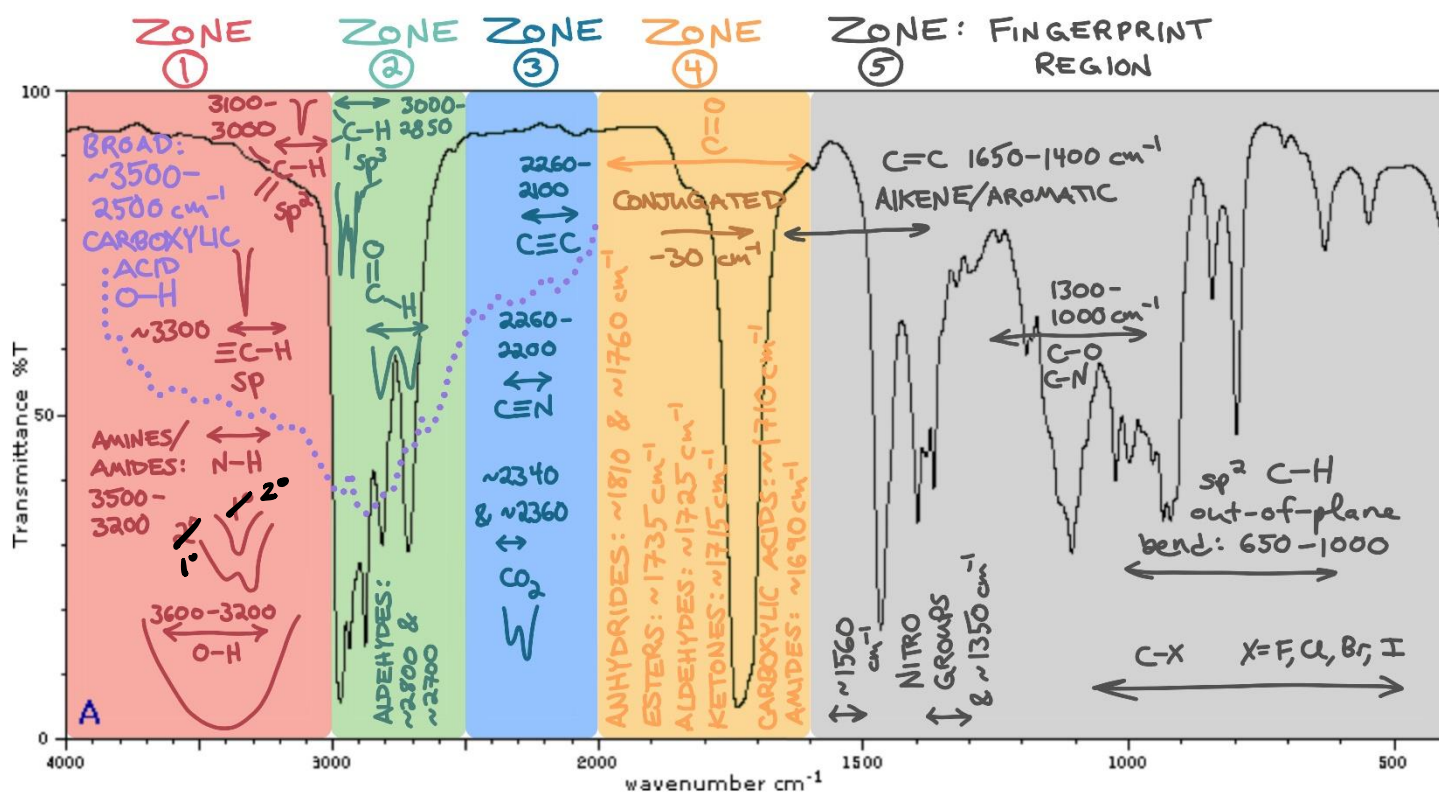
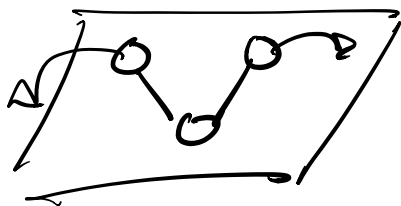
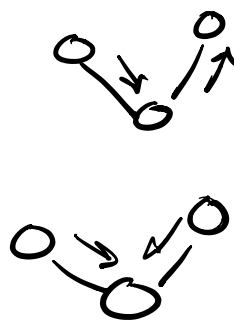
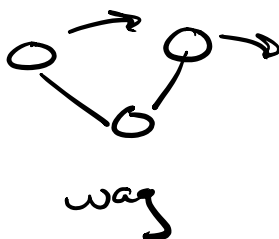
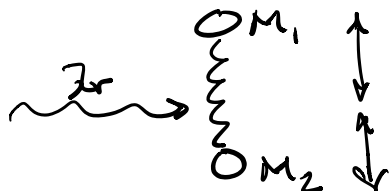


