e-ISSN:2582-7219

INTERNATIONAL JOURNAL OF MULTIDISCIPLINARY RESEARCH IN SCIENCE, ENGINEERING AND TECHNOLOGY

Volume 7, Issue 2, February 2024

INTERNATIONAL STANDARD SERIAL NUMBER INDIA

Impact Factor: 7.521

| ISSN: 2582-7219 | www.ijmrset.com | Impact Factor: 7.521| Monthly Peer Reviewed & Referred Journal |

| Volume 7, Issue 2, February 2024 |

| DOI:10.15680/IJMRSET.2024.0702001 |

IR AND RAMAN SPECTRUM OF PROPAN-1-OL (1-PROPANOL)

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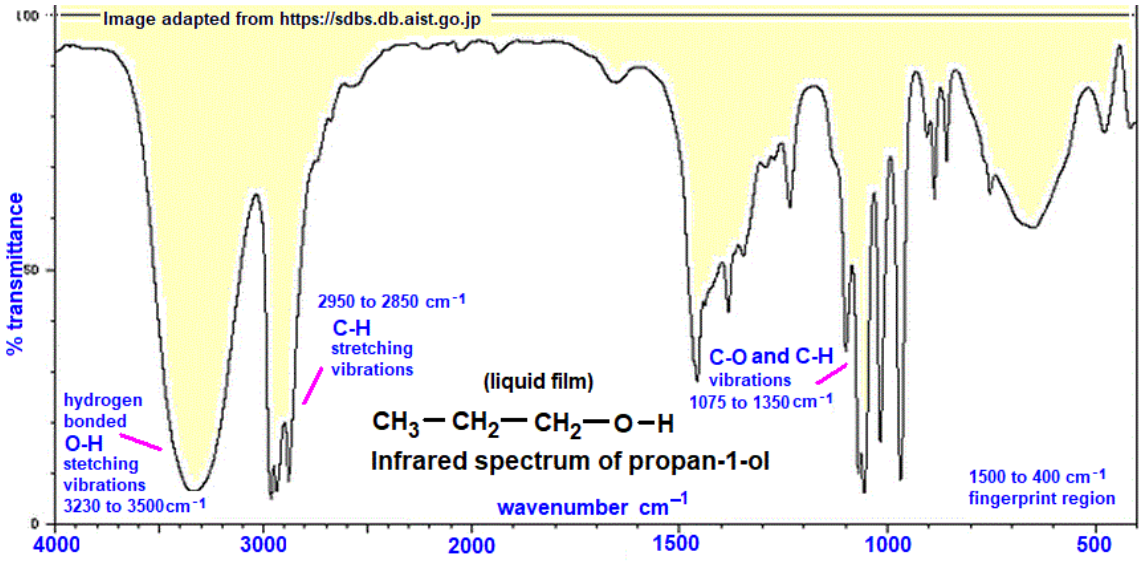
ABSTRACT: Spectra obtained from a liquid film of propan-1-ol. The right-hand part of the of the infrared spectrum of propan-1-ol, wavenumbers ~1500 to 400 cm^{-1} is considered the fingerprint region for the identification of propan-1-ol and most organic compounds. It is due to a unique set of complex overlapping vibrations of the atoms of the molecule of propan-1-ol.

KEYWORDS-IR, Raman, spectrum, propanol, propan-1-ol

I.INTRODUCTION

The most prominent infrared absorption lines of propan-1-ol

For propan-1-ol, the most characteristic absorption is the broad O-H stretching vibration band at wavenumbers ~3500 to 3200 cm^{-1}, the breadth is caused by hydrogen bonding interactions, common to all hydrogen bonded molecules with a hydroxyl group e.g. alcohols and carboxylic acids.[1,2]



C-H stretching vibration absorption occurs ~2900 cm^{-1}, wavenumbers common to any molecule with alkyl groups such as the propyl group in propan-1-ol.

