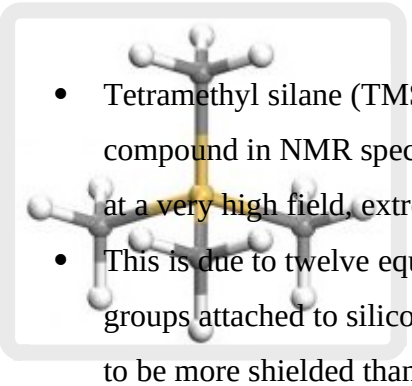
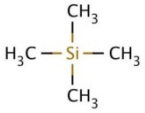
- **Reference Compound**

An ideal reference compound will be that,

1. It gives a strong and sharp singlet signal, in a region different from the region in which the signals of protons from the compound appear.
2. It is chemically inert and does not react with sample.
3. It should have high dissolving power.
4. It can be easily removed from the sample.

Tetramethyl silane (TMS) as internal standard





- Tetramethyl silane (TMS) is commonly used reference compound in NMR spectroscopy. It gives a strong signal at a very high field, extremely right of the NMR spectrum.
- This is due to twelve equivalent hydrogens of four methyl groups attached to silicon in TMS. These protons are said to be more shielded than most of the protons in any organic compounds.
- In TMS electronegativity of Si (1.8) is very low as compared to hydrogen (2.1) and carbon (2.5), hence electron density flows from silicon to methyl groups. Thus these protons becomes more shielded and shows strong, intense peak than any proton in organic compounds.

- **Information from NMR spectrum**

1. The number of signals

It reveals that how many different kinds of equivalent protons present in a molecule.

2. The position of signals

It reveals about the electronic environment of each kind of proton.

3. The intensities of signals

It reveals the relative number of protons in different sets.

4. The splitting of the signals into several peaks

It reveals about the environment of proton with respect to other, nearby protons.

- # The number of signals

The number of signals in the NMR spectrum reveals the number of different sets of equivalent protons in a molecule. In a given molecule protons with same environment absorb, same applied field. While protons with different environment absorb, different applied field.

Thus, '*magnetically equivalent protons are chemically equivalent*'.

1. Equivalent protons

i. The protons having identical chemical environment are called equivalent protons.

ii. These protons constitute a same set of equivalent protons.

iii. They absorb, same field strength, so they have same chemical shift.

iv. Each set of equivalent protons gives one absorption peak.

2. Non-equivalent protons

i. The protons having different chemical environment are called as non-equivalent protons.

ii. These protons constitute a different set of equivalent protons.

iii. They absorb, different field strength, so they have different chemical shift.

iv. They give different absorption peak.

