INFRARED (IR) SPECTROSCOPY
\[ 1 \text{m} = 10^2 \text{cm} = 10^6 \mu \text{m} = 10^9 \text{nm} \]
\[ \tilde{\nu} = \frac{1}{\lambda} \]
\[ \tilde{\nu} = \text{wavenumber (cm}^{-1}\text{)} \]
\[ \tilde{\nu} = 1/10^{-4} \mu \text{m} = 10^4/\mu \text{m} \]

<table>
<thead>
<tr>
<th>Region</th>
<th>Energy (kJ/mol)</th>
<th>Wavenumber (cm(^{-1}))</th>
<th>Wavelength (\mu m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Near IR</td>
<td>150-50</td>
<td>12,800-4000</td>
<td>0.78-2.5</td>
</tr>
<tr>
<td>Mid IR</td>
<td>50-2.5</td>
<td>4000-200</td>
<td>2.5-50</td>
</tr>
<tr>
<td>Far IR</td>
<td>2.5-0.1</td>
<td>200-10</td>
<td>50-1000</td>
</tr>
</tbody>
</table>
The portion of the infrared region most useful for analyses of organic compounds is $4000-666 \text{ cm}^{-1}$.

Photon energies associated with this part of the infrared are not large enough to excite electrons, but may induce vibrational excitation of covalently bonded atoms and groups.

The covalent bonds in molecules (A-B) are not rigid sticks or rods, but are more like stiff springs that can be stretched and bent.
In addition to rotation of groups about single bonds, molecules experience a wide variety of vibrational motions, characteristic of their component atoms. Consequently, organic compounds will absorb infrared radiation that corresponds in energy to these vibrations. Absorption in this region implies the occurrence of vibrational transitions in the molecule while it remains in its ground state.
IR spectroscopy permit chemists to obtain absorption spectra of compounds that are a unique reflection of their molecular structure.
The **complexity** of this spectrum is typical of most infrared spectra, and illustrates their use in **identifying substances**.

**No two compounds have identical IR spectrum, except enantiomers.**

The **inverted display of absorption**, compared with **UV-Visible**, is characteristic of **IR spectra**. Thus a sample that did not absorb at all would record a horizontal line at 100%.

The frequency scale at the bottom of the chart is given in units of **reciprocal centimetres (cm\(^{-1}\))** rather than Hz, because the numbers are more manageable. 

\[ \bar{\nu} = \nu / c \]
Interaction of Molecules with IR Radiation

Vibrational frequencies of molecules correspond to the frequencies of absorbed radiation. I.e. Infrared light is absorbed when the oscillating dipole moment (due to molecular vibration) interacts with the oscillating electrical vector of the infrared beam.

Band intensities are expressed as transmittance \( T \) \( (T=I/I^\circ) \)

\( I = \) intensity of light transmitted
\( I^\circ = \) Intensity of initial light from the source

Band intensities are described as \( w \) (for weak), \( m \) (for medium) and \( s \) (for strong)
Types of Molecular Vibration

- **Two types** of molecular vibration:
- 1) **Stretching**: a rhythmic movement along the bond axis such that the interatomic distance is **increased** or **decreased**.

![Stretching vibrations]

- Symmetric
- Asymmetric
- Symmetric
- Asymmetric
• 2) **Bending**: a change in bond angle between bonds with a common atom or

• the **movement of a group of atoms** with respect to the remainder of the molecule,

• with out movement of the atoms in the group with respect to one another.
Only those vibrations that result in rhythmical change of dipole moment of the molecule are observed in IR.

Homonuclear diatomic molecules such as $\text{H}_2$ or $\text{O}_2$ do not absorb IR radiation (they are IR-inactive), since there is no over-all electric (Dipole) moment in the molecule.
It is not necessary for polyatomic molecules to possess permanent dipole moment in order to exhibit IR absorption, provided that some polar bonds are present in the molecule.

