productive	Unproductive	Neutral	Unpro./Neu.	Pro./Neu.	N/A to Kinetics

Note: This table maps kinetics outcome codes onto the same graphical reasoning code distribution of Table 3. "Unpro./Neu."and "Pro./Neu." color coding indicates that a given code had at least one instance of both an Unproductive and Neutral code or a Productive and Neutral code respectively. If a code emerged during the interview and the code did not give rise to a kinetics outcome code, it is labelled as grey (N/A to Kinetics).

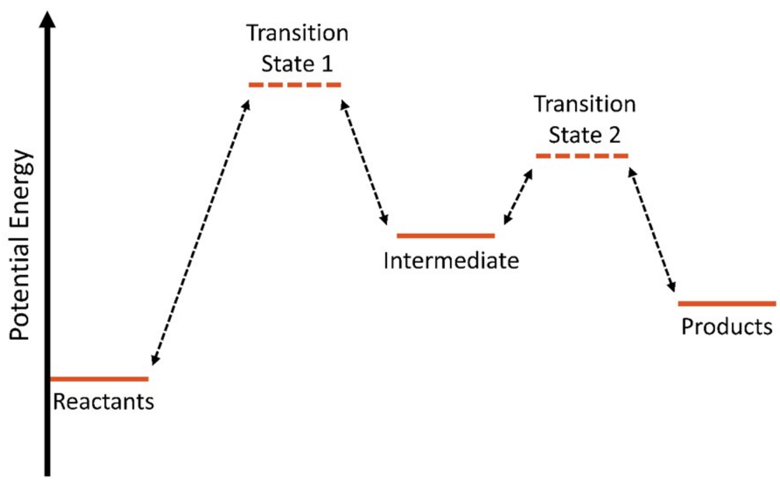

Fig. S2 A states-based RCD depiction including a single intermediate. The inclusion of a solid line to denote the intermediate "state" may be used to distinguish its pseudo-stable nature and lifetime from the dashed transition state lines.

References

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