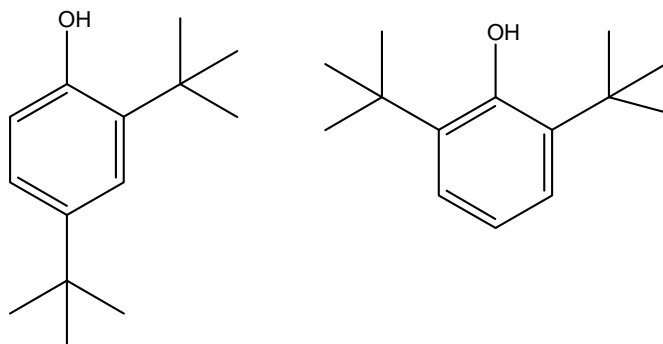


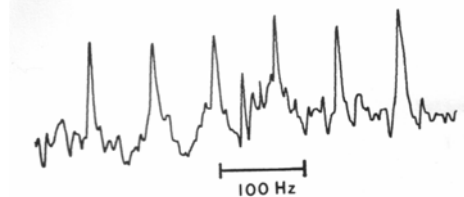
HW 3	Multinuclear NMR	Name:	
Points:	C6800	Date:	
Max. 100 points	Spring 2017	Version A	

1. (5 pts) Photolysis of HSiCl_3 provides a compound with an empirical formula $\text{Si}_5\text{Cl}_{12}$. The product displays two resonances in the ^{29}Si NMR spectra in a 4:1 intensity ratio. Derive structural formula of this molecule.

2. (12 pts) How would you distinguish these two isomers? Give the symmetry point groups of the molecules. Calculate chemical shifts of aromatic carbons (use your table of ^{13}C increments).



3. The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum in the picture belongs to $\text{Li}[\text{Al}(\text{CH}_3)_4]$ in dimethoxyethane.

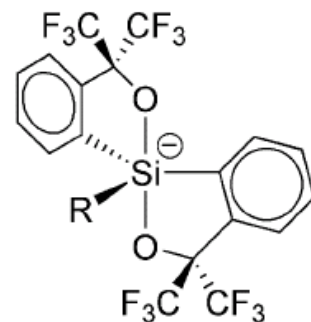


- (10 pts) Explain multiplicity (number of lines) of the signal, intensities of lines in the multiplet, and mark a coupling constant in the spectrum.
- (5 pts) Which property of this molecule allows observing the splitting? Give the symmetry point group.
- (5 pts) How would this spectrum change after turning off $\{^1\text{H}\}$ decoupling?
- (5 pts) Designate this spin system by prime notation (consider only H, C, and Al nuclei).

4. Consider two derivatives of the following anion:

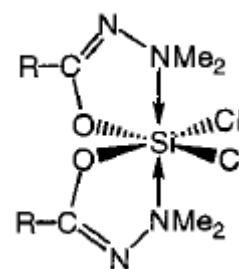
A: R = F, **B:** R = CHMePh

- (2 pts) Draw clearly all symmetry elements present in the anion **A**.
- (6 pts) Give the symmetry point group of anions **A** and **B**.
- (8 pts) Are there any geminal groups in **A**? If yes, what class do they belong to? homotopic (**H**), enantiotopic (**E**) and diastereotopic (**D**)
- (8 pts) How many resonances do you expect in the ^{19}F NMR spectra of **A** and **B**.
- (5 pts) How would you explain, that in **A** there is actually only one signal at room temperature.

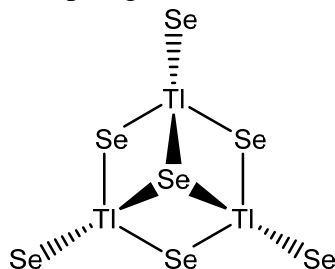


5. (20 pts) How would you explain the number of signals in the ^{29}Si NMR spectra the following molecules:

- R = Ph, -145.9 ;
- R = (R,S)-CHMePh, -146.1 , -146.4 , -146.6 ;
- R = (R)-CHMePh, -146.2 , -146.8 ;



6. (9 pts) The anion $\text{Tl}_3\text{Se}_7^{5-}$ has symmetry point group C_{3v} . Consider the following isotopologue enriched to 100% both in Se = ^{77}Se , and Tl = ^{205}Tl :



Designate this spin system by prime and bracket notations: