5.12 ABX Pattern

AMX, ABX and ABC patterns, and various related spin systems are very common in organic molecules. Below some of the structural types which give patterns of this type.

**AMX Patterns.** Three nuclei coupled to each other and separated by a large chemical shifts compared to the coupling between them can be analyzed in first order fashion (Sect. 5-HMR-3): the A, M and X signals are each a doublet of doublets, and the couplings can be extracted by inspection. How can the assignments for the A and M protons be done in the example below?

**ABX Patterns.** When two of the protons of an AMX pattern approach each other to form an ABX pattern, the characteristic changes in intensities (leaning) are seen, and, as the size of \( J \) approaches the value of \( \nu_{AB} \) more complicated changes arise, so that the pattern can no longer be analyzed correctly by first order methods. A typical ABX spectrum is shown below:

For this spectrum \( \nu_{AB} \) is less than twice \( J \), and a first order (AMX-type) interpretation starts to become imprecise, although, in this particular case, it is unlikely to lead to a substantial misinterpretation. On the other hand, for the spectrum below (which is actually an ABMX, where \( X = ^{19}F \)), the second order effects are so large than a first order interpretation may lead to grossly inaccurate couplings, both in magnitude and sign, and a possible misinterpretation of the structure.
Even more likely to mislead is the ABX pattern below, for which any form of first order analysis could lead to wildly incorrect structure interpretations, or even a "false negative" during synthesis of a molecule (i.e., your reaction was actually successful, but you conclude that if failed because the NMR spectrum does not appear to fit the desired structure).

(C9H13NO)

For these reasons, we will examine ABX patterns in some detail. In the progression from first-order NMR patterns to incomprehensible jungles of peaks, they represent the last stopping point where a complete analysis (by hand or hand calculator) is still possible, and where insights into the problems that arise in the analysis of more complex systems can be achieved. Specifically, ABX patterns are the simplest systems which show the phenomenon sometimes referred to as "virtual coupling" (see Sect. 5-HMR-16) and they are the simplest systems in which both the magnitude and the sign of $J$ coupling constants is significant. Furthermore, as illustrated above, there are several pathological forms of ABX patterns which are sufficiently nonintuitive that the unwary spectroscopist can mis-assign coupling constants and even structures.
Development of an ABX Pattern. Consider the stick diagram below which represents an ABX pattern in which we sequentially turn on first the A-X and then the B-X coupling:

One of the two lines in the A-pattern arises from those molecules with the spin of the X-nucleus aligned against the field ($\beta$) and the other from those which have the X-spin aligned with the field ($\alpha$). Similarly for the B-pattern. Note, however, that the line assignments of the pattern with both $J_{AX}$ and $J_{BX}$ nonzero will be different depending on the relative sign of $J_{AX}$ and $J_{BX}$, as illustrated in the figure. Up to this point the line positions are identical.

The key to understanding ABX patterns is to realize that the $A$ and $B$ nuclei with $X = \alpha$ and those with $X = \beta$ are actually on different molecules, and cannot interact with each other. Thus, when we finally turn on $J_{AB}$, it will be the $X = \alpha$ line of A and the $X = \alpha$ line of B that will couple to form an AB-quartet, similarly the two $X = \beta$ lines will form a second AB-quartet. Since the line intensities and line positions of an AB quartet depend on the “chemical shift” between the nuclei, it is clear that the different relative signs of $J_{AX}$ and $J_{BX}$ will result in different spectra. The ABX pattern is thus the simplest spin system for which the discerning spectroscopist can identify the relative signs of coupling constants by analysis of the pattern. The figure below shows the final AB part of the ABX pattern for the two cases.

Effect of Relative Sign of $J_{AX}$ and $J_{BX}$ on an ABX pattern

<table>
<thead>
<tr>
<th>Same sign</th>
<th>Different signs</th>
</tr>
</thead>
<tbody>
<tr>
<td>$J_{AB} = 13$ Hz</td>
<td>$J_{AB} = 13$ Hz</td>
</tr>
<tr>
<td>$J_{AX} = 5$ Hz</td>
<td>$J_{AX} = 5$ Hz</td>
</tr>
<tr>
<td>$J_{BX} = 10$ Hz</td>
<td>$J_{BX} = -10$ Hz</td>
</tr>
</tbody>
</table>

$\nu_B = 90$ Hz
$\nu_A = 110$ Hz
Solving ABX Patterns

Recognizing an ABX Pattern. A typical ABX spectrum consists of an unsymmetrical 8-line pattern which has 4 doublets with the same separation $J_{AB}$ (each doublet shows strong "leaning"). This is the AB part and integrates to two protons. The X part is a symmetric 6-line pattern, with two of the lines small, and not often seen. $J_{AB}$ and $\nu_X$ are easily found. It integrates to one proton.

The AB part consists of two superimposed ab quartets (8 lines) which have normal intensities and line separations, both of which have identical $J_{AB}$ values. Occasionally one of the ab quartets has $\nu_{ab} = 0$, and appears as a singlet. Such systems appear as a five line pattern, with one ab quartet and a singlet (see Fig. 5-12-4 for an example). There are also several other deceptive forms with one or more lines superimposed.

The X part usually consists of an apparent doublet of doublets, although apparent triplets are not uncommon. There are two other lines which are often too weak to be detected (total of 6 lines). They become large when $J_{AB} > \nu_{AB}$.

First Order "AMX" Type Solution. Many ABX patterns are sufficiently close to AMX (i.e., $\nu_{AB} >> J_{AB}$) that a first-order solution has a good chance of being correct. We identify the distorted doublet of doublets ($J_{AB}$, $J_{AX}$) which make up the A portion, as well as the dd ($J_{AB}$, $J_{BX}$) for B, and begin the analysis by first removing the $J_{AX}$ and $J_{BX}$ couplings, respectively. This leaves us with an AB pattern, which we can solve in the usual way. Since this is a first-order analysis there is no information about the relative signs of $J_{AB}$ and $J_{BX}$.

Exact solution to an ABX Pattern

1. Solve the two AB patterns
2. Then remove $J_{AX}$ and $J_{BX}$ (solve two d)

Note that the approximate analysis at the bottom proceeds in the reverse order as the exact one at the top.

Approximate "AMX" Solution

1. Remove $J_{AX}$ and $J_{BX}$ (solve two dd)
2. Then solve AB pattern

For ABX patterns which are of the "Solution 1" type (see below) this analysis will lead to $J$ and $\delta$ values that are quite close to correct. The errors become larger when $J_{AX}$ and $J_{BX}$ are very different in size (especially if they are different in sign) and, of course, when $\nu_{AB}$ is small compared to $J_{AB}$. However, such an analysis, carelessly applied, can be completely wrong if the system is of the "Solution 2" type.

1 We will use "a" and "b" for the AB-subquartets of the AB part of an ABX pattern
Correct Analysis of ABX Patterns. In order to correctly analyze an ABX pattern of arbitrary complexity we have to reverse the order of extraction of coupling constants compared to the AMX solution above. We have to first solve for $J_{AB}$, and then for $J_{AX}$ and $J_{BX}$. Proceed in the following order:

1. **Identify the two ab quartets.** These can usually be recognized by the characteristic line separations and "leaning." We will use the notation $ab_+$ and $ab_-$ for the two quartets (+ identifies the one with the larger $\nu_{ab}$). Check to make sure that $J_{ab_+} = J_{ab_-}$, and that the ab quartet with the taller middle lines has the shorter outer lines. Note that ABX patterns are not affected by the sign of $J_{AB}$.

If the ABX pattern verges on AMX ($\nu_{AB}/J_{AB} >> 2$), then line intensity patterns will not allow unambiguous choice of ab subquartets. Such systems can normally be analyzed as an AMX pattern, but with the limitation that the relative signs of $J_{AX}$ and $J_{BX}$ is indeterminate. If you complete the full ABX treatment with the wrong assignment of quartets, the signs of $J_{AX}$ and $J_{BX}$ will be wrong, and there will be small errors in their magnitude. This could ultimately lead to a wrong Solution 1/2 assignment (see below) if you use the signs of couplings to make the distinction.

