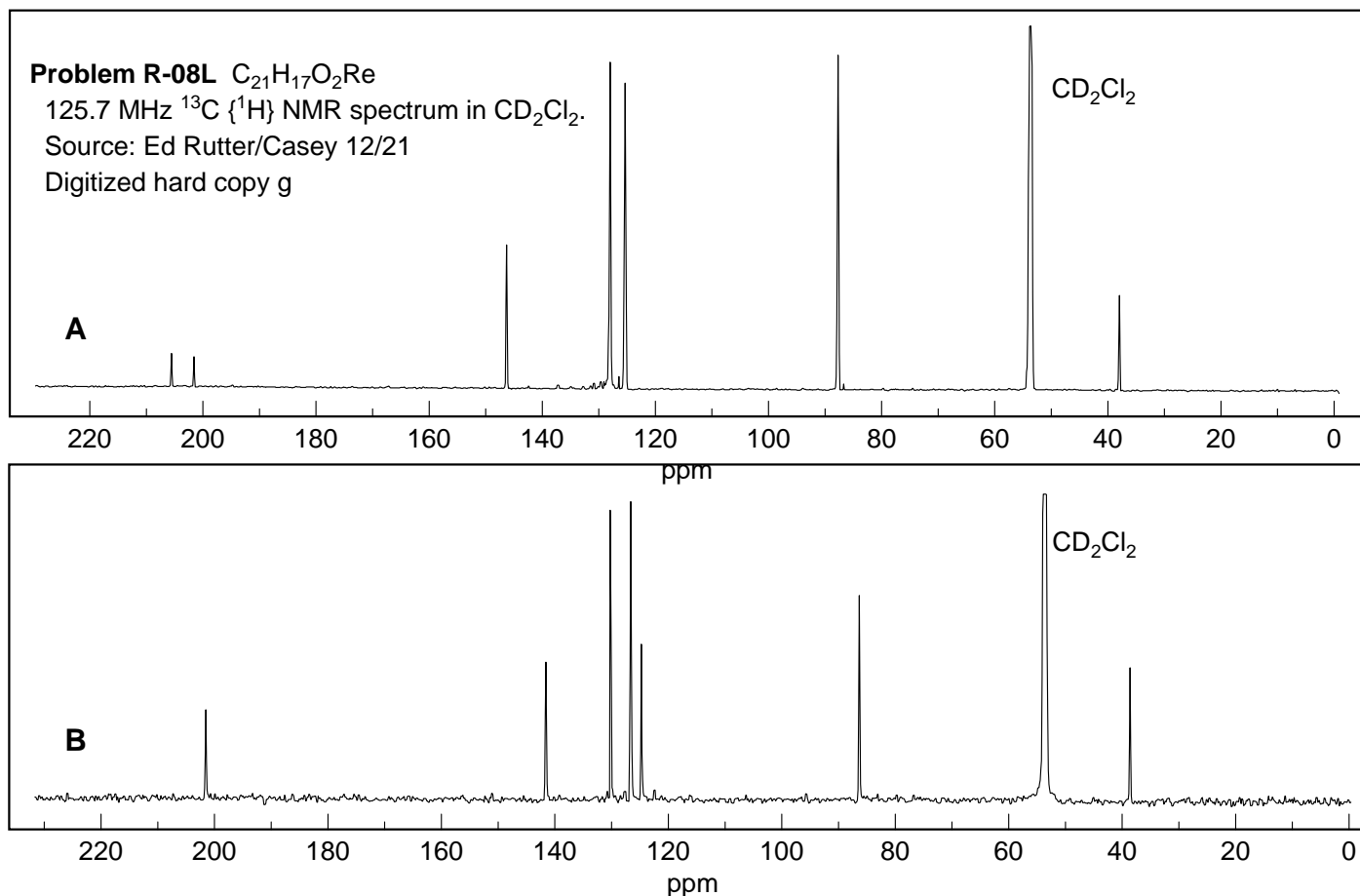
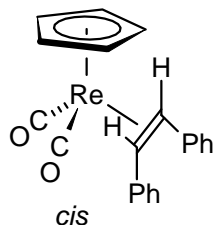
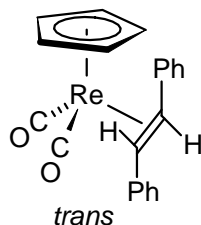


Problem R-08L. This problem requires you to determine which isomer is which from the 125 MHz ^{13}C NMR spectra (CD_2Cl_2 solvent) of cyclopentadienyl dicarbonyl rhenium complexed to *cis* and *trans* stilbene (Ed Rutter/Casey 12/21).

Since you probably don't know too much about ^{13}C shifts of organometallic complexes involving rhenium, here are some hints: vinyl carbon: 40 ppm; cyclopentadiene carbon: 90 ppm; CO carbon: 200 ppm; CD_2Cl_2 : 54 ppm.

