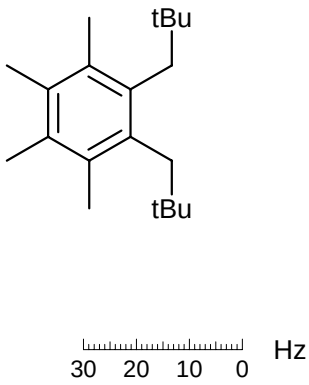
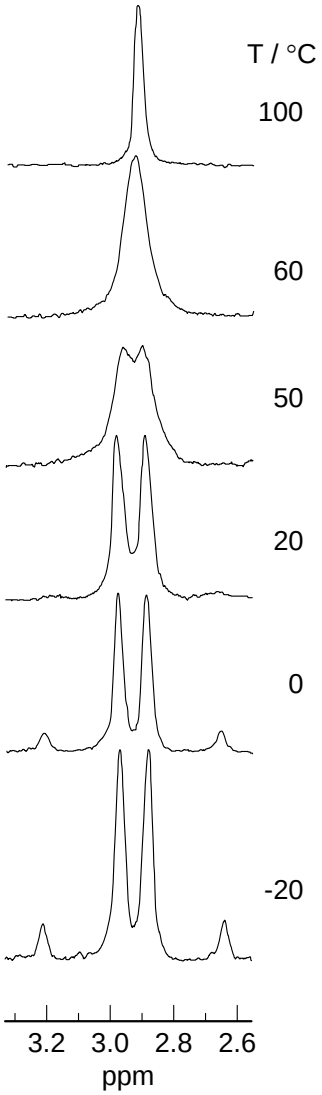
# Problem Set 13

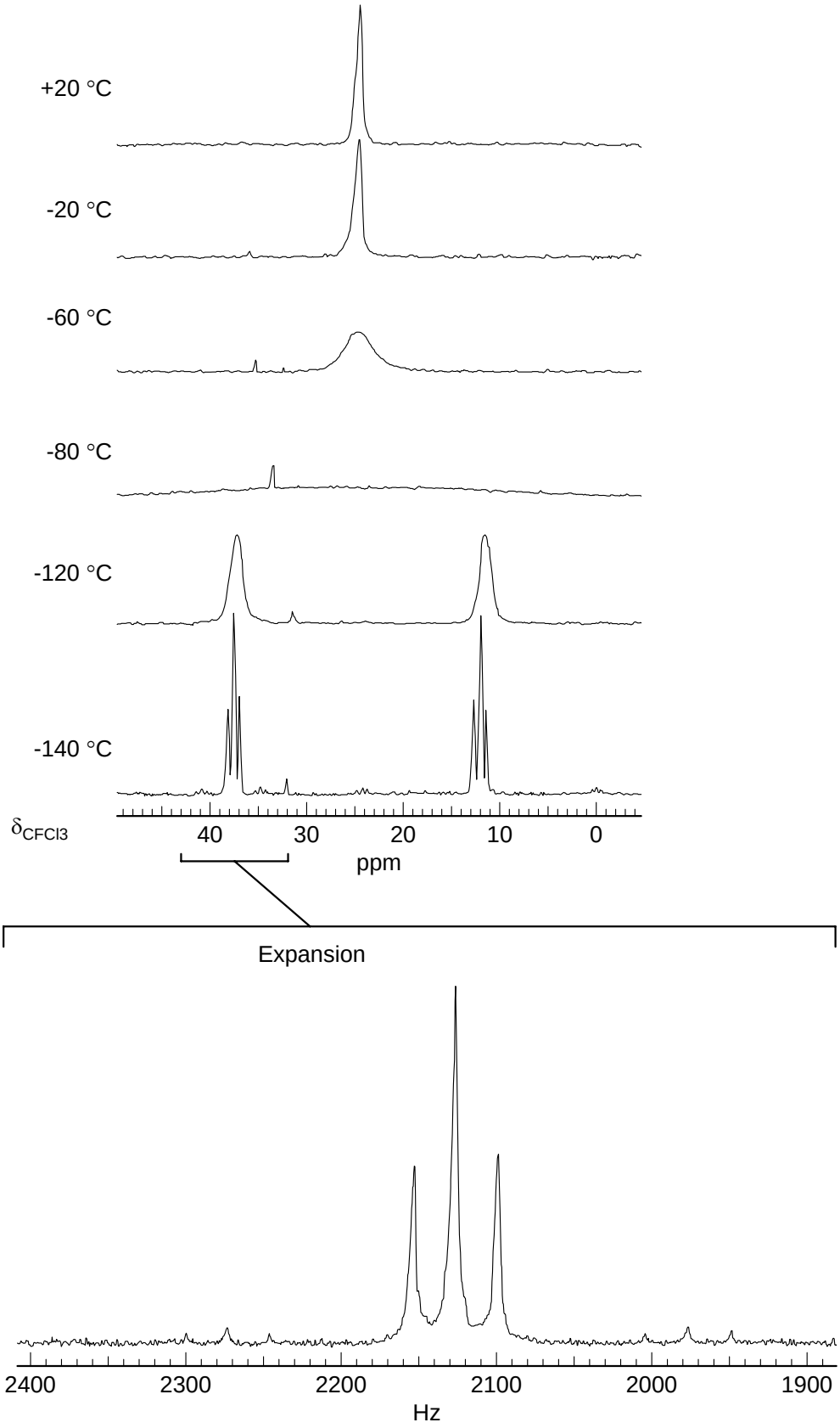
**Problem R-03N** ($C_{20}H_{34}$): Interpret the 60 MHz variable temperature $^{1}H$ NMR spectrum of 1.2-dineopentyl-3,4,5,6-tetramethylbenzene in $CCl_4$. Source: Dix, D. T.; Fraenkel, G.; Karnes, H. A.; Newman, M. S. *Tetrahedron Lett.* **1966**, 517



