

ChemEdXData: experimental and computational data for general and physical chemistry

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Center for Learning Innovation

<http://goo.gl/892xo0>



UNIVERSITY OF MINNESOTA ROCHESTER

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

Remember



Understand



The web

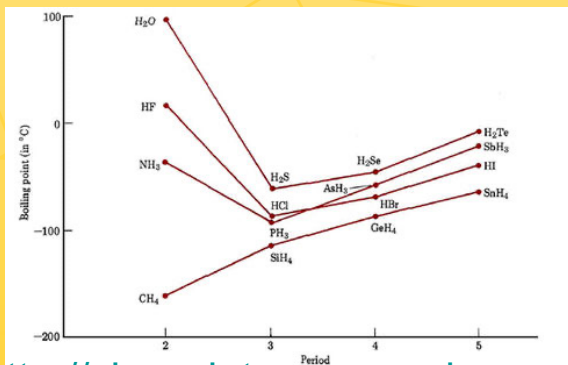
Apply

Unstructured data
Non-linear
Non-sequential
Open-ended

→ 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



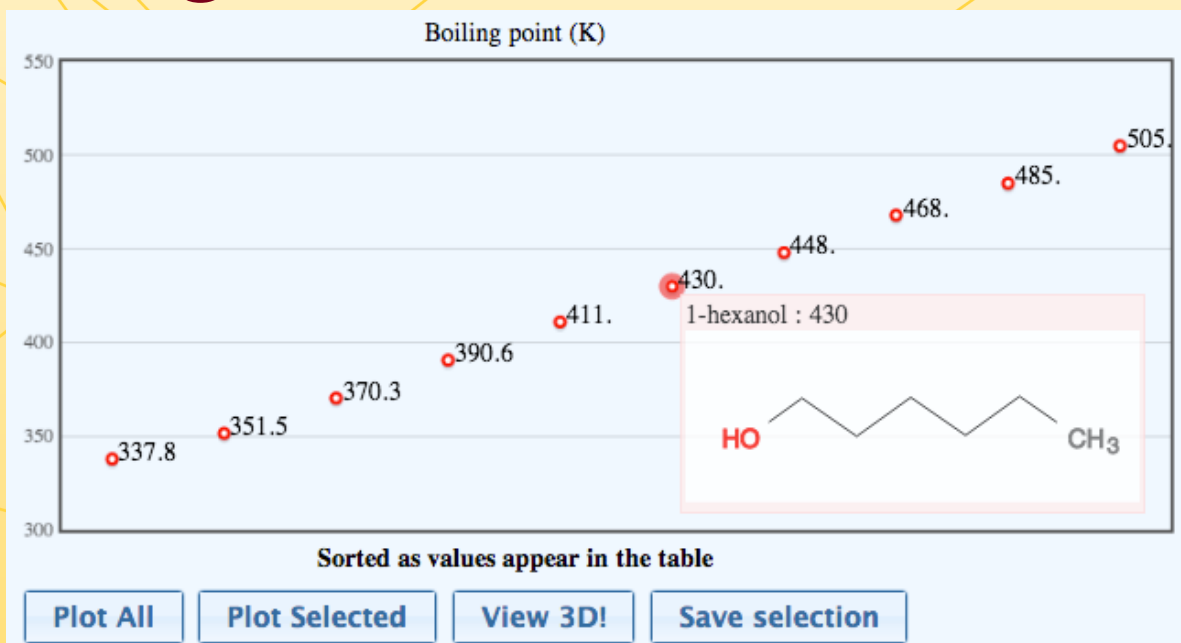
**Skills required: Self-regulation
Self-evaluation**



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Organic molecules

Sorting, filtering tables



Select all Select None Click to select rows

Show 10 entries

Search:

Name	Image	Mol. Wt.	Numb. Carbons	Labels	Boiling point (K)
methanol	<chem>CO</chem>	32.0	1	alcohols, linear	337.8
ethanol	<chem>CCO</chem>	46.1	2	alcohols, linear	351.5
propanol	<chem>CCCO</chem>	60.1	3	alcohols, linear	370.3
1-butanol	<chem>CCCCO</chem>	74.1	4	alcohols, linear	390.6
1-pentanol	<chem>CCCCCO</chem>	88.1	5	alcohols, linear	411.
1-hexanol	<chem>CCCCCCO</chem>	102.2	6	alcohols, linear	430.

