

11.5: INFRARED SPECTRA OF SOME COMMON FUNCTIONAL GROUPS

COMMON GROUP FREQUENCIES SUMMARY

When analyzing an IR spectrum, it is helpful to overlay the diagram below onto the spectrum with our mind to help recognize functional groups.

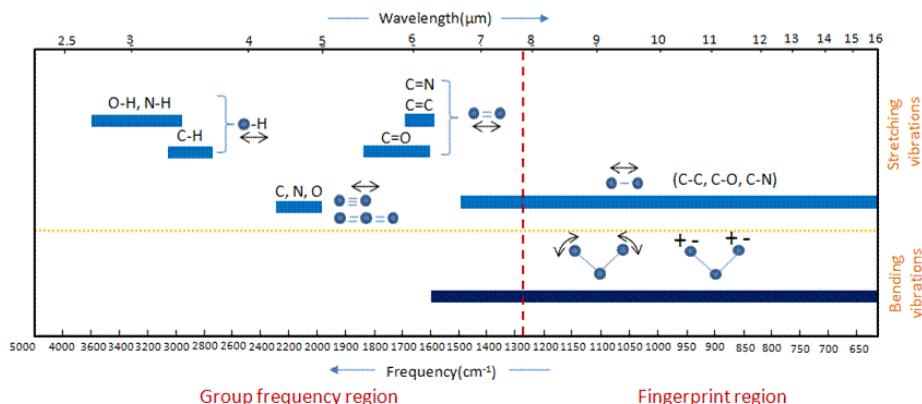


Figure 1. Group frequency and fingerprint regions of the mid-infrared spectrum

The region of the infrared spectrum from 1200 to 700 cm^{-1} is called the fingerprint region. This region is notable for the large number of infrared bands that are found there. Many different vibrations, including C-O, C-C and C-N single bond stretches, C-H bending vibrations, and some bands due to benzene rings are found in this region. The fingerprint region is often the most complex and confusing region to interpret, and is usually the last section of a spectrum to be interpreted. However, the utility of the fingerprint region is that the many bands there provide a fingerprint for a molecule.

GROUP FREQUENCIES - A CLOSER LOOK

Detailed information about the infrared absorptions observed for various bonded atoms and groups is usually presented in tabular form. The following table provides a collection of such data for the most common functional groups. Following the color scheme of the chart, stretching absorptions are listed in the blue-shaded section and bending absorptions in the green shaded part. **More detailed descriptions for certain groups (e.g. alkenes, arenes, alcohols, amines & carbonyl compounds) may be viewed by clicking on the functional class name.** Since most organic compounds have C-H bonds, a useful rule is that absorption in the 2850 to 3000 cm^{-1} is due to sp^3 C-H stretching; whereas, absorption above 3000 cm^{-1} is from sp^2 C-H stretching or sp C-H stretching if it is near 3300 cm^{-1} .

