



# Chem115 Fall 2023 - Ilana Berlin/Lab8: Computational Chemistry I: Molecular Shape/LabReport8

Jason Cody - Oct 23, 2023, 11:02 AM CDT

## Assignment #16 - LabReport8

**i** You cannot edit this entry after it is graded.

Description Molecular Shape  
I worked in a group with Dazzo, Gina  
The work for this assignment My notebook  
is in

**Grade** **9.5 / 10**

Graded on Oct 23, 2023, 11:02 AM CDT

Jason Cody - Oct 01, 2021, 10:37 AM CDT

**TITLE:** (insert experimental title here. All italicized text in parentheses should be followed and then deleted throughout this template).

**Purpose:** (insert experimental purpose here).

**Reference:** Kanley, L. J., *Introduction to Chemistry in the Laboratory*, 20<sup>th</sup> Ed., Lake Forest College, 2021. Experiment 19, Appendix 10. (Edit the experiment title and/or appendix later; add other references, if used, following the same format.)

**Observation and Data:** (Write your clear, concise, complete, just-numeric, precise written descriptions or narrative of the experiment as the experiment is performed. Complete sentences are used throughout.)  
(If needed, insert tables and edit the header: Table 1. Preparation of Standard Solutions. If needed, insert figures and edit this caption below the figure: Figure 1. Beer's Law Plot of B12 Standard Solutions at  $\lambda = 520$  nm. Number tables and figures in order of appearance in the report.)

**Calculations:** (insert sample calculation here, if relevant. Otherwise, delete this section entirely.)

**Conclusion:** (state the quantitative values (percent error and/or CV) to indicate how well the goals of the experiment have been met; answer any questions in the experiments' instructions, too).

**ReportTemplate.docx (15.5 kB)**

Jason Cody - Oct 03, 2020, 12:21 PM CDT

## Date and Title

Ilana Berlin - Oct 09, 2023, 1:57 PM CDT

## Purpose

Jason Cody - Oct 23, 2023, 10:58 AM CDT

Spartan Student v9 will be used to 3D model and examine 3 different sets of molecules, for a total of 14 molecules. Set A, CH<sub>3</sub>Cl, CH<sub>2</sub>Cl<sub>2</sub>, CHCl<sub>3</sub>, and CCl<sub>4</sub>, shows how the differences in molecular dipole moments (in debye) affect the molecule shape. Set B, C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>H<sub>4</sub>, and C<sub>2</sub>H<sub>2</sub>, how the differences in central atom electron domains affect the molecule shape. Set C, CH<sub>3</sub>CH<sub>2</sub>CH<sub>3</sub>, CH<sub>3</sub>OCH<sub>3</sub>, CH<sub>3</sub>CH<sub>2</sub>OH and CH<sub>3</sub>COCH<sub>3</sub>, show how structure of the molecules affect the shape of the molecule and the molecular dipole moment. Set D PF<sub>5</sub>, SF<sub>4</sub>, and ClF<sub>3</sub> show how lone pairs on the central atom affect the molecule shape. **Nicely done.**

Jason Cody - Oct 03, 2020, 12:21 PM CDT

## Reference

Jason Cody - Oct 23, 2023, 10:58 AM CDT

Kateley, L. J., *Introduction to Chemistry in the Laboratory, 20th Ed.*, Lake Forest College, 2021, Experiment 8 Appendix A.

