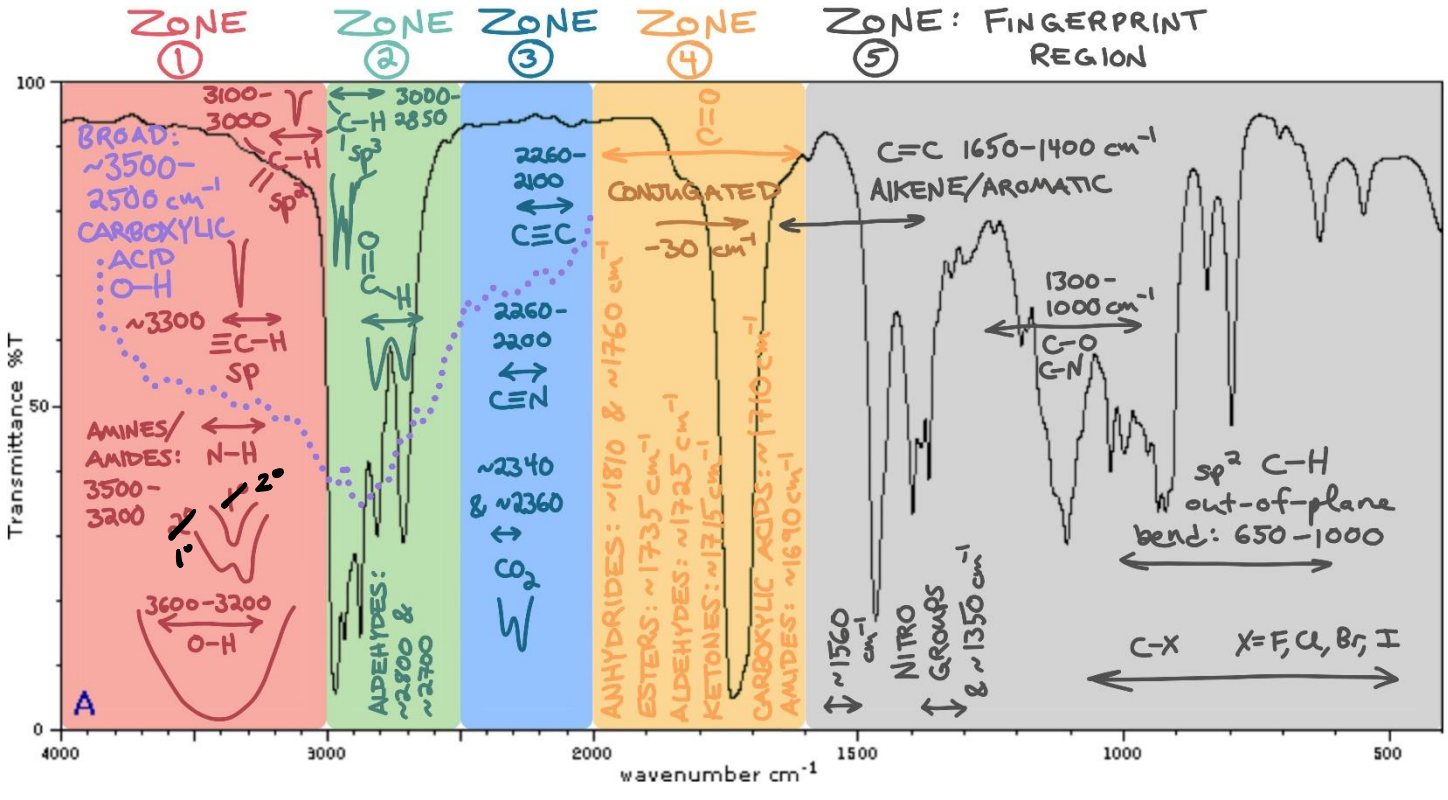
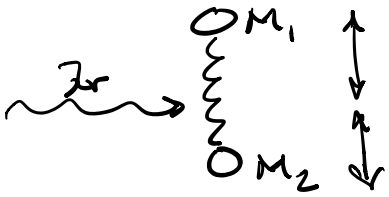
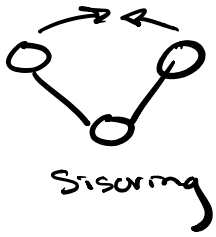
IDENTIFYING the MAJOR FUNCTIONAL GROUP:

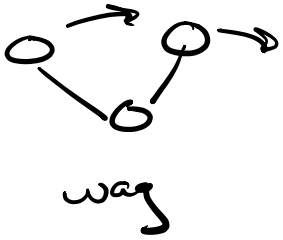
1. Is a carbonyl present? **Check ZONE 4.** If no carbonyl is present, go to step 3.
   - **The C=O double bond gives rise to a strong absorption in ZONE 4: 2000-1600 cm^{-1}. This peak is often the strongest in the spectrum, and characteristic of the type of carbonyl present (see spectrum below).**
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 cm^{-1} with medium intensity**
   - **Aldehydes should also have two signals in ZONE 2: ~2800 & ~2700 cm^{-1}**
   - **Carboxylic acids should have a broad signal that extends from ZONE 1 through ZONE 2: 3500-2500 cm^{-1}**
   - **Amides (primary & secondary) should have a signal in ZONE 1: 3500-3200 cm^{-1}**
3. If C=O is absent, check for:
   - **Alcohols/Phenols have a broad signal in ZONE 1: 3600-3200 cm^{-1}**
   - **Signals for amines also show up in ZONE 1: 3500-3200 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 cm^{-1}**
4. Double bonds and/or aromatic rings:
   - **Phenyl and vinyl sp2 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 cm^{-1} imply an aromatic ring**
5. sp Hybridized Triple bonds:
   - **Nitrile C≡N bonds display in ZONE 3 around 2250 cm^{-1}**
   - **Alkyne C≡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 sp3 hybridized C-H bonds are in ZONE 2 just below 3000 cm^{-1}**

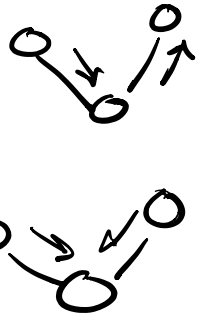


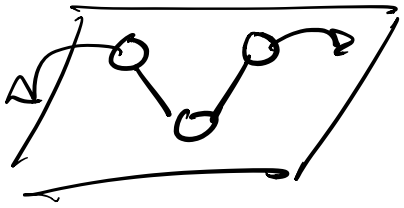
Vibrational frequencies











* Look for Wavelength (cm^{-1})
* Look for Intensity
  - Strong 80-95%T
  - Med 40-70%T
  - Weak < 30%T

