Literature discussion of “The Noble Gases: How Their Electronegativity and Hardness Determines Their Chemistry”

P. Geerlings and co-workers, *J. Phys. Chem. A* **2015**, *119*, 1339-1346.

**Instructions:**

Prior to class, please read the Introduction (Section 1) of the above paper and answer questions 1-3.

1. Using chemical equations, give examples of the processes described by ionization energy and electron affinity and clearly label each.
2. Give the definitions of the chemical properties of both electronegativity and hardness.
3. Electronegativity can be calculated using multiple different scales. Describe how the three most common scales (Pauling, Mulliken, and Allred-Rochow) are calculated or on what measurable properties these scales are based on.
4. What do the authors claim as the problem with the reported electron affinity values, *A*, for the noble gases?
5. What do these reported *A* values imply about the relative stability of anions of the noble gases?
6. To what do the authors ascribe the increase in popularity of the Mulliken scale of electronegativity?

For the following questions, use the data contained in Tables 1-3 in the Results and Discussion, (Section 3) and read the analysis on pages 1343-4.

1. Open an Excel spreadsheet, and copy in the ionization energy, *I*, and electron affinity, *A*, values reported in Tables 1-3 for each element in Groups 16-18. Note that these values are reported in eV/atom. Convert these into kJ/mol for each element.
2. Using the converted values for *I* and *A*, calculate the Mulliken electronegativity for each element using eqn 2. This value can be scaled to match the Pauling electronegativity by dividing cM by 252.4.
3. Generate a plot of the atomic number vs cM values to observe the trend in electronegativity for each group.
4. How well do the calculated values of cM match the reported Pauling electronegativity values for Groups 16 and 17?
5. How do the calculated cM values for the noble gases compare to Groups 16 and 17?
6. How do these values compare to the general trend of electronegativity across the Periodic Table?
7. Based on the cM values, how would you expect the dipole moment to be oriented in known compounds of Xe and F (ie. XeF4)? Does this match the polarities previously reported in the literature?
8. According to the authors, what is the cause of the hardness values of Group 18 elements being higher than the hardness of Group 17 elements?
9. Of the two calculated electronic factors, electronegativity and hardness, which do the authors conclude drives the reactivity of the noble gases? In physical terms, what does this imply about the requirements for noble gases to bond with other elements?