Stretching Vibrations				Bending Vibrations		
Functional Class	Range (cm ⁻¹)	Intensity	Assignment	Range (cm ⁻¹)	Intensity	Assignment
Alkanes	2850-3000	str	CH ₃ , CH ₂ & CH 2 or 3 bands	1350-1470	med	CH ₂ & CH ₃ deformation
				1370-1390	med	CH ₃ deformation
				720-725	wk	CH ₂ rocking
Alkenes	3020-3100	med	=C-H & =CH ₂ (usually sharp)	880-995	str	=C-H & =CH ₂
	1630-1680	var	C=C (symmetry reduces intensity)	780-850	med	(out-of-plane bending)
	1900-2000	str	C=C asymmetric stretch	675-730	med	cis-RCH=CHR
Alkynes	3300	str	C-H (usually sharp)	600-700	str	C-H deformation
	2100-2250	var	C≡C (symmetry reduces intensity)			
Arenes	3030	var	C-H (may be several bands)	690-900	str-med	C-H bending & ring puckering
	1600 & 1500	med-wk	C=C (in ring) (2 bands) (3 if conjugated)			
Alcohols & Phenols	3580-3650	var	O-H (free), usually sharp	1330-1430	med	O-H bending (in-plane)
	3200-3550	str	O-H (H-bonded), usually broad	650-770	var-wk	O-H bend (out-of-plane)
	970-1250	str	C-O			
Amines	3400-3500 (dil. soln.)	wk	N-H (1°-amines), 2 bands	1550-1650	med-str	NH ₂ scissoring (1°-amines)
	3300-3400 (dil. soln.)	wk	N-H (2°-amines)	660-900	var	NH ₂ & N-H wagging (shifts on H-bonding)
	1000-1250	med	C-N			
Aldehydes & Ketones	2690-2840(2 bands)	med str str str str str str	C-H (aldehyde C-H) C=O (saturated aldehyde) C=O (saturated ketone) aryl ketone α, β-unsaturation cyclopentanone cyclobutanone	1350- 1360 1400- 1450 1100	str str med	α-CH ₃ bending α-CH ₂ bending C-C-C bending
	1720-1740					
	1710-1720					
Carboxylic Derivatives	Acids & 2500-3300 (acids) overlap C-H 1705-1720 (acids) 1210-1320 (acids)	str str med-str str str str str str	O-H (very broad) C=O (H-bonded) O-C (sometimes 2-peaks) C=O C=O (2-bands) O-C C=O O-C (2-bands) C=O (amide I band)	1395- 1440 1590- 1650 1500- 1560	med med med	C-O-H bending N-H (1°-amide) II band N-H (2°-amide) II band
Nitriles	2240-2260	med	C≡N (sharp)			
Isocyanates, Isothiocyanates, Diimides, Azides & Ketenes	2100-2270	med	-N=C=O, -N=C=S -N=C=N-, -N ₃ , C=C=O			

RECOGNIZING GROUP FREQUENCIES IN IR SPECTRA - A VERY CLOSE LOOK

HYDROCARBONS

Hydrocarbons compounds contain only C-H and C-C bonds, but there is plenty of information to be obtained from the infrared spectra arising from C-H stretching and C-H bending.

In alkanes, which have very few bands, each band in the spectrum can be assigned:

- C-H stretch from 3000–2850 cm⁻¹
- C-H bend or scissoring from 1470-1450 cm⁻¹
- C-H rock, methyl from 1370-1350 cm⁻¹
- C-H rock, methyl, seen only in long chain alkanes, from 725-720 cm⁻¹

Figure 3. shows the IR spectrum of octane. Since most organic compounds have these features, these C-H vibrations are usually not noted when interpreting a routine IR spectrum. Note that the change in dipole moment with respect to distance for the C-H stretching is greater than that for others shown, which is why the C-H stretch band is the more intense.

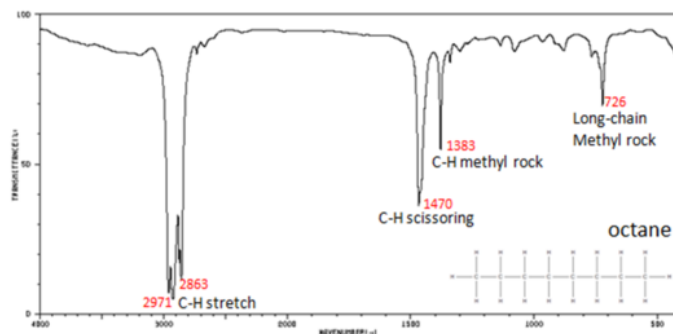


Figure 3. Infrared Spectrum of Octane

In alkenes compounds, each band in the spectrum can be assigned:

- C=C stretch from 1680-1640 cm^{-1}
- =C-H stretch from 3100-3000 cm^{-1}
- =C-H bend from 1000-650 cm^{-1}

Figure 4. shows the IR spectrum of 1-octene. As alkenes compounds, these bands are not specific and are generally not noted because they are present in almost all organic molecules.