Example

\[ \begin{array}{ccc}
\delta^- & 2\delta^+ & \delta^- \\
O &=& C \quad \equiv \quad O
\end{array} \]
• A is **not** IR active
• B, C and D are **IR active**
• its positive and negative electrical centres are no longer coincident,
• a **dipole moment** is temporarily induced.
Simple Harmonic Oscillator

1st Approximation, a covalent bond behaves as a weightless spring and obeys Hooke’s Law: the restoring force acting upon it when it is stretched is proportional to the degree of stretching.

\[ \mathbf{F} = -k \mathbf{x} \]

A molecule can be regarded as a collection of balls and springs, where the balls are the atoms and the springs are the chemical bonds.
Hooke’s law

$$\tilde{\nu} = \frac{1}{2\pi c} \left( \frac{\kappa}{\mu} \right)^{1/2}$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

$\tilde{\nu}$ = wave number of the stretching vibration

$\kappa$ = the force constant (bond strength)

$m_1, m_2$ = masses of atoms joined by the bond

$c$ = speed of light

The exact wave number at which a given vibration occurs is determined by:

1) the strengths of the bonds involved and

2) the masses of the component atoms.
Fundamental Vibrations

• Molecules of $n$ atoms will have $3n$ degrees of freedom.
• Since its atoms may have its movement resolved along $x$, $y$ and $z$ axes.
• Movement of the whole molecule as a rigid unit will take up six of these degrees of freedom,
• three translational and three rotational
• (two rotational in the case of linear molecules).
• So, for vibrational motions where atoms move relative to each other, we have $3n-6$ ($3n-5$ for linear molecules) fundamental vibrations
• (vibrations responsible for number of theoretically expected absorption bands in IR).
H₂O
• Three atoms (non-linear).
• $3 \times 3 = 9$ degrees of freedom.
• $3n-6$ (fundamental vibrations).
• $9 - 6 = 3$ (fundamental vibrations).

CO₂
• Three atoms (linear).
• $3 \times 3 = 9$ degrees of freedom.
• $3n-5$ (fundamental vibrations).
• $9 - 5 = 4$ (fundamental vibrations).
Formaldehyde, $\text{H}_2\text{C}=\text{O}$

Four atoms (non-linear).

$3 \times 4 = \textbf{12 degrees of freedom}.$

$12 - 6 = 6$ (fundamental vibrations).

Gas phase
• In practice, IR spectra do not normally display separate absorption signals for each of the $3n-6$ fundamental vibrational modes of a molecule.

• I) Absorption signals may be increased by:
  • additive and subtractive interactions of the fundamental vibrations (overtones),

• II) Absorption signals, may be decreased by:
  • a) Molecular Symmetry (identical group in the same molecule will have the same value),
  • b) Spectrometer limitations
  • c) Selection rules (only those vibrations which results in a change of dipole moment will show absorption bands).
Band Intensity:

- Described as **w** (for weak), **m** (for medium) and **s** (for strong).
- One selection rule that influences the intensity is that a change in dipole moment should occur for a vibration to absorb infrared radiation.
- Absorption of **C=O bond** stretching are usually very strong.

\[ \delta^+ \xrightarrow{\text{mode}} \delta^- \]

because a large change in the dipole moment takes place in that mode.
Some General Trends

i) **Stretching frequencies** are **higher** than the corresponding **bending frequencies**.

- (It is easier to bend a bond than to stretch or compress it)

ii) **Asymmetrical stretching** frequencies are **higher** than **symmetrical stretching** frequencies.

\[
\bar{\nu} = \frac{1}{2\pi c} \left( \frac{\kappa}{\mu} \right)^{1/2}
\]

\[
\mu = \frac{m_1 m_2}{m_1 + m_2}
\]

iii) Bonds to **hydrogen** have **higher stretching frequencies** than those to **heavier atoms**.

iv) **Triple bonds** have **higher stretching frequencies** than **double bonds**, which in turn have higher frequencies than **single bonds** (except for bonds to hydrogen).
Blue colours refer to stretching vibrations,

Green coloured band encompasses bending vibrations.
• The 1450 to 666 cm\(^{-1}\) region is complex.
• It is difficult to assign all the absorption bands.
• Because of the unique patterns,
  • this region is often called the fingerprint region.
• It is characteristic of the molecule as a whole;
• useful as confirmatory evidence than identification.
• Absorption bands in the 4000 to 1450 cm\(^{-1}\) region are usually due to stretching vibrations of diatomic units,
• and this is sometimes called:
• the group frequency region.
• Useful for identification of functional groups.
Interpretation of IR Spectra

• IR spectroscopy is one of several aids to the elucidation of structures.
• Physical, chemical and other spectroscopic data are necessary.

