# Functional groups

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In organic chemistry, **functional groups** are specific groups of atoms within molecules that are responsible for the characteristic chemical reactions of those molecules. The same functional group will undergo the same or similar chemical reaction(s) regardless of the size of the molecule it is a part of. If we replaced the H-atoms in ethene with $CH_3$ groups, that would be a methyl group.

**Functional groups are attached to the carbon backbone of organic molecules. They determine the characteristics and chemical reactivity of molecules. Functional groups are far less stable than the carbon backbone and are likely to participate in chemical reactions. Six common biological functional groups are**

**hydrogen, hydroxyl, carboxyl, carbonyl, amino, phosphate, and methyl.**

The following is

1. A list of common functional groups. In the formulas, the symbols R and R' usually denotes an attached hydrogen, or a hydrocarbon side chain of any length, but may sometimes refer to any group of atoms.

**The first carbon after the carbon that attaches to the functional group is called the alpha carbon.**

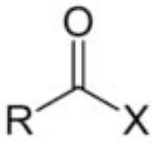
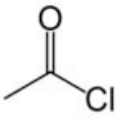
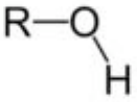
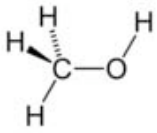
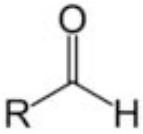
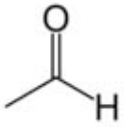
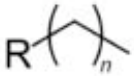
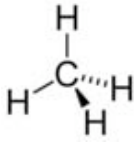
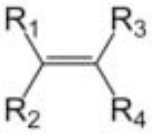
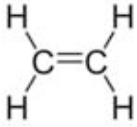
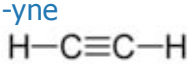
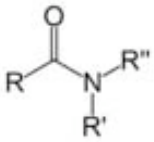
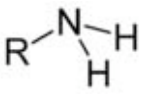
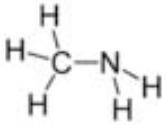
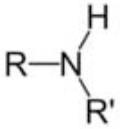
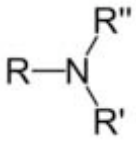
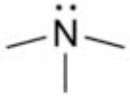
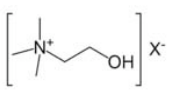
Combining the names of functional groups with the names of the parent alkanes generates a powerful systematic nomenclature for naming organic compounds. Unfortunately not all listings of functional groups agree, and the British system avoids functional groups altogether, maintaining that it is a categorization that obscures what is really going on in organic chemistry.

The non-hydrogen atoms of functional groups are always associated with each other and with the rest of the molecule by covalent bonds. When the group of atoms is associated with the rest of the molecule primarily by ionic forces, the group is referred to more properly as a polyatomic ion or complex ion. And all of these are called radicals, by a meaning of the term *radical* that predates the free radical.

Notice that some important *classes* of molecules, like cyclic aromatics (conjugated hydrocarbon rings) and heterocycles (related) are not listed.

2. A (more useful) table of the main functional groups that are important in elementary biochemistry (but several are omitted).

3. Finally some infrared spectra to show how these types of groups can actually be identified in the spectra of planets and other astronomical objects.

| Chemical class | Group | Formula | Structural Formula | Prefix | Suffix |
|---|---|---|---|---|---|
| Acyl halide | Haloformyl | RCOX |  | haloformyl- | -oyl  |
| Alcohol | Hydroxyl | ROH |  | hydroxy- |  -ol |
| Aldehyde | Aldehyde | RCHO |  | oxo- | -al  |
| **Alkane*** | Alkyl | RH |  | alkyl- |  -ane |
| **Alkene*** | Alkenyl | $R_2C=CR_2$ |  | alkenyl- |  -ene |
| **Alkyne*** | Alkynyl | RC≡CR' |  | alkynyl- | -yne  |
| Amide | Carboxamide | $RCONR_2$ |  | carboxamido- | -amide |
| Amines | Primary amine | $RNH_2$ |  | amino- | -amine  |
| | Secondary amine | $R_2NH$ |  | amino- | -amine |
| | Tertiary amine | $R_3N$ |  | amino- | -amine  |
| | 4° ammonium ion | $R_4N^+$ | | ammonio- | -ammonium  |

