CHM 2000 Sinex

# Molecular Polarity Collaborative Project

A class collaboration activity for 20 molecules - 4 per student to start and maybe more!

Using a variety of carbon compounds, build the structure, optimize geometry, and then minimize energy in Avogadro. *The golden rule for carbon in organic compounds: C always has four and only four bonds!* For organic-type molecules (carbon-based), use the MMFF94 force field.

Produce each structure and have a fellow student proof it and then do the following:

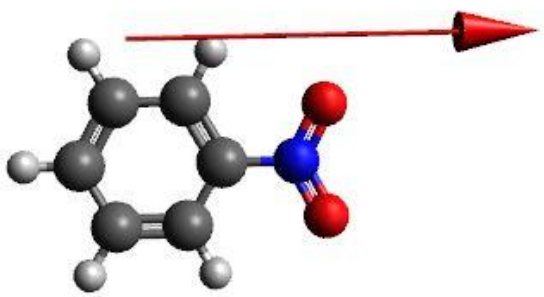
- Dipole moment - calculated by Avogadro (record the value)
- Dipole moment - measured using NIST data (will be given)
- Dipole arrow
- Screen capture the image using a white background, keep tight around the structure, and then save the file! Windows Snipping tool allows you to save screen captures!

Compile a shared document (spreadsheet supplied by your instructor) with the following information for each of your molecules:

1. Chemical name
2. Chemical line formula
3. Chemical structure (use white background) showing dipole arrow (on menu bar: Insert > Image... to get the file into the spreadsheet) Resize your image to fit in the cell!
4. Prepared by (use your initials)
5. Calculated dipole moment from Avogadro
6. Experimental dipole moment from NIST
7. Dummy column to create y = x line
8. Difference (calculated dipole moment - experimental dipole moment)

Link to spreadsheet that all can edit:
https://docs.google.com/spreadsheets/d/1FGe4mvGkQ2e9KSTUhH19TmKZl7kICrA1nwtcRufVN0M/edit?usp=sharing

Nitrobenzene is given as an example in the spreadsheet and shown here to the right.

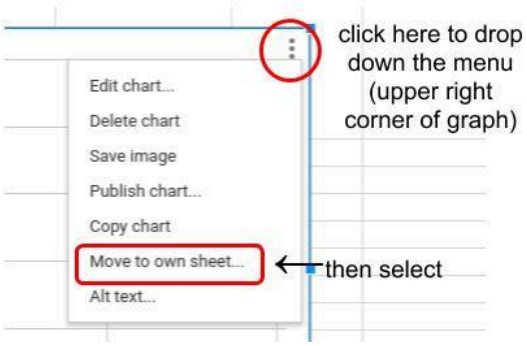


Now build and add your assigned molecules to the spreadsheet.

Compare calculated vs. measured dipole moment (divide the work up amongst the class!)

- Plot calculated dipole moment as a function of measured dipole moment
- Add the y = x comparison line (copy calculated dipole moment column into dummy column) Show only regression line through data with no data points!
- Perform a linear regression on the dipole moments data, plot with equation and r-squared value
- Calculate difference (calculated dipole moment - experimental dipole moment)
- On a seperate plot, plot the difference as a function of measured dipole moment

After inserting a graph, the graph should be moved to its own tab or sheet. See image to the right. This should be done for both plots.




How to use the y = x comparison line. See the following Excelets,

"How do you compare data from two different sources?" at
http://academic.pgcc.edu/~ssinex/excelets/comparison_plots.xls
and/or
"Rulers and Measurement Error", erroneous ruler II tab at
http://academic.pgcc.edu/~ssinex/excelets/Ruler_error.xls

Conclude how good are the Avogadro calculated dipole moment results.

Experimental Dipole Moments: https://cccbdb.nist.gov/diplistx.asp