1
1 1
1 2 1
1 3 3 1
1 4 6 4 1

2

of an A_nX_2 species would also be a 1 : 2 : 1 triplet of splitting J, the only difference that the intensity of the A resonance would be n times as great as that of AX_2.

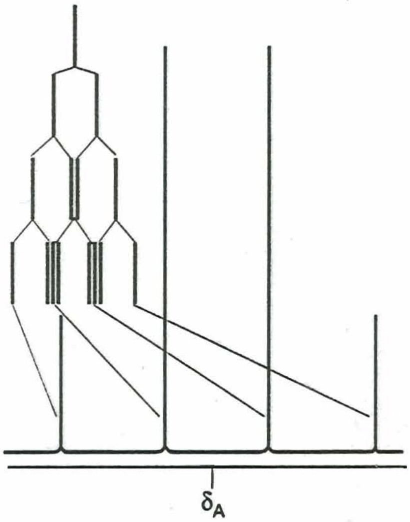
Three equivalent X nuclei (an AX_3 species) split the resonance of A into four li intensity ratio 1 : 3 : 3 : 1 and separation J (Fig. 18.14). The X resonance, though, is doublet of separation J. In general, n equivalent spin-$\frac{1}{2}$ nuclei split the resonance of a n spin or group of equivalent spins into $n+1$ lines with an intensity distribution giv Pascal's triangle (2). The easiest way of constructing the pattern of fine structure is to d diagram in which successive rows show the splitting of a subsequent proton. The proc is illustrated in Fig. 18.15 and was used in Figs. 18.13 and 18.14. It is easily extend molecules containing nuclei with $I > \frac{1}{2}$ (Fig. 18.16).

Example 18.2 Accounting for the fine structure in a spectrum

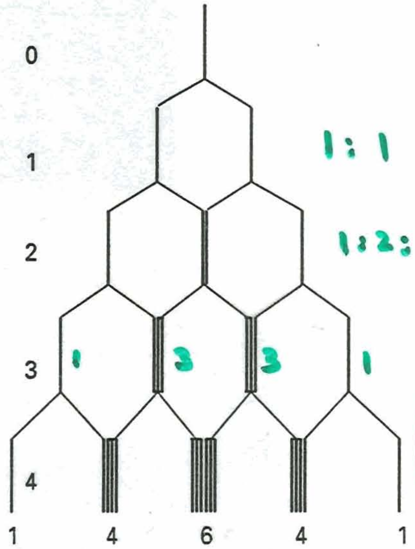
Account for the fine structure in the NMR spectrum of the C–H protons of ethanol.

Method Consider how each group of equivalent protons (for example, three methyl pr split the resonance of the other groups of protons. There is no splitting within grou equivalent protons. Each splitting pattern can be decided by referring to Pascal's tri

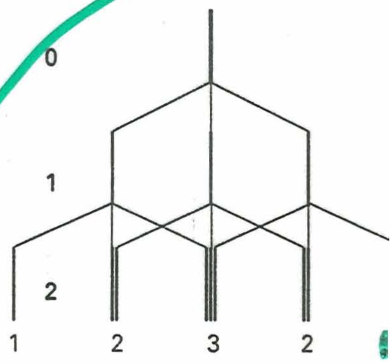
Answer The three protons of the CH_3 group split the resonance of the CH_2 protons 1 : 3 : 3 : 1 quartet with a splitting J. Likewise, the two protons of the CH_2 group sp resonance of the CH_3 protons into a 1 : 2 : 1 triplet with the same splitting J. All the mentioned so far are split into doublets by the OH proton, but the splitting cann detected because the OH protons migrate rapidly from molecule to molecule and their averages to zero.



18.14 The origin of the 1 : 3 : 3 : 1 quartet in the A resonance of an AX_3 species. The third X nucleus splits each of the lines shown in Fig. 18.13 for an AX_2 species into a doublet, and the intensity distribution reflects the number of transitions that have the same energy.



18.15 The intensity distribution of the A resonance of an AX_n resonance can be constructed by considering the splitting caused by 1, 2, ... n protons, as in Figs. 18.13 and 18.14. The resulting intensity distribution has a binomial distribution and is given by the integers in the corresponding row of Pascal's triangle. Note that, although the lines have been drawn side-by-side for clarity, the members of each group are coincident. Four protons, in AX_4, split the A resonance into a 1 : 4 : 6 : 4 : 1 quintet.



18.16 The intensity distribution arising from spin interaction with nuclei with $I = 1$ can b constructed similarly, but each successive nu splits the lines into three equal intensity components. Two equivalent spin-1 nuclei gi to a 1 : 2 : 3 : 2 : 1 quintet.