–OH

Strong

Very Strong

C≡C

C≡N

weak

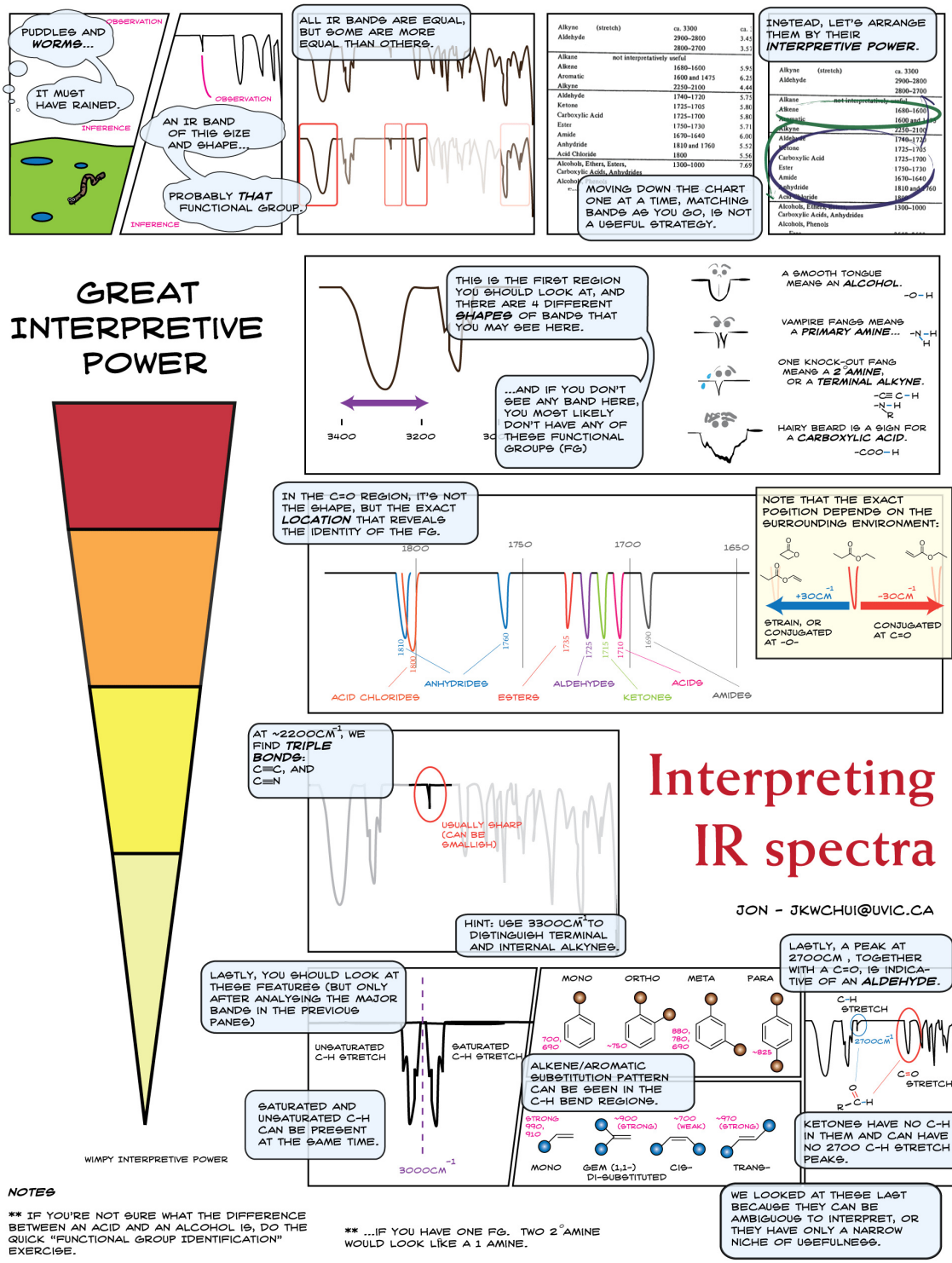
N-H

N-H

H

med

Reactivity

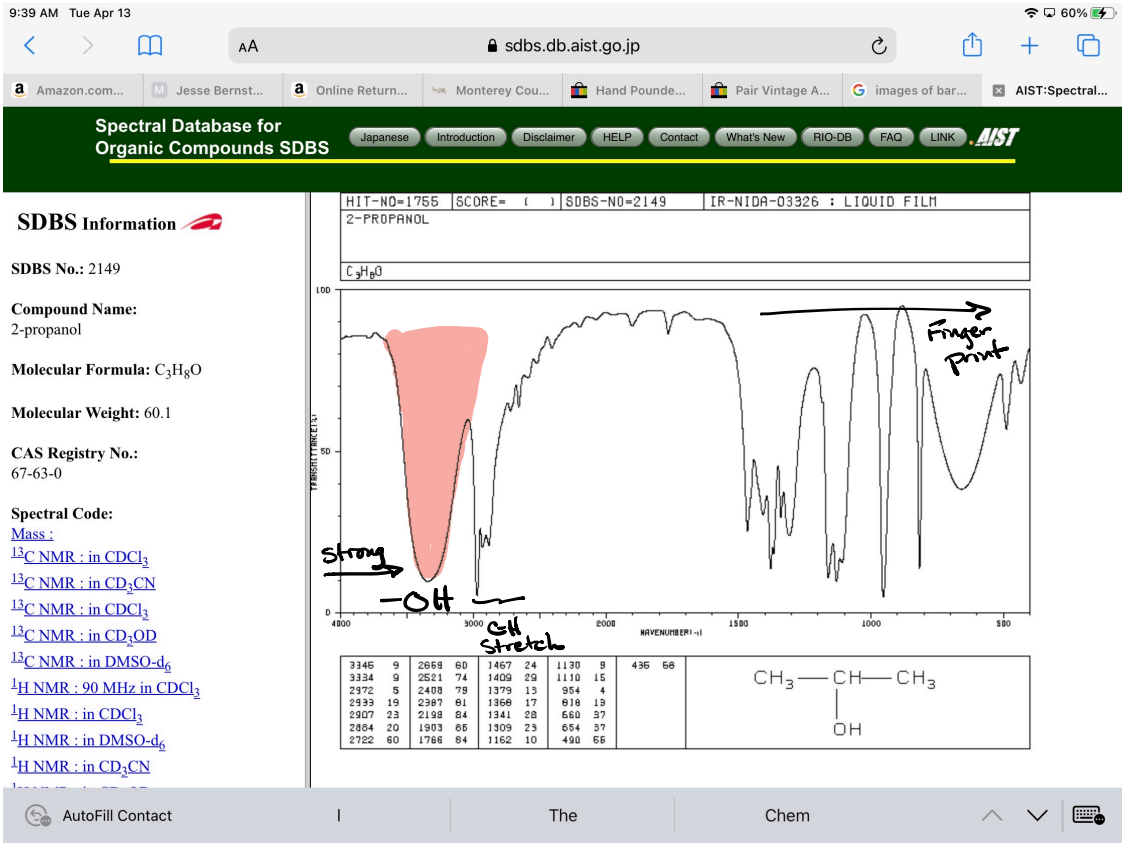


NOTES

** 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.

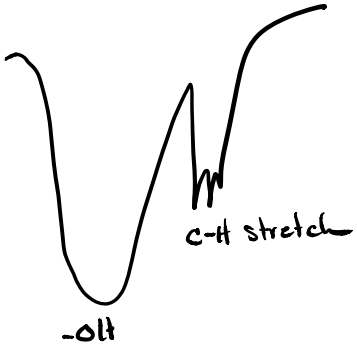
2-propanol

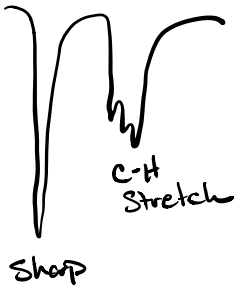


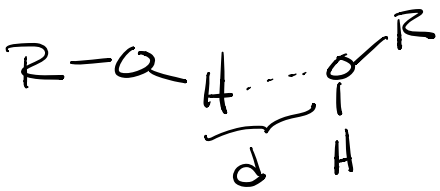
Types of hydroxyl groups

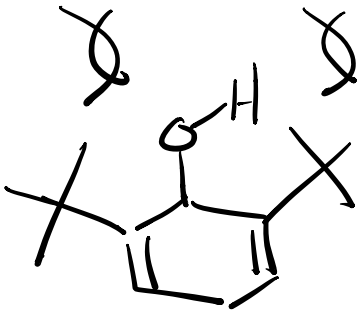
R-OH
Hydrogen Bonding

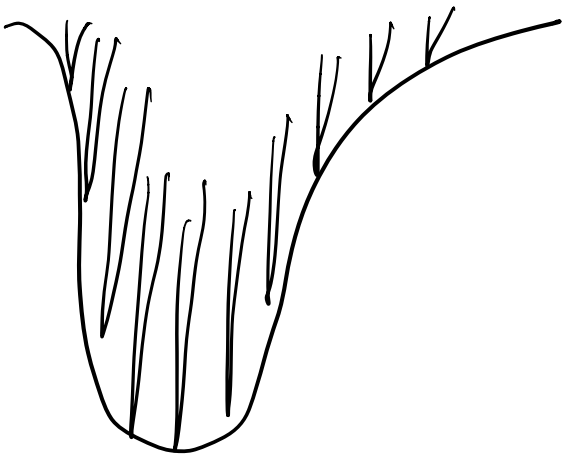
R–OH
non-H-bonding