IDENTIFYING the MAJOR FUNCTIONAL GROUP:

1. Is a carbonyl present? **Check ZONE 4.** If no carbonyl is present, go to step 3.
 - **The C=O double bond gives rise to a strong absorption in ZONE 4: $2000-1600\text{ cm}^{-1}$. This peak is often the strongest in the spectrum, and characteristic of the type of carbonyl present (see spectrum below).**
2. If C=O is present, check for additional peaks to confirm the following types of carbonyls:
 - **Anhydrides have two C=O absorptions near 1810 & 1760 cm^{-1}**
 - Esters should also have C-O stretches in ZONE 5 around $1300-1100\text{ cm}^{-1}$ with medium intensity
 - **Aldehydes should also have two signals in ZONE 2: ~ 2800 & $\sim 2700\text{ cm}^{-1}$**
 - **Carboxylic acids should have a broad signal that extends from ZONE 1 through ZONE 2: $3500-2500\text{ cm}^{-1}$**
 - **Amides (primary & secondary) should have a signal in ZONE 1: $3500-3200\text{ cm}^{-1}$**
3. If C=O is absent, check for:
 - **Alcohols/Phenols have a broad signal in ZONE 1: $3600-3200\text{ cm}^{-1}$**
 - **Signals for amines also show up in ZONE 1: $3500-3200\text{ cm}^{-1}$**
 - i. **Primary amines (RNH_2) display 2 signals**
 - ii. **Secondary amines (R_2NH) display 1 signal**
 - Ethers have signals in ZONE 5 due to C-O stretch: $1300-1000\text{ cm}^{-1}$
4. Double bonds and/or aromatic rings:
 - **Phenyl and vinyl sp^2 C-H stretches occur in ZONE 1 to the left of 3000 cm^{-1}**
 - **Alkenes display weak C=C stretching signals near 1650 cm^{-1}**
 - Medium to strong signals from $1650-1400\text{ cm}^{-1}$ imply an aromatic ring
5. sp Hybridized Triple bonds:
 - **Nitrile $\text{C}\equiv\text{N}$ bonds display in ZONE 3 around 2250 cm^{-1}**
 - **Alkyne $\text{C}\equiv\text{C}$ bonds display in ZONE 3 around 2150 cm^{-1}**
 - i. **Terminal alkynes also have a sharp signal in ZONE 1 around 3300 cm^{-1}**
6. Nitro groups, NO_2 :
 - N=O stretches observed as two signals in ZONE 5 around 1560 & 1350 cm^{-1}
7. Alkanes:
 - **Main signals for sp^3 hybridized C-H bonds are in ZONE 2 just below 3000 cm^{-1}**



Vibrational frequencies



* Look for Wavelength (cm^{-1})

* Look for Intensity

strong 80-95% T

med 40-70% T

weak < 30% T



Strong



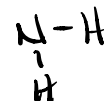
Very Strong



$\text{C}\equiv\text{C}$

$\text{C}\equiv\text{N}$

weak



med



← Reactivity →

PUDDLES AND WORMS...
OBSERVATION

IT MUST HAVE RAINED.
INFERENCE

AN IR BAND OF THIS SIZE AND SHAPE...
OBSERVATION

PROBABLY THAT FUNCTIONAL GROUP.
INFERENCE

ALL IR BANDS ARE EQUAL, BUT SOME ARE MORE EQUAL THAN OTHERS.