**Spartan Student v. 9. (with more details to complete the reference)**

Jason Cody - Oct 03, 2020, 12:21 PM CDT

## Data and Observations

Jason Cody - Oct 23, 2023, 11:01 AM CDT

Figure 1. Sets A and B **OK**

	CH <sub>3</sub> Cl	CH <sub>2</sub> Cl <sub>2</sub>	CHCl <sub>3</sub>	CCl <sub>4</sub>	C <sub>2</sub> H <sub>6</sub>	C <sub>2</sub> H <sub>4</sub>	C <sub>2</sub> H <sub>2</sub>
Name	chloromethane	dichloromethane	trichloromethane	tetrachloromethane	ethane	ethylene	ethyne
Lewis structure							
number of central atom electron domains	4	4	4	4	4,4	3,3	2,2
central atom shape name	tetrahedral	tetrahedral	tetrahedral	tetrahedral	tetrahedral	trigonal plane	linear
3D structure showing dipole moment							
molecular dipole moment (debye)	2.31	2.05	1.40	0.00			
bond lengths (Å)	C-Cl 1.806 C-H 1.076	C-Cl 1.784 C-H 1.072	C-Cl 1.776 C-H 1.072	C-Cl 1.778 C-H 1.069	C-C 1.543 C-H 1.084	C-C 1.315 C-H 1.073	C-C 1.188 C-H 1.051
bond angle (°)	H-C-H 110.81 H-C-Cl 108.1	H-C-H 111.57 H-C-Cl 109.3	H-C-Cl 107.94 Cl-C-Cl 112.09	H-C-Cl 110.96 Cl-C-Cl 109.47	H-C-C 110.80 H-C-H 108.11	H-C-C 121.92 H-C-H 116.16	H-C-C 180
description of location of blue (positive) and red (negative) regions	blue red H, Cl	blue red H, Cl	blue red H, Cl	blue Cl			
electrostatic potential	max: 116.74 min: -82.69	max: 161.29 min: 77.98	max: 195.85 min: -49.79	max: 100.84 min: -26.98			

Figure 2. Sets C and D OK

	CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>	CH <sub>3</sub> OCH <sub>3</sub>	CH <sub>3</sub> CH <sub>2</sub> OH	CH <sub>3</sub> COCH <sub>3</sub>	PF <sub>5</sub>	SF <sub>4</sub>	ClF <sub>4</sub>
Name	propane	dimethyl ether	ethyl alcohol	dimethyl ketone	phosphorus pentafluoride	sulfur tetrafluoride	chlorine trifluoride
Lewis structure							
number of central atom electron domains	C 4 C 4 C 4	C 4 O 4 C 4	C 4 C 4 O 4	C 4 C 3 C 4	5	5	5
central atom shape	c Tetra c Tetra o Bent c Tetra	c Tetra o Bent c Tetra	c Tetr c Tetr o Bent	c Tetr c Tri Plane c Tetra	Trigonal Bi-pyramidal	see-saw	T-shaped
3D structure showing dipole moment							
molecular dipole moment (debye)	0.04	1.85	1.94	3.14	0.00	1.37	1.15
bond lengths (Å)	C-C 1.541 C-O 1.433		C-C 1.525 C-O 1.441	C-C 1.515 C-O 1.211	P-F <sub>ax</sub> 1.538 P-F <sub>eq</sub> 1.566	S-F <sub>ax</sub> 1.580 S-F <sub>eq</sub> 1.617	Cl-F <sub>ax</sub> 1.676 Cl-F <sub>eq</sub> 1.605
bond angles (°)					F <sub>ax</sub> -P-F <sub>ax</sub> 120 F <sub>eq</sub> -P-F <sub>ax</sub> 90 F <sub>eq</sub> -P-F <sub>eq</sub> 180	F <sub>ax</sub> -S-F <sub>ax</sub> 101.78 F <sub>eq</sub> -S-F <sub>ax</sub> 86.78 F <sub>eq</sub> -S-F <sub>eq</sub> 169.77	F <sub>ax</sub> -Cl-F <sub>ax</sub> 171.01 F <sub>eq</sub> -Cl-F <sub>ax</sub> 85.50
electrostatic potential	max: 41.18 min: -24.83	68.28 -240.42	230.17 -247.31	102.24 -230.63	336.44 -81.99	247.77 -116.12	220.45 -130.02
central atom hybridization	All C's sp <sup>3</sup>	Both C's sp <sup>3</sup> O sp <sup>3</sup>	All C's and O sp <sup>3</sup>	End C's sp <sup>3</sup> Middle C sp <sup>2</sup>	sp <sup>3</sup> d	sp <sup>2</sup> d	sp <sup>3</sup> d

