

Learning higher-order thinking skills in General Chemistry: Using “*ChemEd X Data*” to teach *students self-regulation*

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<http://goo.gl/33xlc0>



UNIVERSITY OF MINNESOTA ROCHESTER

President's Council of Advisors on Science and Technology (PCAST) 2010:

instructors during the first two years of college must focus on deeper and transferable knowledge

P. Atkins. Pure Appl. Chem., Vol. 71, No. 6, pp. 927-929, 1999.

“...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”

Atomic size and ionization

Nuclear charge

Electronic shielding

Orbital size

Example Radius:

$r(\text{O}) < r(\text{Cl})$

$r(\text{Li}) > r(\text{Mg})$

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

DATA FIRST!



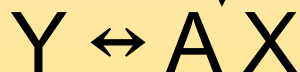
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Structure-property relationships in 1st semester of General Chemistry

Properties of Substance

Substances

Electronic or molecular structure



*(it's never one single factor
... and sometimes they come into conflict)*

Electronic ground state of elements \leftrightarrow Aufbau principle + Hund's rule

Atomic size and ionization energy \leftrightarrow Nuclear charge + shielding + orbital size

Ionic lattice energy of crystal solids \leftrightarrow Cation's and anion's size and charge

Boiling point of molecular solids \leftrightarrow Intermolecular forces + shape + mass

Heat capacity of molecular solids \leftrightarrow Intermolecular forces + bonds + mass



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Data-driven exercises

Static, “precooked”
data

Remember



Understand



The web

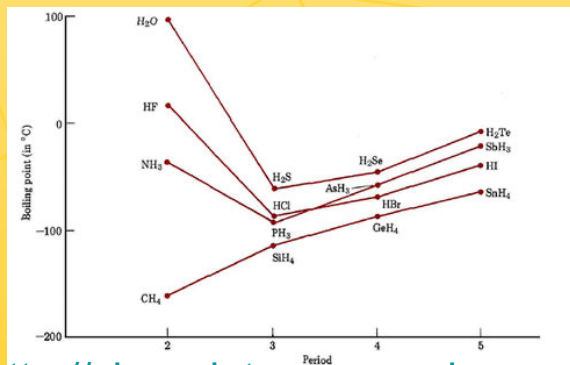
Apply

Unstructured data
Non-linear
Non-sequential
Open-ended

→ Evaluate
Create

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



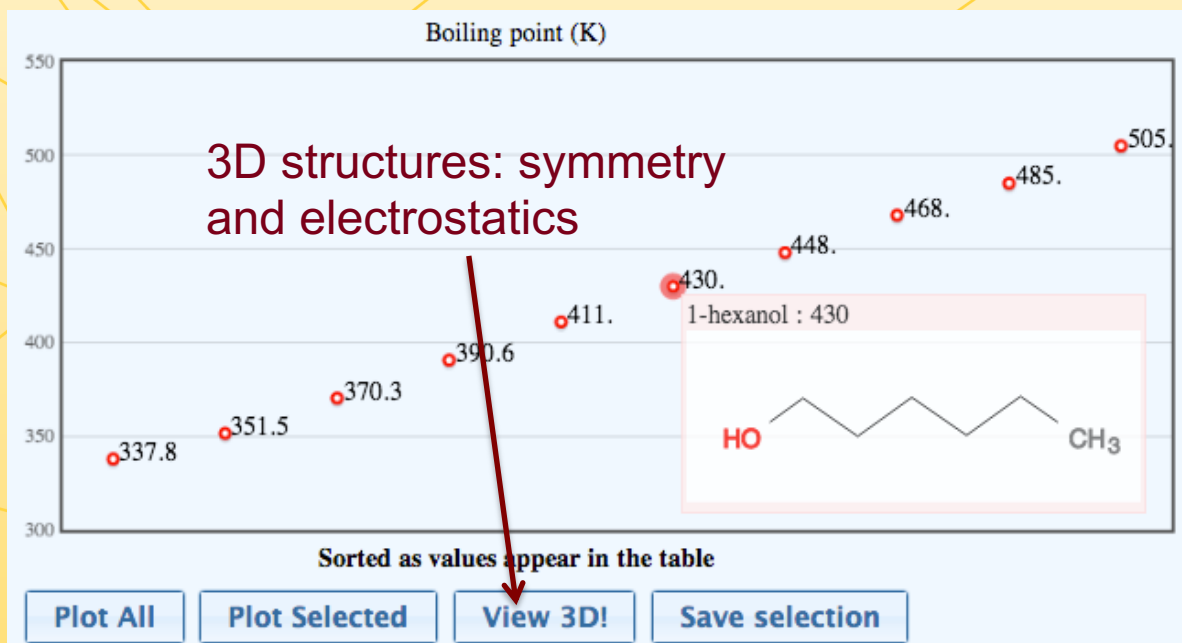
**Skills required: Self-regulation
Self-evaluation**



