ChemEdXData: experimental and computational data for general and physical chemistry

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http://goo.gl/892xo0

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Outline

- Using the web for data-driven exercises
- Bring educational web resources to common places
- ChemData: Make web resources last
- How to use the API
- GoogleSpreadsheets:
  - Resources for General Chemistry
  - Resources for Physical Chemistry

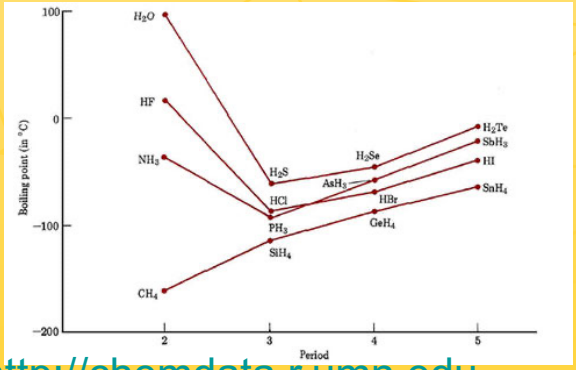
Data-driven exercises

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



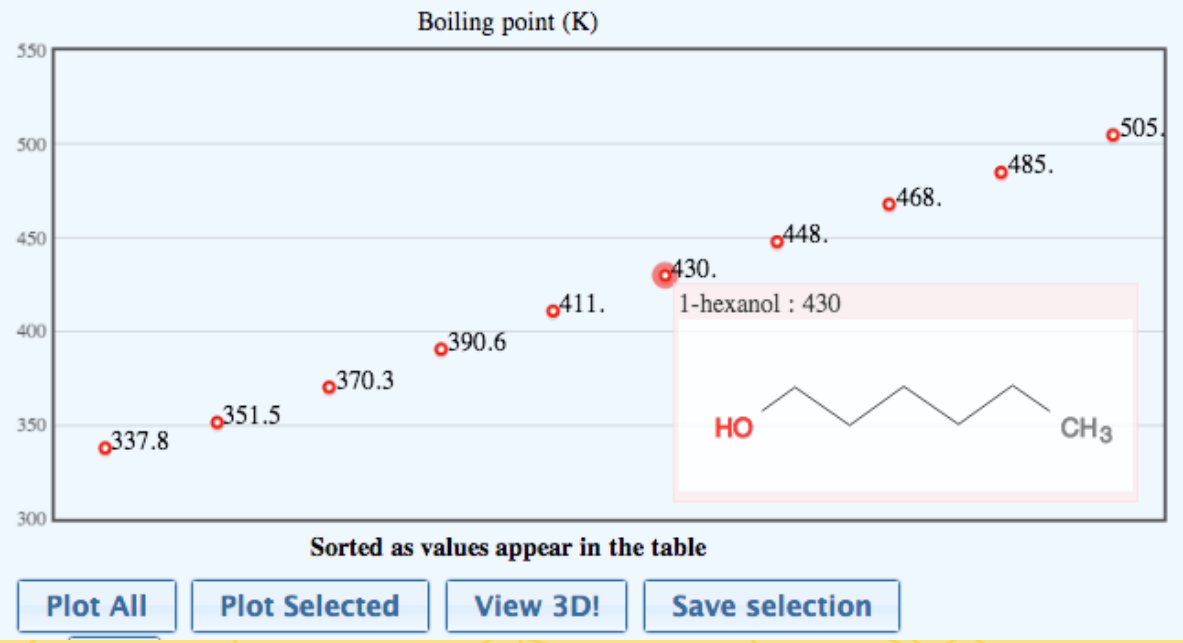
1. Choose some data
2. Represent it
3. Find patterns
4. Find exceptions

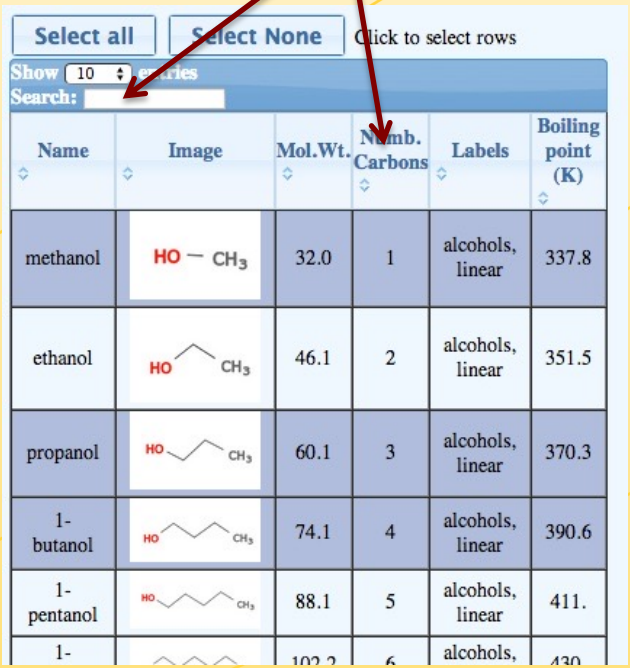
Skills required: Self-regulation
Self-evaluation