Set A: CH<sub>3</sub>Cl, CH<sub>2</sub>Cl<sub>2</sub>, CHCl<sub>3</sub>, and CCl<sub>4</sub>

The general trend for positive and negatives in set A is positive regions near hydrogen atoms and negative regions near chlorine atoms. CCl<sub>4</sub> is the exception to this trend, the positive regions are near the chlorine atoms since there are no hydrogen atoms. The dipoles increases as the number of hydrogen atoms increase. The molecule with the greatest number of chlorine atoms CCl<sub>4</sub> does not have the greatest dipole because the chlorine atoms are evenly distributed and non-polar. The dipole does not need to point along the bond, it points from the most positive to the most negative

region of the atom **molecule?**. the bonds themselves have no affect of the dipole, the atoms attached by the bonds are what affect the dipole.  $\text{CH}_3\text{Cl}$  and  $\text{CHCl}_3$  because both molecules have shapes similar to the shape predicted by the VSEPR (**electron domain**) model.

Set B:  $\text{C}_2\text{H}_6$ ,  $\text{C}_2\text{H}_4$ , and  $\text{C}_2\text{H}_2$

The bond length decrease from single to double to triple but it does not decrease at constant rate because the electronegativity acting on the electrons is not the same for each bond. Decreasing number of hydrogen electrons also increases bond strength as there are less positive forces to repel each other.  $\text{C}_2\text{H}_4$  does not exhibit an ideal trigonal planar structure (as predicted by the VESPR model) as the hydrogens are closer to the equator than they are to the axis as the model predicts. The C-H bonds decrease as the C-C bonds decreases. As the carbons get closer, the hydrogens move further to the other side of the carbon atom and closer to the atom. **OK**

Set C: $\text{CH}_3\text{CH}_2\text{CH}_3$ ,  $\text{CH}_3\text{OCH}_3$ ,  $\text{CH}_3\text{CH}_2\text{OH}$  and  $\text{CH}_3\text{COCH}_3$

The dipolar are effected by the presence and location of the oxygen but it is also effected by the other atoms and the structure of the compound so the dipole does not always point right at the oxygen.  $\text{CH}_3\text{CH}_2\text{OH}$  has a dipole diagonal to oxygen. **OK, the OH scenario is unusual (we'll see more about this later)**. The minimum electrostatic potential increases with the addition of an oxygen atom. The maximum electrostatic potential increases when the oxygen in not on the equator of the atom. **OK**

Set D: $\text{PF}_5$ ,  $\text{SF}_4$ , and  $\text{ClF}_3$

$\text{F}_{\text{eq}}\text{-X-}\text{F}_{\text{eq}}$  bond angle decreases across the the set. The addition of unbonded pairs pushes the equatorial bonds closer together. The same thing happens to the  $\text{F}_{\text{eq}}\text{-X-}\text{F}_{\text{ax}}$  bond angles that also decrease across the set.  $\text{SF}_4$  had the most stable bonds because the bond lengths are the shortest. **OK**

Ilana Berlin - Oct 09, 2023, 3:31 PM CDT

## Conclusions

Jason Cody - Oct 23, 2023, 11:02 AM CDT

$\text{CH}_3\text{Cl}$  and  $\text{CHCl}_3$  closely matched the VESPR **not correct acronym (valence shell electron pair repulsion)** tetrahedral model with bond angles close to  $120^\circ$  and  $90^\circ$ . ??what? Something is confused here.  $\text{C}_2\text{H}_2$  matched the VESPR linear model with a bond angle of  $180^\circ$ . **OK**  $\text{SF}_4$  closely matched the VESPR see-saw model with a  $\text{F}_{\text{eq}}\text{-S-}\text{F}_{\text{eq}}$  of  $169.77^\circ$ , close to  $180^\circ$ . **OK, not close. What about  $\text{PF}_5$ ?**  $\text{C}_2\text{H}_4$  differed the most from the VESPR model of trigonal plane with bond angles of  $108.11^\circ$  and  $110.80^\circ$ .  $\text{CH}_3\text{CH}_2\text{OH}$  also visibly differed from the VESPR bent model.