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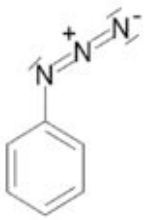
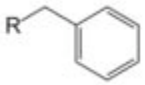
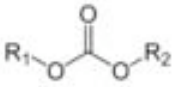
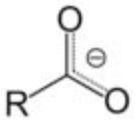
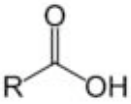
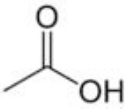
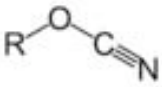
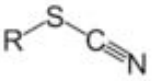
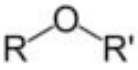
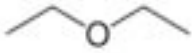
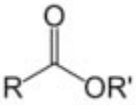
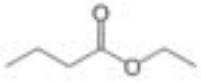
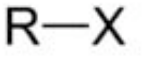
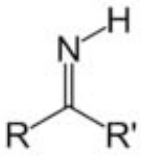
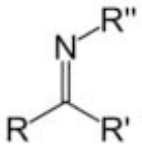
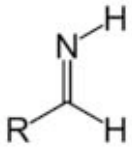
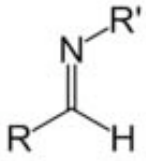
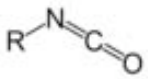
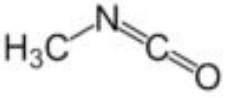
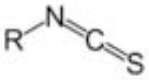
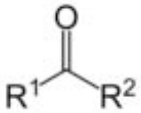
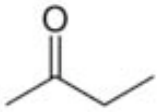
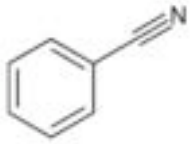
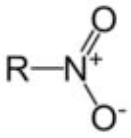
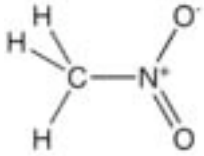
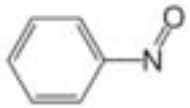
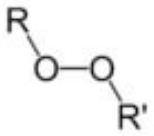
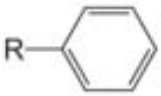
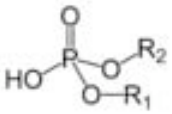
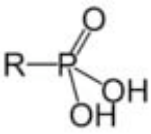
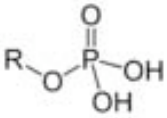
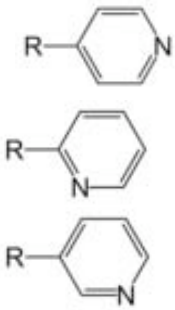
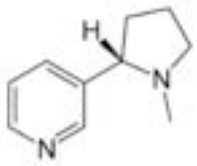
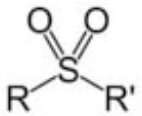
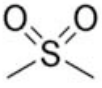
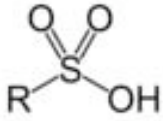
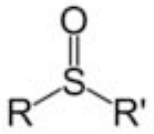
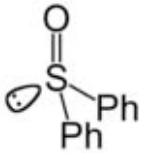
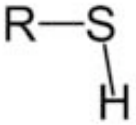
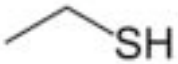
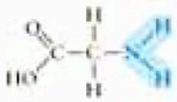
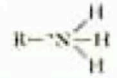
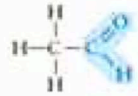
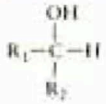
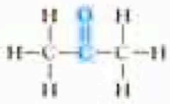
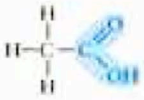
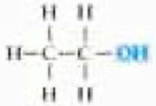
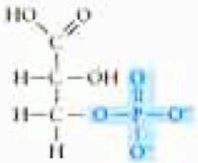
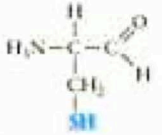
|---|---|---|---|---|---|
| Azo compound | Azo (Diimide) | $RN_2R'$ | | azo- | -diazene  |
| Toluene derivative | Benzyl | $RCH_2C_6H_5$ RBn |  | benzyl- | 1-(*substituent*)toluene |
| Carbonate | Carbonate ester | ROCOOR |  | | alkyl **carbonate** |
| Carboxylate | Carboxylate | $RCOO^-$ |  | carboxy- | -oate |
| Carboxylic acid | Carboxyl | RCOOH |  | carboxy- | -oic acid  |
| Cyanates | Cyanate | ROCN |  | cyanato- | alkyl **cyanate** |
| | Thiocyanate | RSCN |  | thiocyanato- | alkyl **thiocyanate** |
| Ether | Ether | ROR' |  | alkoxy- | alkyl alkyl **ether**  |
| Ester | Ester | RCOOR' |  | | alkyl alkan**oate**  |
| Haloalkane | Halo | RX |  | halo- | alkyl **halide**  |
| Hydroperoxide | Hydroperoxy | ROOH | | hydroperoxy- | alkyl **hydroperoxide** |
| Imine | Primary ketimine | RC(=NH)R' |  | imino- | -imine |

| | | | | | |
|---|---|---|---|---|---|
| | Secondary ketimine | RC(=NR*)R'* |  | imino- | -imine |
| | Primary aldimine | RC(=NH)H |  | imino- | -imine |
| | Secondary aldimine | RC(=NR')H |  | imino- | -imine |
| Isocyanide | Isocyanide | RNC | | isocyano- | alkyl **isocyanide** |
| Isocyanates | Isocyanate | RNCO |  | isocyanato- | alkyl **isocyanate**  |
| | Isothiocyanate | RNCS |  | isothiocyanato- | alkyl **isothiocyanate** |
| Ketone | Ketone | RCOR' |  | keto-, oxo- | -one  |
| Nitrate | Nitrate | $RONO_2$ | | nitrooxy-, nitroxy- | alkyl **nitrate** |
| Nitrile | Nitrile | RCN |  | cyano- | alkane**nitrile** alkyl **cyanide**  |
| Nitrite | Nitrite | RONO | | nitrosooxy- | alkyl **nitrite** |
| Nitro compound | Nitro | $RNO_2$ |  | nitro- |  |

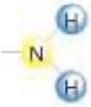
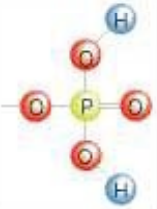
| | | | | | |
|---|---|---|---|---|---|
| Nitroso compound | Nitroso | RNO | | nitroso- |  |
| Peroxide | Peroxy | ROOR |  | peroxy- | alkyl **peroxide** |
| Benzene derivative | Phenyl | $RC_6H_5$ |  | phenyl- | -benzene |
| Phosphine | Phosphino | $R_3P$ | | phosphino- | -phosphane |
| Phosphodiester | Phosphate | $HOPO(OR)_2$ |  | phosphoric acid di(*substituent*) ester | di(*substituent*) hydrogenphosphate **DNA** |
| Phosphonic acid | Phosphono | $RP(=O)(OH)_2$ |  | phosphono- | *substituent* phosphonic acid |
| Phosphate | Phosphate | $ROP(=O)(OH)_2$ |  | phospho- | |
| Pyridine derivative | Pyridyl | $RC_5H_4N$ |  | 4-pyridyl (pyridin-4-yl)<br>3-pyridyl (pyridin-3-yl)<br>2-pyridyl (pyridin-2-yl) | -pyridine  |
| Sulfide | | RSR' | | | di(*substituent*) sulfide |
| Sulfone | Sulfonyl | $RSO_2R'$ |  | sulfonyl- | di(*substituent*) sulfone  |
| Sulfonic acid | Sulfo | $RSO_3H$ |  | sulfo- | *substituent* sulfonic acid |