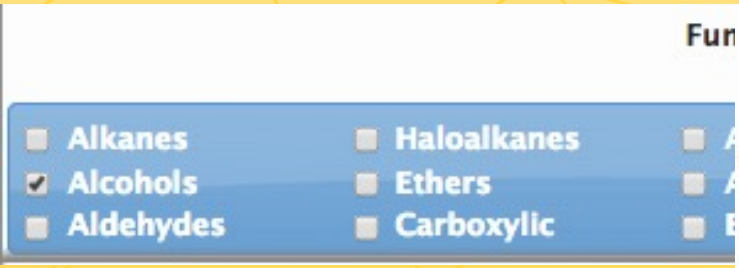
http://chemdata.r.umn.edu

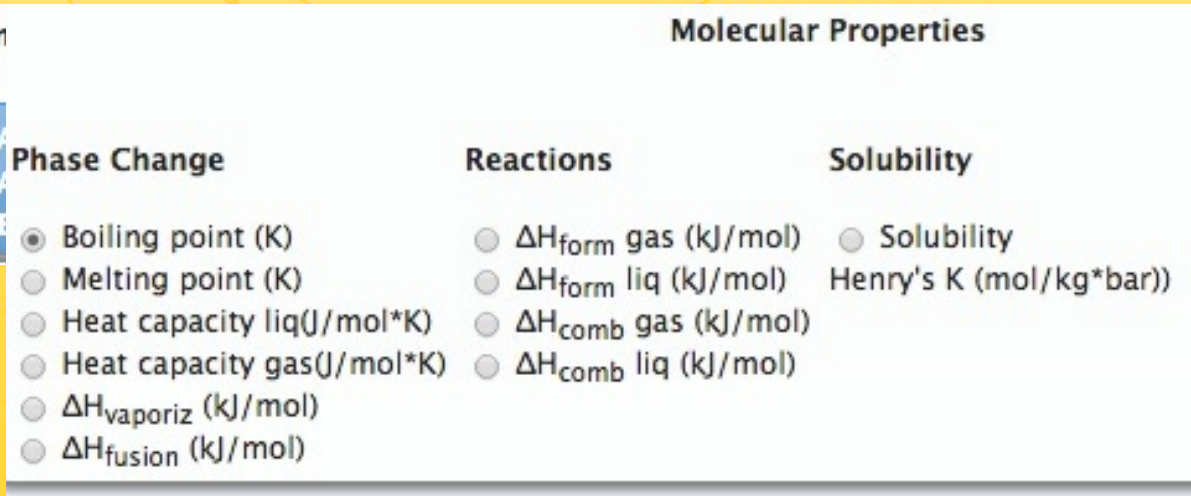
Organic molecules

Sorting, filtering tables









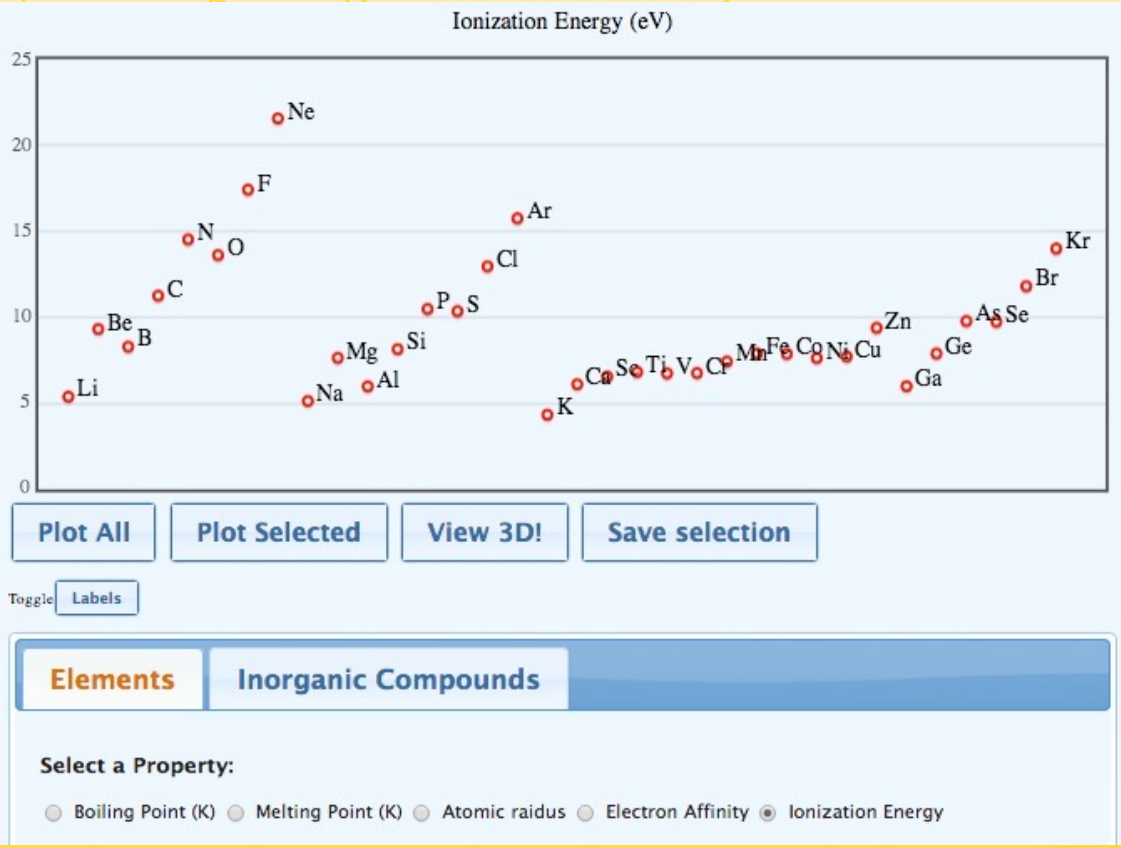
ChemEd X Data

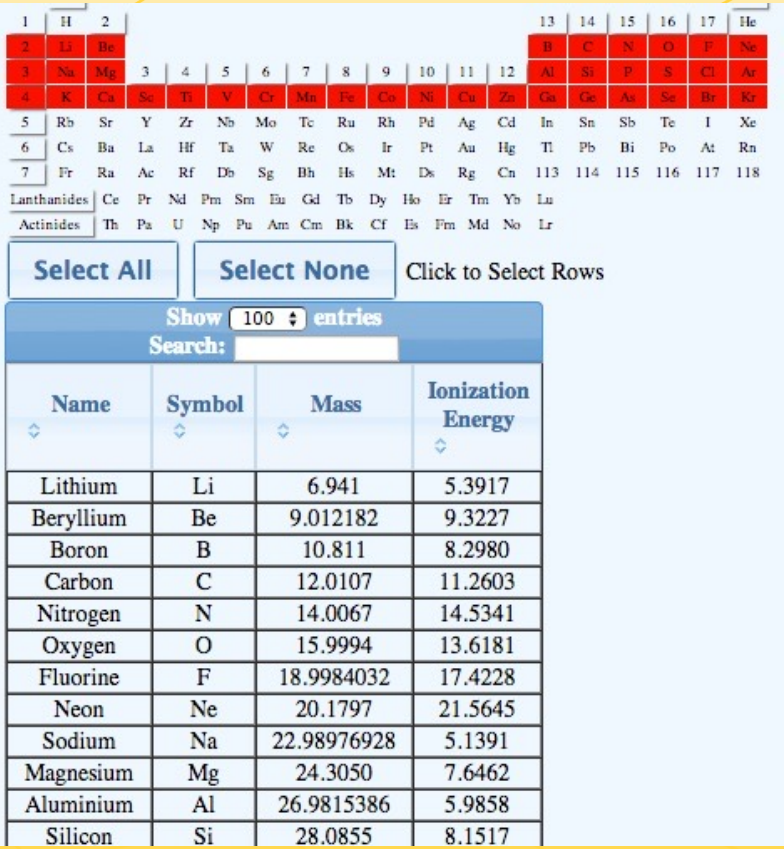
http://chemdata.r.umn.edu

J. Chem. Educ., 91(9), 1501-1504, 2014

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

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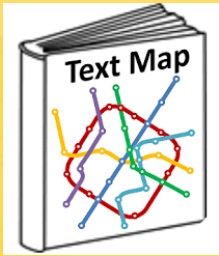