Points to consider during interpretation.
• 1) Begin at the high-frequency end of the chart. (most reliable correlations occur here)
• 2) Use the fingerprint region mainly for confirmation.
• 3) Do not expect to assign every band in the spectrum.
• (only 10-20% of bands can usually be assigned).
4) place more reliance upon negative evidence, (that is absence of absorption in a particular region).
Because the presence of a band may have several possible origins.
5) Continually cross-check the evidence against other spectroscopic methods.
6) Treat published descriptions of band intensities with caution.
7) Study any variation between spectra obtained by different sampling techniques.
### Characteristic Group Frequencies

Tables of characteristic group frequencies are available. (prepared following examination of many compounds).

Precise frequencies of absorption for a group is dependent on its environment within the molecule and on its physical state of measurement.

<table>
<thead>
<tr>
<th>Functional Class</th>
<th>Range (cm(^{-1}))</th>
<th>Intensity</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Alkanes</strong></td>
<td>2850-3000 str</td>
<td>CH(_3), CH(_2) &amp; CH 2 or 3 bands</td>
<td></td>
</tr>
<tr>
<td><strong>Alkenes</strong></td>
<td>3020-3100 med var</td>
<td>=C-H &amp; =CH(_2) (usually sharp)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1630-1680 var</td>
<td>C=C (symmetry reduces intensity)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1900-2000 str</td>
<td>C=C asymmetric stretch</td>
<td></td>
</tr>
</tbody>
</table>
Alkanes

Two types of bonds (C-H and C-C)

Spectra can be interpreted in terms of four vibrations:

- 1) C-H stretching
- 2) C-H bending
- 3) C-C stretching
  - (are weak, and appear in the broad region 1200-800 cm\(^{-1}\))
  - C-C stretching is of little value for identification.
- 4) C-C bending
  - (below 500 cm\(^{-1}\), do not appear in normal spectra).

Thus the most characteristic vibrations are those of C-H stretching and C-H bending.
C-H Stretching Vibration ($\nu$)

**Methyl group**
- Symmetrical stretching ($\nu_s$): $2885-2860\text{cm}^{-1}$
- Asymmetrical stretching ($\nu_{as}$): $2975-2950\text{cm}^{-1}$

**Methylene group**
- Symmetrical stretching ($\nu_s$): $2870-2845\text{cm}^{-1}$
- Asymmetrical stretching ($\nu_{as}$): $2940-2915\text{cm}^{-1}$

**Methine**
- Symmetrical stretching ($\nu_s$): $2890\text{cm}^{-1}$
C-H bending vibration ($\delta$)

Methyl group

Symmetrical bending ($\delta_s$)  
ca. $1375\text{cm}^{-1}$

Asymmetrical bending ($\delta_{as}$)  
ca. $1450\text{cm}^{-1}$

Methylene group

rocking  
$720-725\text{cm}^{-1}$

scissoring  
$1470-1465\text{cm}^{-1}$

wagging  
$1390-1350\text{cm}^{-1}$

twisting
Alkenes

- New modes of vibrations are:
  1) C=C stretching,
  2) C-H stretching (C in olefinic linkage) and
  3) In-plane and out-of-plane bending of the olefinic C-H bond

**C=C stretching**
- 1667-1600 cm\(^{-1}\)
- (moderate to weak)
More alkyl substitution, shift towards high frequency, due to more coupling interaction between C=C and C-C vibrational frequencies.
cis-double bonds which lack the symmetry of the trans structure absorb more strongly.

Internal double bonds absorb more weakly than terminal double bonds, because of pseudo-symmetry.
The C=C stretching vibration is coupled with C-C stretching vibration of the adjacent bonds. Coupling is dependent on bond angle \( \alpha \).
As the angle ($\alpha$) becomes smaller the coupling interaction becomes less until it is minimum at 90° (the attached C-C bond is orthogonal to C=C bond)

![Square and Triangle with labels](image)

1566 cm$^{-1}$ 1641 cm$^{-1}$

In cyclopropene, interaction becomes again appreciable (1641 cm$^{-1}$)
The C=C vibration is strongly coupled to the attached C=C single bond vibration
Effect of Conjugation

Conjugation of a double bond provides a **single bond character** through resonance, which **lowers** force constant $K$, thus a **lower frequency** of vibration.
Olefinic C-H stretching vibration

-C=C-H at 3100-3000 cm\(^{-1}\)

In general, only C-H stretching bonds above 3000 cm\(^{-1}\) result from aromatic, acetylenic or olefinic C-H stretching.