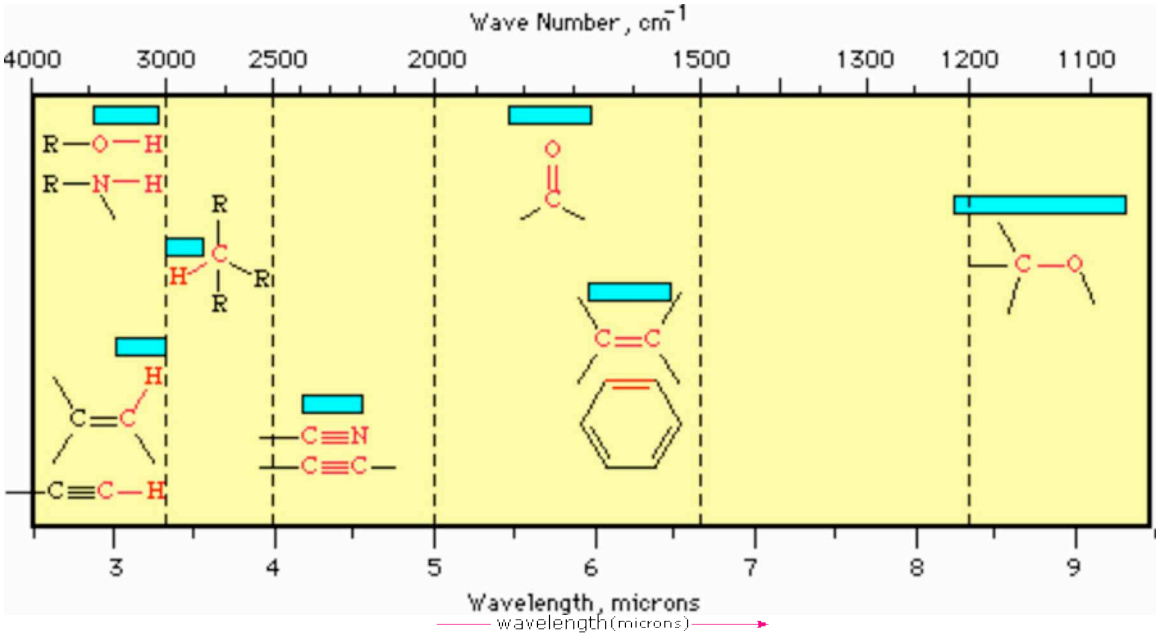
| | | | | | |
|---|---|---|---|---|---|
| Sulfoxide | Sulfinyl | RSOR' |  | sulfinyl- | di(*substituent*) **sulfoxide**  |
| Thiol | Sulfhydryl | RSH |  | mercapto-, sulfanyl- | -thiol  |

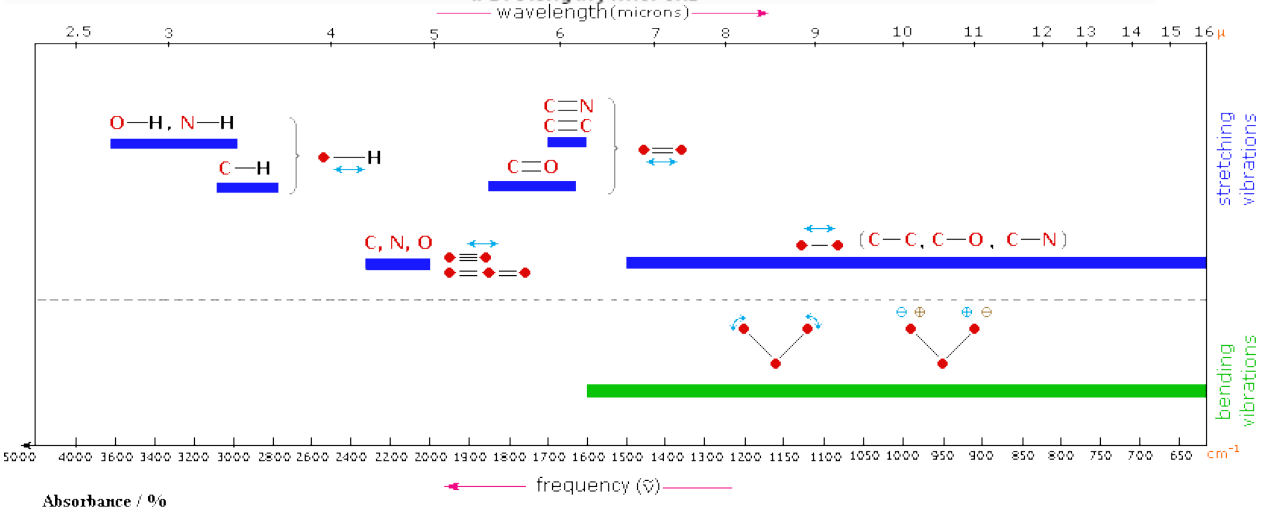
| Functional Group | *Formula | Family of Molecules | Example | Properties of Functional Group |
|---|---|---|---|---|
| Amino |  | Amines |  Glycine (an amino acid) | Acts as a base—tends to attract a proton to form  |
| Carbonyl |  | Aldehydes |  Acetaldehyde | Aldehydes, especially, react with compounds of form $HR_2$ to produce larger molecules with form  |
| |  | Ketones |  Acetone | |
| Carboxyl |  | Carboxylic acids |  Acetic acid | Acts as an acid—tends to lose a proton to form  |
| Hydroxyl |  | Alcohols |  Ethanol | Highly polar, so makes compounds more soluble through hydrogen bonding with water |
| Phosphate |  | Organic phosphates |  3-Phosphoglyceric acid | When several phosphate groups are linked together, breaking O–P bonds between them releases large amounts of energy |
| Sulfhydryl |  | Thiols |  Cysteine | When present in proteins, can form disulfide (S–S) bonds that contribute to protein structure |