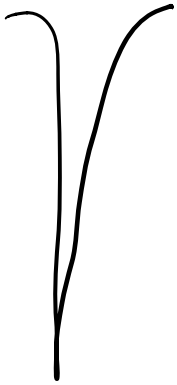








Many frequencies



Sharp
one frequency

Types of Spectra

	OH
CCl_4 film	
neat	
nujol (oil)	
KBr	

9:48 AM Tue Apr 13 61%

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SDBS Information

SDBS No.: 51907

Compound Name:
(R)-2-chlorobutyric acid

Molecular Formula: $C_4H_7ClO_2$

Molecular Weight: 122.5

CAS Registry No.:
54053-45-1

Spectral Code:
Mass :
^{13}C NMR : in $CDCl_3$
^{1}H NMR : in $CDCl_3$
IR : Liquid film

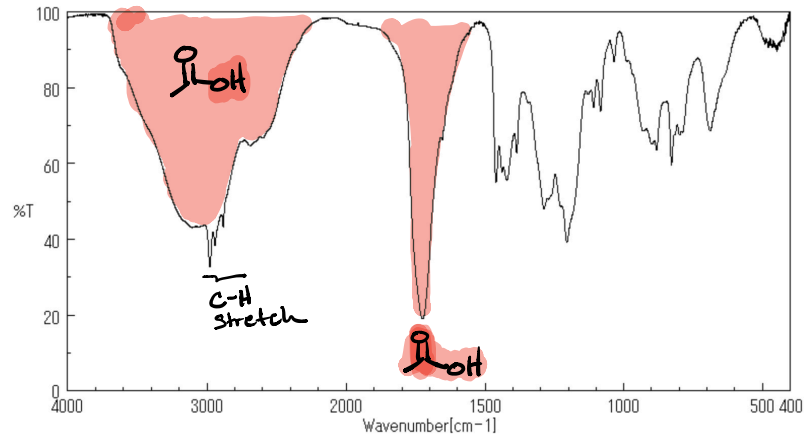
Chemical Information:

Return to Search:
Return to Result:

URL for this Compound:
https://sdbs.db.aist.go.jp/sdbs/cgi-bin/landingpage?sdbsno=51907

External Information:

Spectral Code: IR2007-86327TK
CAS Registry No: 54053-45-1
IR: Liquid film
DOI:



Wave number (cm^{-1}) and Transmittance (T%)

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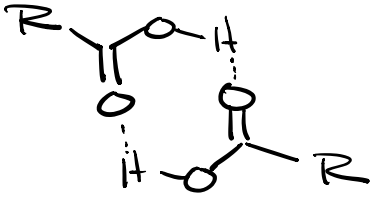
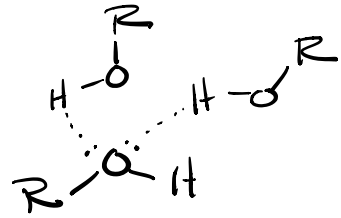
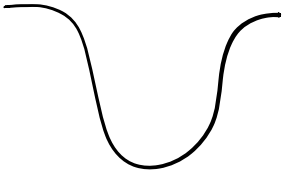
2941	38	1386	63	1035	87