There are wavenumber C-O and C-H vibration absorption bands ~1350 to 1070 cm^{-1} for propan-1-ol.

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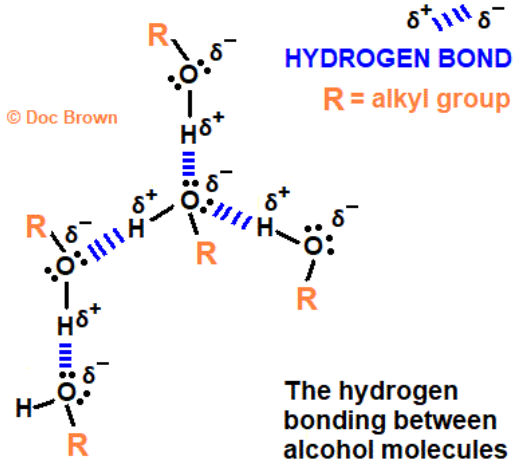
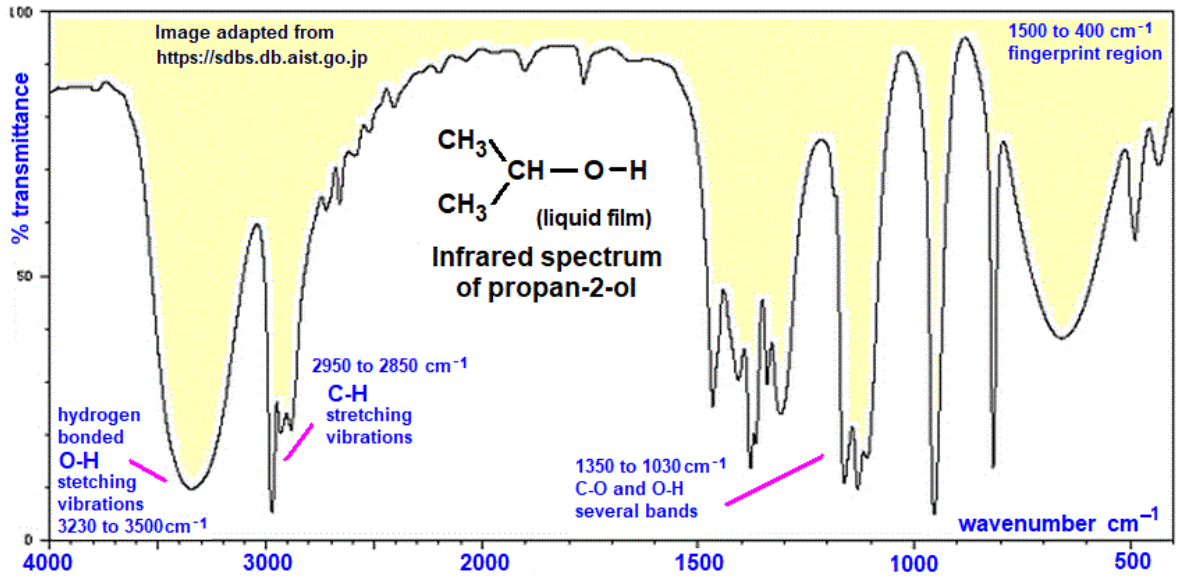
The absence of other specific functional group bands will show that particular functional group is absent from the propan-1-ol molecular structure.[3,4]

1-Propanol (also propan-1-ol, propanol, n-propyl alcohol) is a primary alcohol with the formula $CH_3CH_2CH_2OH$ and sometimes represented as PrOH or n-PrOH. It is a colourless liquid and an isomer of 2-propanol. It is formed naturally in small amounts during many fermentation processes and used as a solvent in the pharmaceutical industry, mainly for resins and cellulose esters, and, sometimes, as a disinfecting agent.



