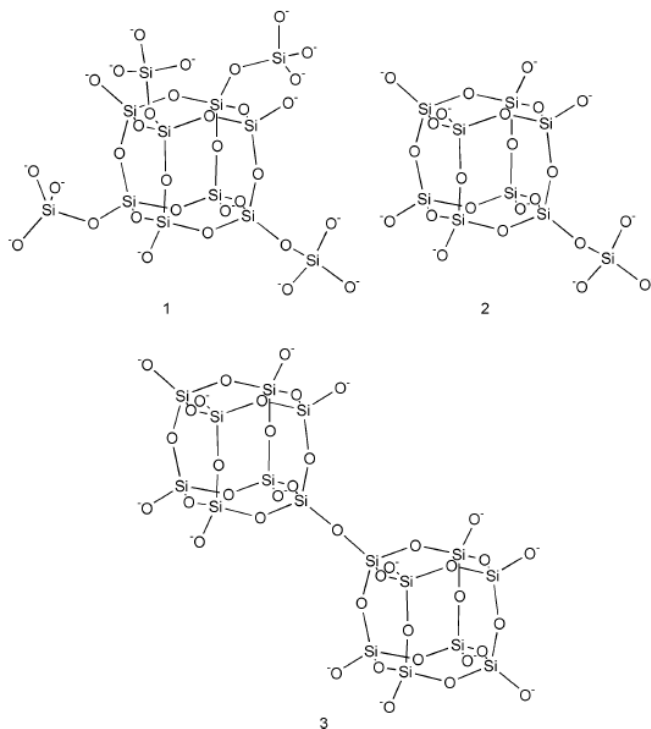
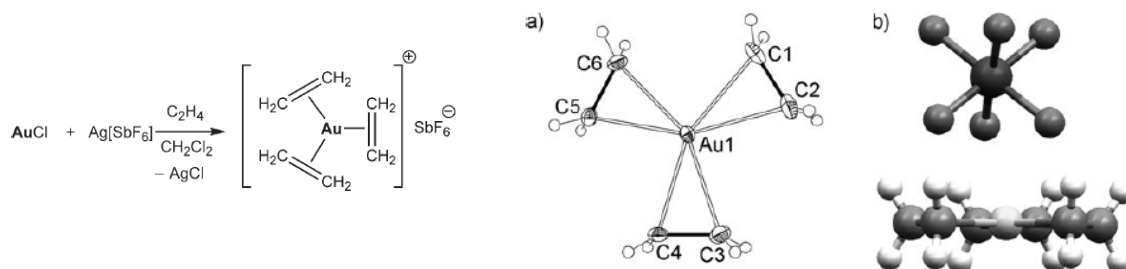


<b>HW 2</b>	<b>Multinuclear NMR</b>	<b>Name:</b>	
<b>Points:</b>	<b>C6800</b>	<b>Date:</b>	
Max. 100 points	<b>Spring 2014</b>	<b>Version A</b>	

1. Predict the number and relative intensity of the signals in the  $^{29}\text{Si}$  NMR spectra of molecules **1–3**. For **1** and **3** give the symmetry point groups.



2. Gold(I) tris(ethylene) complex  $[\text{Au}(\text{C}_2\text{H}_4)_3][\text{SbF}_6]$  was prepared by the following reaction and was structurally characterized.

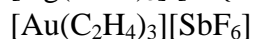


- Draw clearly all symmetry elements present in the cation.
- Give the symmetry point groups of the cation and the anion.
- Is this complex diamagnetic or paramagnetic?
- How many resonances (signals) do you expect in the  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra.
- These resonances are significantly upfield relative to the free ethylene (5.28 / 123.2 ppm). What causes this shielding effect?

$$\Delta\delta(^{13}\text{C}) = \delta(^{13}\text{C})_{\text{complex}} - \delta(^{13}\text{C})_{\text{ethylene}}$$



