Chemistry 416, Dr. Glaser

Multiple Irradiation in NMR Spectroscopy: Difference Decoupling Spectra

Multipe Irradiation

In very complex spectra, decoupling may show little simplification in the spectrum. In such cases it is good to record *difference decoupling spectra*.

* The unaffected peaks don't show up anymore.
* The original peaks show up negative.
* The new (decoupled) peaks show up positive.

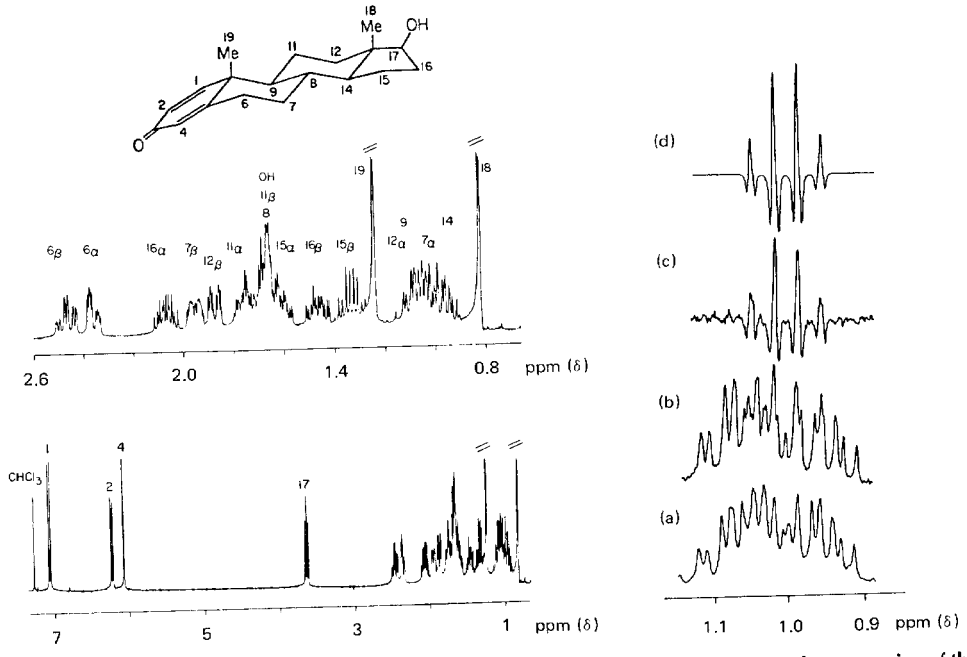

FIGURE 5-8 The 400 MHz spectrum of 1-dehydrotestosterone. The complete spectrum and an expansion of the high-field region are given on the left. On the right are given (a) the coupled spectrum for the δ 0.9–1.1 region, (b) the same region decoupled from the 6α proton, (c) the difference spectrum, and (d) the calculated difference spectrum. [Reproduced with permission from L. D. Hall and J. K. M. Saunders, *J. Am. Chem. Soc.*, **102**, 5703 (1980). Copyright 1980 American Chemical Society.]

Interpret the significance of the spectra (c) and (d). Note that the spectra (a) and (b) would not be useful to deduce anything of significance!!