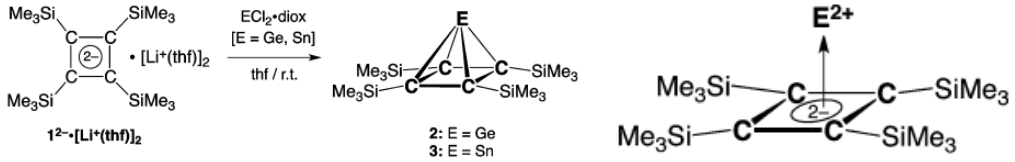
HW 2	Multinuclear NMR	Name:	
Points:	C6800	Date:	
Max. 100 points	Spring 2017	Version A	

1. (2 pts) The ^{119}Sn NMR resonance of the Sn atom at the apex of the square pyramid in **3** was found to be extraordinarily shielded, being observed at −2441.5 ppm. The value closely approaches those of the stannocene derivatives, with their record high-field tin resonances appearing in the range from −2100 to −2300 ppm. Explain these observations considering the two resonance structures of pyramidane **3**, covalent and ionic. Which one is more important?

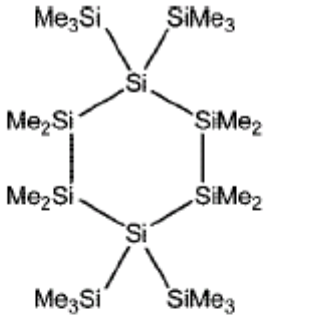


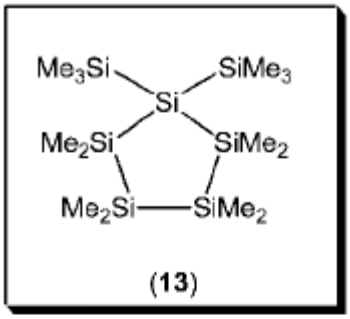
2. (38 pts) Draw all possible complexes $[PF_x(CN)_{6-x}]$ (x = 0 – 6) and predict multiplicities of signals in ^{31}P and ^{19}F NMR spectra (number of resonances, name of a multiplet, and the relative intensities of lines in a multiplet).

x	Molecule	^{31}P	^{19}F
6			
5			
4			

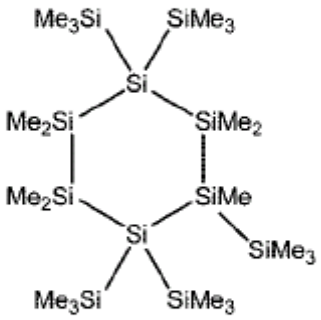
and so on….

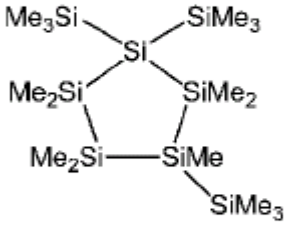
3. (44 pts) Find the symmetry point groups of the following molecules.
How many signals do you expect in the ^{1}H and ^{29}Si NMR spectra.
Mark all geminal groups in these molecules as homotopic (**H**), enantiotopic (**E**) and diastereotopic (**D**).



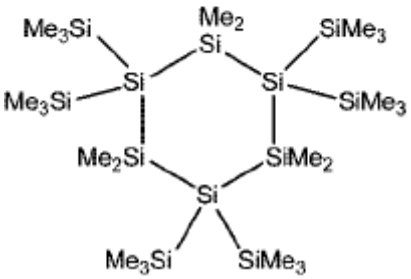


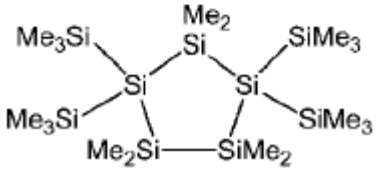
(**13**)



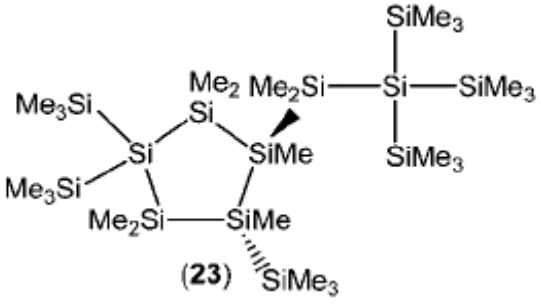


(**14**)



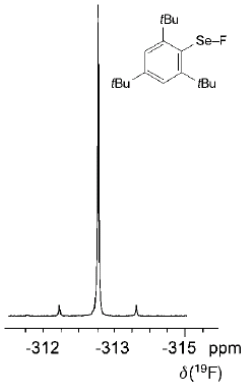


(**15**)



(**23**)

4. (4 pts) Explain the ^{19}F $\{^{1}H\}$ NMR spectrum the following molecule.



5. (12 pts) Calculate relative populations of Te isotopologues of this cation. (Disregard the Se isotopes, use $\sigma = 2$, for the two-fold axis that interchanges the Te atoms)