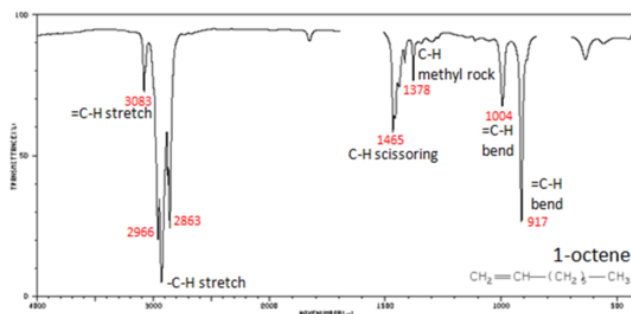


Figure 4. Infrared Spectrum of 1-Octene

In alkynes, each band in the spectrum can be assigned:

- $\text{C}\equiv\text{C}$ stretch from 2260-2100 cm^{-1}
- $\text{C}\equiv\text{C}-\text{H}$: C-H stretch from 3330-3270 cm^{-1}
- $\text{C}\equiv\text{C}-\text{H}$: C-H bend from 700-610 cm^{-1}

The spectrum of 1-hexyne, a terminal alkyne, is shown below.

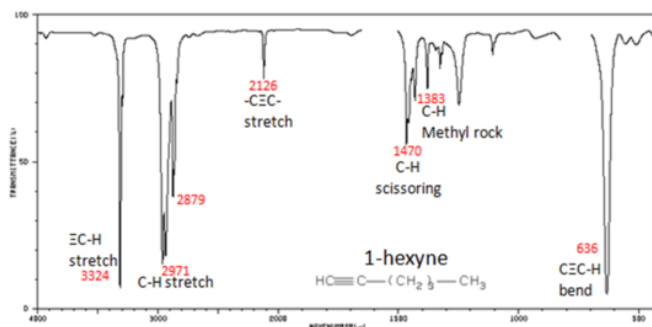


Figure 5. Infrared Spectrum of 1-Hexyne

In aromatic compounds, each band in the spectrum can be assigned:

- C-H stretch from 3100-3000 cm^{-1}
- overtones, weak, from 2000-1665 cm^{-1}
- C-C stretch (in-ring) from 1600-1585 cm^{-1}

- C–C stretch (in-ring) from 1500-1400 cm^{-1}
- C–H "oop" from 900-675 cm^{-1}

Note that this is at slightly higher frequency than is the –C–H stretch in alkanes. This is a very useful tool for interpreting IR spectra. Only alkenes and aromatics show a C–H stretch slightly higher than 3000 cm^{-1} .

Figure 6. shows the spectrum of toluene.

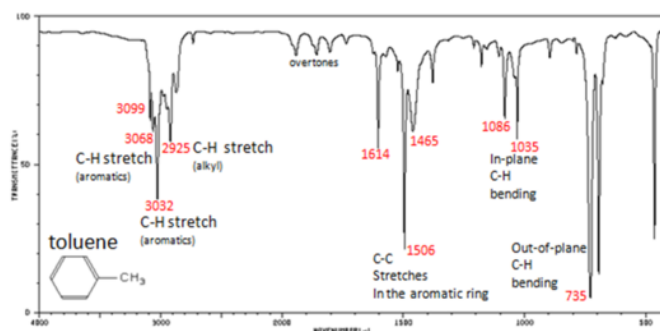


Figure 6. Infrared Spectrum of Toluene

FUNCTIONAL GROUPS CONTAINING THE C-O BOND

Alcohols have IR absorptions associated with both the O–H and the C–O stretching vibrations.

- O–H stretch, hydrogen bonded 3500-3200 cm^{-1}
- C–O stretch 1260-1050 cm^{-1} (s)

Figure 7. shows the spectrum of ethanol. Note the very broad, strong band of the O–H stretch.

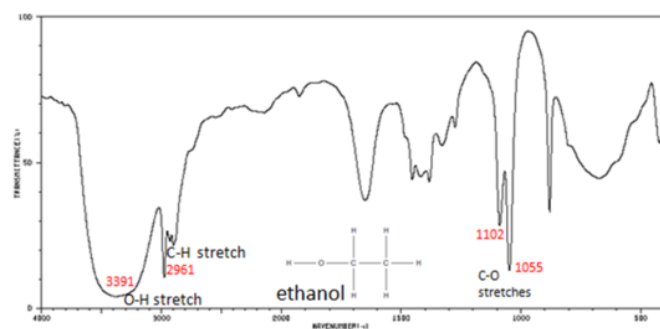


Figure 7. Infrared Spectrum of Ethanol

The carbonyl stretching vibration band C=O of saturated aliphatic ketones appears:

- C=O stretch - aliphatic ketones 1715 cm^{-1}
- ?, ?-unsaturated ketones 1685-1666 cm^{-1}

Figure 8. shows the spectrum of 2-butanone. This is a saturated ketone, and the C=O band appears at 1715.