Fur

Molecular Properties

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

Phase Change

- ☒ 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)

Reactions

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

Solubility

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

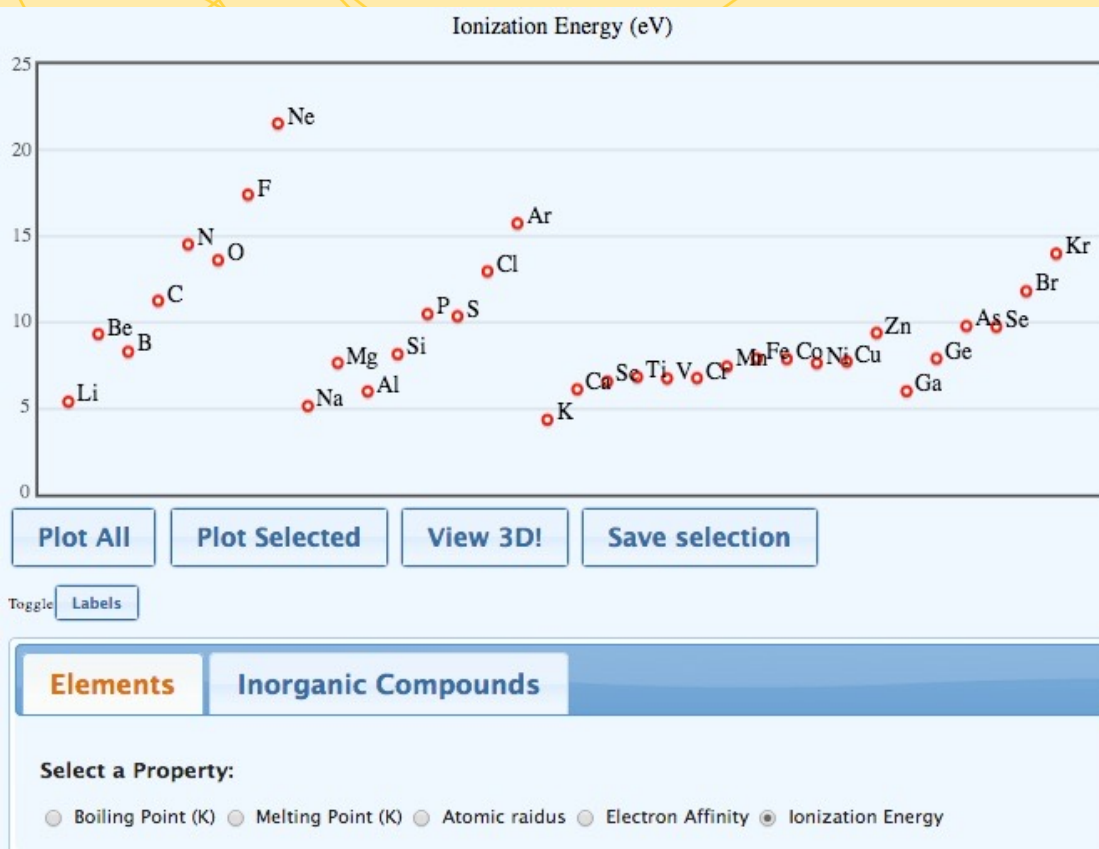
ChemEd X Data

<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/>



1	H	2											13	14	15	16	17	18
3	Li	Be											B	C	N	O	F	Ne
4	Na	Mg	3	4	5	6	7	8	9	10	11	12	Al	Si	P	S	Cl	Ar
5	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
6	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
7	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
8	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	113	114	115	116	117	118
Lanthanides			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
Actinides			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

Select All

Select None

Click to Select Rows

Show 100 entries

Search:

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

ChemEd X Data

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

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

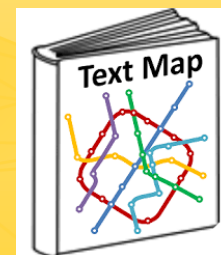
Feedback on ChemEdXData web

- 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



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



Why do we need yet another DB?

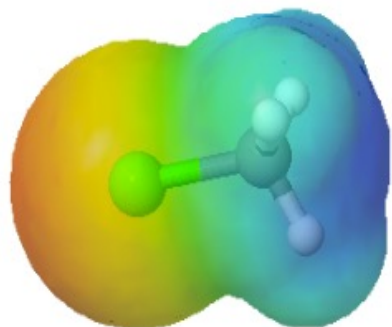
Depending on what you want, one does not need to build a collection or a database.