Another situation in which the choice of ab subquartets can be difficult is in systems verging on ABC, where all of the line intensities are distorted. This is where computer simulations might become necessary.

2. **Solve the two ab quartets.** Treat the ab subquartets as normal AB patterns, and obtain the four "chemical shifts," $\nu_{a+}$, $\nu_{b+}$, and $\nu_{a-}$, $\nu_{b-}$.

\[
\Delta \nu_{ab-} = \delta_- = \frac{(7-1)(5-3)}{2} = 17.5 \\
\frac{\delta_-}{2} = 103.7 \pm 8.76 = 112.5, 94.9 \\
\frac{\delta_+}{2} = 96.25 \pm 8.76 = 107.5, 85.0
\]

At this stage, we know one of the bold lines is a, and the other b, but we do not know which is which.
Similarly for the thin lines.

5-HMR-12.5
3. Identify the correct solution. At this point in the analysis we encounter an ambiguity. We know that each of the ab quartets consists of two a and two b lines, but we do not know which half is a and which is b. There are thus two solutions to all ABX patterns which have two ab quartets.² The two solutions are obtained by pairing up one each of a δ⁺ and a δ⁻ line. The analysis is completed as below:

The relative sign of $J_{AX}$ and $J_{BX}$ is given by the direction of vectors from bold to thin lines (i.e., whether the X = $\alpha$ lines are upfield or downfield of the X = $\beta$ lines).

As part of the solution we obtain the relative signs of $J_{AX}$ and $J_{BX}$. In the example above, this means that for Solution 1 the couplings are either both positive or both negative, and for Solution 2 one is positive and one negative.

The relative signs of $J_{AX}$ and $J_{BX}$ are determined by the way in which the ab quartets overlap. For the statements below, "lines" refers to the $\nu_a$ and $\nu_b$ line positions obtained by solving the ab and $ab_-$ quartets. If the lines of $ab_-$ do not overlap those of $ab_+$, then $J_{AX}$ and $J_{BX}$ have the same sign in Solutions 1 and 2. If the lines of $ab_+$ are inside those of $ab_-$, then $J_{AX}$ and $J_{BX}$ have opposite signs in both Solutions 1 and 2. If the lines of $ab_-$ and $ab_+$ partially overlap, then $J_{AX}$ and $J_{BX}$ have the same signs in one solution, and opposite signs in the other. This is the case for the current example.

Solution 1 is defined as the one with the larger difference between $\nu_a$ and $\nu_b$. Thus Solution 1 always has the least distorted X-part.

---

² The only exceptions are those ABX patterns in which one of the ab quartets has collapsed to a singlet. For these there is only one solution.
Distinguishing Between Solutions 1 and 2. Which solution is the correct one? This determination can be made according to several criteria:

1. **Magnitude of the couplings.** Sometimes one of the solutions gives unreasonable couplings. In the example above, if we are dealing with proton-proton couplings, Solution 2 looks dubious because one of the couplings, $J_{BX}$ at 27.6 Hz, is larger than usually observed for $J_{HH}$. A coupling this large is not impossible for a proton spectrum, but rather unlikely.

2. **Signs of coupling constants.** Sometimes the sign of the coupling constants is definitive. If the structure fragment is known, the signs can sometimes be predicted, and may rule out one solution. For example, all vicinal $J_{HC}$ couplings are positive, geminal $J_{HCH}$ couplings at sp$^3$ carbons are usually negative. A common structure fragment which gives ABX patterns is CHX-CHAHB. Here both $J_{AX}$ and $J_{BX}$ must have the same sign. On the other hand, if the pattern is CHA-CHBHX then the signs must be different. Note, however, that if you misidentified the ab subquartets, then the signs of the coupling constants you calculated may be wrong.