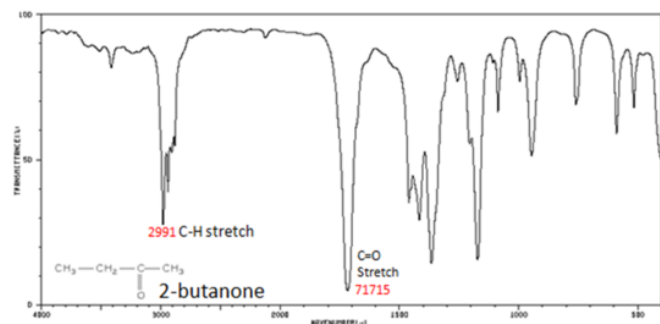


Figure 8. Infrared Spectrum of 2-Butanone

If a compound is suspected to be an aldehyde, a peak always appears around 2720 cm^{-1} which often appears as a shoulder-type peak just to the right of the alkyl C–H stretches.

- H-C=O stretch 2830-2695 cm^{-1}
- C=O stretch:
 - aliphatic aldehydes 1740-1720 cm^{-1}
 - alpha, beta-unsaturated aldehydes 1710-1685 cm^{-1}

Figure 9. shows the spectrum of butyraldehyde.

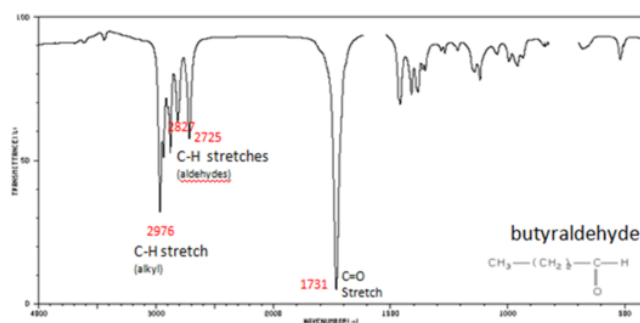


Figure 9. Infrared Spectrum of Butyraldehyde

The carbonyl stretch C=O of esters appears:

- C=O stretch
 - aliphatic from 1750-1735 cm^{-1}
 - α, β -unsaturated from 1730-1715 cm^{-1}
- C-O stretch from 1300-1000 cm^{-1}

Figure 10. shows the spectrum of ethyl benzoate.

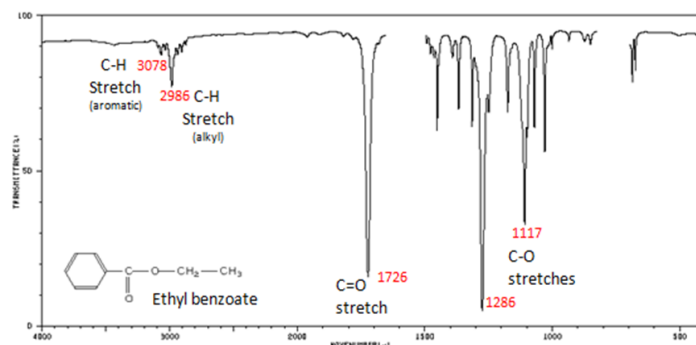


Figure 10. Infrared Spectrum of Ethyl benzoate

The carbonyl stretch C=O of a carboxylic acid appears as an intense band from 1760-1690 cm^{-1} . The exact position of this broad band depends on whether the carboxylic acid is saturated or unsaturated, dimerized, or has internal hydrogen bonding.

- O-H stretch from 3300-2500 cm^{-1}
- C=O stretch from 1760-1690 cm^{-1}
- C-O stretch from 1320-1210 cm^{-1}
- O-H bend from 1440-1395 and 950-910 cm^{-1}

Figure 11. shows the spectrum of hexanoic acid.