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<http://chemdata.r.umn.edu>

Order and filter



Select all Select None Click to select rows

Show 10 entries

Search:

Name	Image	Mol. Wt.	Numb. Carbons	Labels	Boiling point (K)
methanol		32.0	1	alcohols, linear	337.8
ethanol		46.1	2	alcohols, linear	351.5
propanol		60.1	3	alcohols, linear	370.3
1-butanol		74.1	4	alcohols, linear	390.6
1-pentanol		88.1	5	alcohols, linear	411.
1-		102.2	6	alcohols,	430.

Fun

Molecular Properties

- ☐ Alkanes
- ☒ Alcohols
- ☐ Aldehydes
- ☐ Haloalkanes
- ☐ Ethers
- ☐ Carboxylic

Phase Change

Reactions

Solubility

- ☒ Boiling point (K)
- ☐ Melting point (K)
- ☐ Heat capacity liq(J/mol*K)
- ☐ Heat capacity gas(J/mol*K)
- ☐ $\Delta H_{\text{vaporiz}}$ (kJ/mol)
- ☐ ΔH_{fusion} (kJ/mol)

- ☐ ΔH_{form} gas (kJ/mol)
- ☐ ΔH_{form} liq (kJ/mol)
- ☐ ΔH_{comb} gas (kJ/mol)
- ☐ ΔH_{comb} liq (kJ/mol)

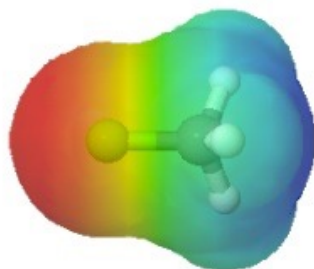
- ☐ Solubility
- ☐ Henry's K (mol/kg*bar)

Select func. groups and properties.
Hundreds of compounds.

