2/2 Good work!

Jigsaw 3D

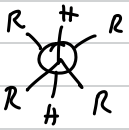
1) $J_{HH} = p_g J_1 + p_t J_2$, $p_g + p_t = 1$ (Formula 3.12 from the course)

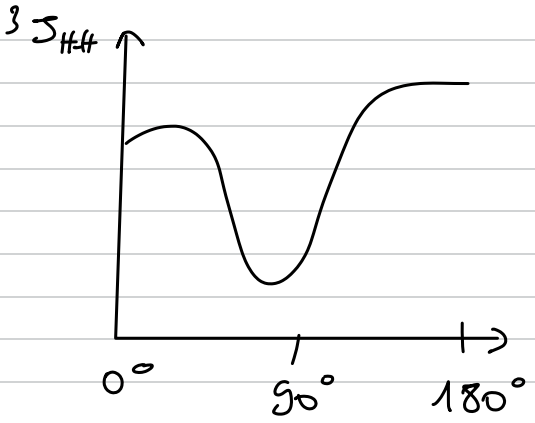
$3.96 = p_g(1.00) + (1-p_g)\ 11.70$

$p_{gauche} = 0.7898 \approx 79\,\%$

$\Rightarrow p_{trans} = 1 - 0.7898 \approx 21\,\%$

2) At 180° we expect a maximum, it corresponds to when the orbitals overlap in the best way, so it's giving the best coupling, like:



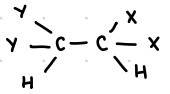


The J-coupling depends on the dihedral angles mainly because of σ-orbitals overlap with the best overlap happening around 180° and the smallest happens around 60° following the "Karplus relation" 3.11 from the course:

$$^3J_{HH} \approx A + B\cos\theta + C\cos^2\theta$$

2/2 Nice job!

Problem 1



$J_{coupling}$ $^1H-^1H$ → 3.96 Hz

$J_1 = 1.9$ Hz → gauche
$J_2 = 11.7$ Hz → trans

we know that $\begin{cases} J_{12} = P_1 J_1 + P_2 J_2 \\ P_1 + P_2 = 1 \end{cases}$

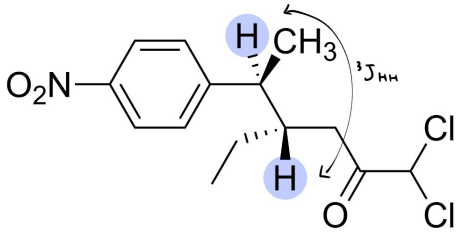
$\Leftrightarrow \begin{cases} 3.96 = (1-P_2)\cdot 1.9 + P_2 \cdot 11.7 \\ P_1 = 1-P_2 \end{cases}$

$\Leftrightarrow \begin{cases} 3.96 = 1.9 + P_2(11.7-1.9) \\ P_1 = 1-P_2 \end{cases}$

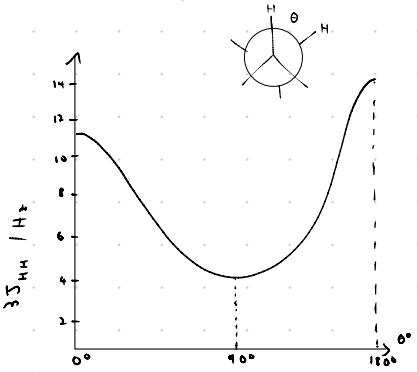
$\Leftrightarrow \begin{cases} \frac{3.96-1.9}{11.7-1.9} = P_2 \\ P_1 = 1-P_2 \end{cases}$

$\Leftrightarrow \begin{cases} P_2 = 0.21 \\ P_1 = 0.79 \end{cases}$

Problem 2



As shown on the sketch and using karplus relation, we see that the angle for the maximum $^3J_{HH}$ constant is 180°, generalised for all H-C-C-H bonds.



⇒ $^3J_{HH}$ values for ring protons depends on if axial/equatorial protons are involved.

Trans $^1H-^1H$ coupling ⇒ 2 times the value of cis-coupling