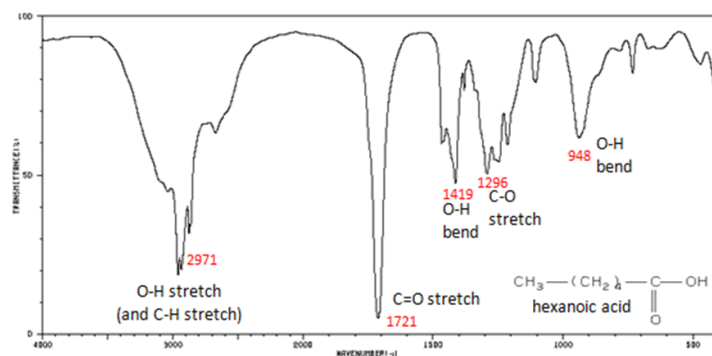


Figure 11. Infrared Spectrum of Hexanoic acid

ORGANIC NITROGEN COMPOUNDS

- N-O asymmetric stretch from $1550\text{--}1475\text{ cm}^{-1}$
- N-O symmetric stretch from $1360\text{--}1290\text{ cm}^{-1}$

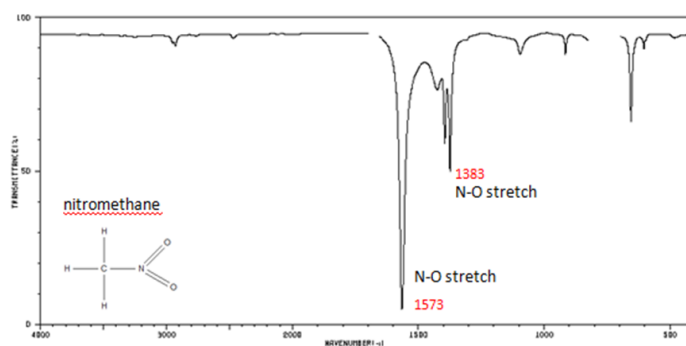


Figure 12. Infrared Spectrum of Nitomethane

ORGANIC COMPOUNDS CONTAINING HALOGENS

Alkyl halides are compounds that have a C-X bond, where X is a halogen: bromine, chlorine, fluorene, or iodine.

- C-H wag ($-\text{CH}_2\text{X}$) from $1300\text{--}1150\text{ cm}^{-1}$
- C-X stretches (general) from $850\text{--}515\text{ cm}^{-1}$
 - C-Cl stretch $850\text{--}550\text{ cm}^{-1}$
 - C-Br stretch $690\text{--}515\text{ cm}^{-1}$

The spectrum of 1-chloro-2-methylpropane are shown below.

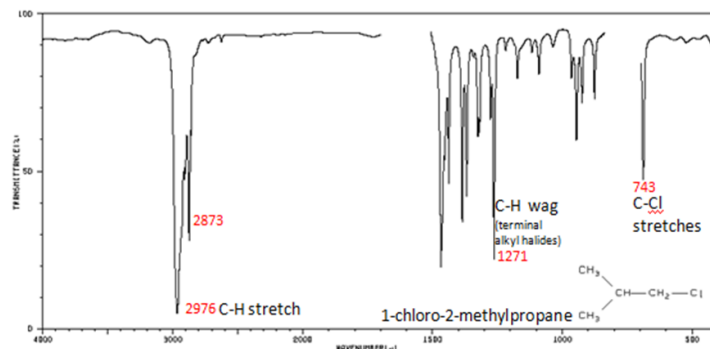


Figure 13. Infrared Spectrum of 1-chloro-2-methylpropane

For more Infrared spectra Spectral database of organic molecules is introduced to use free database. Also, the infrared spectroscopy correlation table is linked on bottom of page to find other assigned IR peaks.

Exercise

1. What functional groups give the following signals in an IR spectrum?

A) 1700 cm^{-1}

B) 1550 cm^{-1}

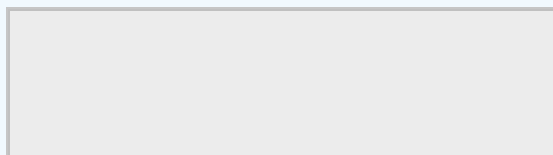
C) 1700 cm^{-1} and $2510\text{--}3000\text{ cm}^{-1}$

