Problem R-10K (C_{42}H_{33}P_3). The proton decoupled $^{31}$P NMR spectrum below is of one of the compounds 1, 2 or 3.

Problem R-10K C_{42}H_{33}P_3
80.96 MHz $^{31}$P {1H} NMR spectrum.
(Source: Peter H. M. Budzelaar)
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(a) Which of the structures is correct? ____. Explain briefly.

(b) What kind of pattern is this (e.g. AA'BB') ______. Analyze the spectrum to obtain all pertinent coupling constants and chemical shifts, and report them below.

(c) What is the proton NMR frequency on this spectrometer? ______
Problem R-10K \((C_{42}H_{33}P_3)\). The proton decoupled \(^{31}P\) NMR spectrum below is of one of the compounds 1, 2 or 3.

(a) Which of the structures is correct? \(\textbf{1}\). Explain briefly.

Should show just a singlet, 2 should show three shifts (AMX or ABX), each a dd. Neither one fits the spectrum

1 would show an AX\(_2\) or AB\(_2\) pattern, this clearly fits

(b) What kind of pattern is this (e.g. AA'BB') \(\textbf{AB}\(_2\)\). Analyze the spectrum to obtain all pertinent coupling constants and chemical shifts, and report them below.

From the integration (as well as general appearance), the left 4 peaks are \(\textbf{A}\), the right 4 peaks \(\textbf{B}\)

\[\nu_A = \nu_3 = -1295.2 \text{ Hz}, \quad \delta_A = -16.0 \text{ ppm}\]

\[\nu_B = (\nu_5 + \nu_7) / 2 = -1417.6 \text{ Hz}, \quad \delta_B = -17.51 \text{ ppm}\]

\[J_{\text{AB}} = (\nu_1 - \nu_4 + \nu_6 - \nu_8) / 3 = 120.2 \text{ Hz}\]

(c) What is the proton NMR frequency on this spectrometer? \(\textbf{200}\)

\[\frac{\gamma_H}{\gamma_P} \times 80.96 = 199.95 \text{ MHz}\]