Olefinic C-H bending vibration

Scissoring vibration (same plane) ca. 1416 cm\(^{-1}\)

Out of plane bending (Twisting and wagging) 1000-650 cm\(^{-1}\)
Strongest in alkenes
Alkynes

Contains \( \text{C} \equiv \text{C} \) group

**Three characteristic bands** are present

1) \( \text{C} \equiv \text{C} \) stretching \((2260-2100 \text{ cm}^{-1})\)

In symmetrical substituted alkynes \( \text{R} - \text{C} \equiv \text{C} - \text{R} \) stretching vibration is **not observed**.

Even in non-symmetrical substituted alkynes stretching vibration is **very weak**, due to *pseudo-symmetry*.

Only in **mono-substituted** alkynes this is observed.
2) C-H stretching

\[
\text{\begin{tabular}{c}
C≡C – H \\
\text{(3300-3250 cm}^{-1})
\end{tabular}}
\]

Observed in \textit{mono-substituted} acetylenes (\textit{Strong band}).

Narrower than \text{hydrogen-bonded} O-H and N-H bands which occurring in the same region.

3) C-H bending

\[
\text{\begin{tabular}{c}
C≡C – H \\
\text{(700-600 cm}^{-1})
\end{tabular}}
\]

Observed in \textit{mono-substituted} acetylenes.
Aromatic Compounds

Show characteristic bands in five regions

1) The C-H stretching appear above 3000 cm\(^{-1}\) (aliphatic C-H stretching (below 3000 cm\(^{-1}\)) .

2) In 2000-1700 cm\(^{-1}\) region, a series of weak combination bands (overtones) appear.

3) Skeletal vibration, representing C=\(\text{C}\) stretching absorb in the 1650-1430 cm\(^{-1}\).

4) The C-H bending bands appear in the regions 1275-1000 cm\(^{-1}\) (in-plane bending) and 5) 900-690 cm\(^{-1}\) (out-of-plane C-H bending). These bands are strong and characteristic of the number of hydrogen atoms in the ring.
Bands of the out-of-plane bending in substituted benzene

Substitution

Mono-

Di-
1,2-
1,3-
1,4-

Tri-
1,2,3-
1,2,4-
1,3,5-

Tetra-
1,2,3,4-
1,2,3,5-
1,2,4,5-

Penta-
Alcohols and Phenols

- Characteristic bands due to O-H and C-O stretching.

**O-H stretching**
- Affected by **hydrogen bonding**
- ‘Free’ hydroxyl groups absorb between
- **3650-3585 cm\(^{-1}\) (strong and sharp).**
- ‘Free’ OH bands are only observed in the vapour phase or very dilute solution of **non-polar** solvents (e.g., CCl\(_4\)).
- Intermolecular H-bonding increases as the **concentration** of the solution increases or when the sample is analysed **neat**.
- This lowers frequency of absorption
- to **3550-3200 cm\(^{-1}\)**.
Reason:

- The **stronger** the hydrogen-bonding
- the **longer** the O-H bond (**more polarized**)  
- the **lower** the **force constant**
- the **lower** the **vibrational frequency**
- the **broader** the band (**H-bonding is not uniform throughout the sample**) and
- the **more intense** (due to **increased polarization** of the O-H bond) the absorption band.
Can IR spectroscopy distinguish these isomers?

**Intramolecular H-bonding** occurs in *O*-Hydroxyacetophenone at 3077 cm$^{-1}$ (lower frequency) (independent of concentration)

*O*-Hydroxyacetophenone

‘free’ hydroxyl peak at 3600 cm$^{-1}$ (Sharp) in dilute solution of CCl$_4$.

*P*-Hydroxyacetophenone

intermolecular H-bonded peak at 3100 cm$^{-1}$ (broad) when run neat sample (high concentration)
Why the difference in absorption position?

