Daily Activities for a Data-Driven Approach to Learning About Molecular Structure and Bonding. Text references are to numbered discussion questions in *Molecular Origami* (University Science Books)

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Day 1: Molecular Shapes and Sigma Bonding

Pick three examples from each of the following sets
(that makes 18 examples, total):

1. linear (AX2)
2. bent (AX2E)
3. bent (AX2E2)
4. trigonal planar (AX3)
5. tetrahedral (AX4)
6. trigonal pyramidal (AX3E)

and, for each set:

a) Determine the overall number of valence electrons for each of the three examples.
b) Draw a proper "sigma" structure (no double bonds) for each example.
c) Discuss the similarity or differences in central atom bonding (number of sigma bonds, number of lone pairs) among the three examples.

Day 2: Molecular Distances and Bonding

1. Find as much evidence as you can in the data arguing for the existence of "double" or "triple" bonds and discuss it. Examples include C=C, C≡C, C=N, C≡N, C=O, C≡O, C=S, S=O, and P=O.
2. Draw appropriate Lewis structures in each case (including double or triple bonds), indicating by each bond the actual distance in pm.
3. Compare these species to ones having single bonds, e.g. ethylene ($H_3C{=}CH_3$) with ethane ($H_3C{—}CH_3$), or acetonitrile (CH_3CN), with ethylamine ($H_3C{—}NH_2$).
4. In the case of H_2SO_4, show evidence for both S=O and S—O; in the case of H_3PO_4, show evidence of P=O and P—O.
5. How does all this relate to the "octet rule."

Day 3: Molecular Angles and Hybridization

1. Carefully compare the angles in five different sets of shapes: linear, bent, trigonal planar, trigonal pyramidal, and tetrahedral. Discuss any salient points or trends.
2. What sort of range of angles are present in each set?
3. Why do you think a specific angle is small while another is large?

Pertinent discussions can be found on pp. 9, 29, 129, 191, and 202.

Day 4: Trends in Molecular Distance

Compare distances to the central atom in the following related compounds and discuss what might be the reason for any trends that you see. (Consider one of the F atoms in F_2 to be central.) Pertinent discussions are shown in brackets.

a) CH_4, NH_3, H_2O, HF [11bcd]
b) CF_4, NF_3, OF_2, F_2 [13d]
c) BH_4^-, CH_4, NH_4^+ [31a,37a]
d) BeF_4^{2-}, BF_4^-, CF_4 [33b,39b]
e) PH_3, SiH_4, H_2S [19cd]
f) NHF_2, CH_2F_2, OF_2 [17bc]
g) PHF_2, SF_2, $S(CH_3)_2$ [25ab]
h) PF_3, POF_3 [21c]
i) NF_3, CHF_3 [13c]
j) IO_3^-, XeO_3, IO_4^-, XeO_4 [27ab,77]

Day 5: Trends in Molecular Angle

Carefully compare the angles in the related compounds shown below and discuss what might be the reason for any trends that you see. Pertinent discussions are given in brackets.

a) CH_4, NH_3, H_2O [11bcd]
b) CF_4, NF_3, OF_2 [13d]
c) BH_4^-, CH_4, NH_4^+ [31b]
d) BeF_4^{2-}, BF_4^-, CF_4 [33b]
e) PH_3, SiH_4, H_2S [19cd]
f) NHF_2, CH_2F_2, OF_2 [17c]
g) NF_3, CHF_3 [13c]
h) OF_2, $O(CH_3)_2$, SF_2, $S(CH_3)_2$ [25ab]
i) PF_3, POF_3 [21c]
j) IO_3^-, XeO_3, IO_4^-, XeO_4 [27a,75]

Day 6: Acid-Base Structure and Reactivity

Discuss each of the following phenomena using ideas of lone pairs, polarized bonds, Lewis dot (or just sigma) structures, and/or molecular orbitals.

1) Ammonia is a weak base.
2) Water is both weakly acidic and weakly basic.
3) BF_3 is a weak acid.
4) BH_3, if it existed, would be a weak acid, not a weak base.
5) H_2CO_3 is acidic, but CO_3^{2-} is basic.
6) $HClO_4$ is a stronger acid than $HClO_3$, which is stronger than $HClO_2$.
7) acetic acid, (structure shown on the right) is considered to be a weak acid, but methanol, CH_3OH, is not.

Day 7: Diatomic Molecules

Read the discussion 47a on page 206. For each of the following sets of diatomic compounds:

a) Determine the total number of valence electrons.
b) Fill in the appropriate energy level diagram using the number of electrons from (a) and determine the bond order.
c) Discuss the bond distances given in your text in relation to bond order. Consider very small differences (1-2 pm) to be insignificant.

1) H_2, H_2^+, He_2^+
2) N_2, N_2^+
3) CN^-, CN, CN^+
4) O_2^{2-}, O_2^-, O_2, O_2^+
5) CO, CO^+
6) NO, NO^+
7) CO, NO^+
8) N_2, NO^+

Day 8: Group Presentations

- 1-4 person groups only
- up to 15 points per person based on complexity of project and success of venture
- work with me for project description
- possibilities include:
  - presentation of advanced topics in Molecular Origami
  - construction of molecules NOT in Molecular Origami
  - enzyme/DNA structure presentation
  - development of interactive web site

The following presentations were made by students:

1) Molecular Web Site Using CHIME
2) CH_4/NH_4^+ Structure/Orbital Comparison Using CAChe
3) A Structural Comparison of Several MF_6^{n-} Ions
4) Three Triangulated Dodecahedra of the form $M(NO_3)_4$
5) The Three Forms of Carbon
6) YVO_4 vs. $ZrSiO_4$: A Comparison of Structure
7) The Structure of Quartz
8) Pyrite vs. Marcasite: Two Forms of FeS_2
9) Structure and Chemistry of Nerve Toxins
10) The Structure and Function of Zinc Fingers