<http://chemdata.r.umn.edu>

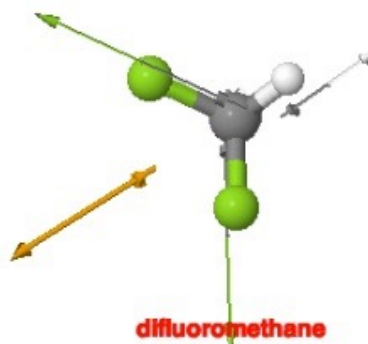
☐ Synchronize mouse ☐ Drag and minimize

Group= C3v



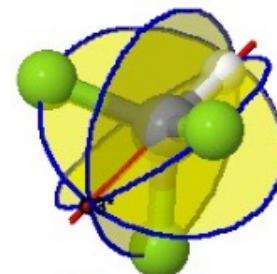
fluoromethane

JSmol



difluoromethane

JSmol



trifluoromethane

JSmol

Show/Hide properties

fluoromethane

☐ MEP ☐ Partial Charges ☐ Molecular Dipole ☐ Bond Dipoles ☐ Symmetry

Show/Hide properties

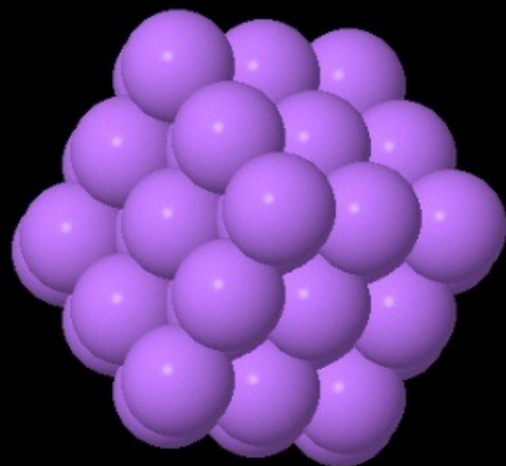
difluoromethane

☐ MEP ☐ Partial Charges ☐ Molecular Dipole ☐ Bond Dipoles ☐ Symmetry

Show/Hide properties

trifluoromethane

☐ MEP ☐ Partial Charges ☐ Molecular Dipole ☐ Bond Dipoles ☐ Symmetry



JSmol

Lithium

Cell Size

☐ Display Unit Cell ☒ Display Lattice

Style

☐ Wireframe
☐ Ball & Stick
☒ Van der Waals

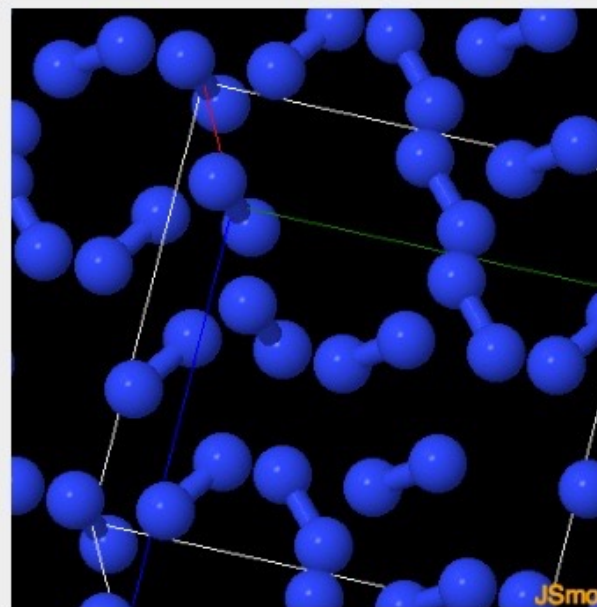
☐ Spin

☐ Display distances in the cell

Popup window

Take a picture

Reset



JSmol

Nitrogen

Cell Size

☐ Display Unit Cell ☒ Display Lattice

Style

☐ Wireframe
☒ Ball & Stick
☐ Van der Waals

☐ Spin

☐ Display distances in the cell

Popup window

Take a picture

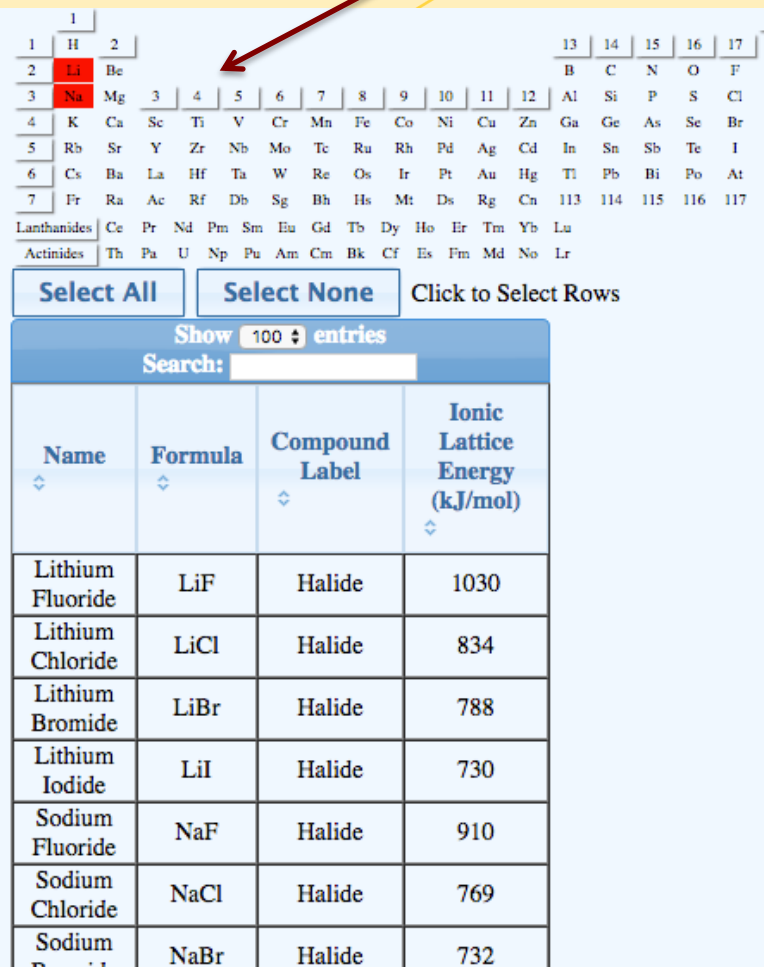
Reset

Experimental and computed data



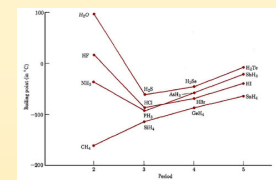
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Periodic table for easy selection

