ChemEd X Data: an open web platform to allow students discover chemical trends

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Center for Learning Innovation

BCCE August 4th 2014

http://chemdata.r.umn.edu/bcce14.pptx

UNIVERSITY OF MINNESOTA Rochester

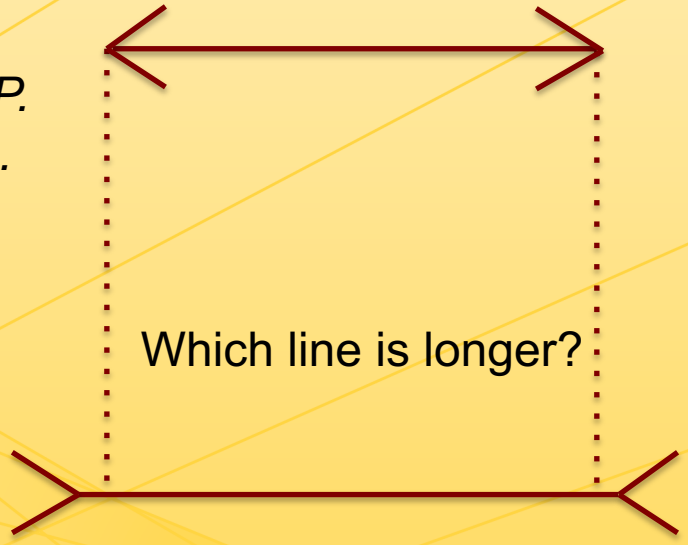
U of Minnesota Rochester

- Our new campus is a “little special”
  - Started accepting students in 2009 (~120/year)
  - One single major in Health Sciences
  - Multiple faculty teaching one course: recitation sessions are spread through the week as personalized one-to-one help
  - Laptop program: all students bring the same laptop model to class
  - No “lecture halls” but discussion
  - Downtown: 3rd and 4th floor of a shopping mall

Chemistry: learning the conflict

"…we should teach them to judge between conflicting influences. That is the essence of our subject, for it is rare that a single property governs the outcome of a reaction. We need to train our students to judge the likely outcome of conflict" P. Atkins. Pure Appl. Chem., Vol. 71, No. 6, pp. 927-929, 1999.

"…I assume there are exceptions to this rule because there is an exception to pretty much every rule in chemistry." Gen Chem student.



Often, we remember older problems and apply to new problems the **older solution**