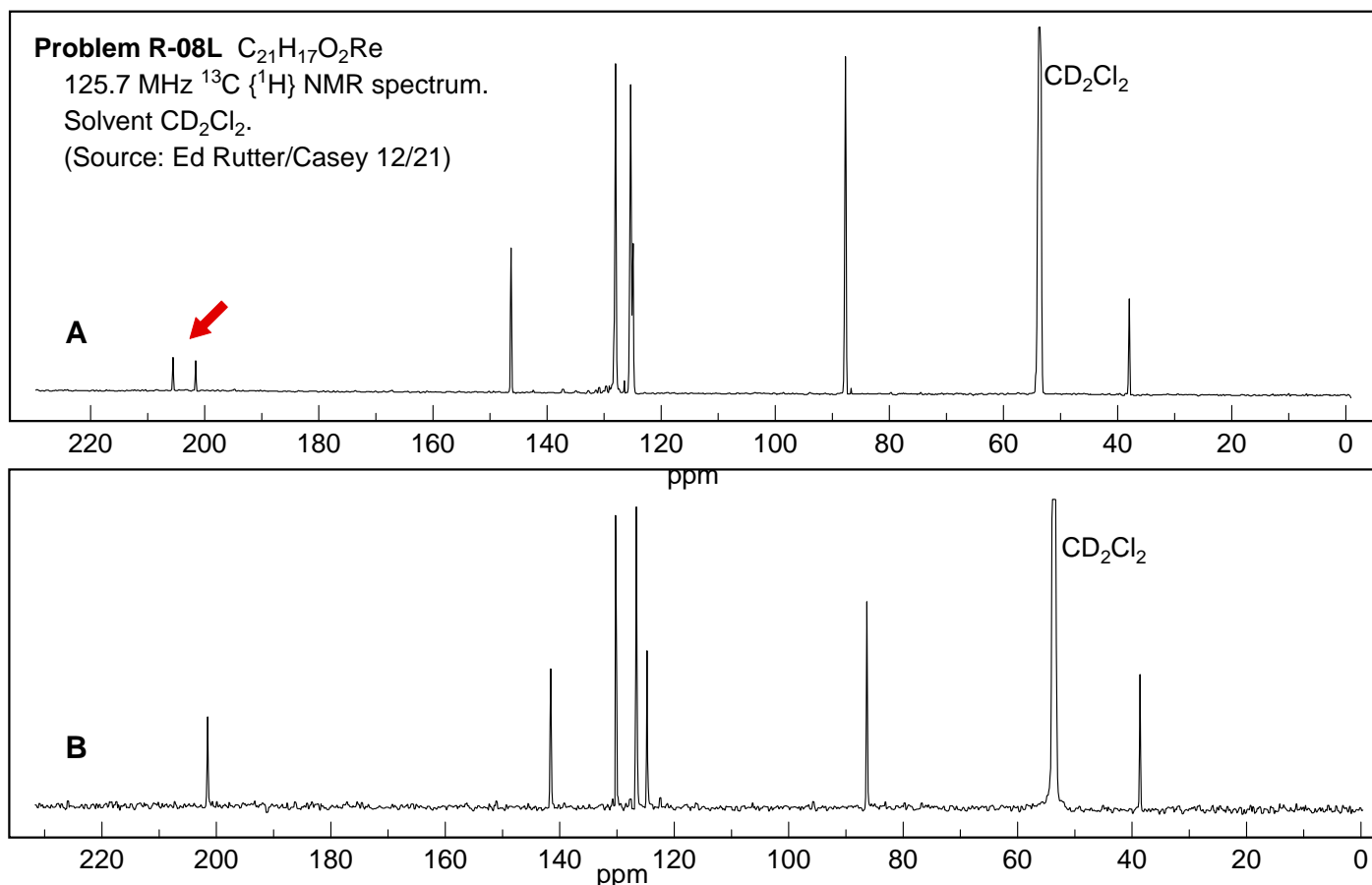
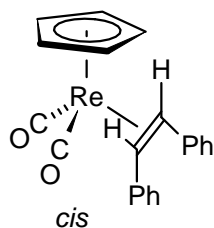
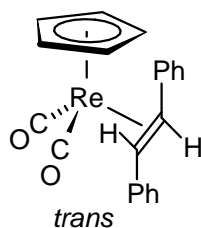


(a) Which spectrum (A or B) corresponds to the *trans*____ and which is the *cis*____? Explain your reasoning.

(b) What can you learn about the freedom of movement of the stilbene ligand from the ^{13}C NMR spectra of the two compounds?

Problem R-08L. This problem requires you to determine which isomer is which from the 125 MHz ^{13}C NMR spectra (CD_2Cl_2 solvent) of cyclopentadienyl dicarbonyl rhenium complexed to *cis* and *trans* stilbene (Ed Rutter/Casey 12/21).

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- 4 (a) Which spectrum (A or B) corresponds to the *trans* A and which is the *cis* B? Explain your reasoning.

The *trans* Re compound is chiral, so the CO groups are diastereotopic

The *cis*-Re compound has a plane of symmetry bisecting the $\text{Re}(\text{CO})_2$ grouping, so the carbonyls are equivalent (enantiotopic).

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- (b) What can you learn about the freedom of movement of the stilbene ligand from the ^{13}C NMR spectra of the two compounds?

1. The ligand must be able to rotate around the Re-olefin bond, otherwise the *trans* compound would show nonequivalent phenyl groups, and there would be two olefinic carbons.

2. The Re cannot move from one face of the olefin to the other on the NMR time scale, otherwise the CO carbons in the *trans* isomer would become equivalent.

3. There is no rapid (NMR time scale) equilibration between the *cis* and *trans* stilbenes, since they give different spectra.

4. The CO ligands are not labile (coming on and off) on the NMR time scale, since that would probably cause averaging of the diastereotopic CO signals in the *trans* isomer

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