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Using ChemEdXData

Example 1: Boiling point of molecular solids



The exercise had several questions classified here according to its cognitive level

Level 1: (*remember*) Recognize intermolecular forces present in molecules

Level 2-3: (*understand*) Mass or dipole in the series of CH_3F , CH_2F_2 , CHF_3 , CF_4

Level 2-3 : (*apply*) Which of the following datasets are good “controlled experiments” or “Control Variable Strategy” (CVS)

$\text{H}_3\text{C} - \text{CH}_3$ Mass: 30.06904; BP=184.6	 Mass: 44.05256; BP=293.9	 Mass: 46.06844; BP=351.5	 Mass: 60.05196; BP=391.2
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Level 4: (*build*) Build a controlled experiment or “Control Variable Strategy” (CVS) to investigate the role of mass in boiling points of molecules

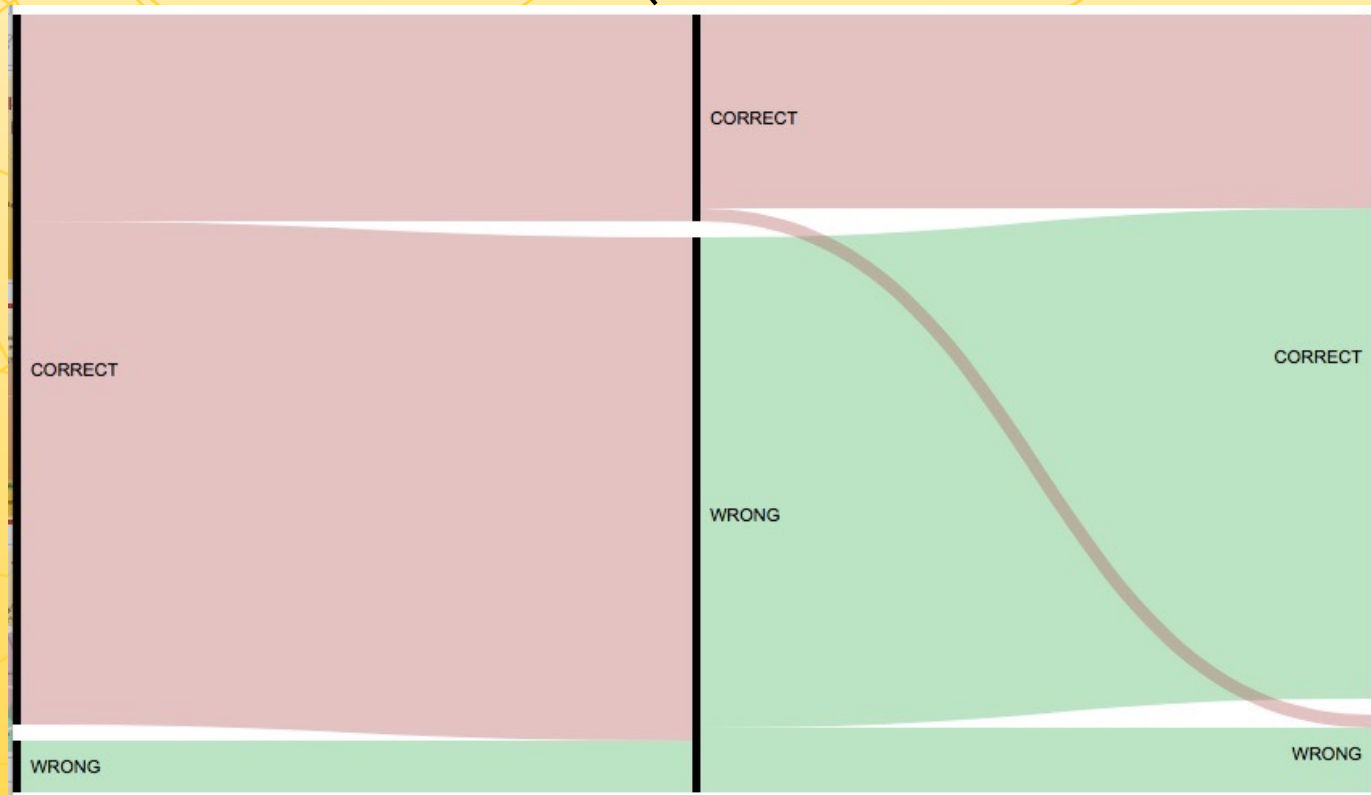
Using ChemEdXData

Example 1: Boiling point of molecular solids

Remember
Intermol Force
Level 1

Build CVS
Role of IMF in BP
Level 4

Apply
Rank IMF in BP
Level 2-3



→ Students cannot build the CVS but they have understood the trend and can successfully answer the ranking