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

Jmol on the fly

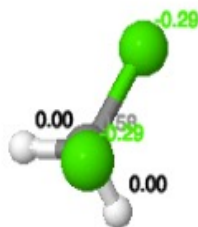
Write any name, formula or identifier in the URL separated by "/"
Example: `jmol.html#ch3cl/dichloromethane/chcl3`

☐ Synchronize mouse ☐ Drag and minimize



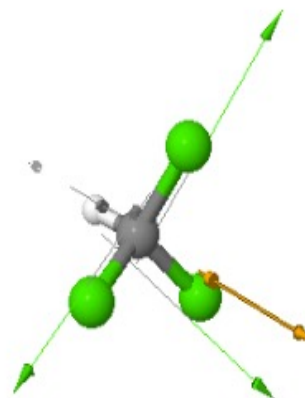
ch3cl

JSmol



dichloromethane

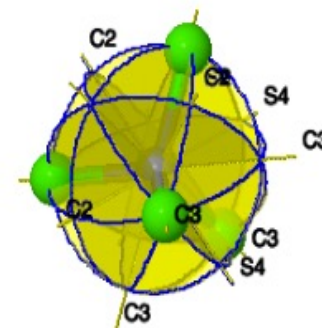
JSmol



chcl3

JSmol

Group= Td



JSmol

Show/Hide properties

ch3cl

MEP Partial Charges Molecular Dipole
Bond Dipoles Symmetry

Show/Hide properties

dichloromethane

MEP Partial Charges Molecular Dipole
Bond Dipoles Symmetry

Show/Hide properties

chcl3

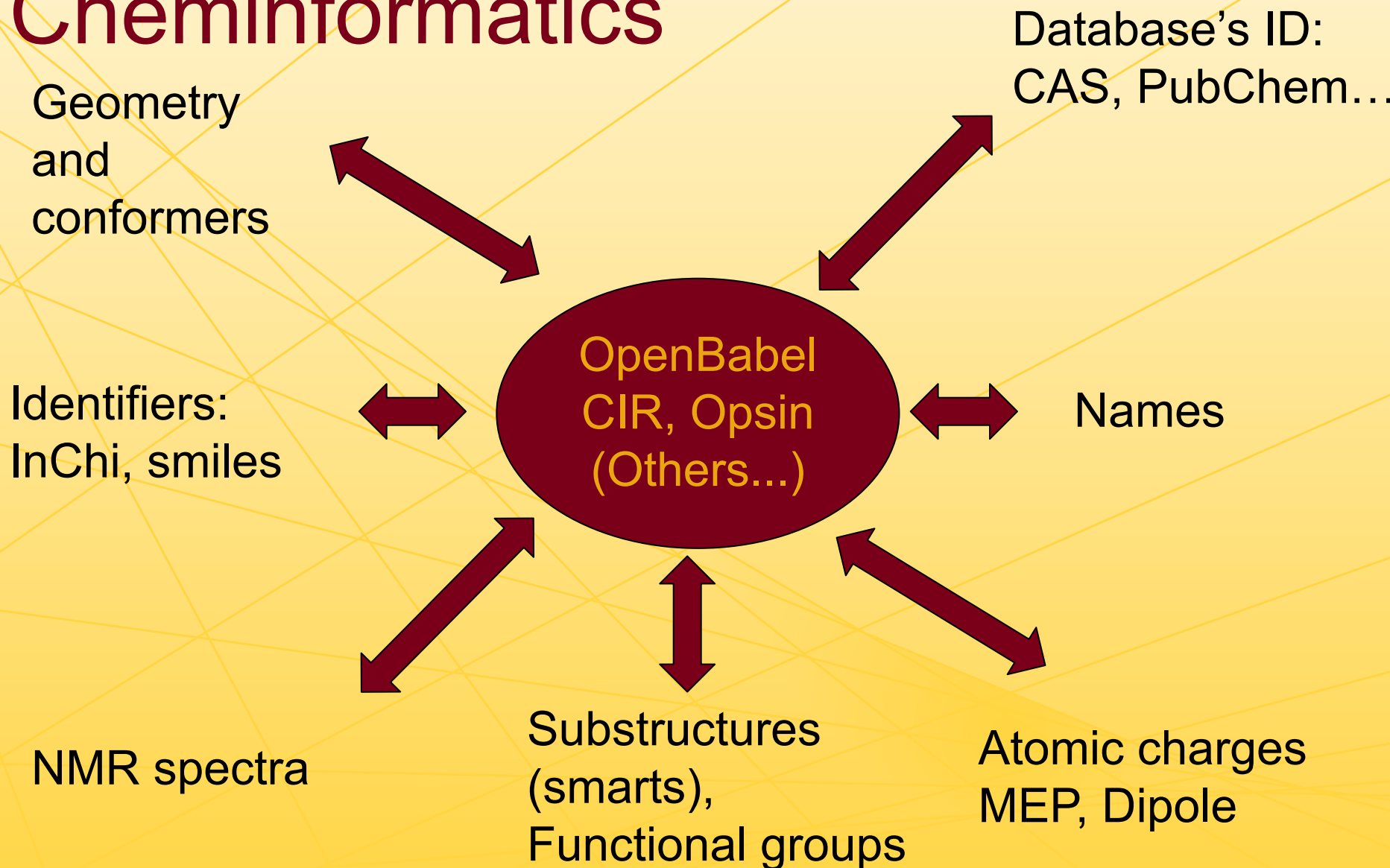
MEP Partial Charges Molecular Dipole
Bond Dipoles Symmetry