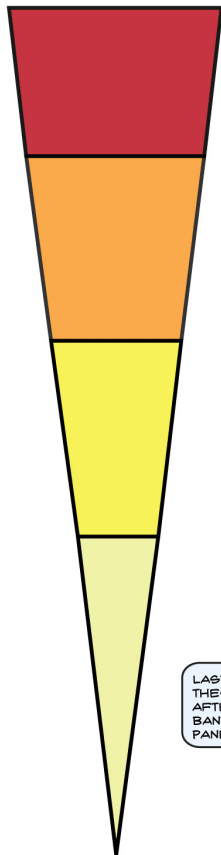
Alkyne (stretch)	ca. 3300	ca. 1.45
Aldehyde	2900-2800	3.43
	2800-2700	3.51
Alkane	not interpretatively useful	
Alkene	1600-1400	5.93
Aromatic	1600 and 1475	6.23
Alkyne	2250-2100	4.44
Aldehyde	1740-1720	5.73
Ketone	1725-1705	5.80
Carboxylic Acid	1725-1700	5.80
Ester	1750-1730	5.71
Amide	1650-1640	6.06
Anhydride	1810 and 1760	5.52
Acid Chloride	1800	5.56
Alcohols, Ethers, Esters, Carboxylic Acids, Anhydrides	1300-1000	7.69
Alcohols	not interpretatively useful	

MOVING DOWN THE CHART ONE AT A TIME, MATCHING BANDS AS YOU GO, IS NOT A USEFUL STRATEGY.

INSTEAD, LET'S ARRANGE THEM BY THEIR INTERPRETIVE POWER.

Alkyne (stretch)	ca. 3300	ca. 1.45
Aldehyde	2900-2800	3.43
	2800-2700	3.51
Alkane	not interpretatively useful	
Alkene	1600-1400	5.93
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Ester	1750-1730	5.71
Amide	1650-1640	6.06
Anhydride	1810 and 1760	5.52
Acid Chloride	1800	5.56
Alcohols, Ethers, Esters, Carboxylic Acids, Anhydrides	1300-1000	7.69
Alcohols, Phenols	not interpretatively useful	

GREAT INTERPRETIVE POWER



THIS IS THE FIRST REGION YOU SHOULD LOOK AT, AND THERE ARE 4 DIFFERENT SHAPES OF BANDS THAT YOU MAY SEE HERE.

...AND IF YOU DON'T SEE ANY BAND HERE, YOU MOST LIKELY DON'T HAVE ANY OF THESE FUNCTIONAL GROUPS (FG)

A SMOOTH TONGUE MEANS AN ALCOHOL... -O-H

VAMPIRE FANGS MEANS A PRIMARY AMINE... -N-H

ONE KNOCK-OUT FANG MEANS A 2° AMINE... OR A TERMINAL ALKYNE... -C#C-H

HAIRY BEARD IS A SIGN FOR A CARBOXYLIC ACID... -COO-H

IN THE C=O REGION, IT'S NOT THE SHAPE, BUT THE EXACT LOCATION THAT REVEALS THE IDENTITY OF THE FG.

NOTE THAT THE EXACT POSITION DEPENDS ON THE SURROUNDING ENVIRONMENT:

STRAIN, OR CONJUGATED AT -O- (+30CM⁻¹)

CONJUGATED AT C=O (-30CM⁻¹)

ACID CHLORIDES	1800
ANHYDRIDES	1760
ESTERS	1735
ALDEHYDES	1725
KETONES	1710
ACIDS	1690
AMIDES	1650

AT ~2200CM⁻¹, WE FIND TRIPLE BONDS: C≡C, AND C≡N

USUALLY SHARP (CAN BE SMALLISH)

HINT: USE 3300CM⁻¹ TO DISTINGUISH TERMINAL AND INTERNAL ALKYNES.

Interpreting IR spectra

JON - JKWCHUI@UVC.CA

LASTLY, YOU SHOULD LOOK AT THESE FEATURES (BUT ONLY AFTER ANALYSING THE MAJOR BANDS IN THE PREVIOUS PAGES)

UNSATURATED C-H STRETCH

SATURATED C-H STRETCH

SATURATED AND UNSATURATED C-H CAN BE PRESENT AT THE SAME TIME.

MONO, ORTHO, META, PARA

ALKENE/AROMATIC SUBSTITUTION PATTERN CAN BE SEEN IN THE C-H BEND REGIONS.

STRONGS 990, 910

~900 (STRONGS)

~700 (WEAK)

~910 (STRONGS)

MONO, GEM (1,1-), DI-SUBSTITUTED, CIS-, TRANS-

LASTLY, A PEAK AT 2700CM⁻¹, TOGETHER WITH A C=O, IS INDICATIVE OF AN ALDEHYDE.