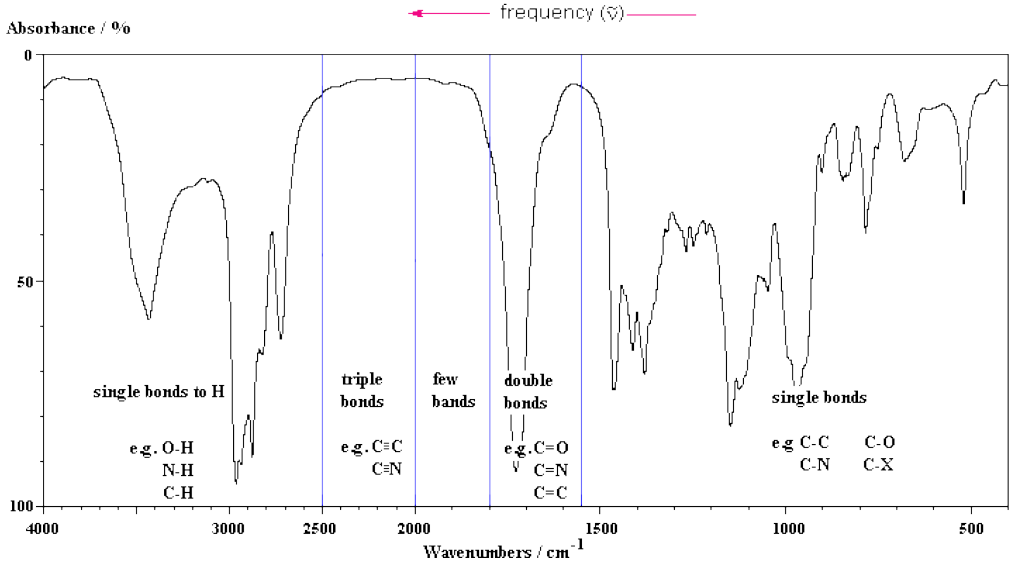
*In these structural formulas, "R" stands for the rest of the molecule

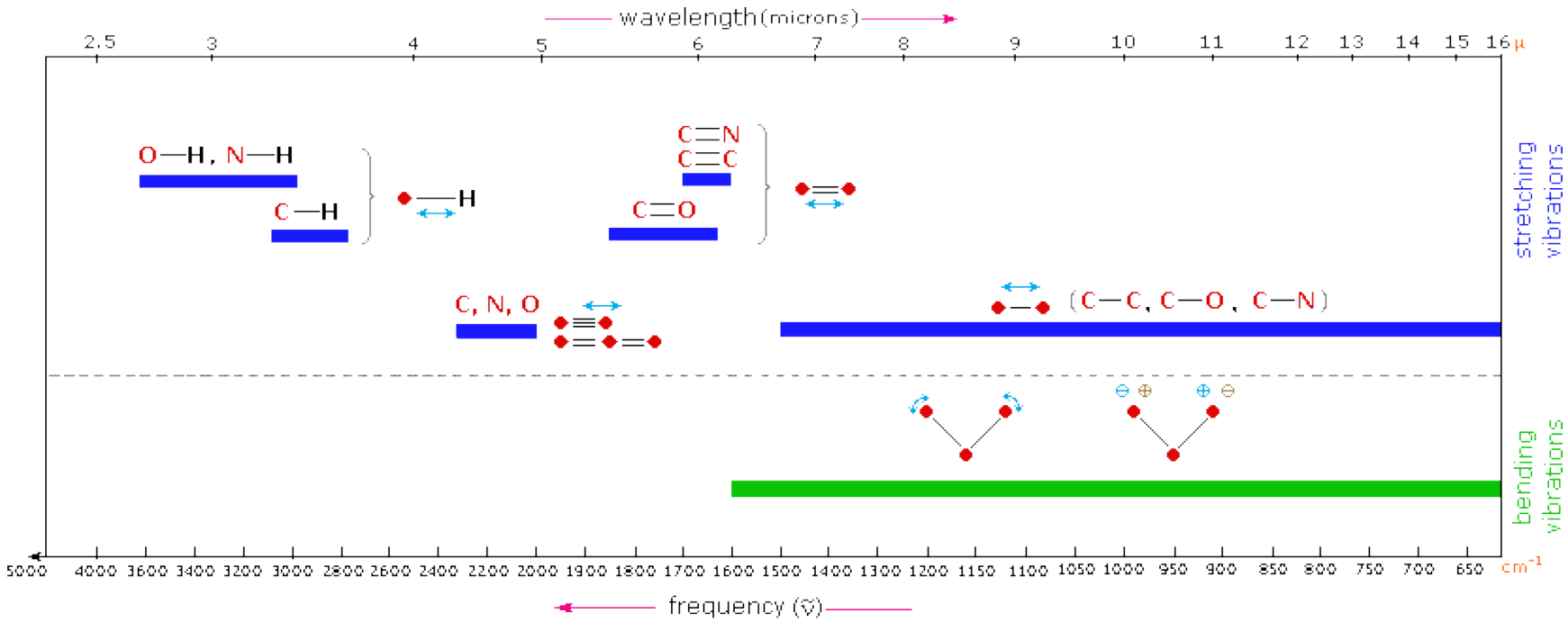
Table 3-1. Important Functional Groups in Biological Molecules

| Group | Structure | Properties | Types of Molecules |
|---|---|---|---|
| **Hydrogen (—H)** |  | Polar or nonpolar, depending on which atom hydrogen is bonded to; involved in condensation and hydrolysis | Almost all organic molecules |
| **Hydroxyl (—OH)** |  | Polar; involved in condensation and hydrolysis | Carbohydrates, nucleic acids, alcohols, some acids, and steroids |
| **Carboxyl (—COOH)** |  | Acidic; negatively charged when $H^+$ dissociates; involved in peptide bonds | Amino acids, fatty acids |
| **Amino (—NH2)** |  | Basic; may bond an additional $H^+$, becoming positively charged; involved in peptide bonds | Amino acids, nucleic acids |
| **Phosphate (—H2PO4)** |  | Acidic; up to two negative charges when $H^+$ dissociates; links nucleotides in nucleic acids; energy-carrier group in ATP | Nucleic acids, phospholipids |
| **Methyl (—CH3)** |  | Nonpolar; tends to make molecules hydrophobic | Many organic molecules; especially common in lipids |