Show/Hide properties

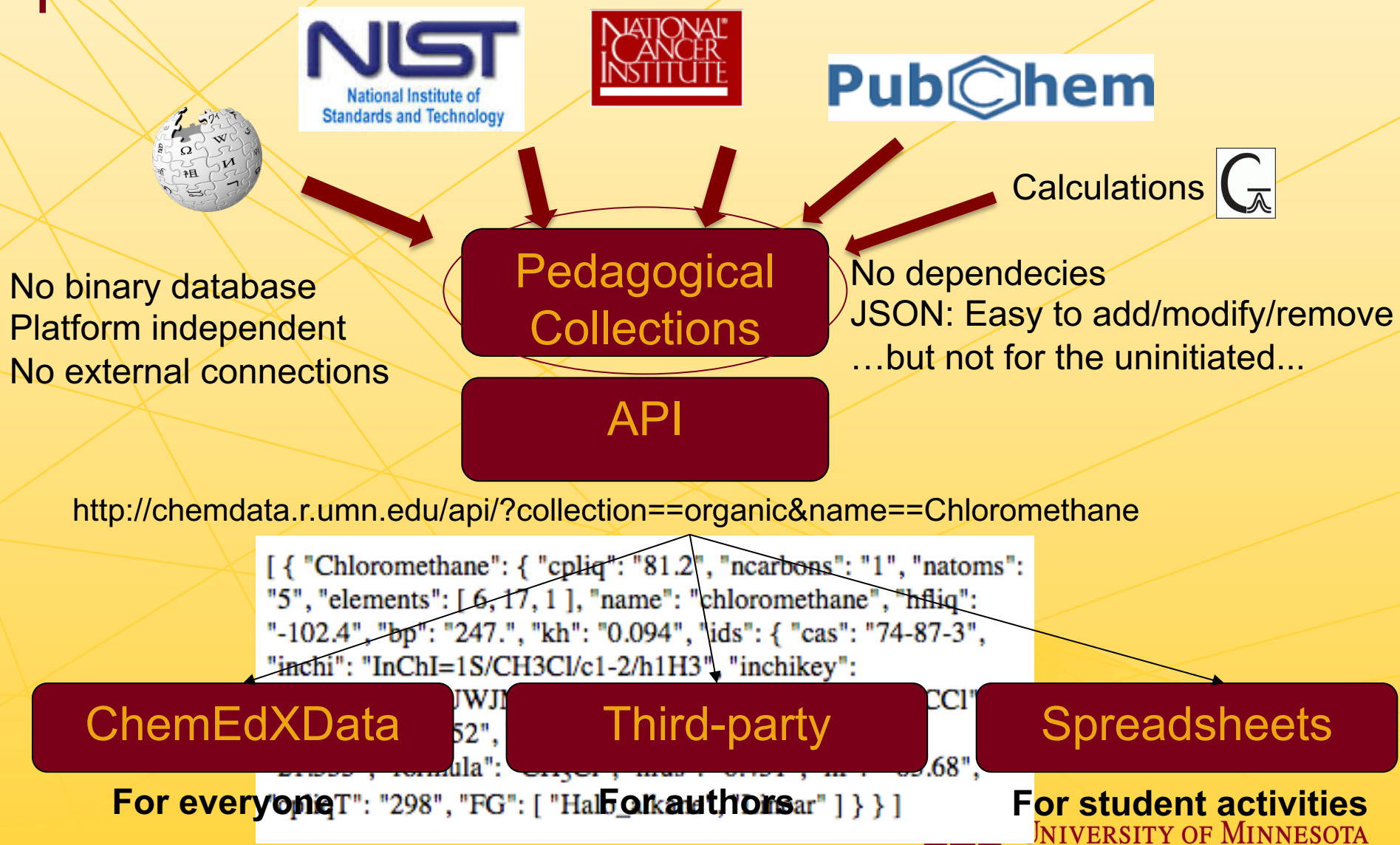
ccl4

MEP Partial Charges Molecular Dipole
Bond Dipoles Symmetry

Cheminformatics



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



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