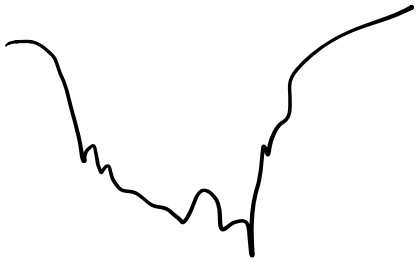




many bond lengths

Dimer
Specific Absorptions





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SDBS Information

SDBS No.: 592

Compound Name:
cyclohexylamine

Molecular Formula: $C_6H_{13}N$

Molecular Weight: 99.2

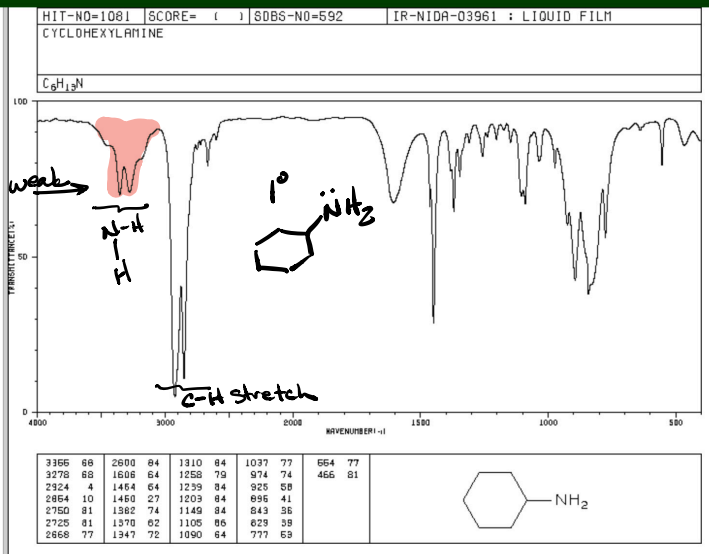
CAS Registry No.:
108-91-8

Spectral Code:
Mass :
^{13}C NMR : in $CDCl_3$
^{1}H NMR : 90 MHz in $CDCl_3$
^{1}H NMR : 400 MHz in $CDCl_3$
IR : CCl_4 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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3278	68	1608	64	1258	79	974	74	466	81
2924	4	1464	64	1239	84	925	58		
2854	10	1450	27	1203	84	895	41		
2750	81	1382	74	1149	84	843	36		
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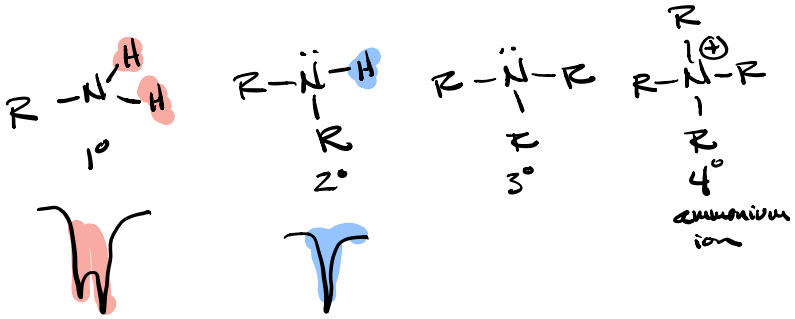

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SDBS Information

SDBS No.: 1672

Compound Name:
dibutylamine

Molecular Formula: $C_8H_{19}N$

Molecular Weight: 129.2

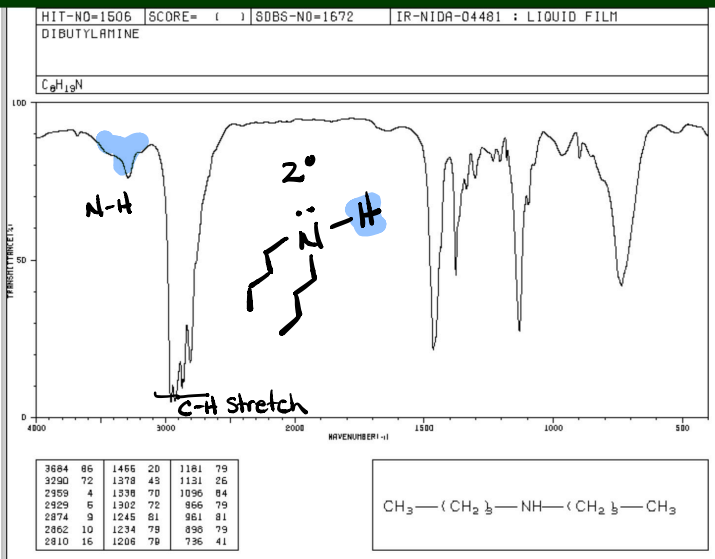
CAS Registry No.:
111-92-2

Spectral Code:
Mass :
^{13}C NMR : in $CDCl_3$
^{1}H NMR : 90 MHz in $CDCl_3$
IR : liquid film
IR : CCl_4 solution