Wave Number, cm-1
4000
3000
2500
2000
1500
1300
1200
1100
R—O—H
R—N—H
C≡N
C≡C—H
3
4
5
6
7
8
9
Wavelength, microns


wavelength (microns)
O—H, N—H
C—H
C≡N
C≡C
C=O
C, N, O
(C—C, C—O, C—N)
stretching vibrations
bending vibrations
frequency (ν)
cm-1


Absorbance / %
0
50
100
single bonds to H
e.g. O-H
N-H
C-H
triple bonds
e.g. C≡C
C≡N
few bands
double bonds
e.g. C=O
C=N
C=C
single bonds
e.g C-C
C-N
C-O
C-X
4000
3000
2500
2000
1500
1000
500
Wavenumbers / cm-1

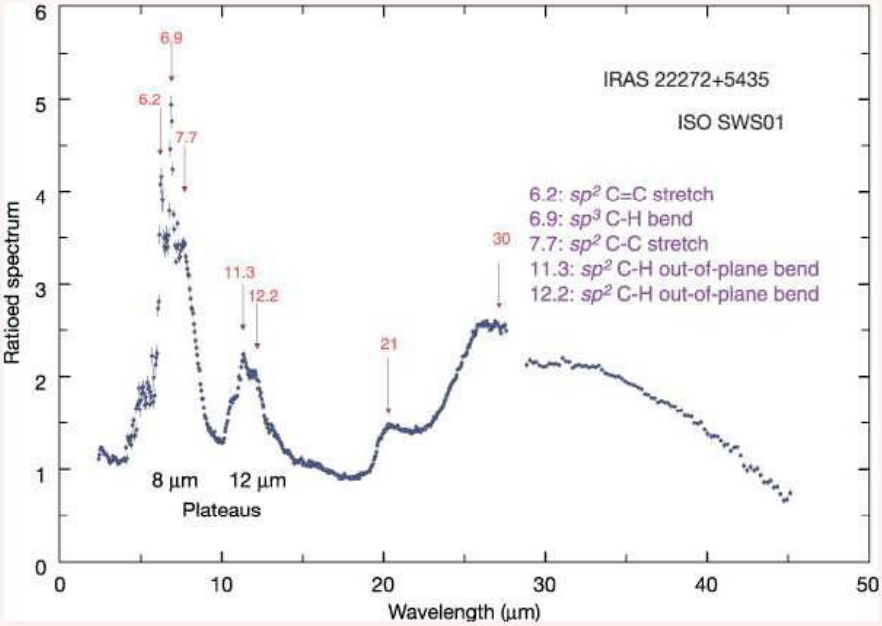

wavelength (microns)
2.5 3 4 5 6 7 8 9 10 11 12 13 14 15 16 μ
O—H, N—H
C—H
—H
C≡N
C=C
C=O
C, N, O
(C—C, C—O, C—N)
stretching vibrations
bending vibrations
5000 4000 3600 3400 3200 3000 2800 2600 2400 2200 2000 1900 1800 1700 1600 1500 1400 1300 1200 1150 1100 1050 1000 950 900 850 800 750 700 650 cm-1
frequency (ν̄)

