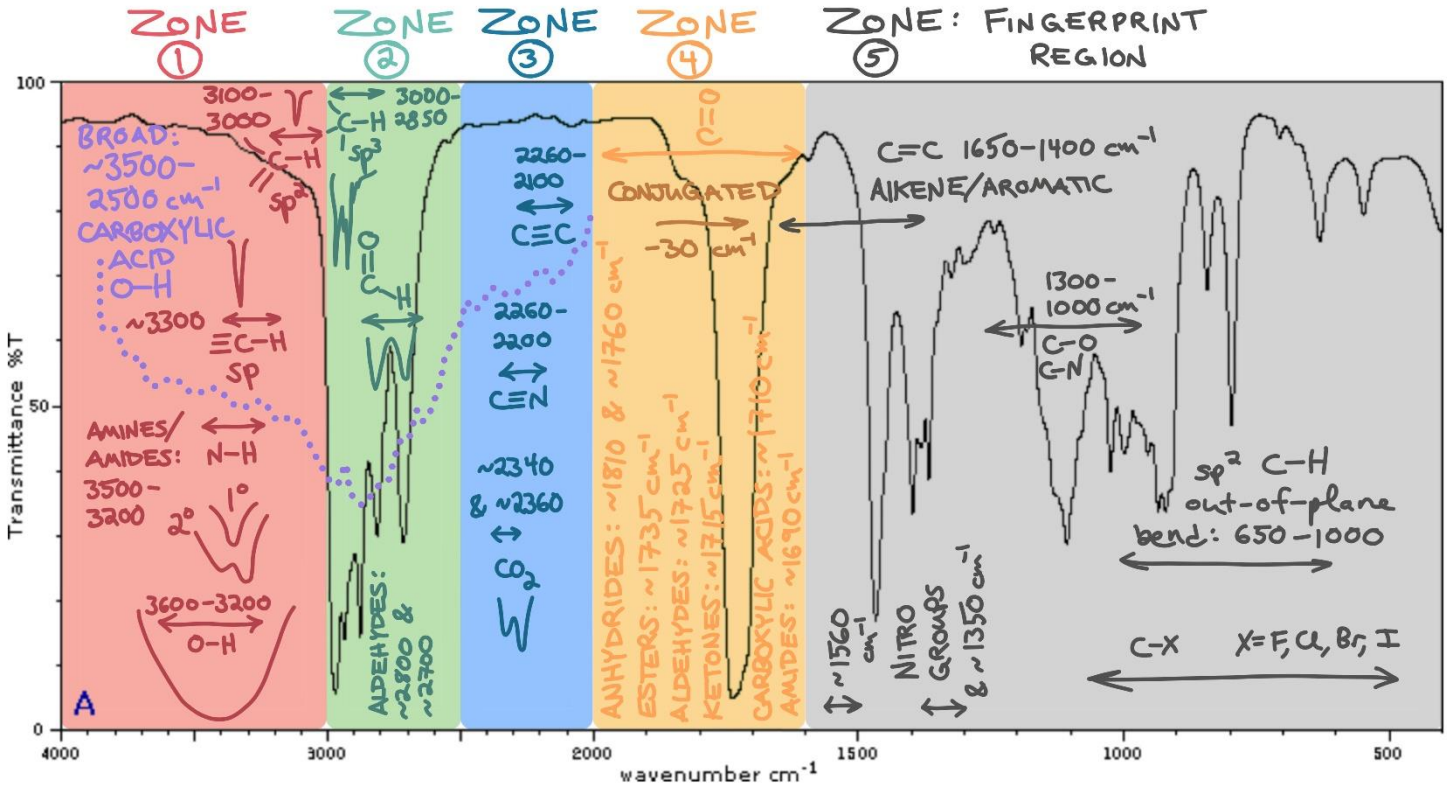
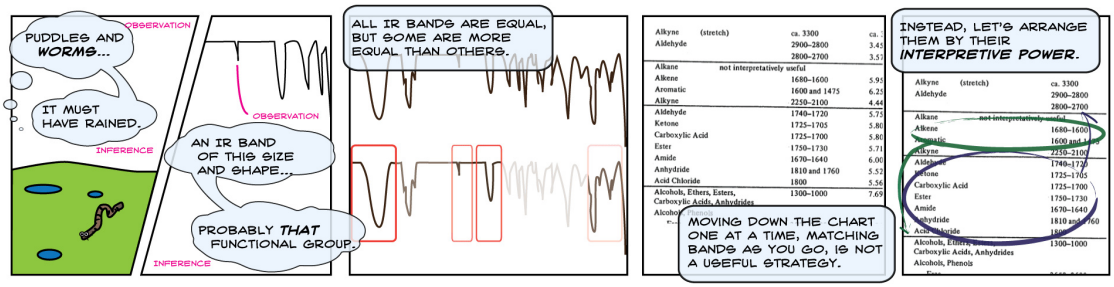
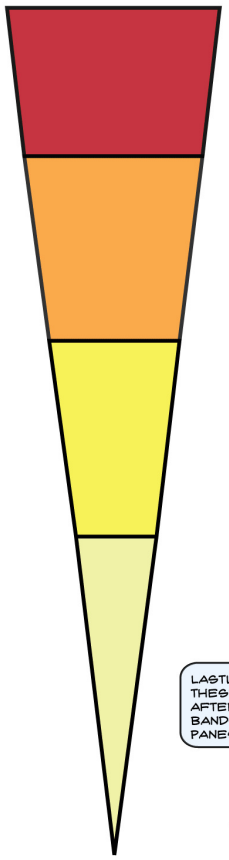
IDENTIFYING the MAJOR FUNCTIONAL GROUP:

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}**

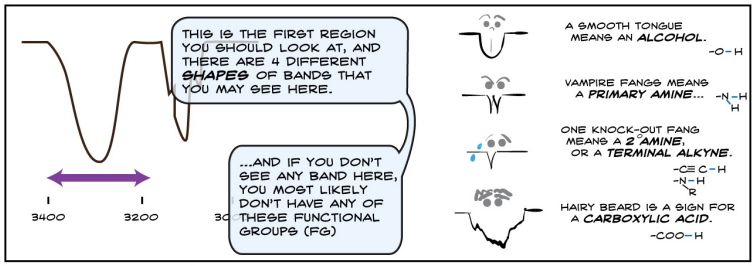


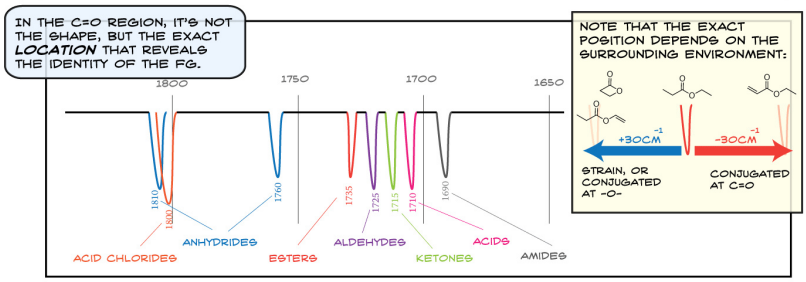


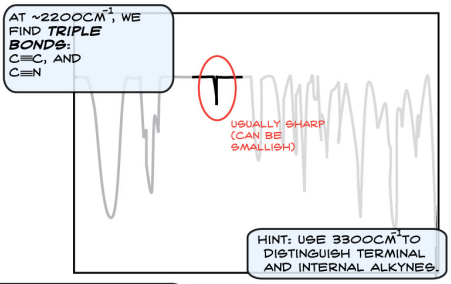
GREAT INTERPRETIVE POWER



WIMPY INTERPRETIVE POWER

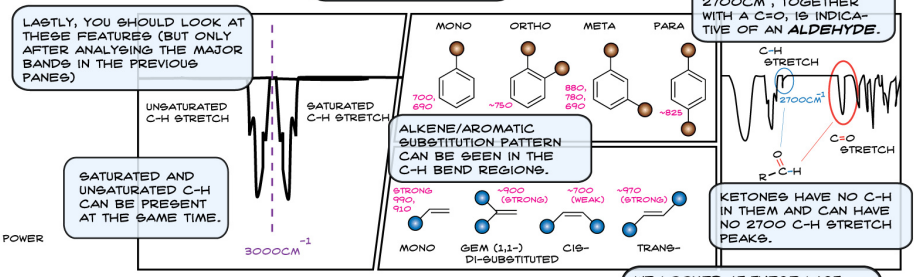






Interpreting IR spectra

JON - JKWCHUI@UVIC.CA

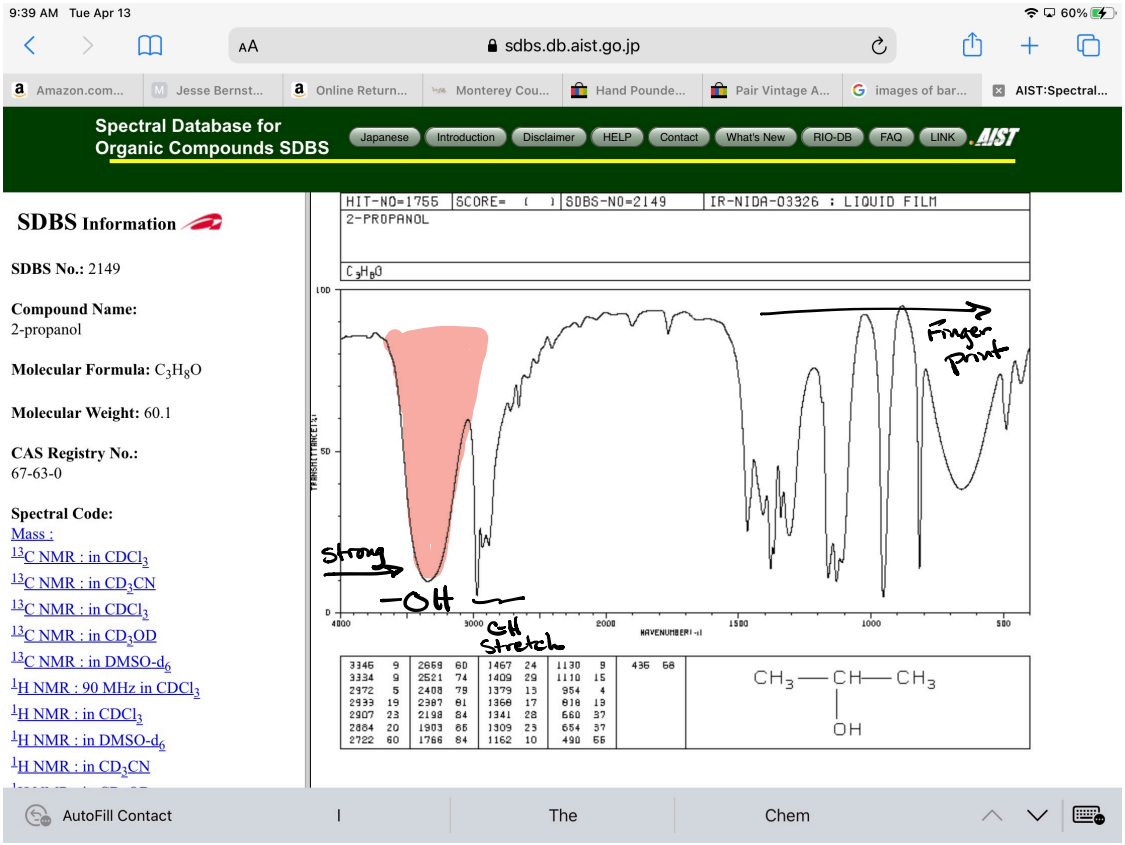


NOTES

** 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.

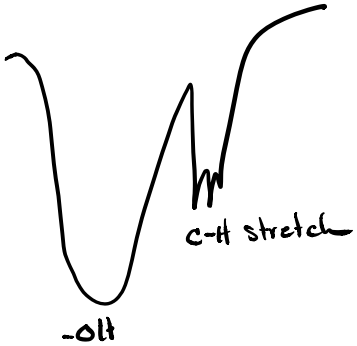
2-propanol

