

INTERPRETING NMR SPECTRA

A T A G L A N C E

WHAT DOES AN NMR SPECTRUM TELL YOU?

- **information about hydrogen atoms** in molecules
- **hydrogen atoms in different environments** respond differently to the field
- each different environment produces a signal in a different position
- tetramethylsilane (TMS) provides the **reference signal** at $\delta = 0$
- the **area under each peak / signal** is proportional to the number of hydrogens
- **signal can be split** according to how many H's are on adjacent atoms

HOW TO WORK OUT AN NMR SPECTRUM

1. Get the formula of the compound
2. Draw out the structure
3. Go to each atom in turn and ask the 'census' questions
4. Work out what the spectrum would look like ... *signals due to H's nearer electronegative atoms (Cl, Br, O) are shifted to higher δ values*

THE BASIC "CENSUS"

Ask each hydrogen atom to...

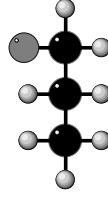
- describe where it lives
- say how many hydrogens live on that atom
- say how many **chemically different** hydrogen atoms live on adjacent atoms

BUT, REMEMBER THAT

Hydrogen atoms on OH groups - ONLY PRODUCE ONE PEAK
- DON'T COUNT AS A NEIGHBOUR

OUR EXAMPLE WILL BE...

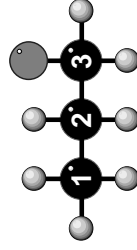
1-BROMOPROPANE C_3H_7Br



"CENSUS"

RESULTS FOR

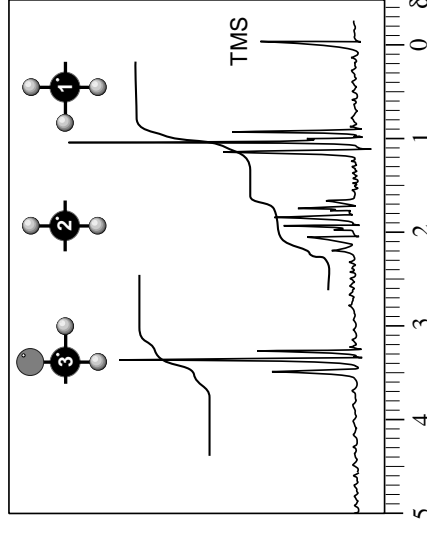
C_3H_7Br



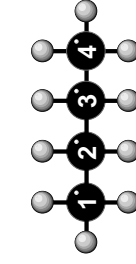
ATOM	UNIQUE DESCRIPTION OF THE POSITION OF H'S ON THE ATOM	NUMBER OF H'S ON ATOM	H'S ON ADJACENT ATOMS	SIGNAL SPLIT INTO
1	On an end carbon atom, two away from the carbon with the bromine on it	3	2	$2+1 = 3$
2	On a carbon atom second from the end and also one away from the carbon with the bromine on it	2	$3+2 = 5$	$5+1 = 6$
3	On an end carbon atom which also has a bromine atom attached to it	2	2	$2+1 = 3$

THE RESULTING SPECTRUM

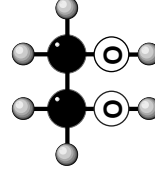
- 3 environments = 3 sets of signals
 - Triplet $\delta = 3.4$
 - Multiplet (sextet) $\delta = 1.9$
 - Triplet $\delta = 1.0$
- Signal for H's on carbon 3 is shifted furthest from TMS due to proximity of the electronegative halogen
- Area ratio from relative heights of integration lines = **2 : 2 : 3**



TWO INTERESTING EXAMPLES INVOLVING SPLITTING



- Quartet and triplet :- ratio of peak areas = 3 : 2
- Carbons 1 & 4 are the same and so are carbons 2 & 3
- The signal for H's on carbon 2 is a quartet - you ignore the two neighbours on carbon 3 because they are chemically identical



- Two singlets :- ratio of peak areas = 2 : 1
- Hydrogens on OH groups only give singlets
- The signal for H's on each carbon are not split, because
 - H's on the neighbouring carbon are chemically identical... and
 - H's on adjacent OH groups do not couple