ChemData Search Interface

Models360 collection

Organic ChemData collection

Elements collection

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

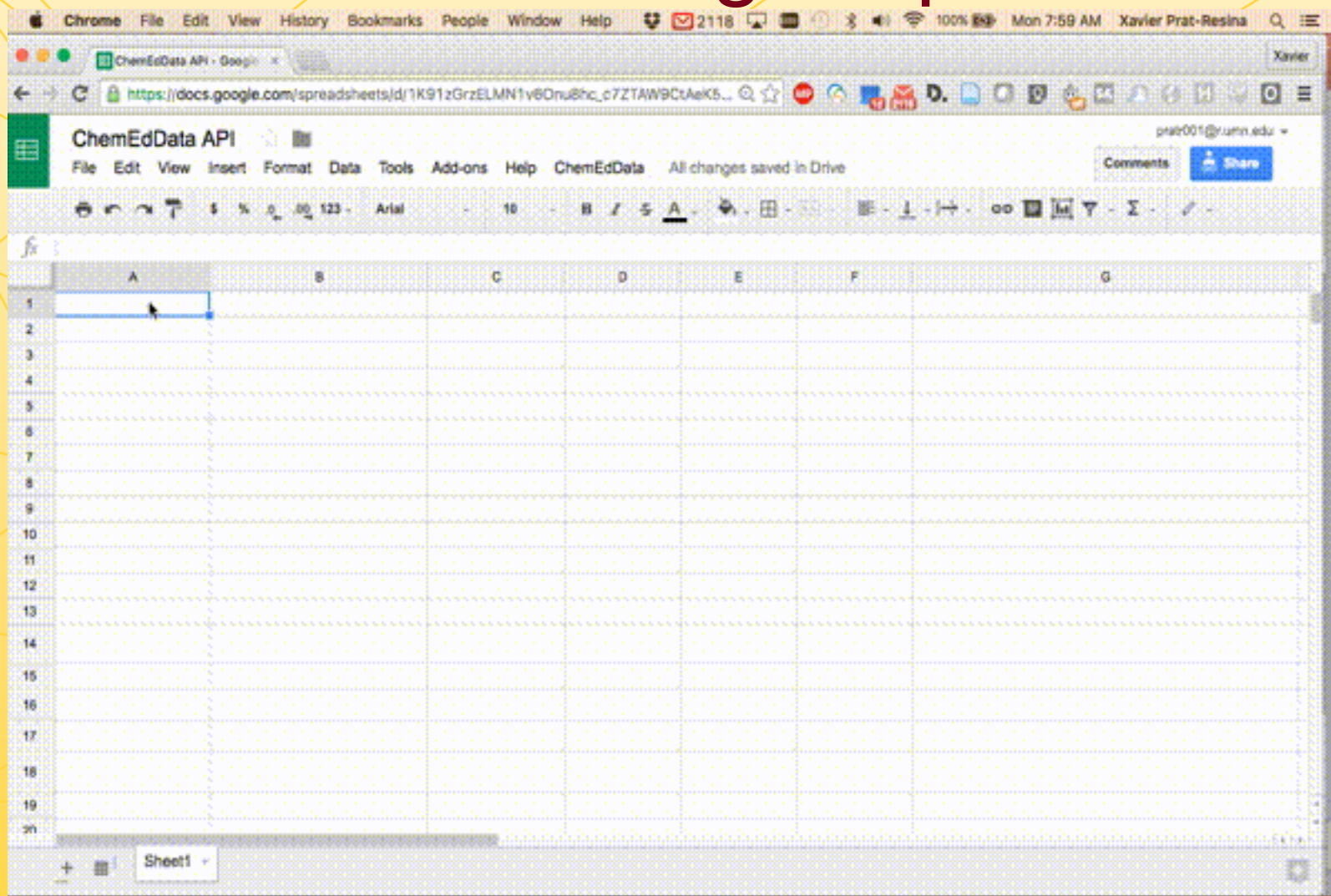
<http://chemdata.r.umn.edu/api/tables.php>