Feedback on ChemEdXData web

- Reviewers: It would be nice if you could plot different functional groups with diff. colors.
- Students: How can I add more sets?
- For educational web resources one must optimize the “user friendliness” and avoid any technical barrier: bring them to common places

For student activities

For authors of resources

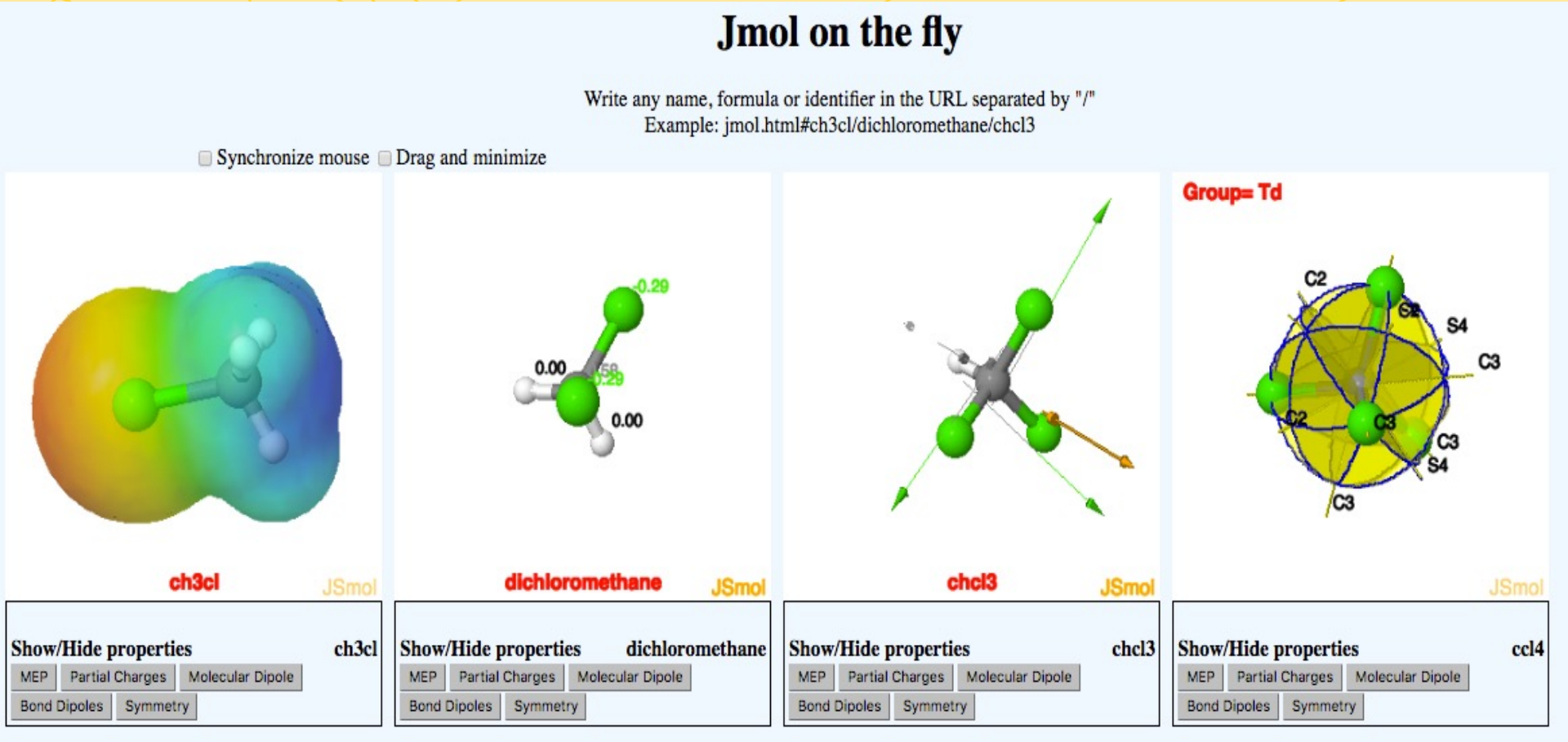


So I’m going to build a new “database”