Chemical Information:

Return to Search:
Return to Result:

URL for this Compound:
https://sdbs.db.aist.go.jp/sdbs/cgi-bin/landingpage?sdbsno=1672



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3290	72	1378	43	1131	26
2959	4	1338	70	1096	84
2929	5	1302	72	966	79
2874	9	1245	81	961	81
2862	10	1234	78	898	79
2810	16	1206	79	736	41

10:02 AM Tue Apr 13

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SDBS No.: 672

Compound Name:
benzaldehyde

Molecular Formula: C_7H_6O

Molecular Weight: 106.1

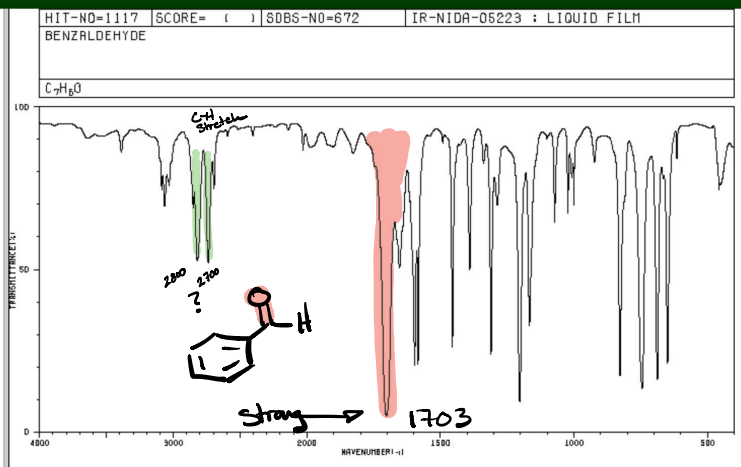
CAS Registry No.:
100-52-7

Spectral Code:
Mass :
^{13}C NMR : in $CDCl_3$
^{1}H NMR : 400 MHz in $CDCl_3$
^{1}H NMR : 90 MHz in $CDCl_3$
IR : liquid film
IR : CCl_4 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://sdbs.db.aist.go.jp/sdbs/cgi-



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3051	72	1909	84	1456	25	1073	62	686	15
2850	86	1901	84	1391	47	1023	64	667	74
2820	50	1828	81	1339	79	1008	74	650	20
2736	50	1703	4	1311	23	1001	65	615	61
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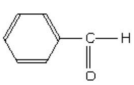

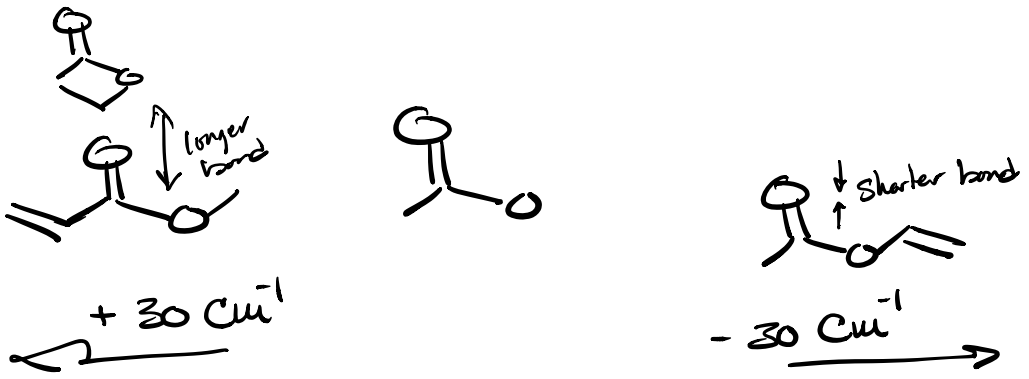

$$\text{wave number} = \frac{1}{\lambda} = \frac{1}{\text{wavelength}}$$