II.DISCUSSION

There are, as expected, differences in the fingerprint region at wavenumbers 1500 to 400 cm^{-1}, but most absorptions for all three molecules are the various C-O and the many C-H vibrational modes. However, there is one characteristic distinguishing absorption only present in the infrared spectra of alcohols, but not in ethers, that is the broad O-H stretching vibration peaking at ~3350 cm^{-1}. There is also another broad absorption band peaking at ~650 cm^{-1} in the alcohol spectra, but not in the ether spectra.[5]



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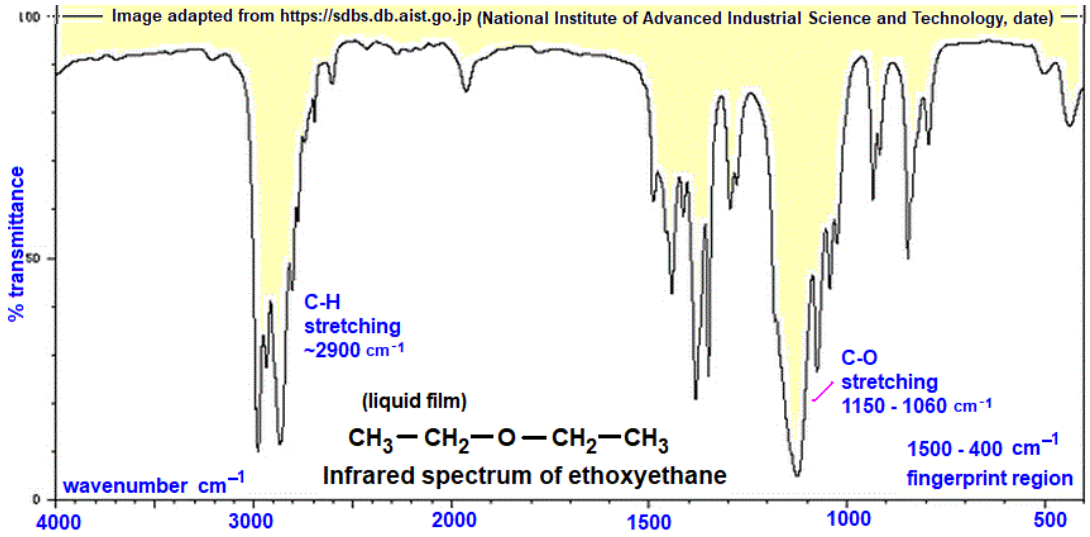
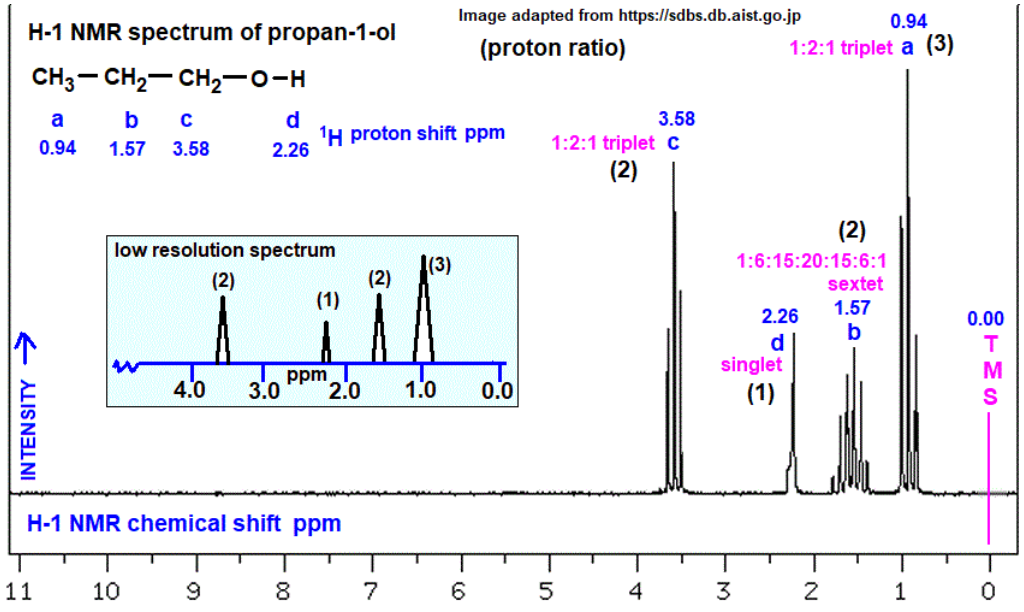