3. **Analysis of the X-Part.** It is important to note that all lines have identical positions in both Solutions 1 and 2. The intensities of the AB part are also identical for both solutions. However, the intensities of the lines in the X-part are always different, and this is the most reliable and general way to identify the correct solution.

For the vast majority of ABX patterns encountered in organic molecules, Solution 1 is correct. Solution 2 spectra are found when A and B are close in chemical shift and the magnitude of $J_{AX}$ and $J_{BX}$ are very different or they have different signs.

**Checking your solution arithmetic.** There are a couple of checks you can run to make sure that there has not been a calculation error:

1. The difference in the centers of the two ab quartets should be half the average of the $J_{AX}$ and $J_{BX}$:

   $$|c_+ - c_-| = \frac{1}{2}[J_{AX} + J_{BX}]$$

2. The average of the two centers should be equal to the average of the two chemical shifts:

   $$\frac{1}{2}|c_+ + c_-| = \frac{1}{2}|\nu_A + \nu_B|$$
**Analysis of the X-Part of ABX Patterns.** The X part of an ABX pattern is maximally a centrosymmetric 6-line pattern. However, in many cases it closely resembles a doublet of doublets, and it is often treated as such. However, the couplings obtained are only approximate. The errors become larger when $J_{AX}$ and $J_{BX}$ differ greatly in size, and especially if they have different signs. The sum of $J_{AX}$ and $J_{BX}$ will be correct, but the individual values will be incorrect, with the errors becoming increasingly larger as $\nu_{AB}$ becomes smaller. The values of $J_{AX}$ and $J_{BX}$ will be completely wrong if we are dealing with a Solution 2 pattern.

The X-part consists of 6 lines, of which only four are usually visible. The two additional lines are often weak, but can be seen in Solution 2 patterns for which $\nu_A$ and $\nu_B$ are close together, and the X-part is consequently significantly distorted. The lines are numbered as follows: the two most intense are 9 and 12, they are separated by $J_{AX} + J_{BX}$. The inner pair of the remaining lines are 10 and 11, their separation is $2D_+ - 2D_-$. The outer lines (often invisible) are 14 and 15, separated by $2D_+ + 2D_-$. Line 13 has intensity of zero. These line assignments are not always straightforward: sometimes lines 10 and 11 are on top of each other, resulting in a triplet-like pattern, sometimes 10 and 11 are very close to 9 and 12, to give a doublet.

<table>
<thead>
<tr>
<th>Line</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>$J_{AX} + J_{BX}$</td>
</tr>
<tr>
<td>10</td>
<td>$2D_+ - 2D_-$</td>
</tr>
<tr>
<td>11</td>
<td>$2D_+ + 2D_-$</td>
</tr>
<tr>
<td>12</td>
<td>$J_{AX} + J_{BX}$</td>
</tr>
<tr>
<td>13</td>
<td>$\nu_{X}$</td>
</tr>
<tr>
<td>14</td>
<td>$\nu_{X}$</td>
</tr>
<tr>
<td>15</td>
<td>$\nu_{X}$</td>
</tr>
</tbody>
</table>

To carry out an intensity calculation we define lines 9 and 12 to have intensity 1 ($i_9 = i_{12} = 1.0$), and proceed as outlined below:

### Solution 1

\[
\begin{align*}
\Phi_{1+} &= 0.5 \arcsin(J_{AB}/2D_+) \\
&= 0.5 \arcsin(13.0/26.0) = 15.0 \\
\Phi_{1-} &= 0.5 \arcsin(J_{AB}/2D_-) \\
&= 0.5 \arcsin(13.0/21.9) = 18.2 \\
i_{10} &= i_{11} = \cos^2(\Phi_{1+} - \Phi_{1-}) \\
&= \cos^2(15.0 - 18.2) = 0.997 \\
i_{14} &= i_{15} = \sin^2(\Phi_{1+} - \Phi_{1-}) \\
&= \sin^2(15.0 - 18.2) = 0.003
\end{align*}
\]