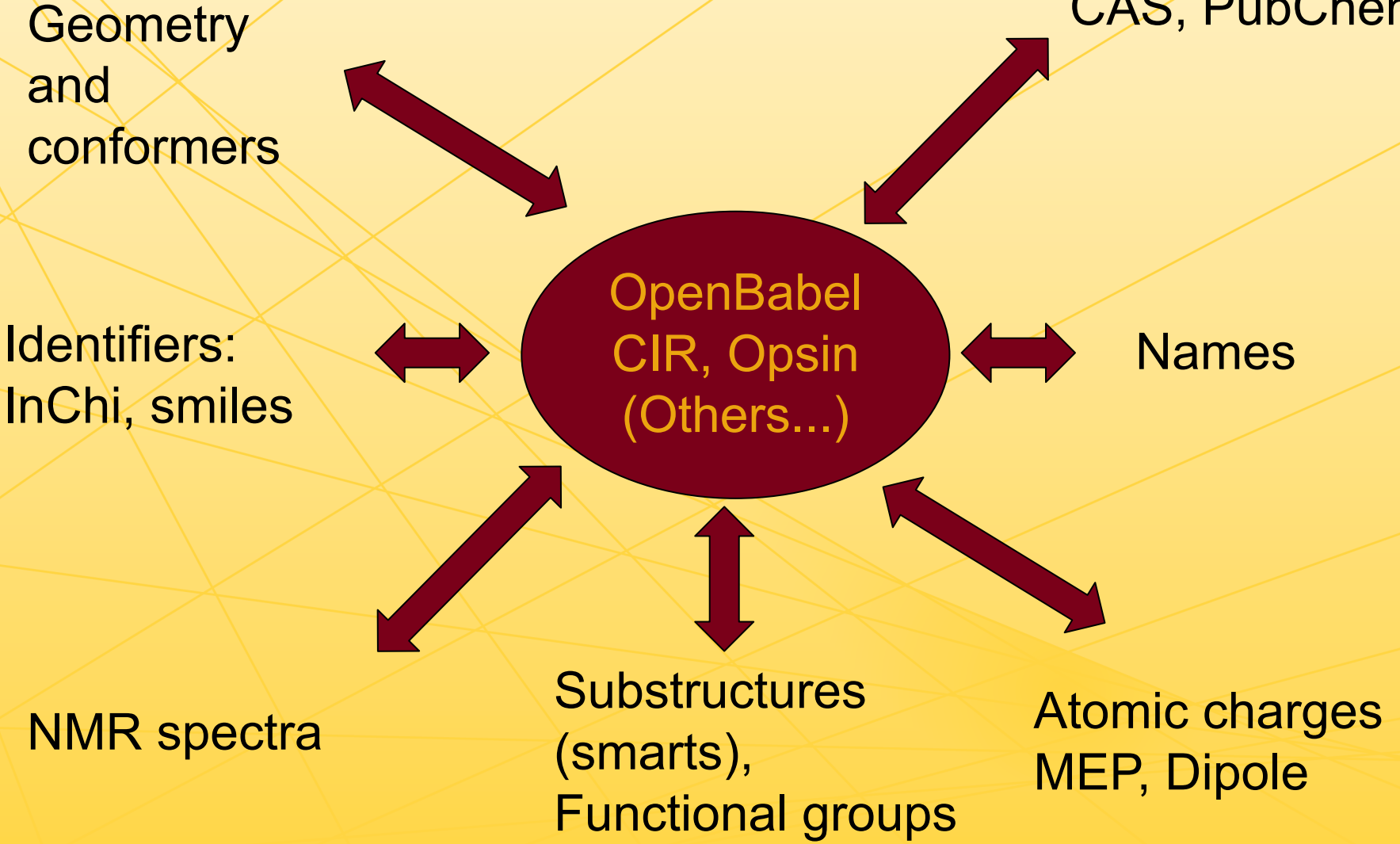
Why do we need yet another DB?

Depending on what you want, one does not need to build a collection or a database.

http://chemdata.r.umn.edu/jmol/#ch3cl/dichloromethane/chcl3/ccl4



Cheminformatics



How to bring educational data to common places and make them last?

Calculations

No binary database
Platform independent
No external connections

Pedagogical Collections

API

No dependecies
JSON: Easy to add/modify/remove
…but not for the uninitiated...

http://chemdata.r.umn.edu/api/?collection==organic&name==Chloromethane

[{ "Chloromethane": { "cpliq": "81.2", "ncarbons": "1", "natoms": "5", "elements": [6, 17, 1], "name": "chloromethane", "hfliq": "-102.4", "bp": "247.", "kh": "0.094", "ids": { "cas": "74-87-3", "inchi": "InChI=1S/CH3Cl/c1-2/h1H3", "inchikey":

ChemEdXData

Third-party

Spreadsheets

For everyone **For authors** **For student activities**

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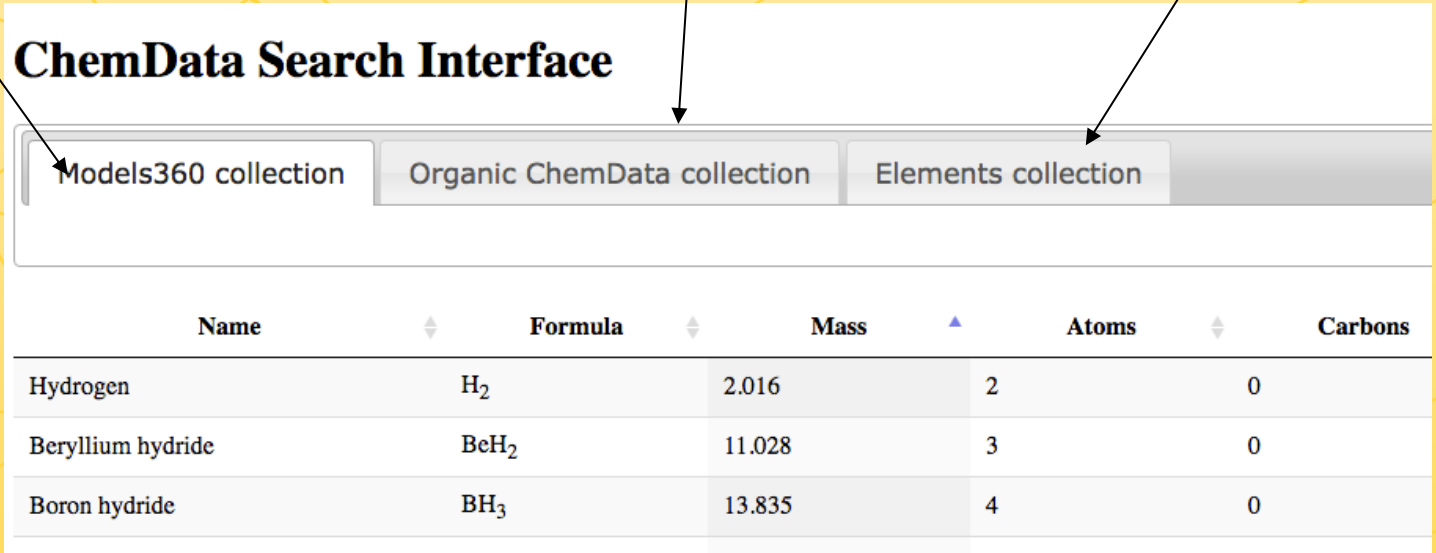
API: ChemData Collections