For student activities



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ChemData on Google Spreadsheets



ChemData+GoogleSpreadsheets

The screenshot shows the Google Sheets interface with the ChemEdData add-on menu open. The menu is divided into two main sections. The top section contains options for data retrieval: 'ChemEd Data tutorial', 'Experimental organic' (with a right-pointing arrow), 'Computed' (with a right-pointing arrow), 'Elements' (with a right-pointing arrow), and 'Units, standards and sources'. The bottom section is a scrollable list of specific chemical categories: 'List all alkanes', 'List all alkanes', 'List all alkynes', 'List all alcohols', 'List all haloalkanes', 'List all ketones', 'List all aldehydes', 'List all amines', 'List all carboxylic', 'List all esters', and 'List all ethers'. A second, smaller menu is open to the right of the 'Experimental organic' option, listing various physical and chemical properties: 'Mass', 'Molecular image', 'Number of atoms', 'Number of carbons', 'List all compounds' (with a right-pointing arrow), 'Boiling point', 'Melting point', 'Enthalpy vaporization', 'Enthalpy fusion', 'Enthalpy formation', 'Enthalpy combustion', 'Heat capacity gas Cp', and 'Heat capacity liquid Cp'. The background shows a Google Sheet with a single cell containing the letter 'C'.

Tools Add-ons Help ChemEdData Last edit was made 1 minute ago by Xavier Prat-Resina Comments Share

Arial 10

ChemEd Data tutorial

Experimental organic ►

Computed ►

Elements ►

Units, standards and sources

List all alkanes

List all alkanes

List all alkynes

List all alcohols

List all haloalkanes

List all ketones

List all aldehydes

List all amines

List all carboxylic

List all esters

List all ethers

Mass

Molecular image

Number of atoms

Number of carbons

List all compounds ►

Boiling point

Melting point

Enthalpy vaporization

Enthalpy fusion

Enthalpy formation

Enthalpy combustion

Heat capacity gas Cp

Heat capacity liquid Cp



ChemData+GoogleSpreadsheets

The screenshot shows the Google Sheets interface with the ChemEdData add-on menu open. The menu is titled 'ChemEdData' and indicates 'Last edit was made 5 minutes ago by Xavier Prat-Resina'. The main menu has four items: 'ChemEd Data tutorial', 'Experimental organic', 'Computed', and 'Elements'. The 'Elements' item is selected, opening a sub-menu with the following options: 'List all elements', 'Atomic mass', 'Name', 'Period', 'Group', 'Electronegativity', 'First ionization energy', 'Multiple ionization energies', 'Electron affinity', 'Atomic radius' (which is highlighted), 'Melting point', 'Boiling point', 'Density', 'Heat capacity', and 'Abundance'. A second sub-menu is open for 'Atomic radius', showing options: 'Empirical', 'Covalent', 'Computed', 'Van der Waals', and 'List all ionic radii'. The background shows a Google Sheet with columns labeled 'C' and 'G'.



Data-driven exercises in PChem

The screenshot shows the ChemEdData web application interface. At the top, there is a navigation bar with 'Tools', 'Add-ons', and 'Help' menus. The 'ChemEdData' menu is open, displaying a list of options: 'ChemEd Data tutorial', 'Experimental organic', 'Computed', 'Elements', and 'Units, standards and sources'. The 'Computed' option is selected, opening a sub-menu. This sub-menu lists various data types: 'Mass', 'Number of atoms', 'Dipole moment', 'List all computed', 'Total Thermodynamic data at 298K', 'Translational data', 'Rotational data', and 'Vibrational data'. The last three options are circled in red. Below the sub-menu, there is a list of specific data types: 'List all frequencies', 'List all IR intensities', 'Zero Point Energy', 'Vibrational internal energy U', 'Vibrational Heat capacity Cv', and 'Vibrational Entropy S'. The background of the application shows a grid with a 'C' in one of the cells.