### Solution 2

\[
\begin{align*}
\Phi_{2+} &= \Phi_{1+} \\
&= 15.0 \\
\Phi_{2-} &= 90 - \Phi_{1-} \\
&= 90 - 18.2 = 71.8 \\
i_{10} &= i_{11} = \cos^2(\Phi_{2+} - \Phi_{2-}) \\
&= \cos^2(15.0 - 71.8) = 0.30 \\
i_{14} &= i_{15} = \sin^2(\Phi_{2+} - \Phi_{2-}) \\
&= \sin^2(15.0 - 71.8) = 0.70
\end{align*}
\]

On the following two pages is another complete worked example of an ABX pattern solution. The "eyeball method" is the one described in the previous pages, the "formula method" is the one commonly presented in NMR books. We recommend the "eyeball method" because it follows the actual coupling tree in a systematic manner, whereas the "formula method" extracts the information in a mathematically correct but non-intuitive fashion. Both will give identical answers.

5-HMR-12.8
1. Pick two quartets in the AB part. The quartet with the largest effective chemical shift is the + quartet, the other the - quartet, i.e. \( \delta_+ > \delta_- \); D+ > D-; ab+: [2], [4], [6], [8]; ab-: [1], [3], [5], [7].


\[
\Delta \nu_{ab+} = \delta_+ = \sqrt{(8-[2])(6-[4])} = 12.2 \text{ Hz}; \quad \Delta \nu_{ab-} = \delta_- = \sqrt{(7-[1])(5-[3])} = 10.4 \text{ Hz}
\]

\[
c_+ = ([6]+[4])/2 = 221.5 \\
2D_+ = [8]-[4] = 16.6
\]

\[
c_- = ([5]+[3])/2 = 215.2 \\
2D_- = [5]-[1] = 15.2
\]

3e. Calculate the line positions (solve ab+, ab-)

\[
c_+ \pm \delta_+/2 = 221.5 \pm 12.2/2 \\
v_{a+} = 227.5, \quad 215.4 \\
\]

\[
c_- \pm \delta_-/2 = 215.2 \pm 10.4/2 \\
v_{a-} = 220.4, \quad 210.0
\]

We don't know at this point which line is a and which line is b.

4e. The two solutions for the AB part are obtained by pairing up one each of a \( \delta_+ \) and a \( \delta_- \) line, i.e. each ab+, ab- is half A and half B, but don't know which. Thus:

**Solution 1**

\[
\nu_A = \frac{227.6 + 220.4}{2} = 224.0 \text{ Hz} \\
\nu_B = \frac{215.4 + 210.0}{2} = 212.7 \text{ Hz}
\]

\[
J_{AX} = 7.2 \text{ Hz} \\
J_{BX} = 5.4 \text{ Hz}
\]

**Solution 2**

\[
\nu_A = \frac{227.6 + 210.0}{2} = 218.8 \text{ Hz} \\
\nu_B = \frac{220.4 + 215.4}{2} = 217.9 \text{ Hz}
\]

\[
J_{AX} = 17.6 \text{ Hz} \\
J_{BX} = -5.0 \text{ Hz}
\]

4f. Solution 1

\[
\nu_A + \nu_B = c_+ + c_- = 436.7 \\
\nu_A - \nu_B = 1/2(\delta_+ - \delta_-) = 11.3
\]

\[
|J_{AX} + J_{BX}| = 2(c_+ - c_-) = 12.6 \\
|J_{AX} - J_{BX}| = \delta_+ - \delta_- = 1.8
\]

Add and subtract each pair of equations:

\[
\nu_A = \frac{436.7 + 11.3}{2} = 224.0 \text{ Hz} \\
\nu_B = \frac{436.7 - 11.3}{2} = 212.7 \text{ Hz}
\]

\[
J_{AX} = \frac{12.6 + 1.8}{2} = 7.2 \text{ Hz} \\
J_{BX} = \frac{12.6 - 1.8}{2} = 5.4 \text{ Hz}
\]