Quantum calculations:
Vibrations, MO, Dipoles
918 molecules

Organic: Experimental data
BP, MP, ΔH, C_v, K
355 molecules

Elements:
cov, ionic radii, MP, BP
consecutive IE, density

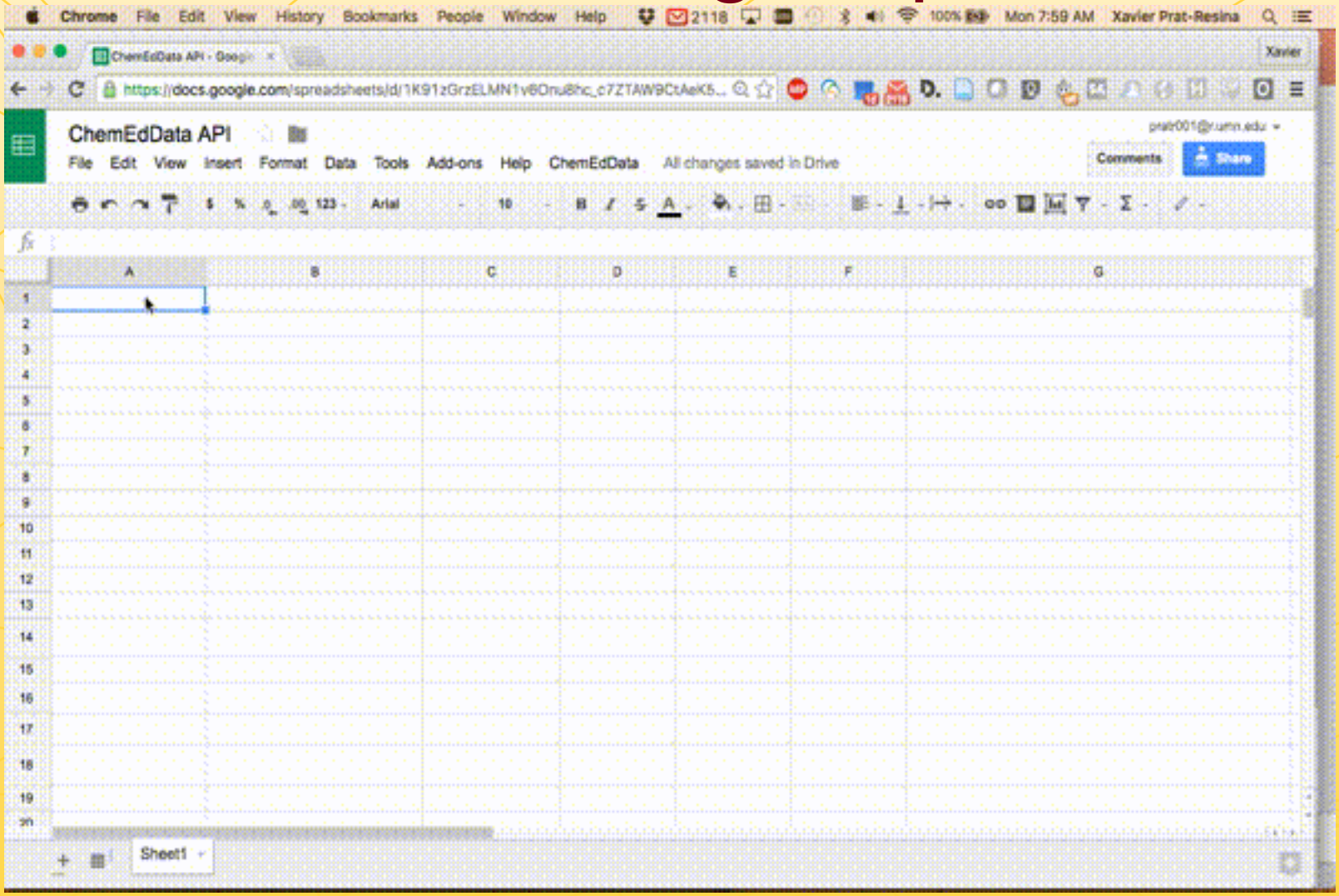


Name	Formula	Mass	Atoms	Carbons
Hydrogen	H_2	2.016	2	0
Beryllium hydride	BeH_2	11.028	3	0
Boron hydride	BH_3	13.835	4	0