C-H STRETCH

C=O STRETCH

R-C-H

KETONES HAVE NO C-H IN THEM AND CAN HAVE NO 2700 C-H STRETCH PEAKS.

NOTES

** IF YOU'RE NOT SURE WHAT THE DIFFERENCE BETWEEN AN ACID AND AN ALCOHOL IS, DO THE QUICK "FUNCTIONAL GROUP IDENTIFICATION" EXERCISE.

** ...IF YOU HAVE ONE FG. TWO 2° AMINE WOULD LOOK LIKE A 1 AMINE.

WE LOOKED AT THESE LAST BECAUSE THEY CAN BE AMBIGUOUS TO INTERPRET, OR THEY HAVE ONLY A NARROW NICHE OF USEFULNESS.

2-propanol 

9:39 AM Tue Apr 13 60%

AA sdb.s.db.aist.go.jp

Amazon.com... Jesse Bernst... Online Return... Monterey Cou... Hand Pounde... Pair Vintage A... images of bar... AIST:Spectral...

Spectral Database for Organic Compounds SDBS Japanese Introduction Disclaimer HELP Contact What's New RIO-DB FAQ LINK AIST

SDBS Information

SDBS No.: 2149

Compound Name:
2-propanol

Molecular Formula: C₃H₈O

Molecular Weight: 60.1

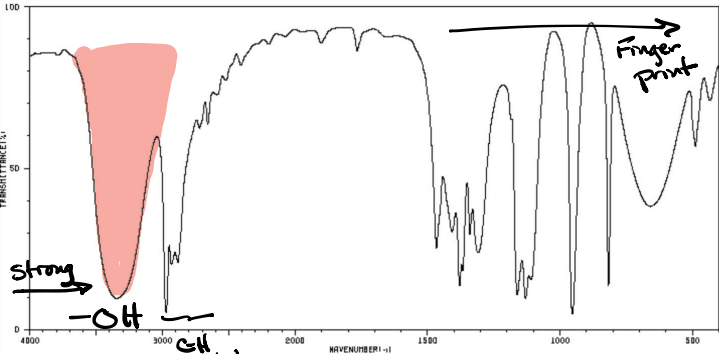
CAS Registry No.:
67-63-0

Spectral Code:
[Mass](#)
[¹³C NMR : in CDCl₃](#)
[¹³C NMR : in CD₂CN](#)
[¹³C NMR : in CDCl₃](#)
[¹³C NMR : in CD₂OD](#)
[¹³C NMR : in DMSO-d₆](#)
[¹H NMR : 90 MHz in CDCl₃](#)
[¹H NMR : in CDCl₃](#)
[¹H NMR : in DMSO-d₆](#)
[¹H NMR : in CD₂CN](#)

HIT-NO=1755 SCORE= () SDBS-NO=2149 IR-NIDA-03326 : LIQUID FILM

2-PROPANOL

C₃H₈O



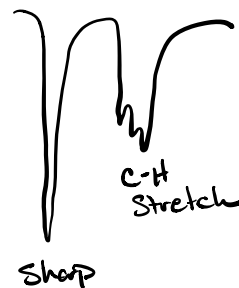
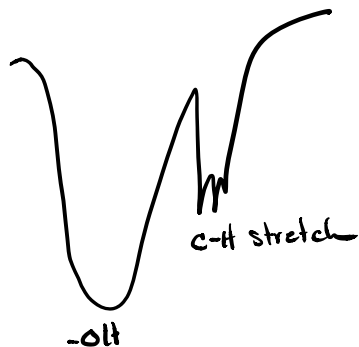
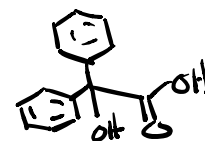
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3334	9	2521	74	1409	29	1110	15		
2972	5	2408	79	1379	15	954	4		
2933	19	2387	81	1368	17	818	19		
2907	23	2198	84	1341	28	660	37		
2864	20	1903	85	1309	23	654	37		
2722	60	1786	84	1162	10	490	66		