2,6-di-<i>t</i>-butylphenol in which steric hindrance prevents hydrogen-bonding,
No H-bonded hydroxyl band is observed, not even in spectra of neat samples.
• **C-O stretching** appear at 1300-1000 cm\(^{-1}\).
• **O-H bending** also occurs but such bands couple with other vibrations and produce complex bands in the fingerprint region (1420-1330 cm\(^{-1}\)).
Carbonyl Compounds

- show strong C=O stretching absorption band in the region 1870-1540 cm\(^{-1}\).
- High intensity and relatively free from interfering bands.
- One of the easiest bands to recognise.
- Neat sample of saturated aliphatic ketone,
- 1715 cm\(^{-1}\) as ‘normal’.

\[ R -\quad\overset{\text{aliphatic ketone}}{\text{C}\text{=O}\quad R'} \quad (1715 \text{ cm}^{-1}) \]

Change in the environment of the carbonyl can either lower or raise the absorption frequency.
Factors affecting position of C=O absorption

1) The physical state of measurement (solid, neat, dilute solution, conc. solution);
2) Electronic effect of substituents;
3) Conjugation;
4) Hydrogen bonding;
5) Ring strain.
1) Physical State

- Non-polar solvents increase absorption frequency.
- Polar solvents decrease absorption frequency.
- Due to solvent-carbonyl interaction.
- Overall range of solvent effect does not exceed 25 cm$^{-1}$.
2) Electronic Effect of Substituents

- Replacement of an alkyl group of a saturated aliphatic ketone by a heteroatom (X) shifts the carbonyl absorption.
- The direction of the shift depends on whether inductive effect or resonance effect predominates.

\[
\begin{align*}
\text{Inductive Effect} & : \\
X & \quad R \\
\text{Resonance Effect} & : \\
X^- & \quad R \\
\end{align*}
\]
Inductive effect reduces the length of the C=O bond
- increases its force constant
- the frequency of absorption will increase.

Resonance effect increases the length of the C=O bond
- reduces its force constant.
- the frequency of absorption will decrease.
Substituent effects **predominantly** inductive

aliphatic ketone, 1715 cm⁻¹

<table>
<thead>
<tr>
<th>X</th>
<th>C=O absorption (cm⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>1869</td>
</tr>
<tr>
<td>Cl</td>
<td>1815-1785</td>
</tr>
<tr>
<td>Br</td>
<td>1812</td>
</tr>
<tr>
<td>OH</td>
<td>1760</td>
</tr>
<tr>
<td>OR</td>
<td>1750-1735</td>
</tr>
</tbody>
</table>
Substituent effects **predominantly** resonance

**aliphatic ketone, 1715 cm\(^{-1}\)**

<table>
<thead>
<tr>
<th>X</th>
<th>C=O absorption (cm(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{NH}_2)</td>
<td>1695-1650</td>
</tr>
<tr>
<td>(\text{SR})</td>
<td>1710-1690</td>
</tr>
</tbody>
</table>
3) Conjugation

Conjugation lowers the stretching frequency of carbonyl by 15-40 cm\(^{-1}\).
This is because the carbonyl bond order (double bond character) is reduced and hence the force constant falls (reduces).
1685 cm\(^{-1}\)

\[
\text{MeO} 
\]

1650 cm\(^{-1}\)

\[
\text{MeO} \quad \text{O} 
\]

1715 cm\(^{-1}\)

1700 cm\(^{-1}\)

Increased conjugation with carbonyl group

Decreased conjugation with carbonyl group

Lowers frequency

Increases frequency
(E)-3-Methyl-4-phenylbut-3-en-2-one

Shows two C=O bands at 1674 and 1699 cm\(^{-1}\). Why?

Steric effects in s-cis reduces co-planarity of the conjugated system and reduces the effect of conjugation.
How can you distinguish the two isomers using IR?

Heptane-2,4-dione

\[ \text{36\%} \quad 1725 \text{ cm}^{-1} \]

Heptane-2,6-dione

\[ 1715 \text{ cm}^{-1} \]

\[ \text{64\%} \quad 1613 \text{ cm}^{-1} \]

\[ 3077 \text{ cm}^{-1} \text{ for O-H stretching (H-bonded)} \]
4) Hydrogen Bonding

H-bonding reduces C=O stretching frequency. This is because the carbonyl bond order is reduced and the force constant falls.
5) Ring Strain

The bond angle ($\alpha$) influences the absorption frequency of C=O.
In non-cyclic ketones and in cyclohexanone $\alpha = 120^\circ$
In strained rings in which $\alpha < 120^\circ$
The energy of C=O stretching increases,
Hence stretching frequency is increased.
Aldehydes

\[ \text{C}=\text{O} \] stretching vibrations of \textbf{aldehydes} absorb at slightly \textbf{higher frequencies} than that of ketones.