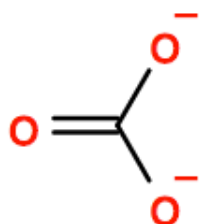
U, Cv, S
 Θ_{rot} ,
ZPE



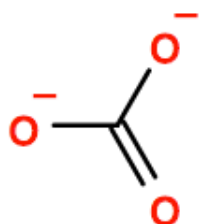
Calculated resonant structures

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

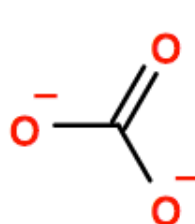
NRT:
Weinhold's
Natural
Resonance
Theory



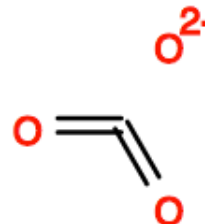
30.44%



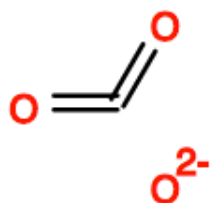
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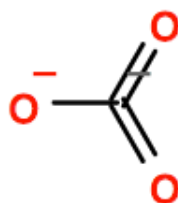
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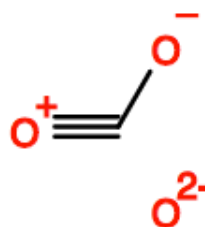
1.45%



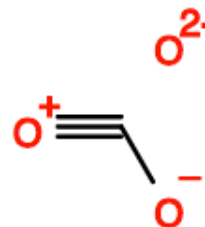
1.45%



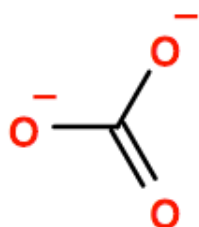
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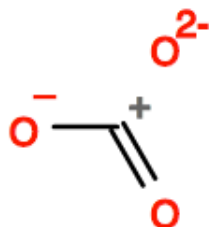
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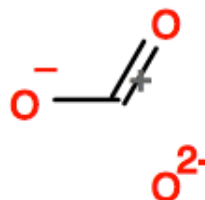
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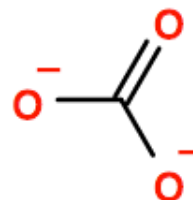
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0.72%



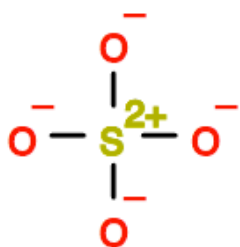
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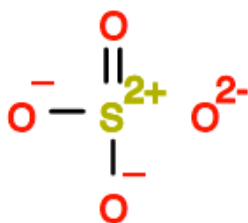
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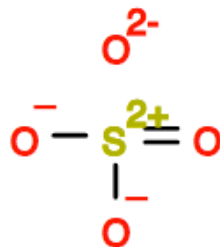
Calculated resonant structures



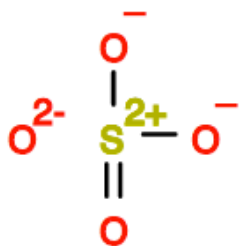
53.16%



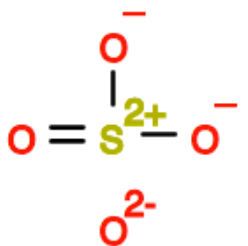
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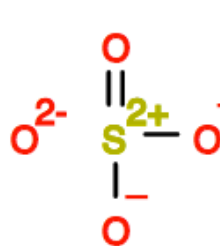
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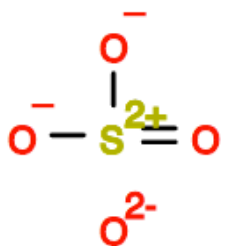
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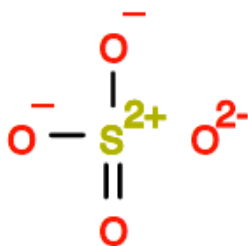
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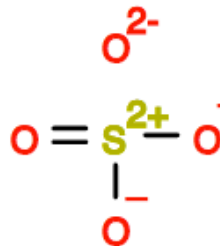
5.81%



5.81%



5.81%



5.81%

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



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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.

