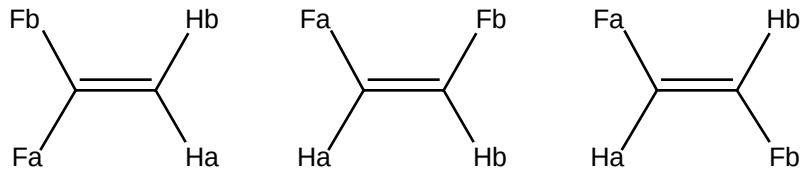
Chemistry 416, Winter Semester 1996, Dr. Glaser
Quiz III: "NMR Spectroscopy", Friday, May 5, 1996, 20 minutes, announced

Your Name:

Question 1. Coupling in Difluoroethene Isomers. (12 points)



(a) In lecture, we talked about the 1,1-isomer and we decided that H_a and H_b are chemically _____ (equi., not equiv.) because they were related by _____ (no, a C_s, a c_2) symmetry element. The term "homotopic" _____ (would, would not) apply to H_a and H_b. Moreover, it is clear that H_a and H_b _____ (are, are not) magnetically equivalent and hence the ^{1}H-NMR spectrum will be _____ (simple, complex). (5 points)

(b) Now let's turn to the two 1,2-isomers. The atoms H_a and H_b in the *cis* isomer are chemically equivalent because of the _____ symmetry element. Because of this chemical equivalence, the H nuclei are chemical shift equivalent and they _____ (are, are not) magnetically equivalent. The *trans* isomer can be described as a _____ (A_2X_2, AA'XX') spin system.

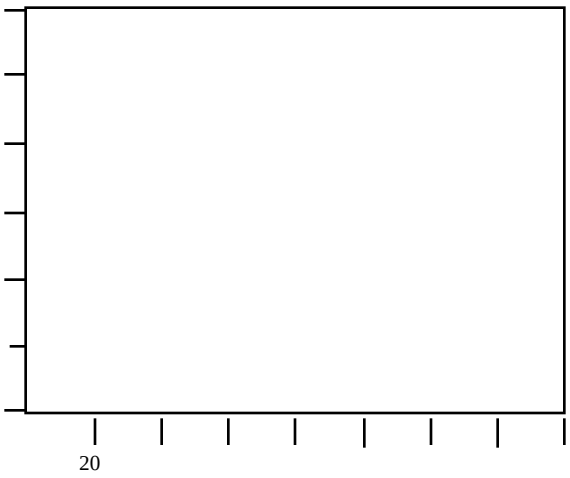
(c) For ethene the geminal coupling constant is about ____ (2.5, 5, 7.5, 10) Hz. The vicinal coupling constant depends on the stereochemical relation: The *cis* coupling is _____ (smaller, larger) than the *trans* coupling and the *trans* coupling is about _____ (8, 16, 24, 32) Hz. The fluorine substituents are expected to _____ (increase, decrease) the geminal coupling constant.

OVER

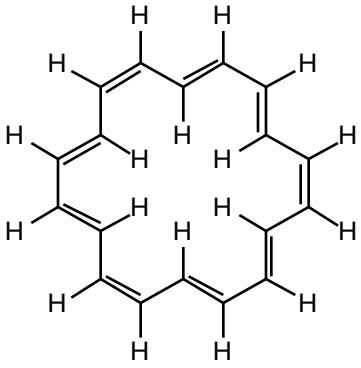
Points for Question 1:	/12		
Points for Question 2:	/10		
Points for Question 3:	/8	Total Points:	/30

Question 2. Karplus Equation. (10 points)

Draw the Karplus correlation in the space provided. The vertical axis shows the coupling constant in Hertz. Provide reasonable labels to the y-axis. Using a Newman projection, indicate to the right what parameter is shown on the x-axis.



Question 3. Ring Current Effects. (8 points)



A spectacular example of shielding and deshielding by ring currents is furnished by some of the annulenes. At low temperatures, the protons outside of ring of [18]annulene are strongly _____ and occur at much _____ (lower, higher) chemical shift and those inside are strongly _____ and occur _____ (downfield, upfield) of TMS. (2 points each)

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