III.RESULTS

The 1H NMR spectra of all three molecules give different integrated proton ratios for the different ^{1}H chemical environments i.e. the proton ratios are as follows: propan-1-ol 3:2:2:1; propan-2-ol 6:1:1 and methoxyethane 3:2:3. Therefore, all three can be distinguished by their ^{1}H NMR spectra.



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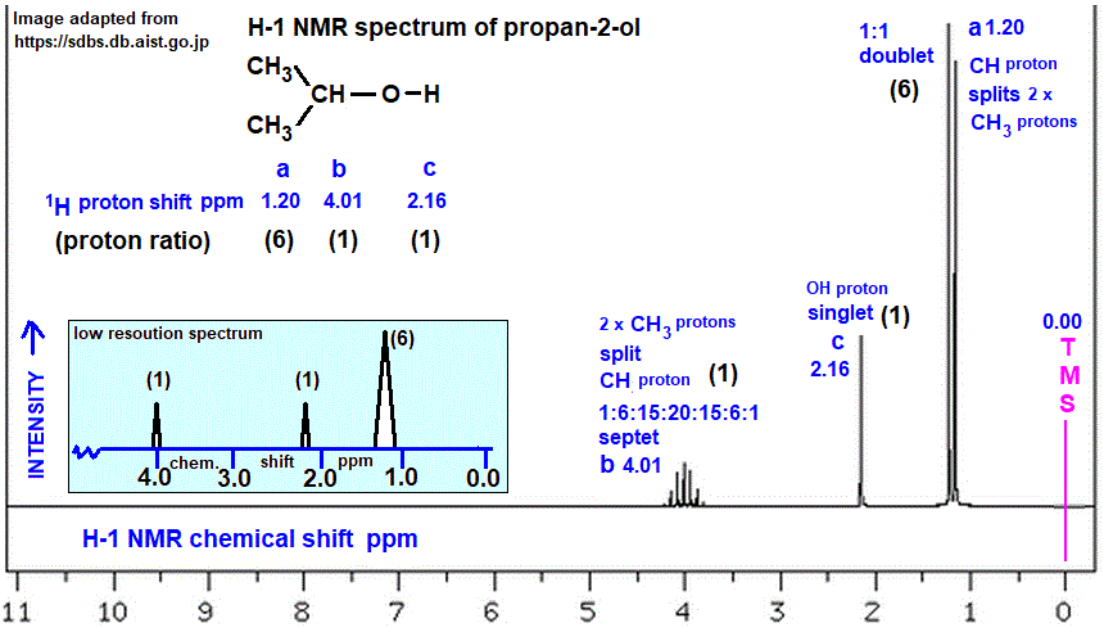

