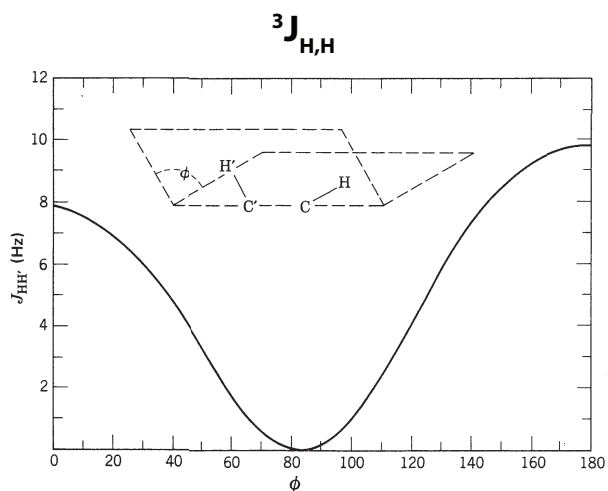
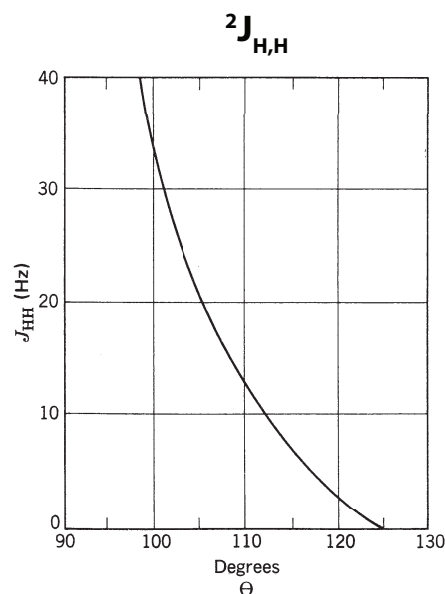


# Karplus Relationships

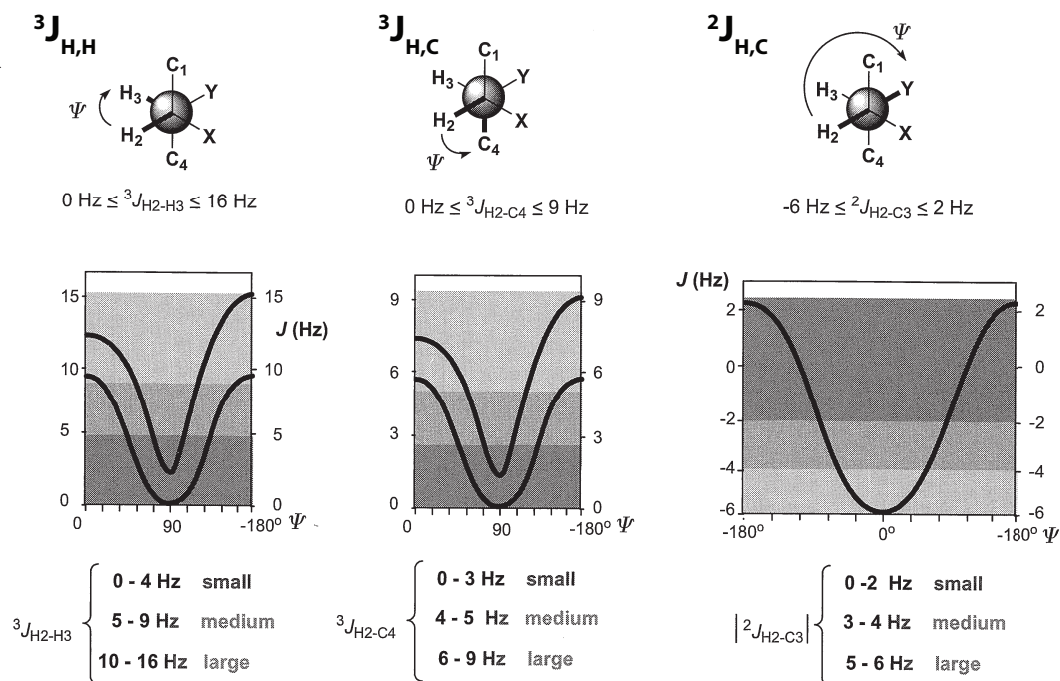


**FIGURE 3.57** The vicinal Karplus correlation. Relationship between dihedral angle ( $\phi$ ) and coupling constant for vicinal protons.



**FIGURE 3.58** The geminal Karplus correlation.  $J_{HH}$  for  $\text{CH}_2$  groups as a function of  $>\text{H}-\text{C}-\text{H}$ . Note the zero coupling at about  $125^\circ$ .

Silverstein, R., et. al. (2005). "Spectrometric Identification of Organic Compounds," 7th Ed. New York: Wiley.



General equation for B bond  $^1\text{H}-^1\text{H}$  coupling constants  

$$^3J_{\text{HH}} = A + B (\cos \psi) + C (\cos 2\psi).$$

**FIGURE 4.7** Relationship between coupling constants ( $^3J$ ,  $^2J$ ) and dihedral angle  $\psi$ . Upper curves represent original Karplus equation, lower curves are the Altona equation for heteroatom-substituted carbon chains.

Crews, P., et. al. (2010). "Organic Structure Analysis," 2nd Ed. New York: Oxford.