In an ever changing world older solutions may not be that useful

higher-order thinking is more important than ever

Data-driven learning

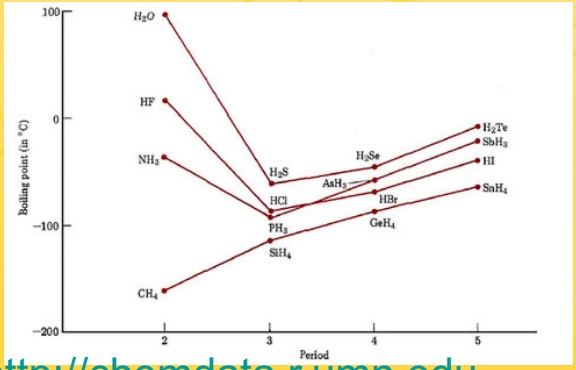
Static, "precooked" data

The web
- Unstructured data
- Non-linear
- Non-sequential
- Open-ended

Remember → Understand → Apply → Analyze → Evaluate

1. Look at this graph
2. See what I want you to see
3. Explain how everything perfectly fits
4. No exceptions

1. Choose some data
2. Represent it
3. Find patterns
4. Find exceptions



Skills required: Self-regulation
Self-evaluation

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Unstructured open data

Chem Ed X Data

Unstructured but easy to represent, parse and sort data

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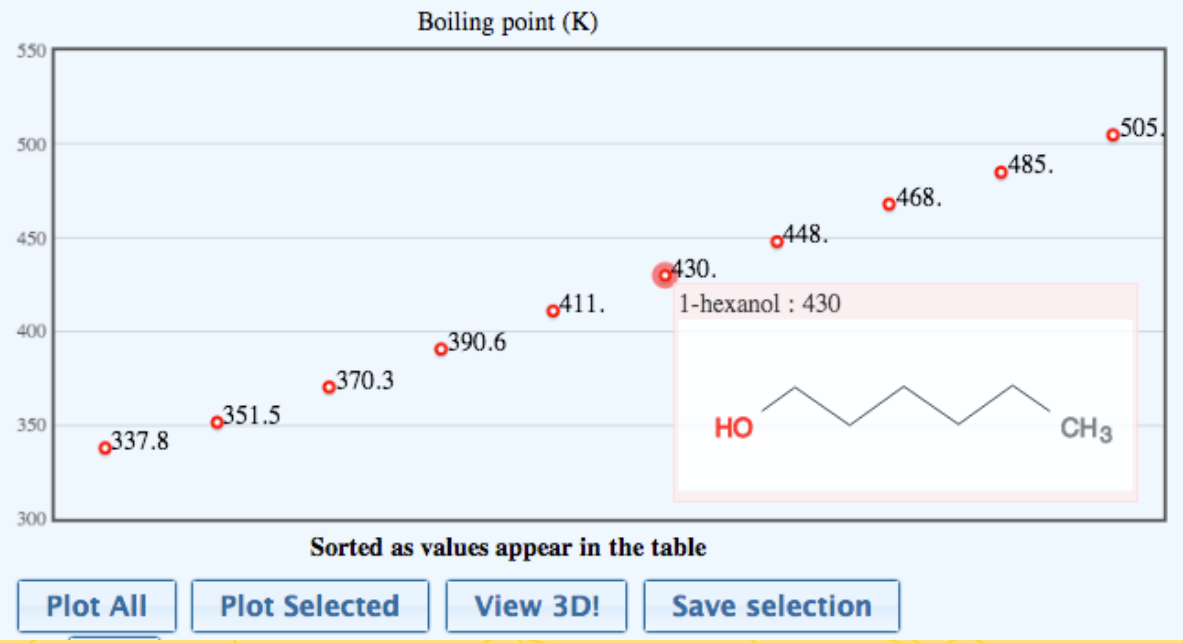
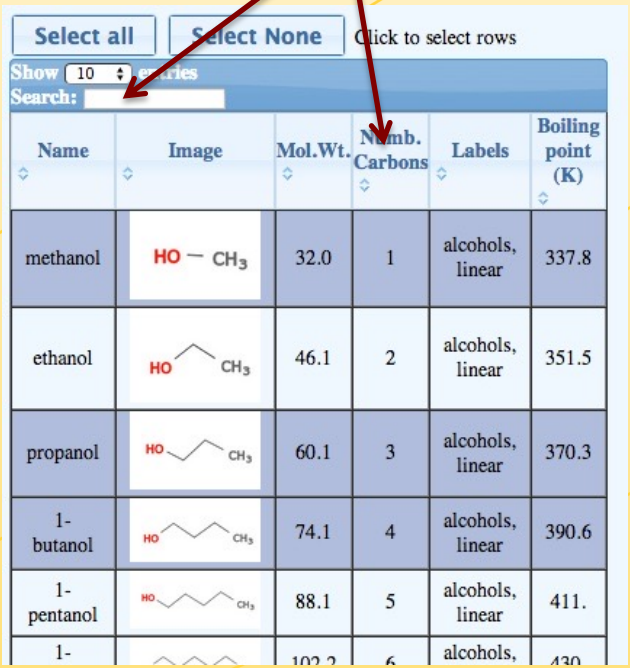
Elements, Organic/inorganic comp, reactions (Ac/Base, Redox, Solub)

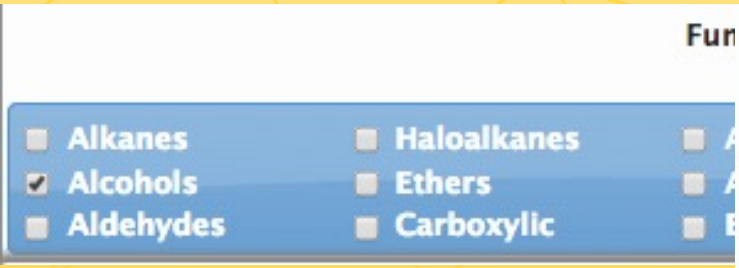
Data	Topic
Ionization energies, atomic radius	Atomic structure
Bond energies, bond length	Chemical bond
ΔH_{vap}, T_{boil}, dipoles	Intermolecular interactions
pKa, Ksp	Ionic equilibria
E^{o}_{red}	Electrochemistry