# PAH features

EMISSION COMPONENTS: PROPERTIES AND ASSIGNMENTS

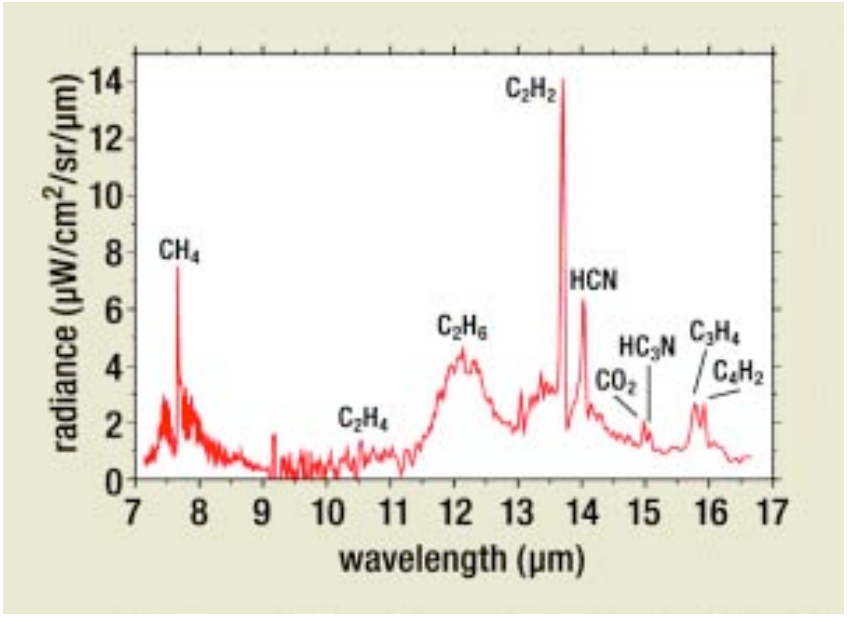
| $\nu$ ($cm^{-1}$) | $\lambda$ (microns) | FWHH ($cm^{-1}$) | Assignment |
|---|---|---|---|
| | | Major Bands | |
| 3040 | 3.29 | 30 | Aromatic C-H stretch ($v = 1 \rightarrow v = 0$) |
| 1615 | 6.2 | 30 | Aromatic C-C stretch |
| 1315–1250 | 7.6–8.0 | 70–200 | Blending of several strong aromatic C-C stretching bands |
| 1150 | 8.7 | ... | Aromatic C-H in-plane bend |
| 890 | 11.2 | 30 | Aromatic C-H out-of-plane bend for nonadjacent, peripheral H atoms |
| | | Minor Features | |
| 3085 | 3.24 | ... | Overtone and/or combination involving fundamentals in the 1810–1050 $cm^{-1}$ (5.52–9.52 $\mu$m) range |
| 2995 | 3.34 | ... | Overtone and/or combination involving fundamentals in the 1810–1050 $cm^{-1}$ (5.52–9.52 $\mu$m) range |
| 2940 | 3.4 | "20" | Aromatic C-H stretch ($v = 2 \rightarrow v = 1$) |
| 2890 | 3.46 | ... | Overtone/combination band involving fundamentals in the 1810–1050 $cm^{-1}$ (5.52–9.52 $\mu$m) range, aromatic C-H stretch (high $v$), aliphatic C-H stretch,? |
| 2850 | 3.51 | ... | Aromatic C-H stretch ($v = 3 \rightarrow v = 2$), aliphatic C-H stretch, overtone/combination band involving fundamentals in the 1810–1050 $cm^{-1}$ (5.52–9.52 $\mu$m) range |
| 2810 | 3.56 | ... | Aromatic C-H stretch (high $v$), aldehydic C-H stretch, overtone/combination band involving fundamentals in the 1810–1050 $cm^{-1}$ (5.52–9.52 $\mu$m) range |
| 1960–1890 | 5.1–5.3 | 30 | Combination of C-H out-of-plane and in-plane bend,? |
| 1785–1755 | 5.6–5.7 | 40 | Overtone of 885 $cm^{-1}$ (11.3 $\mu$m) band; aromatic C-C stretch; Carbonyl C-O stretch,? |
| 1470–1450 | 6.8–6.9 | 30 | Aromatic C-C stretch, aliphatic C-H deformation |
| 840 | 11.9 | ... | C-H out-of-plane bend for doubly adjacent H atoms |
| 790 | 12.7 | ... | C-H out-of-plane bend for triply adjacent H atoms |
| | | Broad Components | |
| 2940 | 3.5 | | Overlap of C-H stretching modes, shifted by anharmonic effects, |
| 3115–2740[a] | 3.21–3.65[b] | "300" | with overtones and combinations of C-C stretch fundamentals in the 1670–1250 $cm^{-1}$ (6–8 $\mu$m) region, aliphatic C-H stretch?,? |
| ~1200 | ~8.5 | "400" | Blending of many weak aromatic C-C stretching bands |
| 1810–1050[a] | 5.52–9.52[b] | | |
| 880 | 12 | "160" | Overlap of many aromatic C-H out-of-plane bending |
| 950–740[a] | 10.5–13.5[b] | | modes for nonadjacent as well as doubly and triply adjacent peripheral H-atoms |
| Red–Near-IR Continuum | | | Electronic transitions between low-lying levels in ionized and complexed PAHs and amorphous carbon particles |
| Mid-IR Continuum | | | Quasi-continuum formed by overlapping overtone and combination bands |