\textbf{Hyperconjugation} (which reduces vibrational frequency) is \textbf{higher in ketones} than in aldehydes.

Electronegative substituents on \textbf{\( \alpha \)-carbon} increases the frequency of carbonyl absorption.
Carboxylic acids

In liquid or solid state and in solutions (>0.01M), carboxylic acids exist as dimers due to strong H-bonding.

Monomers of saturated aliphatic carboxylic acids absorb at 1760 cm\(^{-1}\).

Dimerized saturated aliphatic carboxylic acids absorb at 1720-1706 cm\(^{-1}\).

O-H stretching at 3000 cm\(^{-1}\) (very broad, intense)
Amines

N-H stretching

\[ \text{H-N-H} \]
\[ v_s 3400 \text{ cm}^{-1} \]
\[ v_{as} 3500 \text{ cm}^{-1} \]

\[ \text{H-N-R} \]
\[ v 3550 - 3310 \text{ cm}^{-1} \]

Shifted to lower frequency by hydrogen bonding
N-H bands are weaker and sharper than O-H bands.

N-H bending

\[ \text{H-N-H} \]
\[ \text{scissoring 1650 - 1580 cm}^{-1} \]
\[ \text{(medium to strong)} \]

\[ + \text{H-N-H} + \text{H} \]
\[ - \text{H-N-H} + \text{H} \]

Wagging 909-666 cm\(^{-1}\)
\[ \text{(medium to strong)} \]

The position is affected by H-bonding
Nitriles

\[
\begin{array}{c}
R \equiv \equiv \equiv N \\
\end{array}
\]

Aliphatic nitriles absorb near $2260-2240\text{cm}^{-1}$. Conjugation (aromatic nitriles) at $2240-2222\text{cm}^{-1}$. 
Index of Hydrogen Deficiency

(Double Bond Equivalence)

gives the sum of the number of \( \pi \)-bonds and rings

\[
\text{Index of hydrogen deficiency} = \left( \frac{\text{Number of H's in reference } (C_nH_{2n+2})}{2} \right) - \left( \frac{\text{Number of H's in compound}}{2} \right)
\]

Note: a saturated acyclic alkane (i.e. molecular formula: \( C_nH_{2n+2} \)) is used as the reference.

e.g. A compound X has a molecular formula \( C_7H_{12} \)

the reference compound has 16 Hydrogens

\[
\therefore \text{Index of hydrogen deficiency} = \frac{16 - 12}{2} = 2
\]
the compound contains either 2 \( \pi \)-bonds, 1 \( \pi \)-bond and 1 ring, or 2 rings

possible formulas include:

Which are easily distinguished by \(^1\text{H} \text{ NMR spectroscopy}

Another way of expressing this is that for a molecular formula: \( C_nH_m \)

\[
\text{Index of hydrogen deficiency} = \frac{2n + 2 - m}{2}
\]
Effect of Heteroatoms

Group VII elements \((X = F, Cl, Br, I)\) are equivalent to one proton in the reference. i.e. the number of H's in the reference formula must be corrected by subtracting 1 for each \(X\) present.

Group VI elements \((Y = O, S)\): no correction to the reference formula is necessary.

Group V elements \((Z = N, P)\): the number of H's in the reference formula must be corrected adding 1 for each \(Z\) present.
\[ \text{For a molecular formula: } C_nH_mX^X Y^Y Z^Z \]

\[
\text{Index of hydrogen deficiency} = \frac{2n + 2 + z - x - m}{2}
\]

\text{Example}

\[ C_{10}H_6N_2Br_4Cl_2 \]

\[
\text{Index of hydrogen deficiency} = \frac{(20 + 2) + 2 - 6 - 6}{2} = 6
\]

the exact structure has not yet been fully identified, but it probably has a structure such as:

- [Diagram of the chemical structure]

- [Detailed chemical structure diagram]