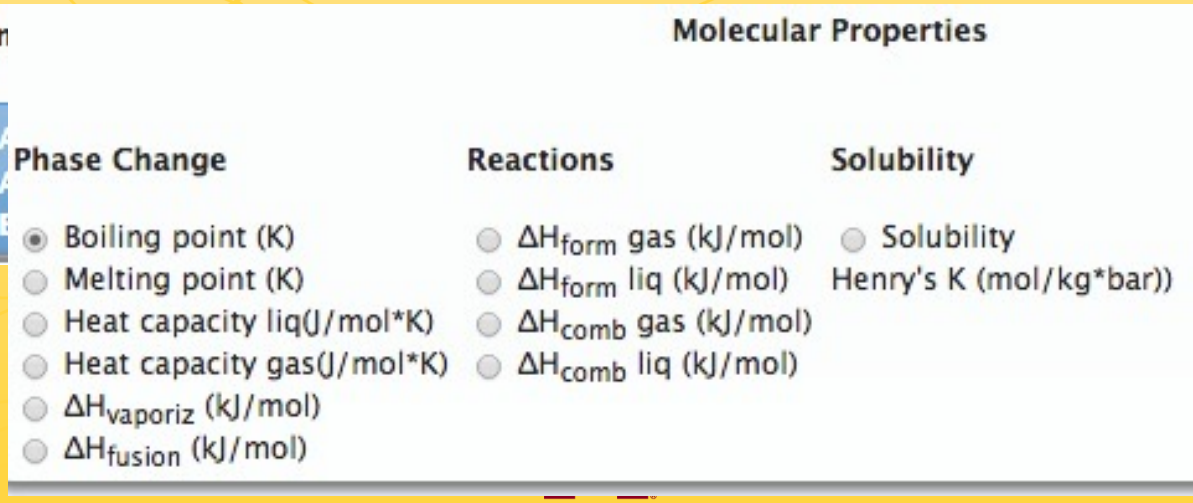
Organic molecules

Sorting, filtering tables









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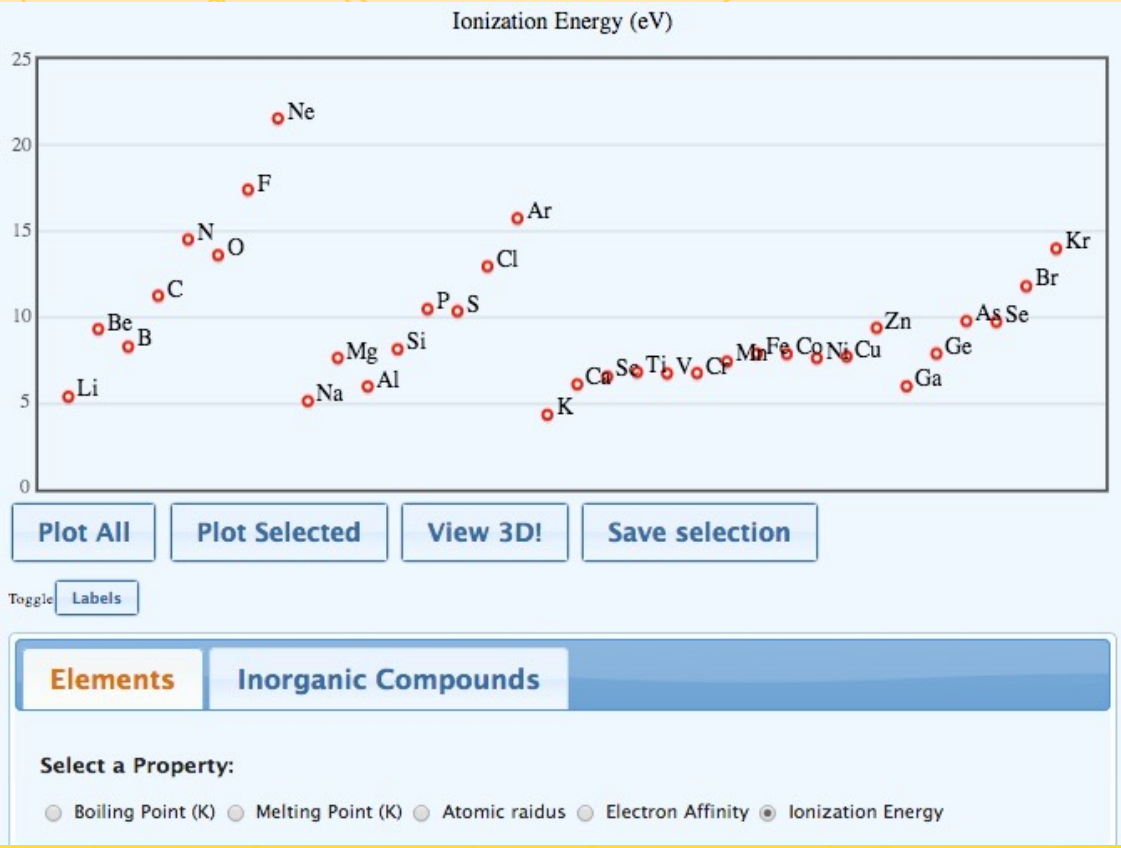
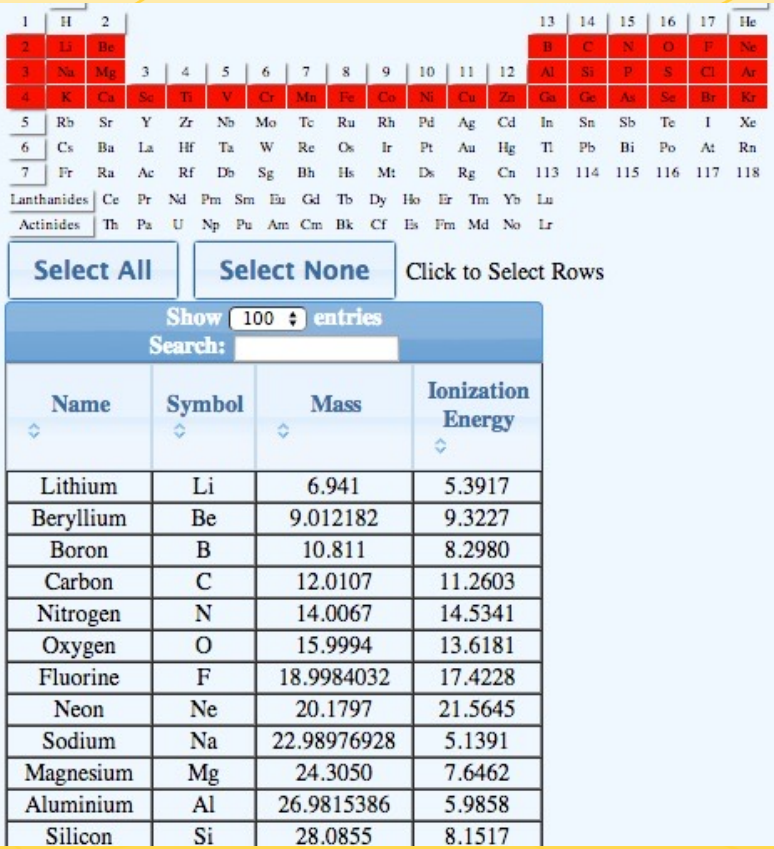
Periodic table trends

