

# Spin System Notation

Capital letters A, B, C, M, A, X, Y, .....

➤ Same letter = same chemical shift ( $A_3, B_2, X_6, \dots$ )

➤ Different letters = different chemical shifts

Letters close in the alphabet (A, B, C, ...)

J [Hz] of the same magnitude as  $\Delta\nu$  [Hz]

Letters separated in the alphabet (A, M, X, ...)

large separation of chemical shifts

-different nuclei ( $^1\text{H}, ^{31}\text{P}, ^{195}\text{Pt}, \dots$ )

-same nuclei but  $\Delta\nu$  [Hz] much larger than J

!!  $\Delta\nu$  [Hz] depends on  $B_0$  !!

Two situations:

a) Complete equivalence =

chemical shift equivalence (isochronous nuclei)

+ magnetic (spin-coupling) equivalence (isotachous)

Magnetic equivalence = each member of one group of spins is coupled equally to all members of any other group

$A_2B_2, A_2X_2, \dots$

b) Chemical shift equivalence, magnetic inequivalence

$AA'BB', AA'XX', AA'A''XX'X'', \dots$

## Prime vs. Bracket Notation

$AA'BB'$

$A_2B_2$

$AA'BXX'$

$AA'X_3X_3'$

$[AB]_2$

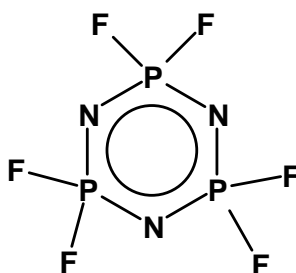
$[A_2B_2]$

$[AX]_2B$

$[AX_3]_2$

$AA'A''XX'X''X'''X^4X^5$

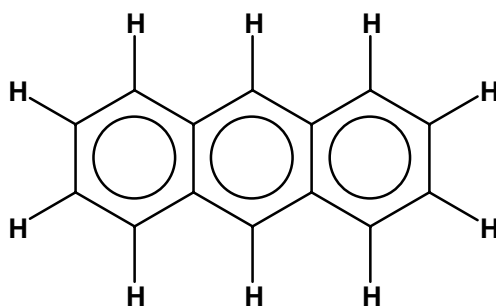
$[A[X]_2]_3$



$^{31}\text{P}$  &  $^{19}\text{F}$  NMR

$BB'AA'CC'A''A'''B''B''$

$[[AB]_2C]_2$

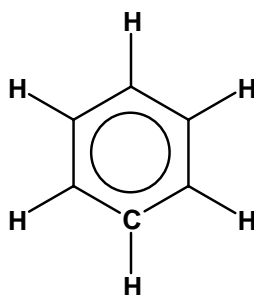


$^1\text{H}$  NMR

considering isotope  
shift:

$ABB'CC'DX$

$A[BC]_2DX$



$^{13}\text{C}$  NMR