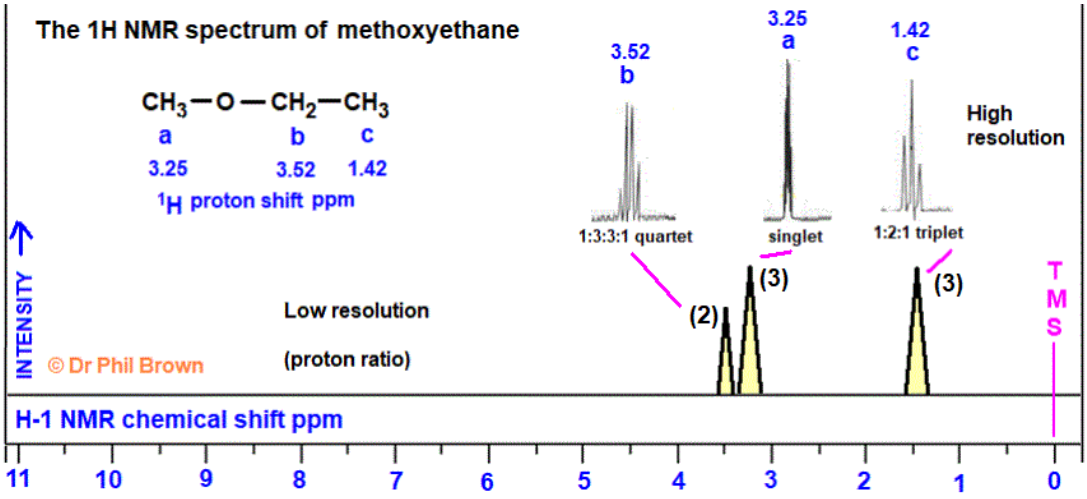

1-Propanol shows the normal reactions of a primary alcohol. Thus it can be converted to alkyl halides; for example red phosphorus and iodine produce n-propyl iodide in 80% yield, while PCl_3 with catalytic $ZnCl_2$ gives n-propyl chloride. Reaction with acetic acid in the presence of an H_2SO_4 catalyst under Fischer esterification conditions gives propyl acetate, while refluxing propanol overnight with formic acid alone can produce propyl formate in 65% yield. Oxidation of 1-propanol with $Na_2Cr_2O_7$ and H_2SO_4 gives a 36% yield of propionaldehyde, and therefore for this type of reaction higher yielding methods using PCC or the Swern oxidation are recommended. Oxidation with chromic acid yields propionic acid.[6]

IV.CONCLUSION

The spectrum of the complex refractive index in the 12,000–100cm−1 region was determined for liquid Propan-1-ol from transmission studies. In the MIR region, very thin layers with thicknesses of a few micrometers had to be used to obtain reliable data. Liquid Propan-1-ol is totally associated via hydrogen bonds. To obtain information on the

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aggregation low-temperature IR spectra in argon matrixes were recorded. An attempt to elucidate the structure of formed adducts was made. FT-Raman spectra of the liquid are also reported. Identifications for numerous bands observed in the liquid phase were proposed basing on literature data and results of DFT calculations.

1-Propanol is manufactured by catalytic hydrogenation of propionaldehyde. Propionaldehyde is produced via the oxo process by hydroformylation of ethylene using carbon monoxide and hydrogen in the presence of a catalyst such as cobalt octacarbonyl or a rhodium complex.

$H_2C{=}CH_2 + CO + H_2 \rightarrow CH_3CH_2CH{=}O$

$CH_3CH_2CH{=}O + H_2 \rightarrow CH_3CH_2CH_2OH$

A traditional laboratory preparation of 1-propanol involves treating n-propyl iodide with moist Ag_2O.

Safety

1-Propanol is thought to be similar to ethanol in its effects on the human body, but 2–4 times more potent according to a study conducted on rabbits. Many toxicology studies find oral acute LD_{50} ranging from 1.9 g/kg to 6.5 g/kg (compared to 7.06 g/kg for ethanol). It is metabolized into propionic acid. Effects include alcoholic intoxication and high anion gap metabolic acidosis. As of 2011, one case of lethal poisoning was reported following oral ingestion of 500mL of 1-propanol. Due to lack of long term data, the carcinogenicity of 1-propanol in human beings is unknown.

1-Propanol as fuel

1-Propanol has high octane number and is suitable for engine fuel usage. However, propanol is too expensive to use as a motor fuel. The research octane number (RON) of propanol is 118, and anti-knock index (AKI) is 108.[7]

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