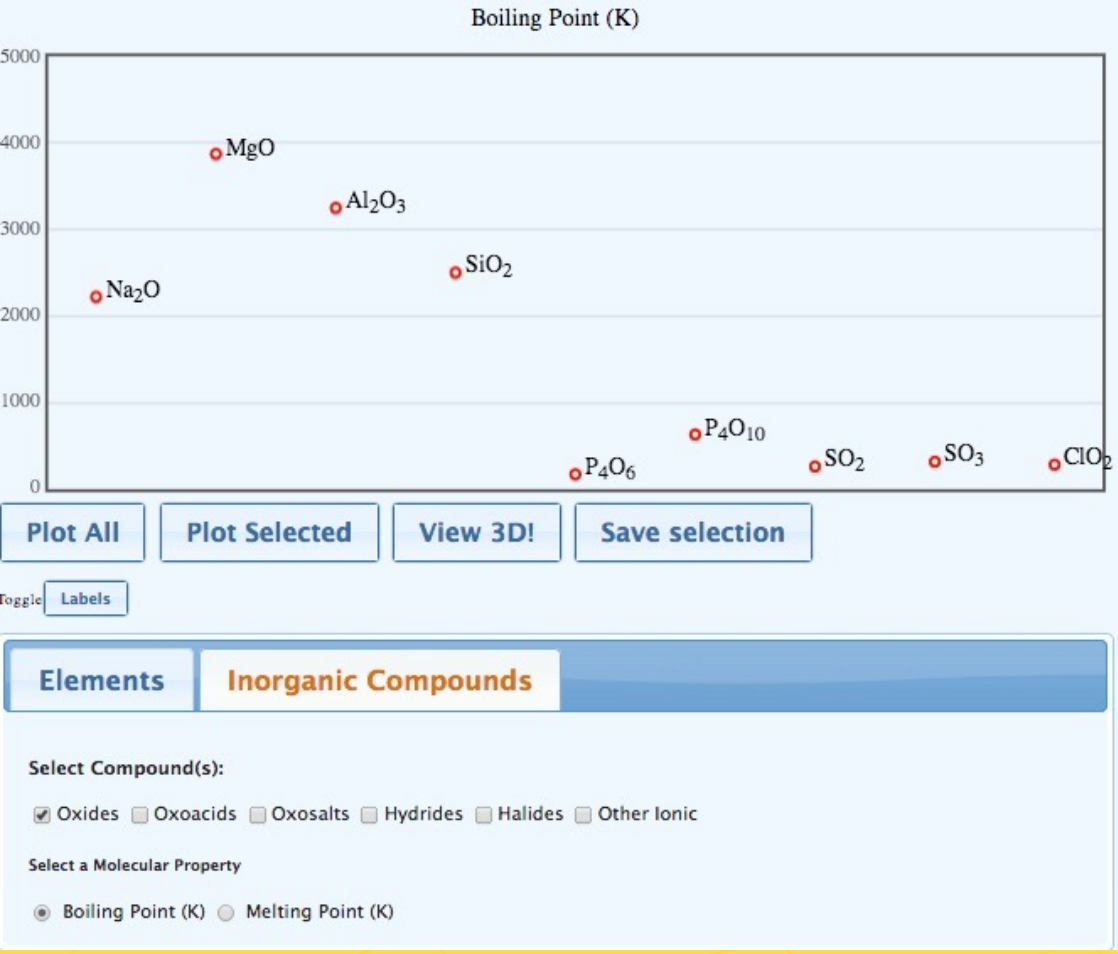
Based on “Periodic Table Live” graphs http://www.chemeddl.org/resources/ptl/charts/