**Solution 2**

\[
\nu_A = \frac{436.7 + 0.9}{2} = 218.8 \text{ Hz} \\
\nu_B = \frac{436.7 - 0.9}{2} = 217.9 \text{ Hz}
\]

\[
J_{AX} = \frac{12.6 + 22.6}{2} = 17.6 \text{ Hz} \\
J_{BX} = \frac{12.6 - 22.6}{2} = -5.0 \text{ Hz}
\]

* Same for both solutions
5. Analyzing the X Part

Solution 1 and Solution 2 are defined such that Solution 1 has the larger $\nu_A - \beta_B$ value (i.e., the larger chemical shift difference between the A and B nuclei). Hence Solution 1 always corresponds to the one with the least distorted X part. To properly identify the correct solution in ambiguous cases it is necessary to do an intensity calculation. The six X lines are numbered as follows: the two most intense are 9 and 12, they are separated by $J_{AX} + J_{BX}$. The inner pair of lines are 10 and 11, their separation is $2D_+ + 2D_-$. The outer pair of lines (often invisible) are 14 and 14, separated by $2D_+ - 2D_-$. Line 13 has intensity 0.

Define the intensity of lines 9 and 12 = 1.0, and calculate the relative intensity of lines 10 and 14:

### Solution 1

\[
\Phi_{1+} = \frac{1}{2} \arcsin \left( \frac{J_{AB}}{2D_+} \right) = \frac{1}{2} \arcsin \left( \frac{11.2}{16.6} \right) = 21.2^\circ
\]

\[
\Phi_{1-} = \frac{1}{2} \arcsin \left( \frac{J_{AB}}{2D_-} \right) = \frac{1}{2} \arcsin \left( \frac{11.2}{15.2} \right) = 23.7^\circ
\]

\[
i_{10} = i_{11} = \cos^2 (\Phi_{1+} - \Phi_{1-}) = \cos^2 (21.2 - 23.7) = 0.995
\]

\[
i_{14} = i_{15} = \sin^2 (\Phi_{1+} - \Phi_{1-}) = \sin^2 (21.2 - 23.7) = 0.0019
\]

### Solution 2

\[
\Phi_{2+} = 21.2^\circ
\]

\[
\Phi_{2-} = 90 - \Phi_{1-} = 90 - 23.7 = 66.3^\circ
\]

\[
i_{10} = i_{11} = \cos^2 (\Phi_{2+} - \Phi_{2-}) = \cos^2 (21.2 - 66.3) = 0.498
\]

\[
i_{14} = i_{15} = \sin^2 (\Phi_{2+} - \Phi_{2-}) = \sin^2 (21.2 - 66.3) = 0.502
\]
A Simple ABX Pattern as $\nu_{AB}$ is Changed

$\nu_{AB} = 52.00$

$\nu_{AB} = 32.00$

$\nu_{AB} = 22.00$

$\nu_{AB} = 12.00$

$\nu_{AB} = 12.00$

$\nu_{AB} = 5.00$

$\nu_{AB} = 3.00$

$J_{AB} = -11.20$

$J_{AX} = 7.20$

$J_{BX} = 5.40$

5-HMR-12.11
Effect of Relative Sign of $J_{AX}$ and $J_{BX}$ on ABX pattern

$J_{AB} = 13$ Hz
$J_{AX} = 10$ Hz
$J_{BX} = 5$ Hz
$J_{BX} = -5$ Hz

$\nu_A = 70$ Hz
$\nu_B = 130$ Hz
$\Delta \nu_{AB} = 60$ Hz

$\nu_A = 85$ Hz
$\nu_B = 115$ Hz
$\Delta \nu_{AB} = 30$ Hz

$\nu_A = 90$ Hz
$\nu_B = 110$ Hz
$\Delta \nu_{AB} = 20$ Hz

$\nu_A = 95$ Hz
$\nu_B = 105$ Hz
$\Delta \nu_{AB} = 10$ Hz
ABX with Accidental Coincidences

\[ \nu_{AB} = 18 \]
\[ J_{AB} = 11.20 \]
\[ J_{AX} = 7.20 \]
\[ J_{BX} = 5.40 \]

\[ \nu_{AB} = 13.2 \]
\[ J_{AB} = 11.20 \]
\[ J_{AX} = 7.20 \]
\[ J_{BX} = 5.40 \]

\[ \nu_{AB} = 12 \]
\[ J_{AB} = 11.20 \]
\[ J_{AX} = 7.20 \]
\[ J_{BX} = 5.40 \]

\[ \nu_{AB} = 3 \]
\[ J_{AB} = 11.20 \]
\[ J_{AX} = 7.20 \]
\[ J_{BX} = 5.40 \]
ABX with Accidental Coincidences