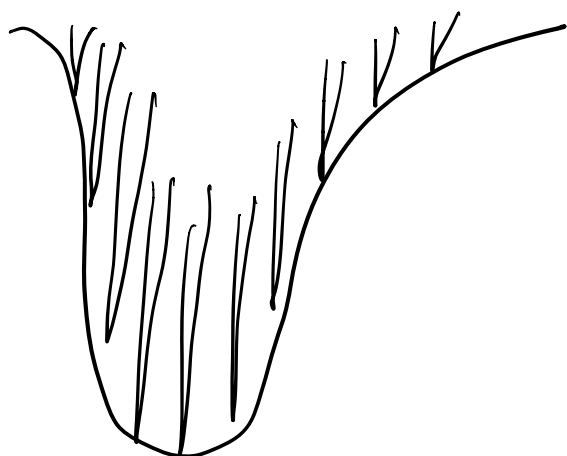
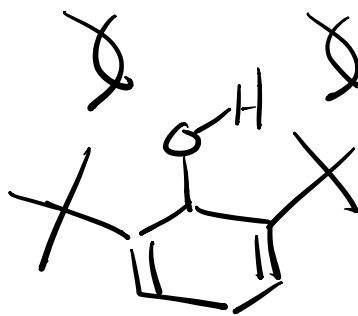
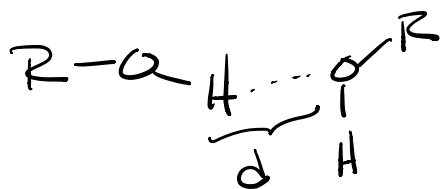
CH₃—CH—CH₃
 |
 OH

Types of hydroxyl groups

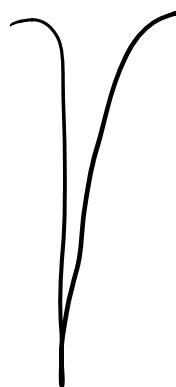
R-OH
Hydrogen Bonding

R-OH
non-H-bonding





many frequencies



Sharp
one frequency

Types of spectra

	OH
CCl ₄ film	
neat	
nujol (oil)	
KBr	

SDBS Information

SDBS No.: 51907

Compound Name:
(R)-2-chlorobutyric acid

Molecular Formula: C₄H₇ClO₂

Molecular Weight: 122.5

CAS Registry No.:
54053-45-1

Spectral Code:

- [Mass:](#)
- [¹³C NMR: in CDCl₃](#)
- [¹H NMR: in CDCl₃](#)
- [IR: Liquid film](#)

[Chemical Information:](#)

- [Return to Search:](#)
- [Return to Result:](#)

URL for this Compound:

<https://sdb.s.db.aist.go.jp/sdb.s/cgi-bin/landingpage?sdb.sno=51907>

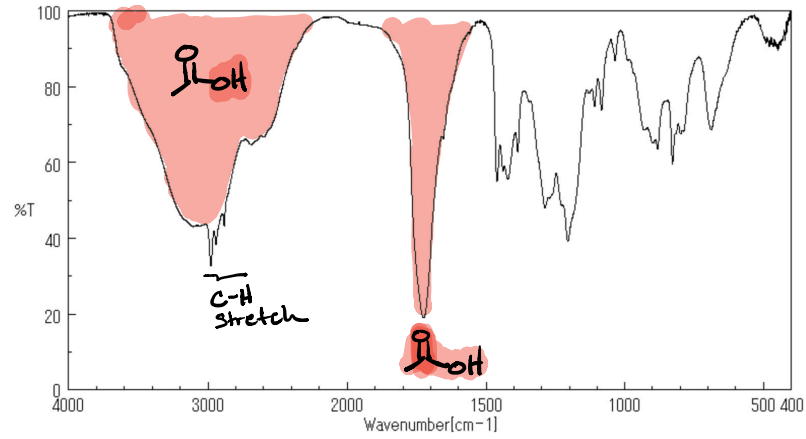
External Information:

Spectral Code: IR2007-86327TK

CAS Registry No: 54053-45-1

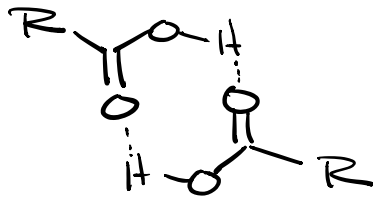
IR: Liquid film

DOI:

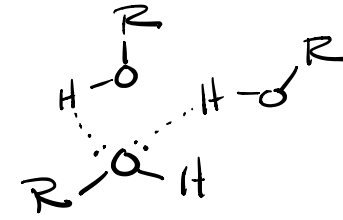


Wave number (cm⁻¹) and Transmittance (T%)

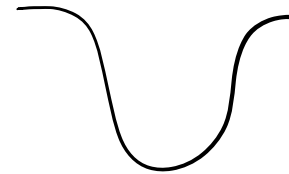
2978	33	1420	56	1084	74
2941	38	1386	63	1035	87
2882	42	1288	48	981	64



Dimer
Specific Absorptions



many bond lengths



SDBS Information

SDBS No.: 592

Compound Name:
cyclohexylamine

Molecular Formula: C₆H₁₃N

Molecular Weight: 99.2

CAS Registry No.:
108-91-8

Spectral Code:

Mass:

¹³C NMR : in CDCl₃

¹H NMR : 90 MHz in CDCl₃

¹H NMR : 400 MHz in CDCl₃

IR : CCl₄ solution

IR : liquid film

Raman : 4880 A, 100M, liquid

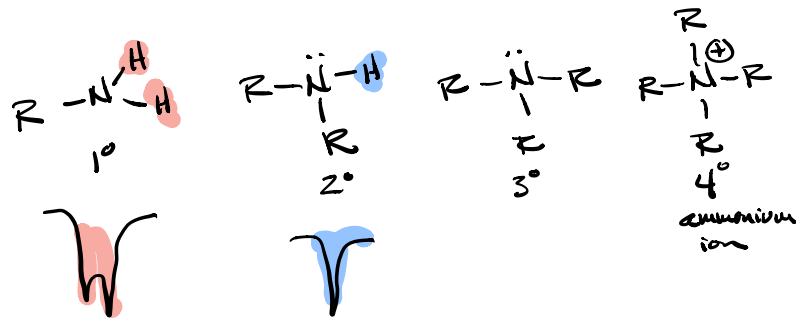
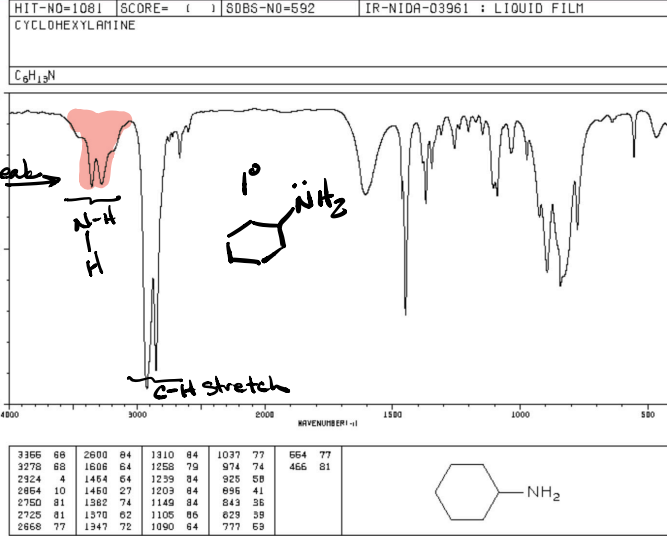
Chemical Information:

[Return to Search:](#)

[Return to Result:](#)

URL for this Compound:

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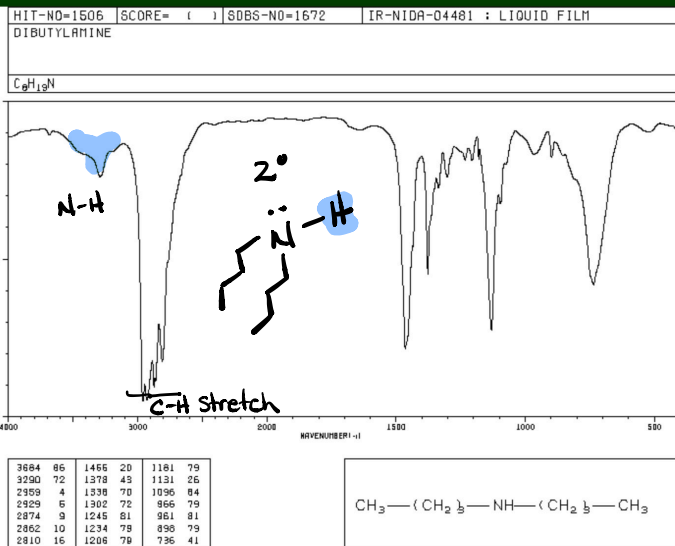