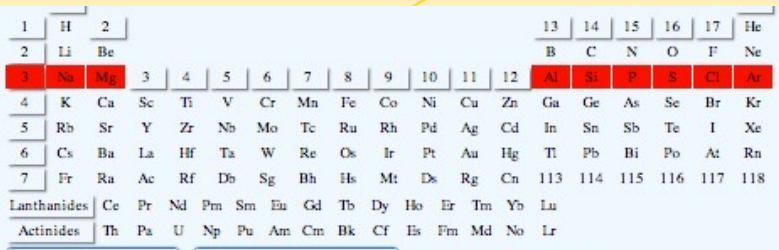




Name	Symbol	Mass	Ionization Energy
Lithium	Li	6.941	5.3917
Beryllium	Be	9.012182	9.3227
Boron	B	10.811	8.2980
Carbon	C	12.0107	11.2603
Nitrogen	N	14.0067	14.5341
Oxygen	O	15.9994	13.6181
Fluorine	F	18.9984032	17.4228
Neon	Ne	20.1797	21.5645
Sodium	Na	22.98976928	5.1391
Magnesium	Mg	24.3050	7.6462
Aluminium	Al	26.9815386	5.9858
Silicon	Si	28.0855	8.1517

Inorganic molecules





Show 100 entries
Search:

Name	Formula	Compound Label	Boiling Point (K)
Sodium Oxide	Na_2O	Oxide	2223
Magnesium Oxide	MgO	Oxide	3873
Aluminum Oxide	Al_2O_3	Oxide	3250
Silicon Dioxide	SiO_2	Oxide	2503
Phosphorus(III) Oxide	P_4O_6	Oxide	173.1
Phosphorus(V) Oxide	P_4O_{10}	Oxide	633
Sulfur Dioxide	SO_2	Oxide	263
Sulfur Trioxide	SO_3	Oxide	318
Chlorine Dioxide	ClO_2	Oxide	284

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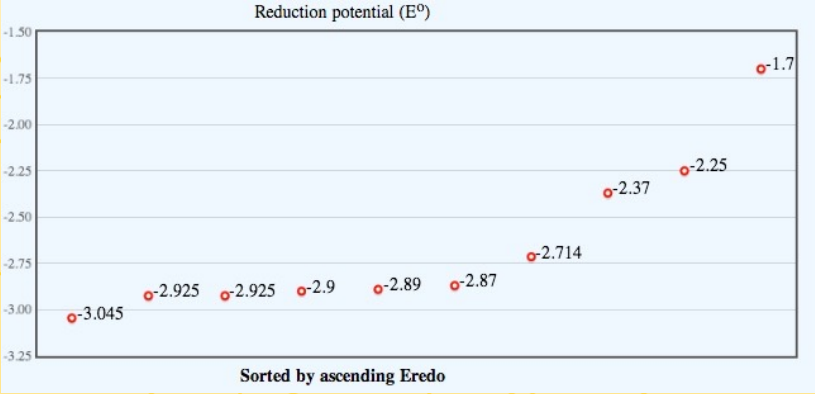
Reaction data

Redox reactions



Select all | Select None | Click rows to select (Shift fo

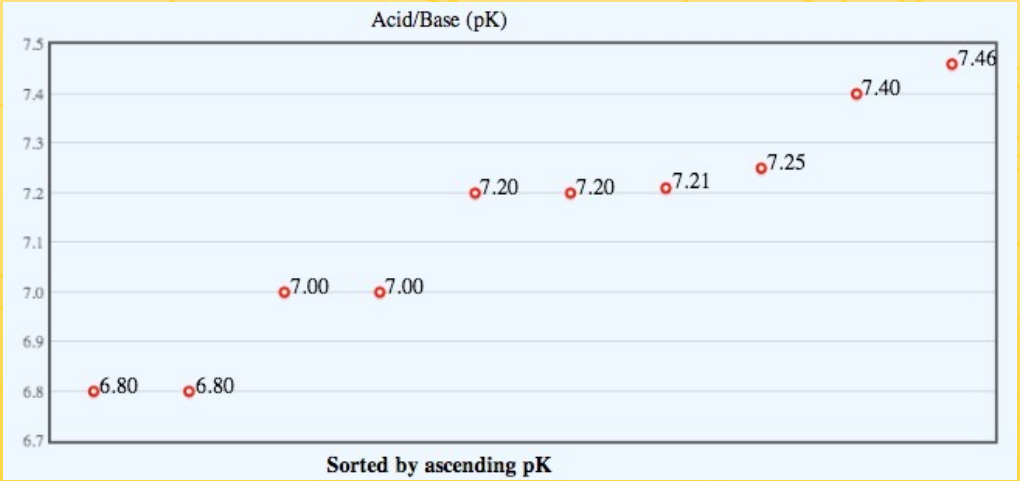
Show 10 entries

Search:

Reactants	Products	Labels	E_{red}^{o}
$Li^{(+)}_{(aq)} + e^{(-)}$	$Li_{(s)}$	redox	-3.045
$Rb^{(+)}_{(aq)} + e^{(-)}$	$Rb_{(s)}$	redox	-2.925
$K^{(+)}_{(aq)} + e^{(-)}$	$K_{(s)}$	redox	-2.925
$Ba^{(2+)}_{(aq)} + 2\ e(-)$	$Ba_{(s)}$	redox	-2.9
$Sr^{(2+)}_{(aq)} + 2\ e^{(-)}$	$Sr_{(s)}$	redox	-2.89
$Ca^{(2+)}_{(aq)} + 2\ e^{(-)}$	$Ca_{(s)}$	redox	-2.87
$Na^{(+)}_{(aq)} + e^{(-)}$	$Na_{(s)}$	redox	-2.714
$Mg^{(2+)}_{(aq)} + 2\ e^{(-)}$	$Mg_{(s)}$	redox	-2.37
$H_{2(g)} + 2\ e^{(-)}$	$2\ H^{(-)}_{(aq)}$	redox	-2.25
$SiO_3^{(2-)}_{(aq)} + 3\ H_2O + 4\ e^{(-)}$	$Si_{(s)} + 6\ OH^{(-)}_{(aq)}$	redox	-1.7

Showing 1 to 10 of 115 entries

Acid-Base reactions



Select all | Select None | Click rows to select (Shift for multiple)

Show 10 entries

Search:

Reactants	Products	Labels	pK
$HPO_4^{(2-)} + H_2O$	$H_2PO_4^{(-)} + OH^{(-)}$	Weak base	6.80
$SO_3^{(2-)} + H_2O$	$HSO_3^{(-)} + OH^{(-)}$	Weak base	6.80
$H_2S + H_2O$	$HS^{(-)} + H_3O^{(+)}$	Weak acid	7.00
$HS^{(-)} + H_2O$	$H_2S + OH^{(-)}$	Weak base	7.00
$Cu(H_2O)_5OH^{(+)} + H_2O$	$Cu(H_2O)_6^{(2+)} + OH^{(-)}$	Weak base	7.20
$HSO_3^{(-)} + H_2O$	$SO_3^{(2-)} + H_3O^{(+)}$	Weak acid	7.20
$H_2PO_4^{(-)} + H_2O$	$HPO_4^{(2-)} + H_3O^{(+)}$	Weak acid	7.21
$H_2AsO_4^{(-)} + H_2O$	$HAsO_4^{(2-)} + H_3O^{(+)}$	Weak acid	7.25
$SeO_3^{(2-)} + H_2O$	$HSeO_3^{(-)} + OH^{(-)}$	Weak base	7.40
$HOCl + H_2O$	$OCl^{(-)} + H_3O^{(+)}$	Weak acid	7.46

