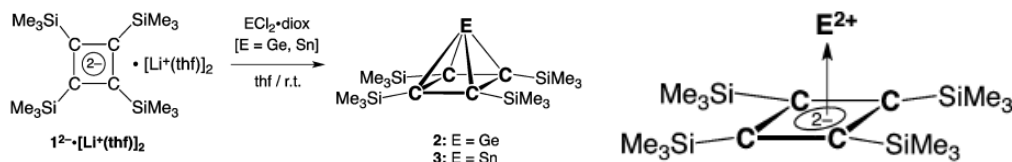
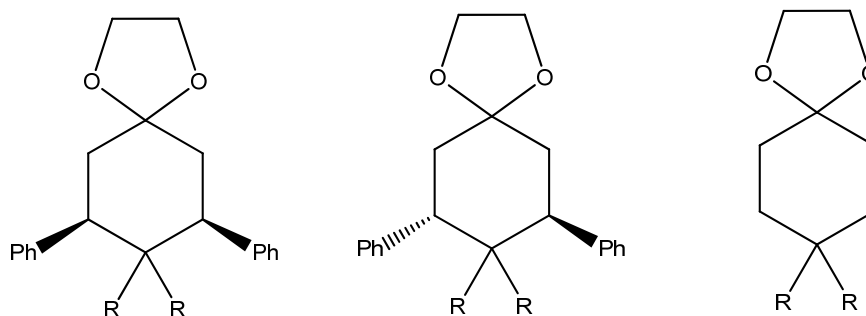


HW 2	Multinuclear NMR	Name:	
Points:	C6800	Date:	
Max. 100 points	Spring 2018	Version A	

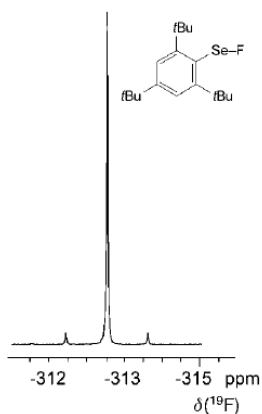
1. (3 pts) The ^{119}Sn NMR resonance of the Sn atom at the apex of the square pyramid in **3** was found to be extraordinarily shielded, being observed at -2441.5 ppm. The value closely approaches those of the stannocene derivatives, with their record high-field tin resonances appearing in the range 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. (15 pts) Mark geminal protons of CH_2 in the following molecule as homotopic (**H**), enantiotopic (**E**) and diastereotopic (**D**). Find the symmetry point group of each molecule:



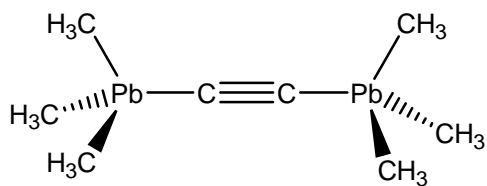
3. (4 pts) Explain the ^{19}F $\{^1\text{H}\}$ NMR spectrum the following molecule, mark all peaks, spin interaction constants and give relative intensities:



4. (38 pts) Draw schematically all possible complexes $[\text{PF}_x(\text{CN})_{6-x}]$ ($x = 0 - 6$) and give the label of the corresponding point group. 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 Point group	^{31}P	^{19}F
6			
5			
4			
3			
2			
1			
0			

5. (6 pts) Calculate relative populations of ^{207}Pb isotopologues in the molecule of plumbane:



6. (4 pts) Values of interaction constants in following anions recalculate for other NMR active isotopes of Ga, In and Tl.

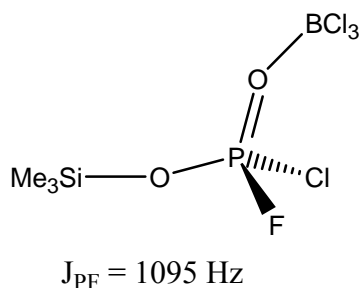
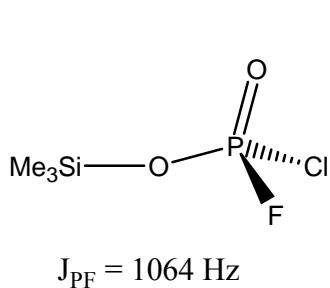
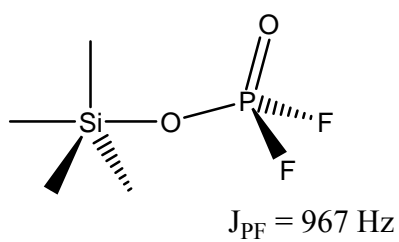
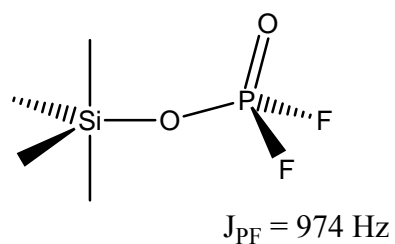
$$[\text{GaF}_6]^{3-} \quad {}^1J(^{71}\text{Ga-F}) = 245.4 \text{ Hz}$$

$$[\text{Ga}(\text{CF}_3)_4]^- \quad {}^2J(^{71}\text{Ga-F}) = 150.2 \text{ Hz}$$

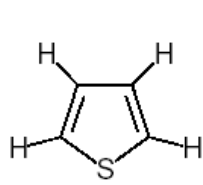
$$[\text{InF}_6]^{3-} \quad {}^1J(^{115}\text{In-F}) = 420.0 \text{ Hz}$$

$$[\text{Tl}(\text{CF}_3)_4]^- \quad {}^2J(^{205}\text{Tl-F}) = 2072 \text{ Hz}$$

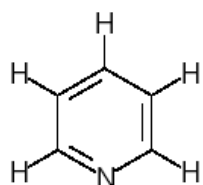
7. (4 pts) Explain differences between values of interaction constants:



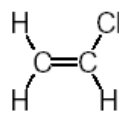
8. (26 pts) Classify spin systems (magnetic in/equivalence) in proton NMR spectra of following molecules. Give both prime and bracket notation labels:



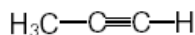
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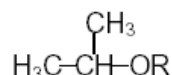
b



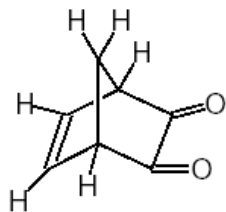
c



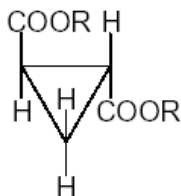
d



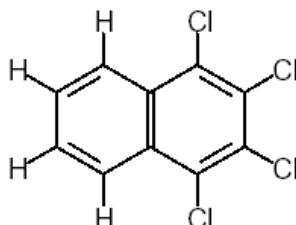
e



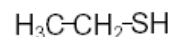
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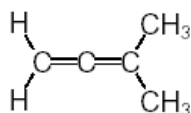
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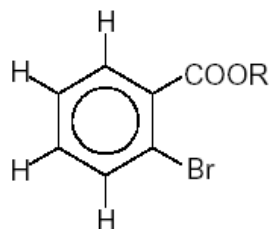
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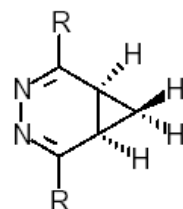
i



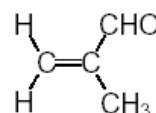
j



k



l



m

	Prime	Bracket		Prime	Bracket
A			H		
B			I		
C			J		
D			K		
E			L		
F			M		
G					