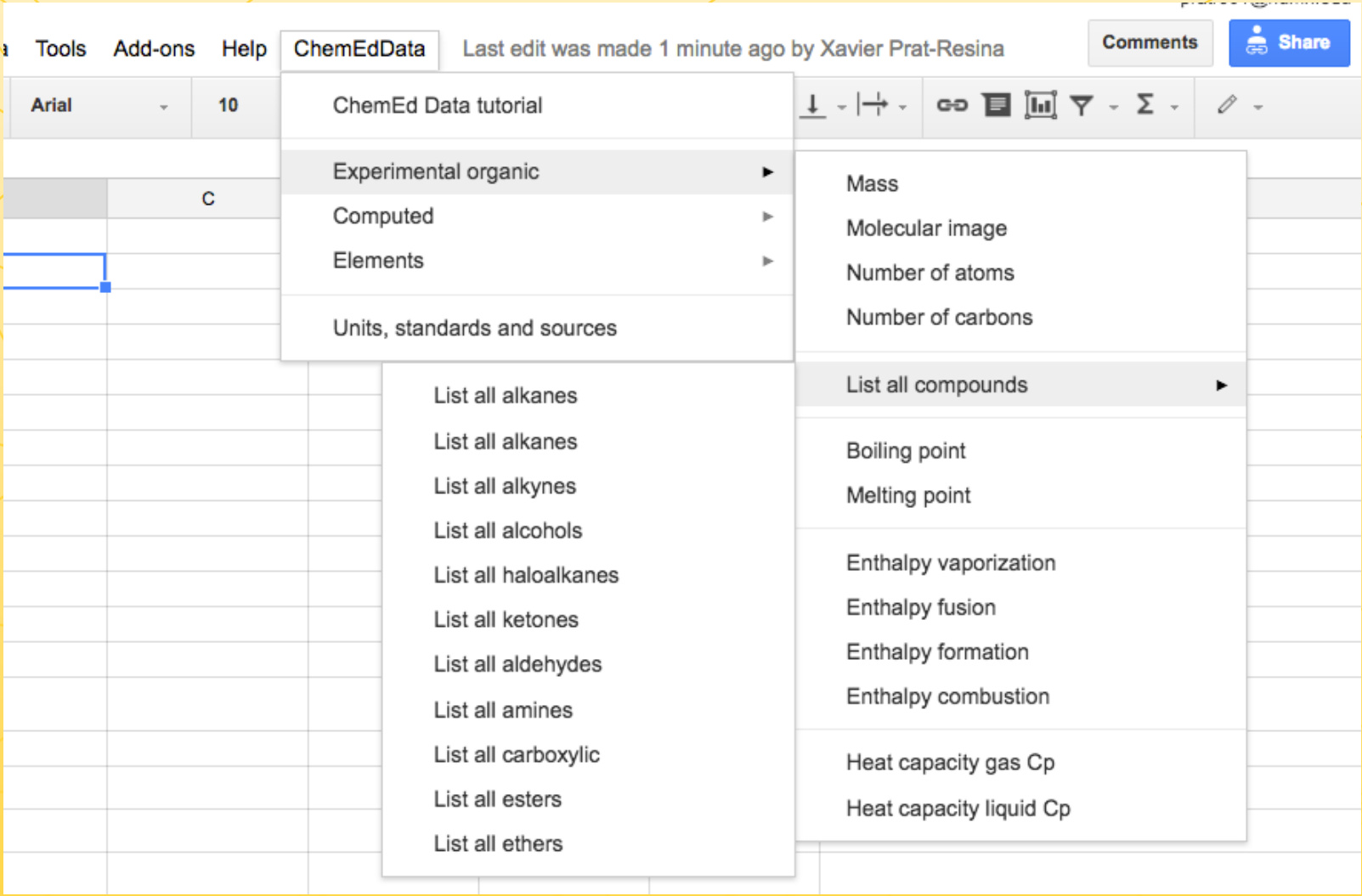
http://chemdata.r.umn.edu/api/tables.php