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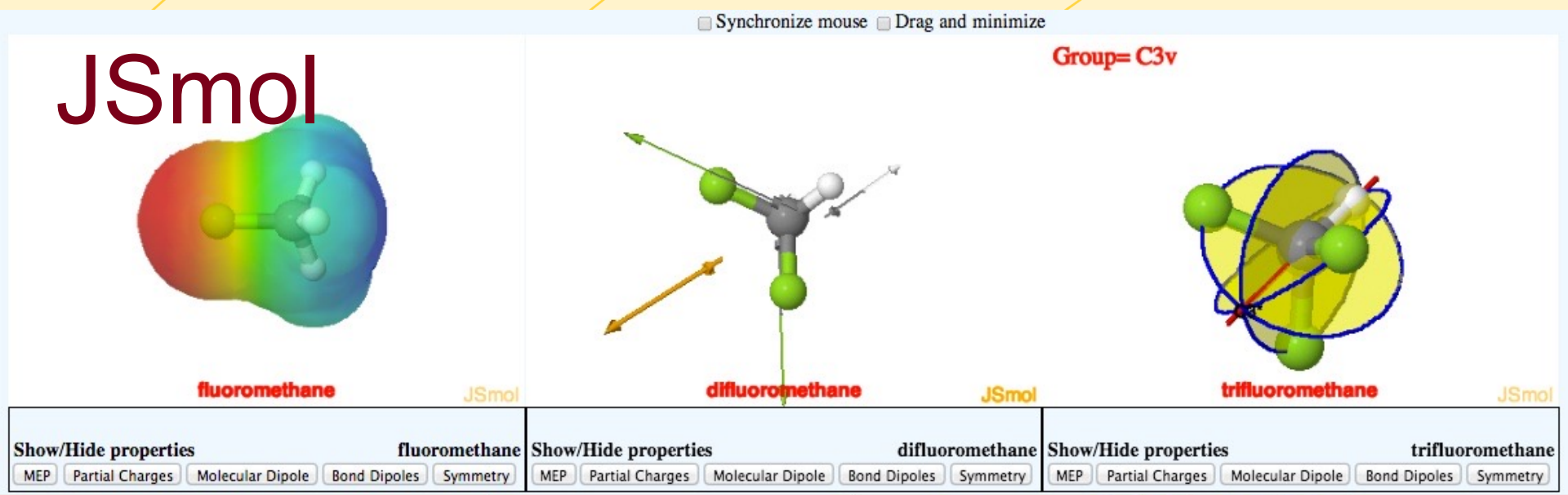
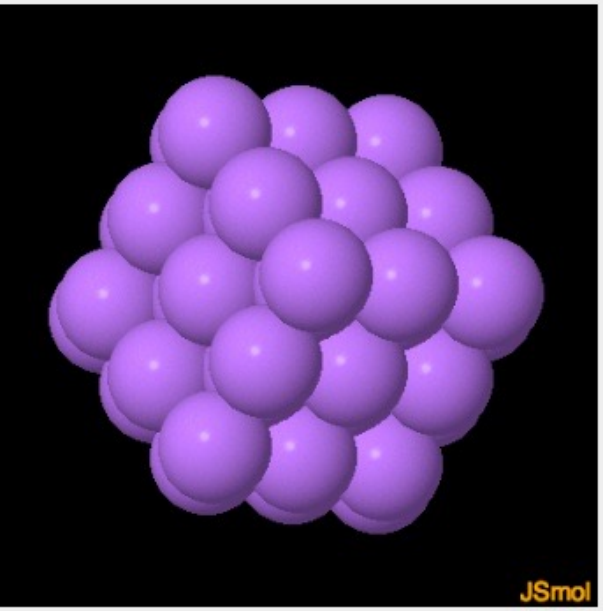
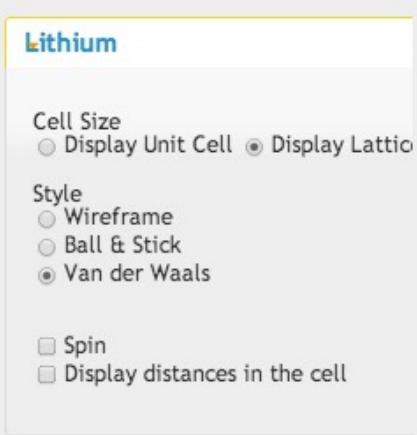
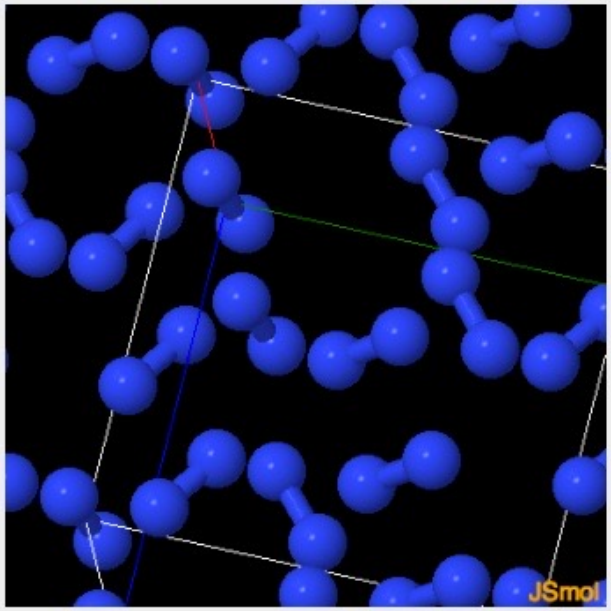
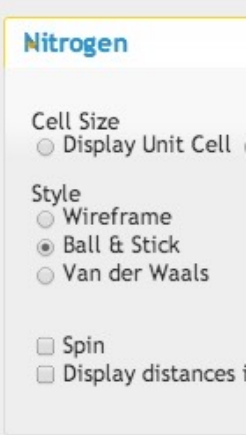
JSmol