## Pre-Planetary Nebula

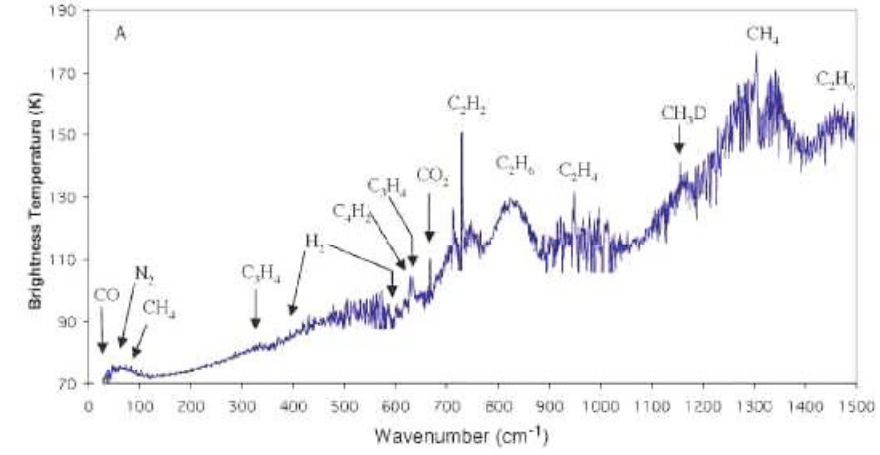


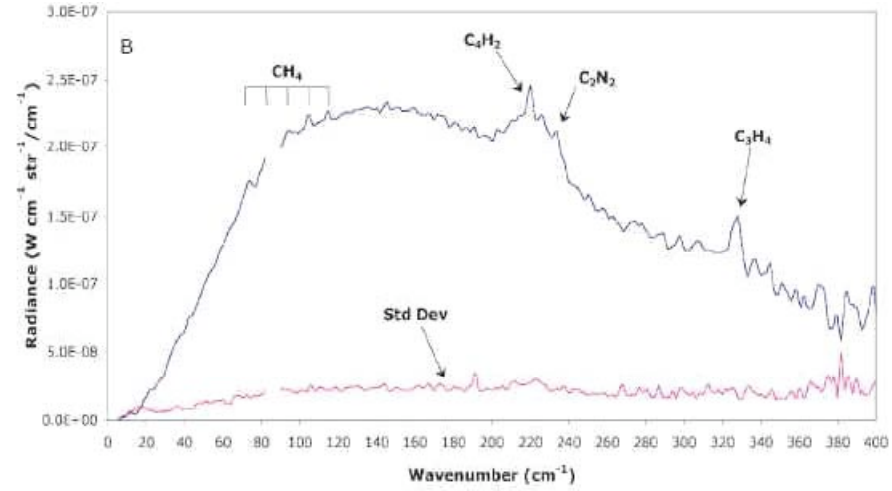

This continuum-removed ISO SWS01 spectrum of the PPN IRAS 22272 + 5435 shows the 8- and 12-µm emission plateaus due to the in-plane and off-plane bending modes of aliphatic side groups attached to an aromatic carbonaceous compound, for which the narrow emission features and their peak wavelengths are marked on the spectrum. Also shown are the unidentified emission features at 21 and 30 µm (ref. 36). The error bars are $1^{\sigma}$ deviation of data points from different scans and detectors over each wavelength resolution element.

## Titan



# Titan


A
Brightness Temperature (K)
Wavenumber (cm-1)
CO
N2
CH4
C3H4
H2
C4H2
C3H4
CO2
C2H2
C2H6
C2H4
CH3D
CH4
C2H6


B
Radiance (W cm-1 str-1/cm-1)
Wavenumber (cm-1)
CH4
C4H2
C2N2
C3H4
Std Dev

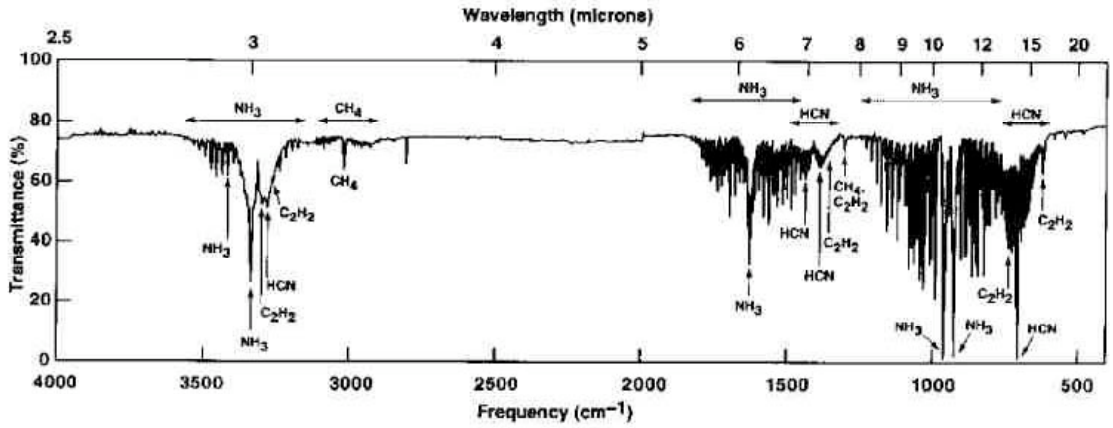



FIG. 5. The gas-phase products for Titan tholin analog synthesis. These simple molecules, which are breakdown products of the initial $CH_4/N_2$ mixture, are composed generally of hydrocarbons and nitrogen-containing species. They may be polymerized into solid tholin under the glow discharge mechanism described in this paper. The gas phase displays a rich chemistry with varied building blocks for Titan tholin analogs.