**Problem R-312**. Below are presented variable temperature 56.4 MHz $^{19}F$ NMR spectra of $SeF_4$. From your knowledge of structure of compounds like $SF_4$ and $SeF_4$ interpret the NMR spectra.

What conclusion can be drawn form the observation that the +20 °C spectrum does not show the weak peaks flanking the low temperature triplets (see expansion)? (*Z. Anorg. Allg. Chem.* **1975**. *416*, 12).



**Problem R-99P** ($C_{63}H_{85}B_2O_{15}P_5Pt$). This problem requires you to interpret the 36.43 MHz $^{31}P$ variable temperature NMR spectra of a platinum phosphite complex $Pt[P(OCH_3)_3]_5^{++}$ $2BPh_4^-$. The spectrum was taken with proton decoupling.

(a) Analyze the low temperature (-151 °C) spectrum. Explain the origin of each of the marked peaks a to e with reference to the structure of the compound. Report coupling constants. Use the form $^nJ_{X-Y}$ = 00.0 Hz. In your drawings, feel free to use "P" for the $P(OCH_3)_3$ group. Hint: make sure you consider the NMR active isotope(s) of platinum.

Peak a:

Peak b:

Peak c:

Peak d:

Peak e:

(b) What molecular process is responsible for the changes in the NMR spectrum as a function of temperature? Is it intra- or intermolecular? Explain how you know.

(c) For the spectra at -98 °C and -69 °C, explain why peak f is broad and peak h is relatively sharp (at still higher temperature both f and h become sharp).

**Problem R-99P** ($C_{63}H_{85}B_2O_{15}P_5Pt$).

Temperature dependent 36.43 MHz {$^1H$} $^{31}P$ NMR Spectra

$Pt[P(OCH_3)_3]_5^{2+}$ $2B(C_6H_5)_5^-$

Solvent: $CHClF_3$

(Source: *J. Am. Chem. Soc.* **1974**, *96*, 5760