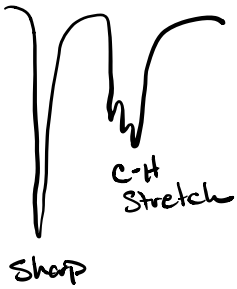


Types of hydroxyl groups

R-OH
Hydrogen Bonding

R–OH
non-H-bonding





9:48 AM Tue Apr 13 61%

AA sdbs.db.aist.go.jp

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Spectral Database for Organic Compounds SDBS

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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

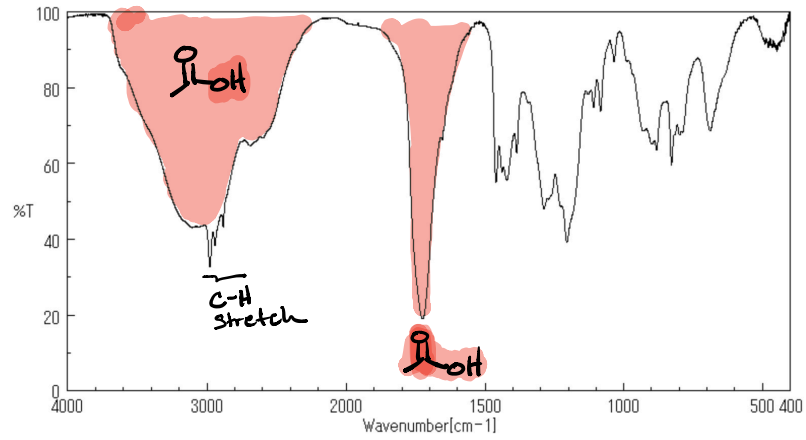
Chemical Information:

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:



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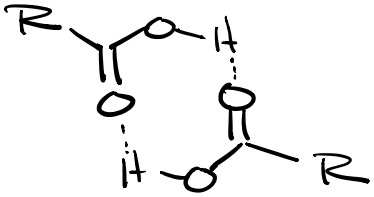
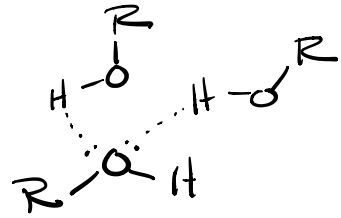
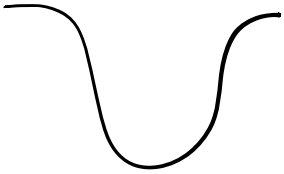
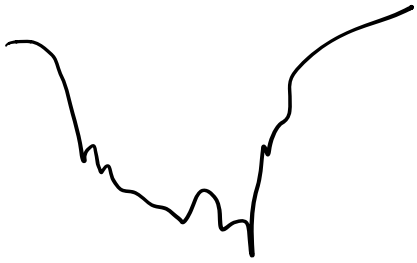




many bond lengths

Dimer
Specific Absorptions





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62%

AA

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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:

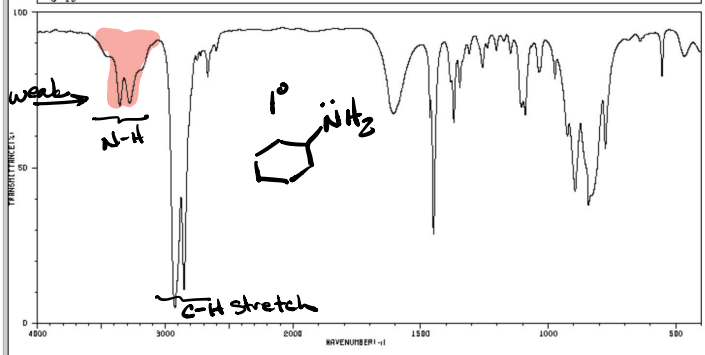
Return to Search:
Return to Result:

URL for this Compound:

HIT-NO=1081 | SCORE= ( ) | SDBS-NO=592 | IR-NIDA-03961 : LIQUID FILM

CYCLOHEXYLAMINE

$C_6H_{13}N$



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2854	10	1450	27	1203	84	895	41		
2750	81	1382	74	1149	84	843	36		
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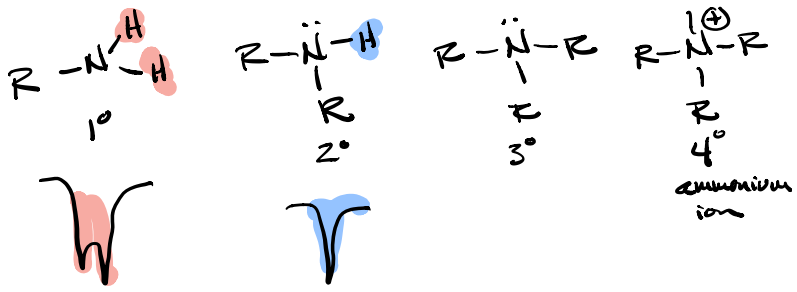

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SDBS Information

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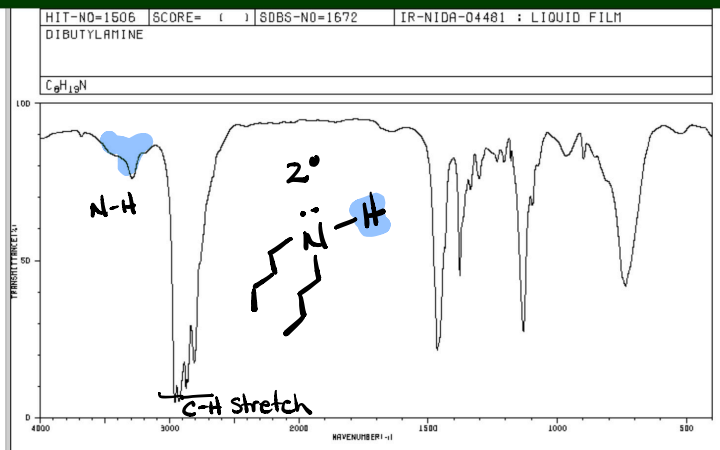
URL for this Compound:
https://sdbs.db.aist.go.jp/sdbs/cgi-bin/landingpage?sdbsno=1672



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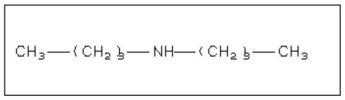

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SDBS No.: 672

Compound Name:
benzaldehyde

Molecular Formula: C_7H_6O

Molecular Weight: 106.1

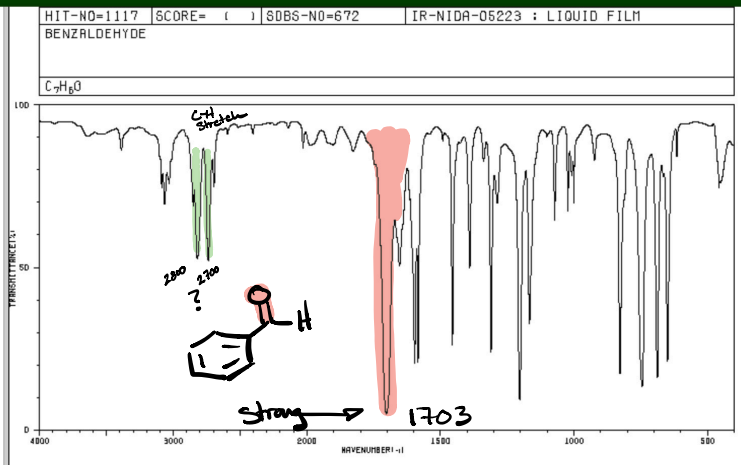
CAS Registry No.:
100-52-7

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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