

In-Class Exercise Solutions: Deciphering Multiplets with Many *J*'s

¹H NMR, 250 MHz, acetone- d_6

b. It's pretty clear based on chemical shift that **d** represents the methyl group, and because J = 5.1 Hz is the only large coupling constant resonance **d** shows, **a** must be the proton α to the methyl group. So, of the two -CH₂-protons, which is **b** and which is **c**?

Looking at the structure of the molecule, the dihedral angle between proton **a** and its two neighbors at 0° and ~140°. I would expect that $\phi = 0^{\circ}$ would maximize *J* (according to the Karplus equation), and $\phi = 140^{\circ}$ would minimize *J*. So, I think that proton **b** is *cis* to proton **a**, and proton **c** is *trans* to proton **a**.