Solution 1 = Solution 2

$\nu_{AB} = 3$
$J_{AB} = 10.2$
$J_{AX} = 5.0$
$J_{BX} = -2.0$

$\nu_{AB} = 4$
$J_{AB} = 2.0$
$J_{AX} = 17.0$
$J_{BX} = 10.0$

$\nu_{AB} = 14$
$J_{AB} = 8.0$
$J_{AX} = 8.0$
$J_{BX} = 8.0$

$\nu_{AB} = 0$
$J_{AB} = 12.0$
$J_{AX} = 2.0$
$J_{BX} = 12.0$

Solution 1 = Solution 2

$\nu_{AB} = 0.5(J_{AX} - J_{BX})$

$\nu_{AB} = 0.5(J_{AX} - J_{BX})$

$\nu_{AB} = 0.5(J_{AX} - J_{BX})$

$\nu_{AB} = 0.5(J_{AX} - J_{BX})$
ABX of the Vinyl Type

$J_{AB} = 2.50$
$J_{AX} = 16.80$
$J_{BX} = 10.00$
$\Delta \nu_{AB} = 25 \text{ Hz}$

Mimic:

\[
\begin{array}{c}
\text{H}_X \\
\text{H}_B \\
\text{H}_A
\end{array}
\]

300 MHz NMR

$\nu_A$
$\nu_B$

$\Delta \nu_{AB} = 10 \text{ Hz}$

$\Delta \nu_{AB} = 5 \text{ Hz}$

$\Delta \nu_{AB} = 3 \text{ Hz}$

$\Delta \nu_{AB} = 1 \text{ Hz}$

ppm

5.9  5.8  5.7  5.6  5.5  5.4  5.3  5.2  5.1  5.0  4.9  4.8

5-HMR-12.15
ABX Going to ABC

$\nu_C = 270.00$

$J_{AB} = -13$

$J_{AC} = 9$

$J_{BC} = 2$

$\nu_A = 60$

$\nu_B = 70$

$\nu_C$ varies

$H_C$

$H_B H_A$

$\nu_C = 210.00$

$\nu_C = 170.00$

$\nu_C = 120.00$

$\nu_C = 100.00$

$\nu_C = 90.00$

$\nu_C = 80.00$

ppm

5-HMR-12.16
ABX Going to $A_2X$

$J_{AB} = 8 \quad \nu_A = 10$

$J_{AC} = 0.8 \quad \nu_B \text{ varies}$

$J_{BC} = 2.3 \quad \nu_C = 180$

$\Delta \nu_{AB} = 15$

$\Delta \nu_{AB} = 8$

$\Delta \nu_{AB} = 6$

$\Delta \nu_{AB} = 4$

$\Delta \nu_{AB} = 2$

$\Delta \nu_{AB} = 1$

Hz
ABX\textsubscript{m}Y\textsubscript{n}Z\textsubscript{o} Patterns

Identify the protons that are shown
Sample ABX Spectra

300 MHz $^1$H NMR spectrum in DMSO$_d$$_6$
Source: Aldrich Spectral Viewer/Reich

300 MHz $^1$H NMR spectrum in CDCl$_3$
Source: Aldrich Spectral Viewer/Reich
Sample ABX Spectra

300 MHz $^1$H NMR spectrum in methanol-d$_4$ C$_{23}$H$_{48}$ClNO$_2$
Source: Aldrich Spectral Viewer/Reich

300 MHz $^1$H NMR spectrum in CDCl$_3$
Source: Aldrich Spectral Viewer/Reich