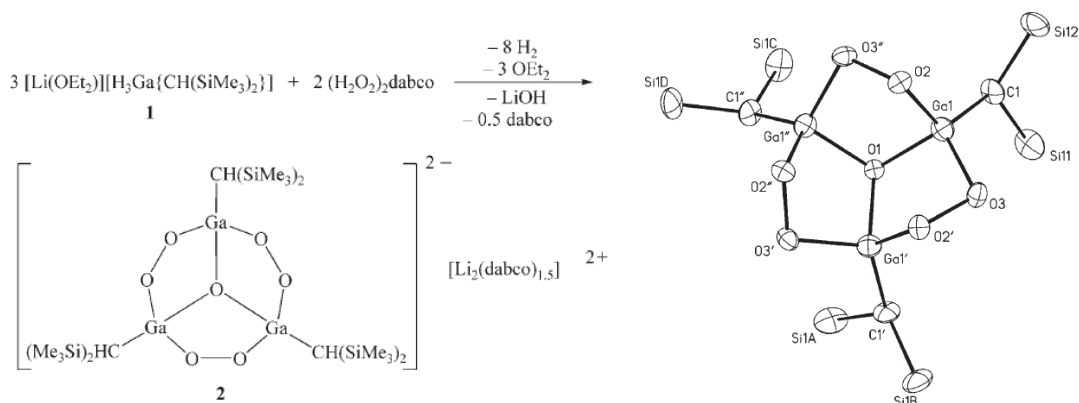
$$-7.0 \text{ ppm}$$



$$-30.7 \text{ ppm}$$

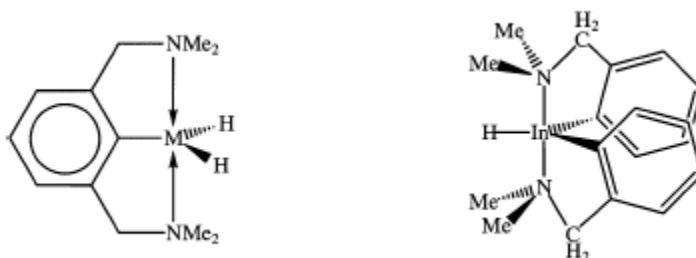
- What are the  $^{13}\text{C}$  NMR chemical shifts of the two complexes?

3. Alkyl gallium peroxide anion was synthesized by the following procedure:

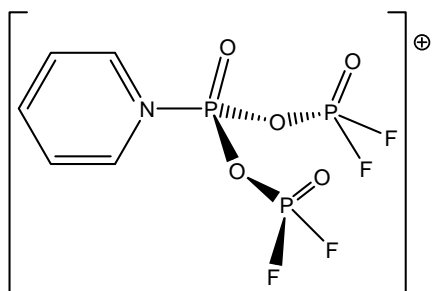


- Draw clearly all symmetry elements present in the anion.
- Give the symmetry point group of the anion.
- Are there any geminal groups? Assign them as Homo-, enantio-, or diastereotopic.
- How many resonances (signals) do you expect in the  $^1\text{H}$ ,  $^{13}\text{C}$ , and  $^{29}\text{Si}$  NMR spectra.

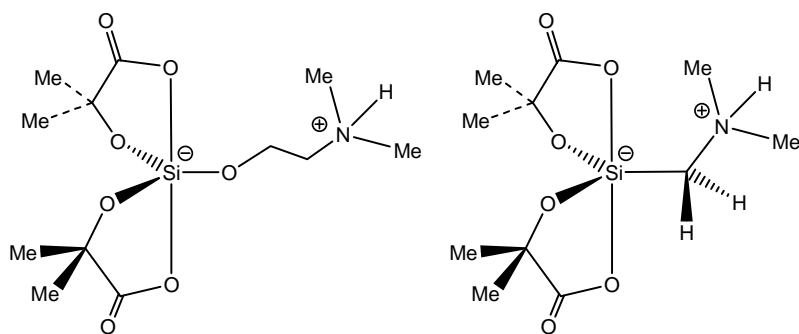
4. How many signals of the  $\text{NMe}_2$  and  $\text{CH}_2$  groups do you expect in the following compounds:



5. a) How many signals do you expect in  $^{19}\text{F}$  and  $^{31}\text{P}$  NMR spectra of the following compound:



b) How many signals do you expect in the  $\text{CH}_3$  and  $\text{CH}_2$  regions in  $^1\text{H}$  NMR:



c) How many signals do you expect in the CH<sub>2</sub> and SiMe<sub>3</sub> region in <sup>1</sup>H, <sup>13</sup>C, and <sup>29</sup>Si NMR spectra when:

i) R = methyl, ii) R = 2-butyl