For student activities

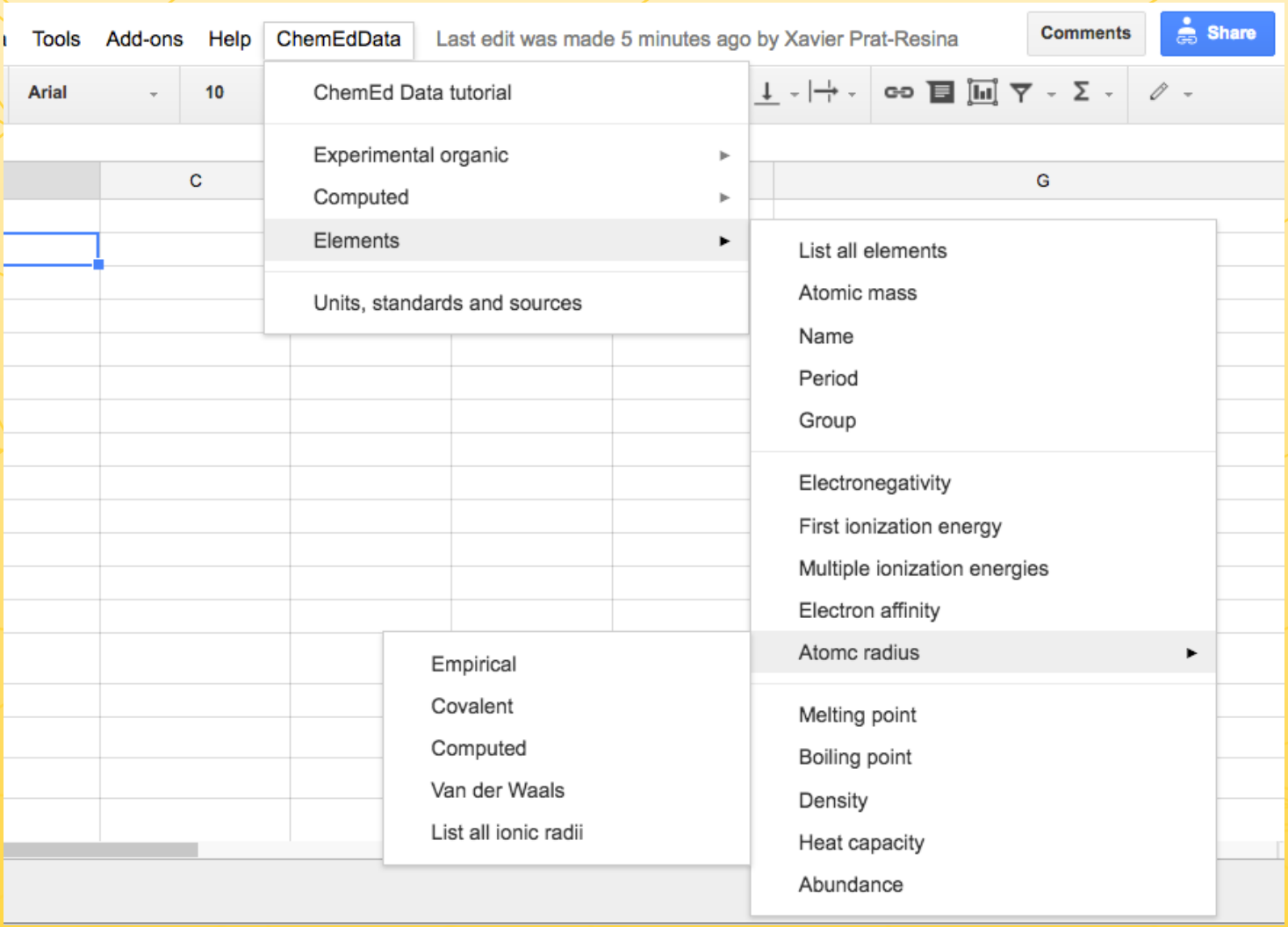
ChemData on Google Spreadsheets



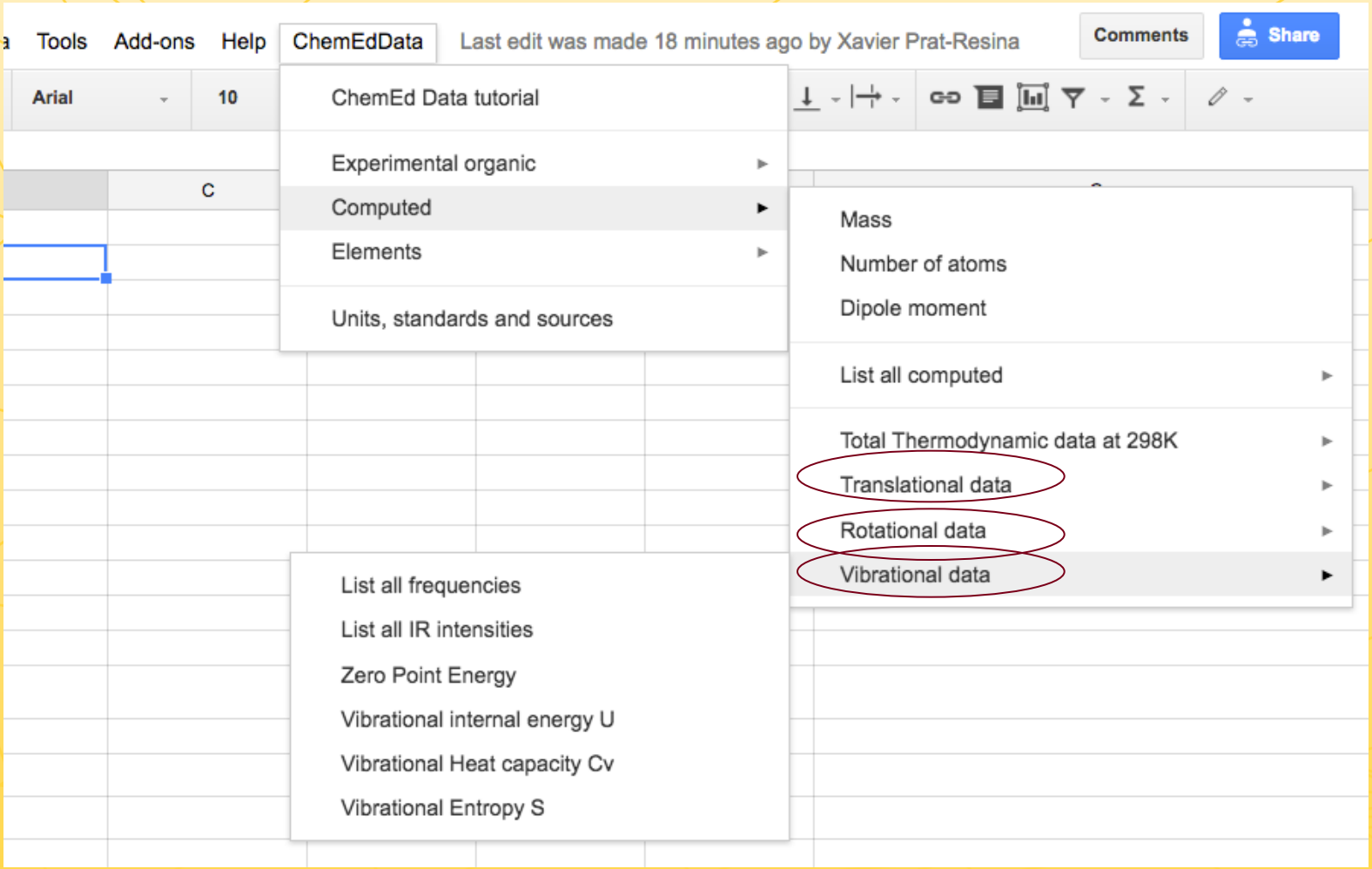
ChemData+GoogleSpreadsheets



ChemData+GoogleSpreadsheets



Data-driven exercises in PChem



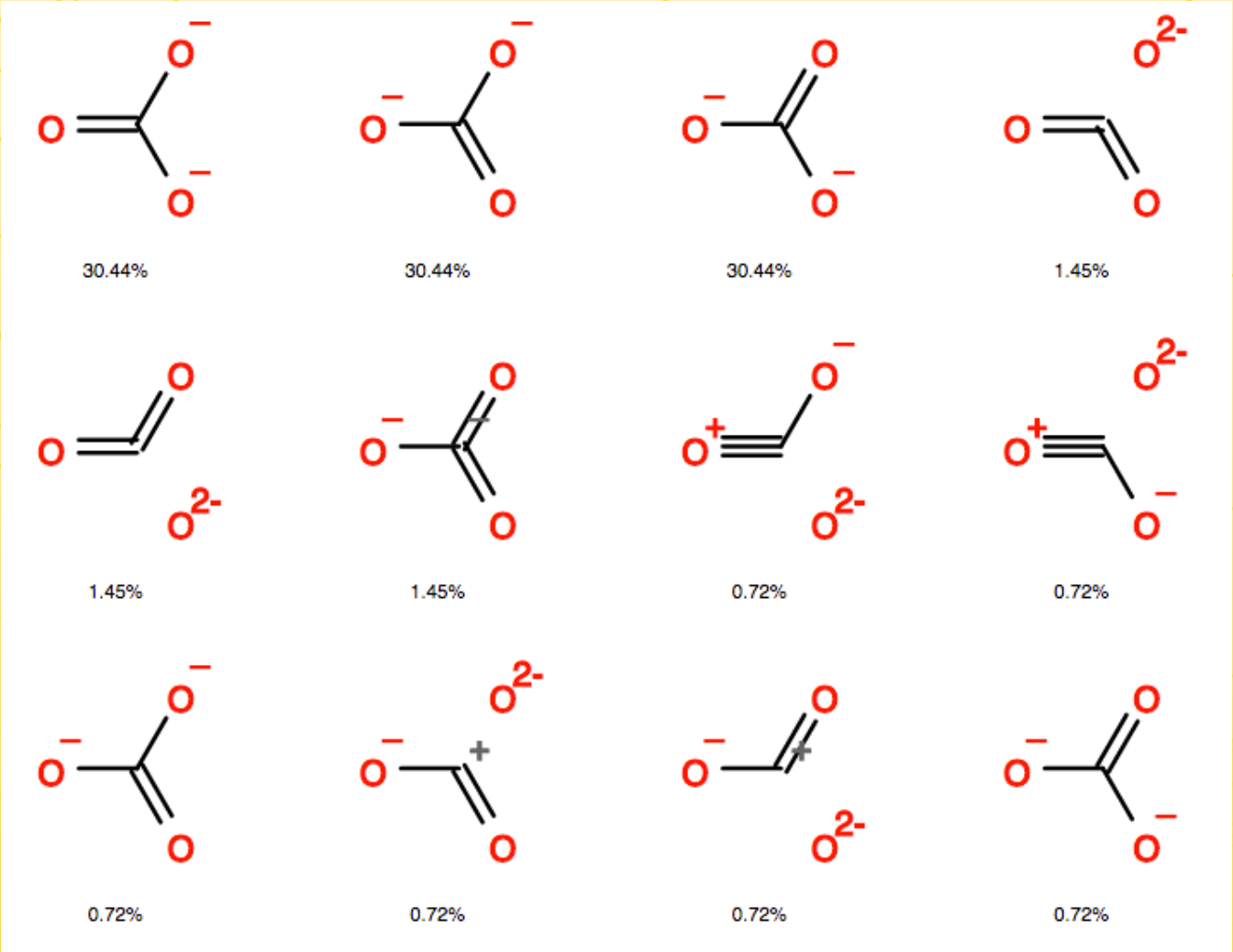
U,Cv,S

Θ_{rot},

ZPE

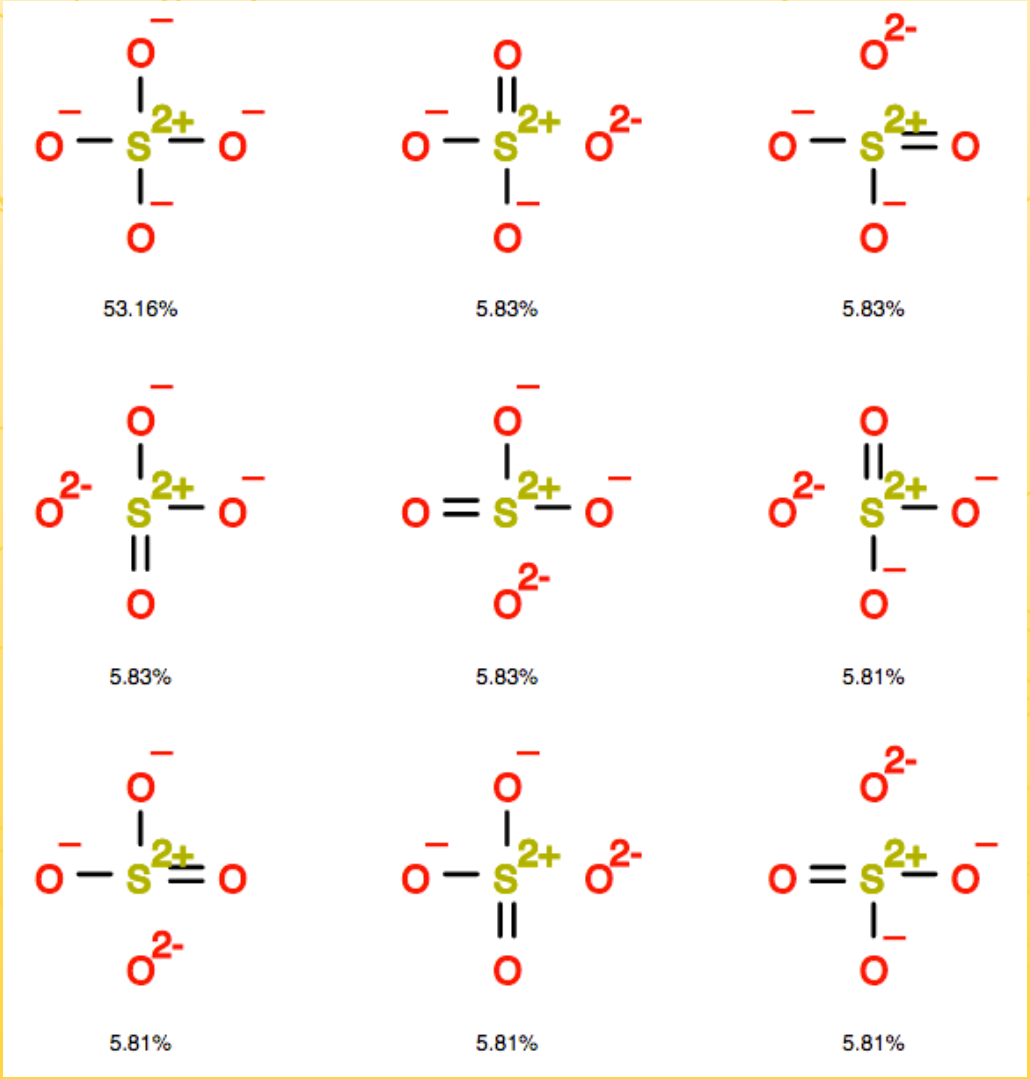
Calculated resonant structures

http://chemdata.r.umn.edu/api/?collection==models360&name==Carbonate%20ion&image==nrt



NRT: Weinhold's Natural Resonance Theory

Calculated resonant structures



http://chemdata.umr.umn.edu/api/?collection==models360&name==sulfate%20ion&image==nrt

Conclusions

- ChemEdXData works on the web but we need to bring Chemistry resources to “common places”
- The ChemData API is designed to make resources last longer, open and independent.
- It can be used in the class for data-driven exercises in General Chemistry and Physical Chemistry using Google SpreadSheets.