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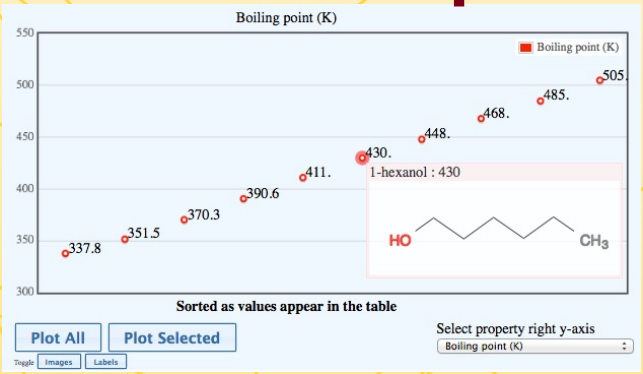
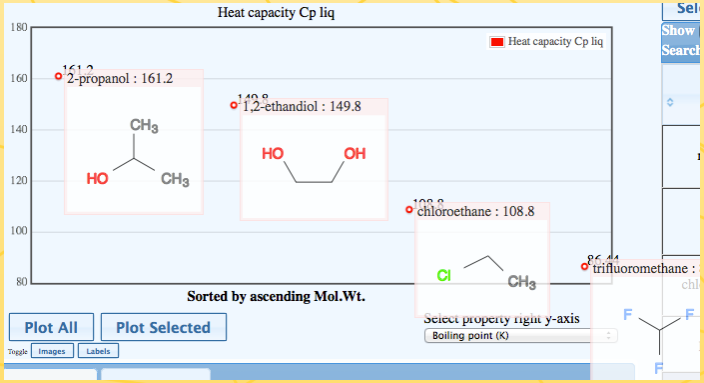
Different questions, different levels



Explanatory questions (pre-selected sets of data. One right answer).
"Why do these molecules show this trend for property X?"



Problem solving questions:(pre-selected sets of data. One right answer)
"If the heavier the molecule the larger the heat capacity. Why does the heat capacity decrease in the following set of data?"

Show evidence: (open-ended)
Choose a set of molecules that show that hydrogen bonds are stronger than dipole-dipole interaction but much weaker than ionic bonds.

Building knowledge: (open-ended)
Choose a set of data to describe what molecular properties have an influence in heat of combustion.

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Implementation

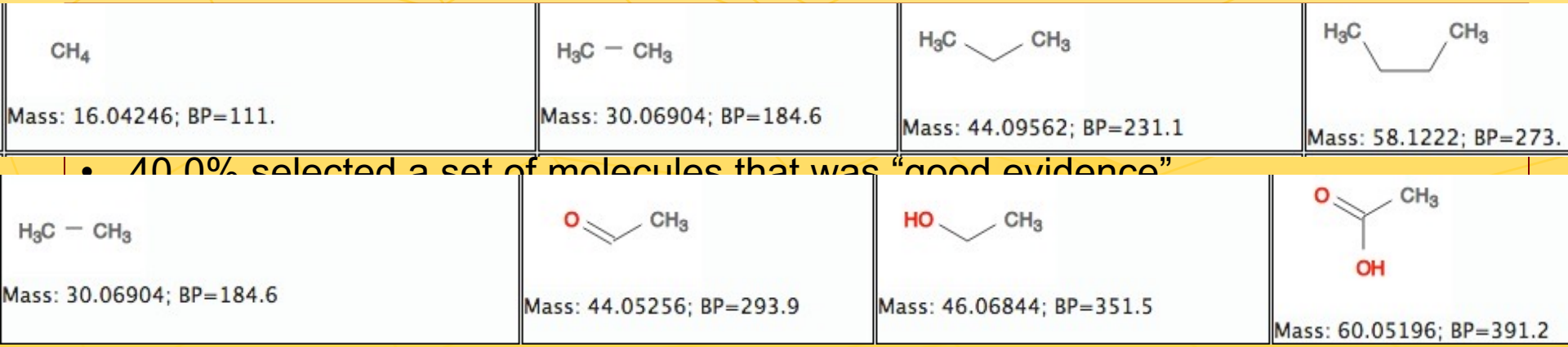
Questions with one right answer. Two kinds of skills:

1. Skill 1: Design an experiment where you minimize correlation vs causation
2. Skill 2: Interpret the experiment without “external interference”.

What is the effect of mass on boiling points? Select a set of molecules that is evidence of your statement. (one right answer)

→100% students gave the correct answer

- 69.8% selected a set of molecules that was “good evidence”
- Out 30.2% who didn’t. 12.7% chose a set of molecules that was proving the opposite of what they said. The right answer for the wrong reason.



- 40.0% selected a set of molecules that was “good evidence”

Implementation

Questions without a right answer. Three kinds of skills:

1. Design an experiment where you minimize correlation vs causation
2. Interpret the experiment without “external interference”.
3. Identify the existence of exceptions.

What has a stronger influence? A heavy molecule with a weak intermolecular force or a light molecule with a strong intermolecular force? Are there exceptions?

- 60.3% said mass has a stronger influence
- 39.7% said intermolecular forces have a stronger influence
- 50.8% chose molecules that was evidence of their statement
- Out of the other 49.2%: 39.7% was inconclusive, but 9.5% was evidence of the opposite and didn’t acknowledge the existence of exceptions.

Conclusions

- Collected properties of organic / Inorganic compounds and reactions
- Representations in plots and 3D Jsmol
- Download data
  ChemEd X Data dataset. figshare. http://dx.doi.org/10.6084/m9.figshare.1121665
- Paper: JCE ASAP
  http://pubs.acs.org/doi/abs/10.1021/ed500316m

- Future directions
  - Include more data to align them with more Chemistry topics
  - Quantitative assessment