2. How can you distinguish the following pairs of compounds through IR analysis?

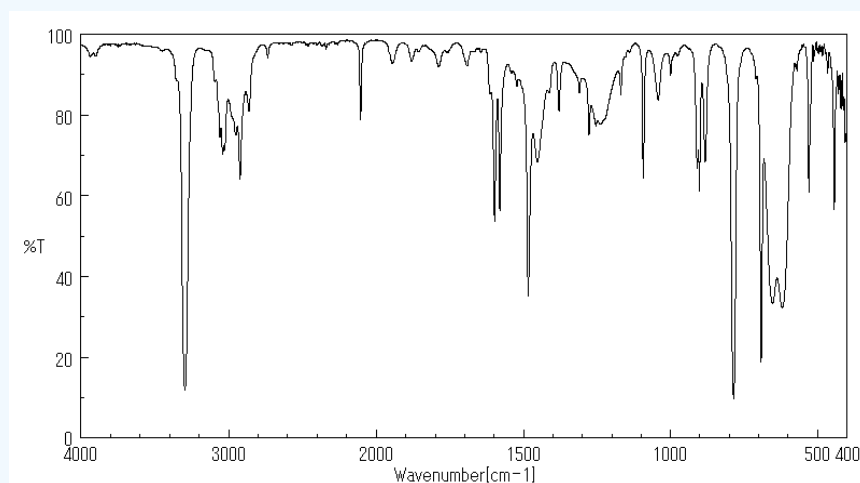
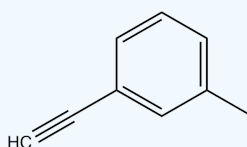
A) CH_3OH (Methanol) and $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$ (Diethylether)

B) Cyclopentane and 1-pentene.

C)

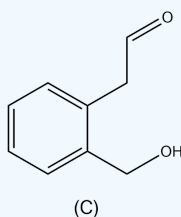
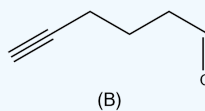
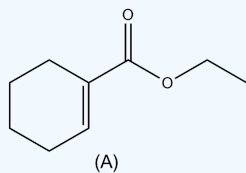


3. The following spectra is for the accompanying compound. What are the peaks that you can identify in the spectrum?



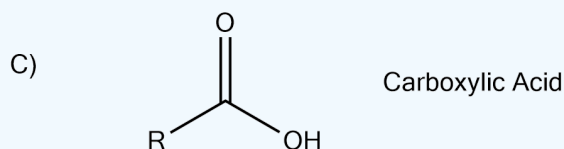
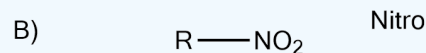
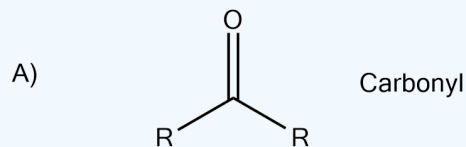
Source: SDBSWeb : <http://sdb.sdb.aist.go.jp> (National Institute of Advanced Industrial Science and Technology, 2 December 2016)

4. What absorptions would the following compounds have in an IR spectra?



Answer

1.



2.

A) A OH peak will be present around 3300 cm^{-1} for methanol and will be absent in the ether.

B) 1-pentene will have a alkene peak around 1650 cm^{-1} for the C=C and there will be another peak around 3100 cm^{-1} for the sp^2 C-H group on the alkene

C) Cannot distinguish these two isomers. They both have the same functional groups and therefore would have the same peaks on an IR spectra.

3.

Frequency (cm-1) Functional Group

3200 C≡C-H

2900-3000 C-C-H, C=C-H

2100 C≡C

1610 C=C

(There is also an aromatic undertone region between 2000-1600 which describes the substitution on the phenyl ring.)

4.

A)

Frequency (cm-1) Functional Group

2900-3000 C-C-H, C=C-H

1710 C=O

1610 C=C

1100 C-O

B)

Frequency (cm-1) Functional Group

3200 C≡C-H

2900-3000 C-C-H, C=C-H

2100 C≡C

1710 C=O

C)

Frequency (cm-1) Functional Group

3300 (broad) O-H

2900-3000 C-C-H, C=C-H

2000-1800 Aromatic Overtones

1710 C=O

1610 C=C

CONTRIBUTORS AND ATTRIBUTIONS

- [Dr. Dietmar Kennepohl](#) FCIC (Professor of Chemistry, [Athabasca University](#))
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- William Reusch, Professor Emeritus ([Michigan State U.](#)), [Virtual Textbook of Organic Chemistry](#)

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