## Tholins

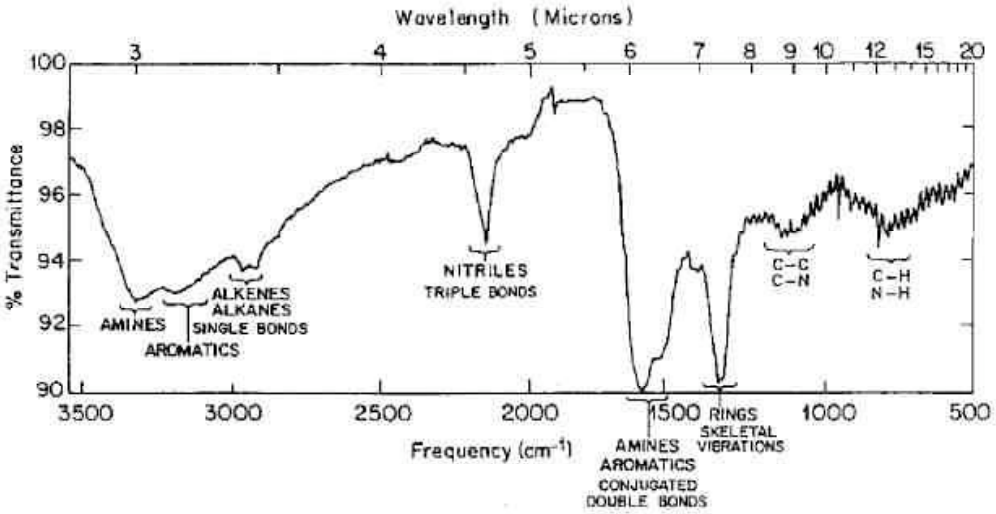
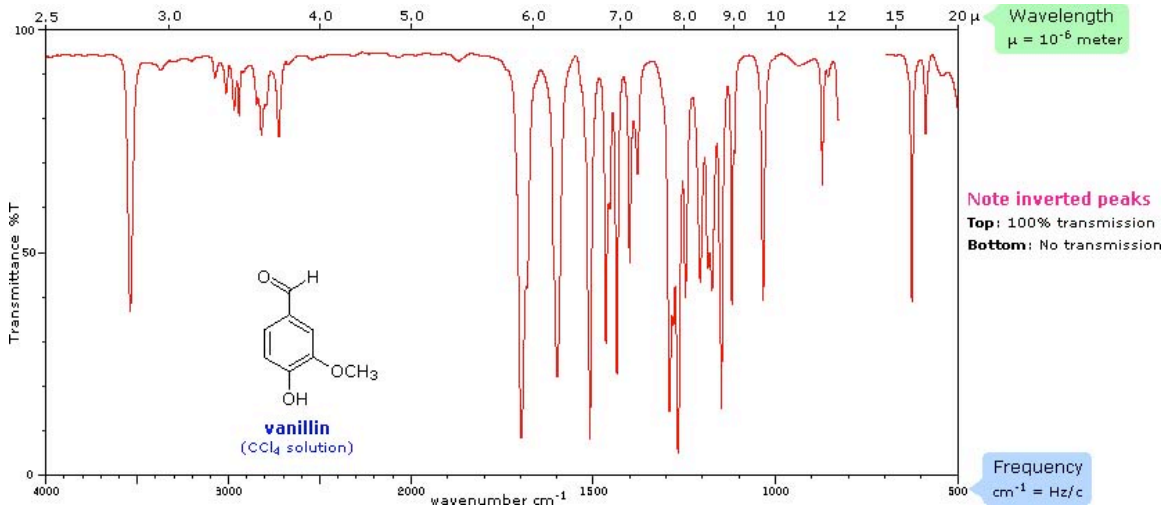
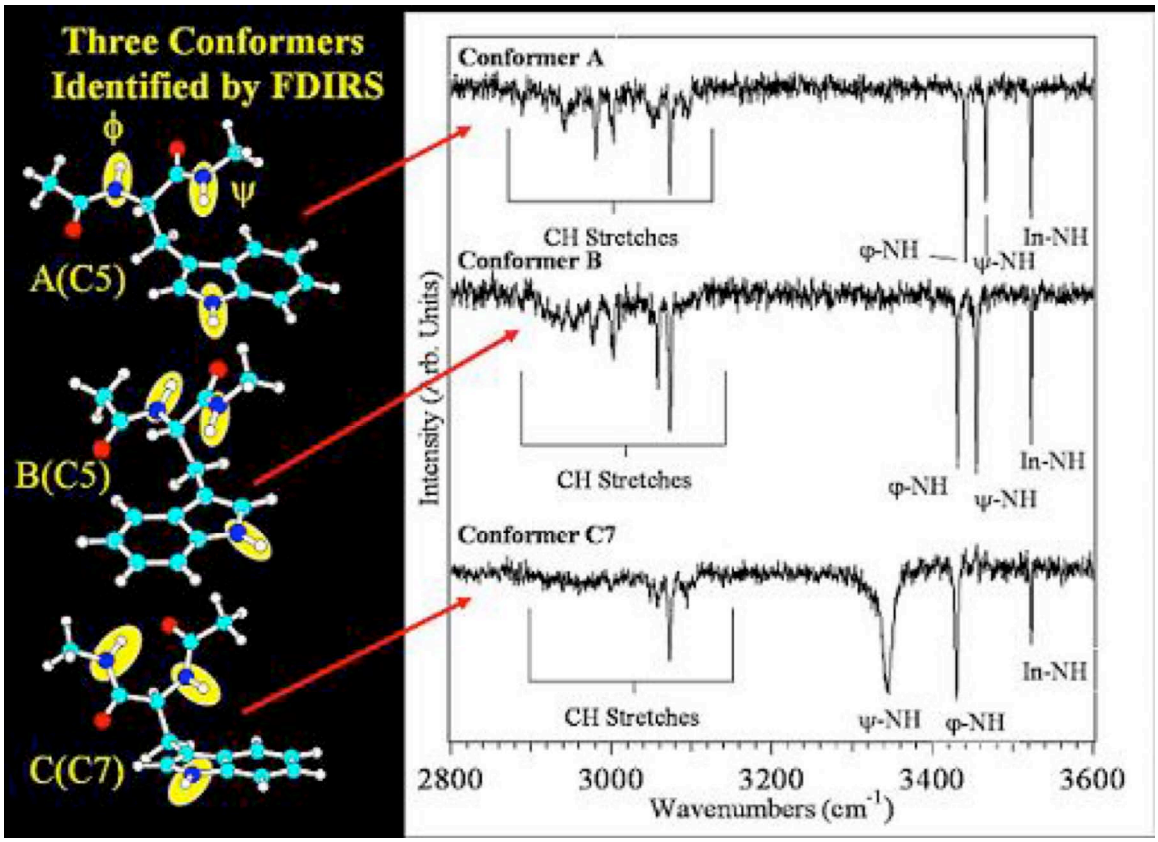



FIG. 2. The IR spectrum of solid tholin material, displaying the chemical nature of the monomer units comprising this complex polymer. Tholins appear to be a complex mixture of heterocyclic hydrocarbons, nitriles, amines, and aliphatic structures from their IR signature. Each region of this IR spectrum is a distinct spectral signature denoting a very specific bond or molecular group (see Table II and Allamandola *et al.* 1989).

# Vanilla


2.5
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10
12
15
20 μ
Wavelength
μ = 10-6 meter
100
50
0
Transmittance %T
4000
3000
2000
1500
1000
500
wavenumber cm-1
Frequency
cm-1 = Hz/c
Note inverted peaks
Top: 100% transmission
Bottom: No transmission
O
H
OCH3
OH
vanillin
(CCl4 solution)


Three Conformers
Identified by FDIRS
ϕ
ψ
A(C5)
B(C5)
C(C7)
Conformer A
CH Stretches
φ-NH
ψ-NH
In-NH
Conformer B
CH Stretches
φ-NH
ψ-NH
In-NH
Conformer C7
CH Stretches
ψ-NH
φ-NH
In-NH
Intensity (Arb. Units)
2800
3000
3200
3400
3600
Wavenumbers (cm-1)