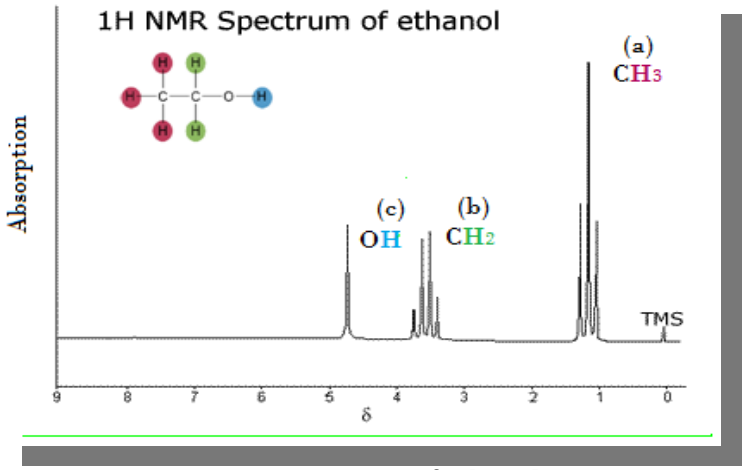


Fig. NMR spectrum of ethanol

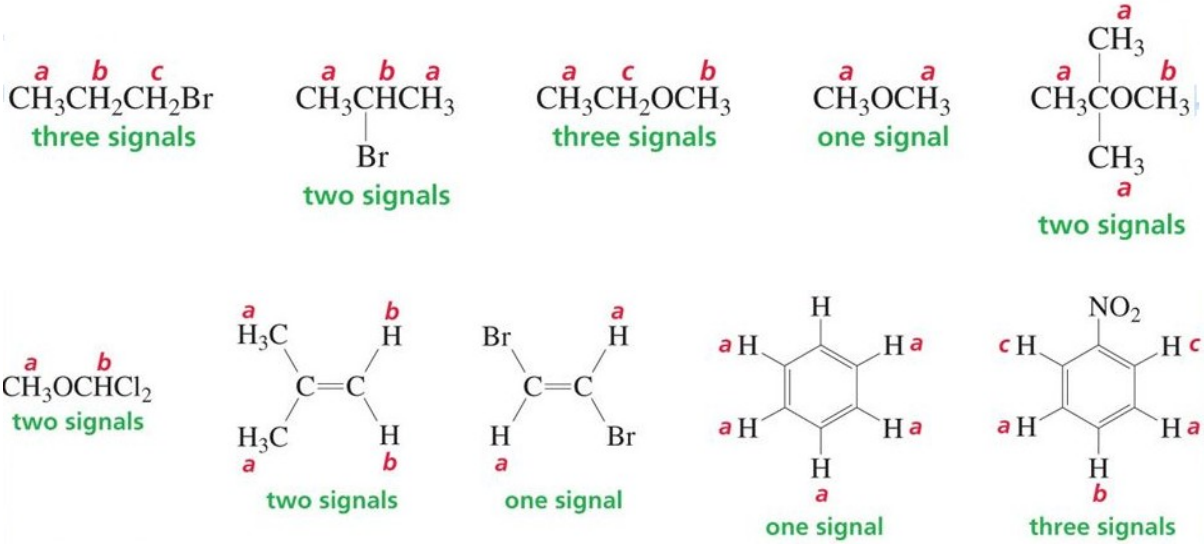
Eg. $CH_3 - CH_2 - OH$ ⟶ 3 sets of equivalent protons

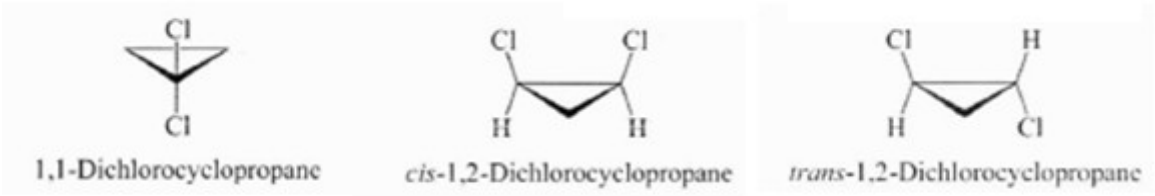
a b c 3 NMR signals

set a ⟶ $-CH_3$ group protons

set b ⟶ $-CH_2$ group protons

set c ⟶ -OH group protons





How many signals would you expect to see in the ^{1}H NMR spectrum of each of the following compounds?

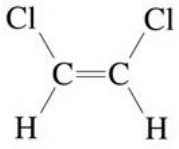
a. $CH_3CH_2CH_2CH_3$

b. $BrCH_2CH_2Br$

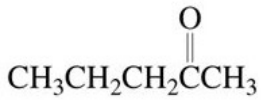
c. $CH_2{=}CCl_2$

d.

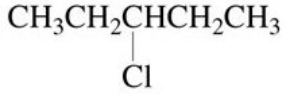
e.



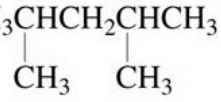
f.



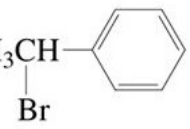
g.



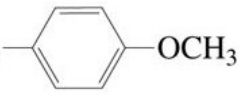
h.



i.

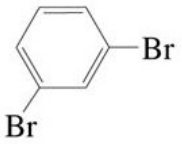


j.

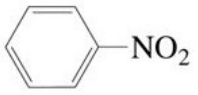


k.

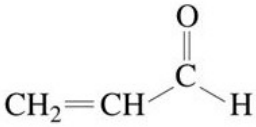
l.



m.



n.



o.