Problem R-13I (C_{16}H_{27}NO_{2}). This problem requires that you determine the stereochemistry of a cyanohydrin (R. Corcoran). The fully coupled 75.6 MHz $^{13}$C NMR spectrum (CDCl$_3$) shown below is of a $\approx$1:4 mixture of two isomers. Source: R, Corcoran, U. Wyoming.

(a) Which carbons are responsible for the signals near 122 ppm? Analyze them.

(b) Which isomer is the major one? Explain your reasoning using a conformational drawing.
Problem R-13I \((C_{16}H_{27}NO_2)\). This problem requires that you determine the stereochemistry of a cyanohydrin (R. Corcoran, U. Wyoming). The fully coupled 75.6 MHz \(^{13}\text{C} \) NMR spectrum (CDCl\(_3\)) shown below is of a \(\approx 1:4\) mixture of two isomers.

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This is the CN group. The C would be coupled only to the adjacent CH\(_2\) protons - all other Hs are 4 or more bonds away.

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122.8  CN carbon, t, \(^3J_{\text{CH}} = 1.7 \text{ Hz} \) (major isomer)
121.7  CN carbon, dd, \(^3J_{\text{CH}} = 9.0, 3.7 \text{ Hz} \) (minor isomer)

(b) Which isomer is the major one? Explain your reasoning using a conformational drawing.

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The CN carbon should show approximately equal small couplings \( (^3J_{\text{eqH(eq)}} \) and \( ^3J_{\text{axH(ax)}} \) ) to the CH\(_2\) ax and eq protons. The major isomer has an approximate triplet, with \( J = 1.7 \text{ Hz} \).

A second argument can be made based on gamma effect on the CN chemical shift: isomer B has an axial CN group, which should therefore be upfield of the equatorial one. This leads to same assignment - Minor is B. However, the chemical shift difference is only 1.1 ppm, so this argument is not as strong as the coupling argument, and one would need some confirmation that \( \gamma \)-effects operate reliably on CN carbons.