HW 4	Multinuclear NMR	Name:	
Points:	C6800	Date:	
Max. 100 points	Spring 2014	Version A	

1. Fluorinated ethers are used as anestethics.
a) (10 pts) Give number of signals, integral intensities, splitting patterns (multiplicity) and relative intensities of lines in the multiplets (consider only ^{1}H and ^{19}F and maximum three-bond scalar coupling).
b) (10 pts) In compounds B to D find and classify the geminal groups (H, E, D).

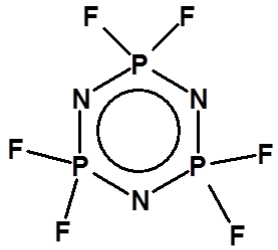
A) Isoflurane $CF_3CHClOCHF_2$

B) Desflurane $CF_3CHFOCHF_2$

C) Enflurane $CHClFCF_2OCHF_2$

D) Sevoflurane $(CF_3)_3CHOCH_2F$

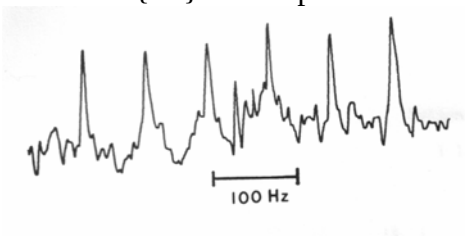
2. (12 pts) Find all possible coupling constants and write a proper label $^{n}J_{AB}$ for each of them. Consider only ^{31}P and ^{19}F nuclei:



^{31}P & ^{19}F NMR

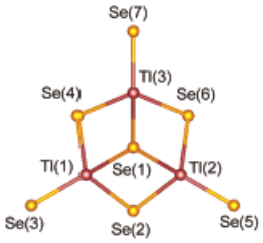
3. (8 pts) Photolysis of $HSiCl_3$ provides a compound with an empirical formula Si_5Cl_{12}. The product displays two chemical shifts in the ^{29}Si NMR spectra in a 4:1 intensity ratio. Derive structural formula of this molecule.

4. The $^{13}C\{^{1}H\}$ NMR spectrum in the picture belongs to $Li[Al(CH_3)_4]$ in dimethoxyethane.



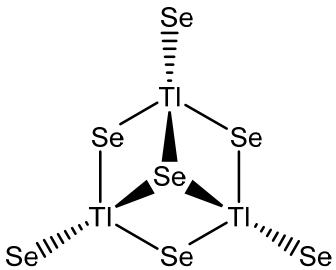
a) (10 pts) Explain multiplicity of the signal, intensities of lines in the multiplet, and mark a coupling constant in the spectrum.
b) (5 pts) Which property of this molecule allows observing the splitting? Give the symmetry point group.
c) (5 pts) How would this spectrum change after turning off decoupling.

5. Consider NMR spectra of the anion $Tl_3Se_7^{5-}$ (its symmetry point group is C_{3v}) in liquid NH_3, at –68 °C:



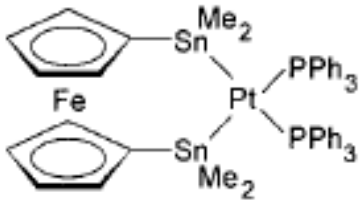
a) (10 pts) Calculate abundances of isotopomers of Tl (disregard Se nuclei).

b) (10 pts) Consider the following isotopomer (enriched to 100% both in Se = ^{77}Se, and Tl = ^{205}Tl):



Designate this spin system by prime and bracket notations:

6. (10 pts) Draw $^{31}P\{^{1}H\}$ NMR spectrum of following compound, consider maximum two-bond scalar couplings with isotopes in natural abundance, mark the coupling constants in the spectrum:



7. (10 pts) Calculate abundances of isotopomers (^{77}Se) in the following cyclic molecule. (Hint: Abundance for the whole molecule in a product (×) of abundance for site A and abundance for site B):