The same it's true for the effect of mass and shape



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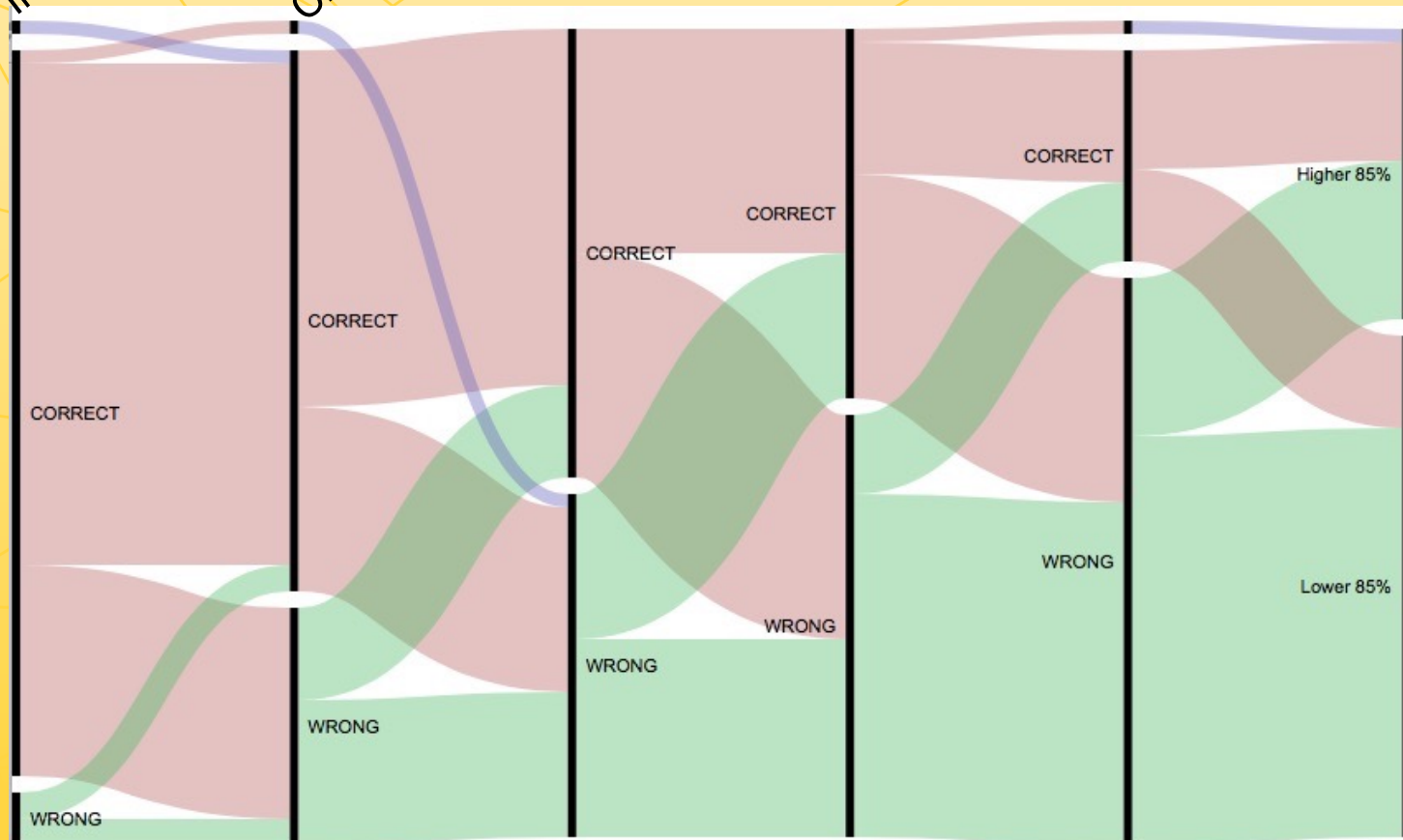
Example 1: Boiling point of molecules

Level 1
Remember
Intermol Forc.

Level 2-3
Mass or dipole?
 CH_xF_y
Recognize
good CVS

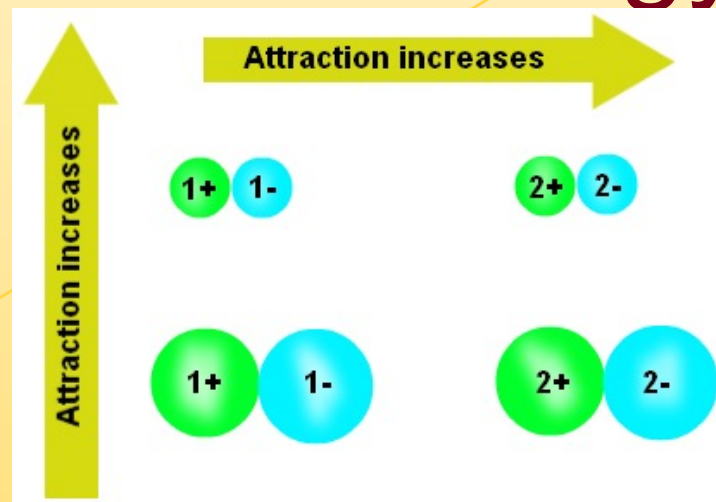
Level 4
Build CVS
Mass role
Build CVS
IMF role

Final course
grade



Using ChemEdXData

Example 2: Ionic lattice energy of crystal solids



The exercise had several questions classified here according to its cognitive level

Level 1: (*remember*) Coulomb's law, size and charge of ions

Level 2-3: (*understand/apply*) Predict substances with highest ionic lattice energy

Level 4: (*evaluation*) Recognize limit of prediction when there is a conflict between factors

Example 2: Ionic lattice energy of crystal solids

Coulombic
Interaction

Charge and size
of ions

Predict with
no conflict

Predict: recogn.
limit of prediction

Can this theory
explain experiment

Final course
grade

Wrong

Wrong

Wrong

Correct

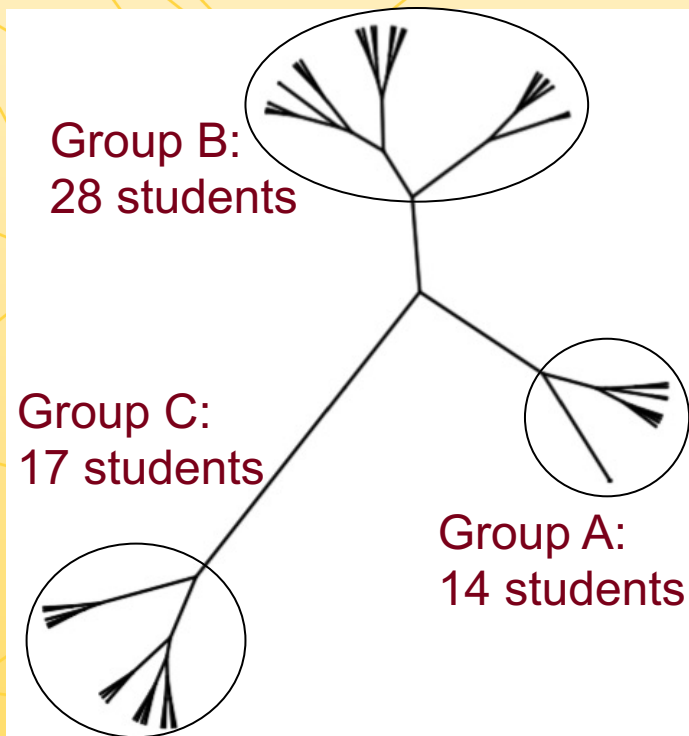
Correct

Correct

Based on what you answered above, the compound with the strongest bond energy (ionic lattice energy is)

NaF / CsI / Cant' predict

Example 2: Ionic lattice energy of crystal solids



	Group B n = 28	Group C n = 17	Group A n = 14
Course Grade	81.0±9.2	79.0±6.2	88.0±5.5
Ionic energy survey	62.7±14.2	31.7±9.3	88.1±12.9
Conflicting factors questions	14.3±26.2	8.8±19.1	85.7±22.6

Hierarchical cluster analysis (Ward's minimum variance method)
using the results for the “Ionic lattice energy” survey



Conclusions

- ChemEd X Data was used to practice higher-level cognitive skills in introductory courses and collect student data for its analysis.
 - Using data-first students learn by themselves
- We have identified several activities as higher-level such as:
 - Learning “Control of variable strategies” in boiling point of molecules and identifying the limit of predictability in ionic bond models.
 - Students who do well in identifying “limits of predictability” obtain the highest course grades



ChemEdXData on GSpreadsheets

