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STRUCTURAL AND SAFETY CHARACTERIZATION OF 3-METHYLPENTAN-1-OL

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1. ABSTRACT

This study presents an integrated analysis of 3-methylpentan-1-ol (C_{6}H_{14}O), focusing on its structural identification through high-resolution ^1H NMR spectroscopy and its industrial safety profile. We examine the electronic environment of its fourteen protons and the symmetry-breaking effects of the C3 chiral center. Furthermore, a toxicological assessment confirms its safety as a fragrance ingredient under current exposure levels.

KEYWORDS: ^1H NMR, 3-methylpentan-1-ol, Chirality, Fragrance Safety.

1. INTRODUCTION

3-Methylpentan-1-ol is a branched primary alcohol known for its unique organoleptic properties, including chocolate and wine-like notes. It occurs naturally in various foods, such as apples, cheese, and brandy. Its molecular structure consists of a pentane backbone with a methyl branch at the third carbon (CH_{3}CH_{2}CH(CH_{3})CH_{2}CH_{2}OH).

2. ^1H NMR Spectroscopic Analysis

The ^1H NMR spectrum is a critical diagnostic tool for elucidating the electronic environment and connectivity of the molecule's fourteen protons.

2.1. Chemical Shift Assignments

* Alpha-Methylene (C_{1}-H_{2}): Due to the inductive effect of the hydroxyl group, these protons resonate downfield at \delta 3.66–3.74 ppm as a triplet.
* Hydroxyl Proton (-OH): Appears as a broad singlet between \delta 1.5–5.0 ppm, highly sensitive to solvent and concentration.
* Aliphatic Region (\delta 1.04–1.81 ppm): This cluster contains the C_{2} and C_{4} methylene protons and the C_{3} methine proton.
* Methyl Groups (\delta 0.89–0.92 ppm): This region includes a doublet for the C_{3}- methyl branch and a triplet for the terminal C_{5}-methyl.

2.2. Impact of Chirality

The C_{3} carbon is a stereocenter, meaning the molecule exists as two enantiomers. This chirality makes the C_{2} and C_{4} methylene protons diastereotopic. These protons are magnetically non-equivalent and exhibit complex multiplets rather than simple triplets at high resolution.

3. Safety and Toxicological Evaluation

According to the Research Institute for Fragrance Materials (RIFM), 3-methyl-1-pentanol is safe for its intended use.

3.1. Human Health Assessment

* Genotoxicity: The compound is non-genotoxic based on BlueScreen assays and read- across data.
* Repeated Dose Toxicity: The NOAEL (No Observed Adverse Effect Level) is established at 1250 mg/kg/day.
* Skin Sensitization: Human clinical tests (HRIPT) at 0.5% concentration show no sensitization potential.
* Phototoxicity: No significant UV absorbance was found between 290–700 nm, indicating no phototoxic risk.

3.2. Environmental Safety

* Aquatic Risk: The risk quotient (PEC/PNEC) is < 1, indicating no significant risk to the aquatic environment.
* Bioaccumulation: The substance is not persistent or bioaccumulative according to IFRA standards.

4. CONCLUSION

The ^1H NMR spectrum of 3-methylpentan-1-ol provides a detailed fingerprint of its branched structure, specifically through the deshielding of alpha-protons and the complexity induced by chirality. Combined with its robust safety profile, these analytical markers support its continued use in the

global chemical and fragrance industries.

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