SDBS Information

SDBS No.: 1672
Compound Name: dibutylamine
Molecular Formula: C₈H₁₉N
Molecular Weight: 129.2
CAS Registry No.: 111-92-2
Spectral Code:
[Mass](#);
[¹³C NMR : in CDCl₃](#)
[¹H NMR : 90 MHz in CDCl₃](#)
[IR : liquid film](#)
[IR : CCl₄ solution](#)

[Chemical Information](#)
[Return to Search](#)
[Return to Result](#)

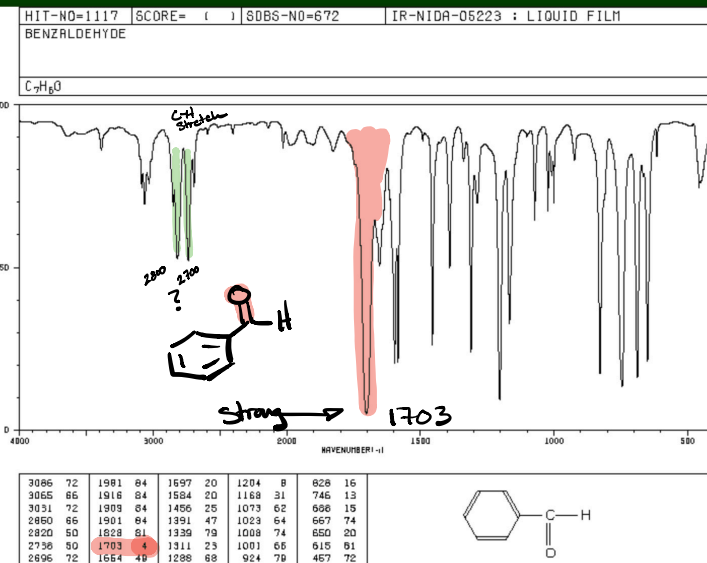
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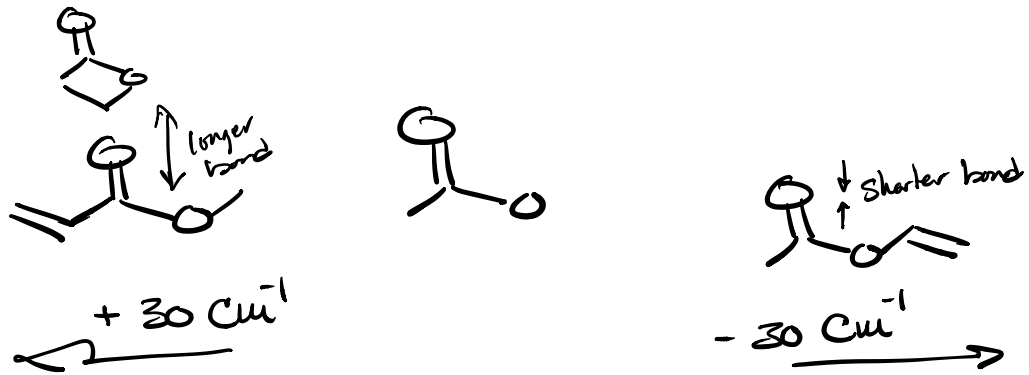


SDBS No.: 672
Compound Name: benzaldehyde
Molecular Formula: C₇H₆O
Molecular Weight: 106.1
CAS Registry No.: 100-52-7
Spectral Code:
[Mass](#);
[¹³C NMR : in CDCl₃](#)
[¹H NMR : 400 MHz in CDCl₃](#)
[¹H NMR : 90 MHz in CDCl₃](#)
[IR : liquid film](#)
[IR : CCl₄ solution](#)
[Raman : 4880 A.150M.liquid](#)
[ESR : ANION RADICAL](#)
[ELECTROLYTIC REDUCTION IN DME](#)

[Chemical Information](#)
[Return to Search](#)
[Return to Result](#)

URL for this Compound:
<https://sdb.s.db.aist.go.jp/sdb/s/cgi-bin/landingpage?sdbno=672>





$$\text{wave number} = \frac{1}{\lambda} = \frac{1}{\text{wavelength}}$$