Structural Isomerism Oxidation and Synthesis Reactions of Alcohols

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Structural isomers are compounds that have the same molecular formula but differ in the way their atoms are connected. The formula $C_4H_{10}O$ can represent alcohols or ethers, and the original assignment focuses mainly on identifying alcohol isomers, predicting their oxidation products, examining dehydration reactions, preparing an ether by Williamson synthesis, and selecting Grignard reagents for alcohol formation. The original reasoning contains several useful ideas, including the distinction between primary, secondary, and tertiary alcohols and the one-step S_N2 mechanism of Williamson ether synthesis. It also contains naming and reaction errors that should be corrected while preserving the sequence of the assignment. (Clayden et al., 2012; McMurry, 2021; Solomons et al., 2016)

There are seven constitutional isomers with the formula $C_4H_{10}O$: four alcohols and three ethers. The four alcohols are butan-1-ol, butan-2-ol, 2-methylpropan-1-ol, and 2-methylpropan-2-ol. The three ethers are ethoxyethane, 1-methoxypropane, and 2-methoxypropane. The original essay discusses compounds C, D, and E as butan-1-ol, butan-2-ol, and 2-methylpropan-1-ol. Those assignments will be retained, while the missing tertiary alcohol and ether isomers are acknowledged for completeness.

Structural Isomerism in $C_4H_{10}O$

Butan-1-ol has a straight chain of four carbon atoms with the hydroxyl group attached to carbon 1. Its condensed formula is $CH_3CH_2CH_2CH_2OH$. Butan-2-ol has the same carbon chain but the hydroxyl group is attached to carbon 2: $CH_3CH(OH)CH_2CH_3$. These compounds are position isomers because the functional group occupies a different position on the same carbon skeleton.

2-Methylpropan-1-ol has a branched carbon skeleton: $(CH_3)_2CHCH_2OH$. It is a chain isomer of butan-1-ol and butan-2-ol because the carbon framework differs. The fourth alcohol, 2-methylpropan-2-ol, has the formula $(CH_3)_3COH$ and is a tertiary alcohol. The three ethers contain a C–O–C linkage rather than an O–H group. Their existence demonstrates functional-group isomerism, because alcohols and ethers share the formula $C_4H_{10}O$ but belong to different functional classes.

Classification of the Alcohols

An alcohol is classified according to the number of carbon groups attached to the carbon bearing the hydroxyl group. Butan-1-ol is primary because the hydroxyl-bearing carbon is attached to one other carbon. Butan-2-ol is secondary because that carbon is attached to two other carbons. 2-

Methylpropan-1-ol is also primary, even though the molecule is branched, because the carbon bonded to OH is connected to only one carbon. 2-Methylpropan-2-ol is tertiary because the hydroxyl-bearing carbon is attached to three carbon groups.

This classification determines oxidation behavior. Primary alcohols can be oxidized first to aldehydes and then to carboxylic acids. Secondary alcohols form ketones. Tertiary alcohols resist ordinary oxidation because the hydroxyl-bearing carbon does not carry a hydrogen atom that can be removed without breaking a carbon–carbon bond. (Clayden et al., 2012; McMurry, 2021; Solomons et al., 2016)

Oxidation With Collins Reagent

The original essay refers to CrO_3/pyridine, commonly associated with Collins reagent. Under controlled, anhydrous conditions, this reagent oxidizes primary alcohols to aldehydes and secondary alcohols to ketones while reducing the risk of further oxidation of an aldehyde to a carboxylic acid. Chromium(VI) reagents are hazardous and require appropriate laboratory controls, but the reaction remains useful for understanding selectivity.

Compound C, butan-1-ol, is oxidized to butanal, $CH_3CH_2CH_2CHO$. Compound D, butan-2-ol, is oxidized to butan-2-one, also called butanone, $CH_3COCH_2CH_3$. The original essay incorrectly names a product "but-2-nal." An aldehyde carbon must be at the end of a chain and is assigned carbon 1, so but-2-nal is not an appropriate name. A secondary alcohol such as butan-2-ol forms a ketone, not an aldehyde.

Compound E, 2-methylpropan-1-ol, is oxidized to 2-methylpropanal, $(CH_3)_2CHCHO$. If the fourth alcohol, 2-methylpropan-2-ol, were treated under ordinary Collins oxidation conditions, no normal carbonyl product would be expected. The three relevant initial oxidation products are therefore butanal, butanone, and 2-methylpropanal.

Further Oxidation of Primary Alcohol Products

Primary alcohols can undergo further oxidation when stronger aqueous oxidants or prolonged conditions are used. Butanal is oxidized to butanoic acid, $CH_3CH_2CH_2COOH$. 2-Methylpropanal is oxidized to 2-methylpropanoic acid, $(CH_3)_2CHCOOH$. The original essay names the second acid as 2-methylbutanoic acid, but that compound contains five carbon atoms and cannot be formed by ordinary oxidation of a four-carbon alcohol. Oxidation changes the functional group without increasing the carbon count.

Butanone, the product of butan-2-ol oxidation, does not undergo ordinary further oxidation to one four-carbon carboxylic acid because ketones lack the aldehydic hydrogen. Strong oxidative cleavage may break carbon–carbon bonds and produce smaller products, but that is different from the simple aldehyde-to-acid oxidation pathway. This distinction explains why primary and secondary alcohols give different final products.

Dehydration of Butan-1-ol

Alcohol dehydration removes the hydroxyl group and a hydrogen from an adjacent carbon to form an alkene and water. The reaction is commonly performed with acid and heat, though the mechanism and ease depend on alcohol class. Butan-1-ol can form but-1-ene because the carbon adjacent to the hydroxyl-bearing carbon is carbon 2. Under strongly acidic conditions, some but-2-ene may also appear through rearrangement or isomerization, but the direct structural prediction from a primary alcohol is but-1-ene.

The original essay assigns compound K as but-1-ene. That assignment is appropriate if the question expects the direct elimination product. But-1-ene has no E/Z geometric isomerism because one carbon of the double bond carries two hydrogen atoms.

Dehydration of Butan-2-ol

Butan-2-ol can lose a hydrogen from either adjacent carbon. Removal from carbon 1 produces but-1-ene, while removal from carbon 3 produces but-2-ene. But-2-ene exists as two geometric isomers because each double-bond carbon is attached to two different groups. These are cis-but-2-ene and trans-but-2-ene, more systematically named (Z)-but-2-ene and (E)-but-2-ene.

The product mixture can therefore contain but-1-ene, cis-but-2-ene, and trans-but-2-ene, corresponding to the original assignment of K, M, and N. According to Zaitsev’s rule, the more substituted alkene, but-2-ene, is usually favored under ordinary acid-catalyzed dehydration conditions. Trans-but-2-ene is generally more stable than cis-but-2-ene because the larger methyl groups are farther apart, reducing steric repulsion. The mixture is not expected to contain equal quantities of all three products.

Dehydration of 2-Methylpropan-1-ol

Compound E, 2-methylpropan-1-ol, has only one distinct adjacent carbon from which the necessary hydrogen can be removed. The alkene product is 2-methylpropene, $CH_2=C(CH_3)_2$. The original essay refers to “2-methyl butene,” which would contain five carbon atoms and is therefore inconsistent with the four-carbon starting alcohol.

2-Methylpropene does not show E/Z isomerism because the terminal double-bond carbon carries two hydrogen atoms. It is the single constitutional alkene expected from direct dehydration of 2-methylpropan-1-ol.

Hydration of 2-Methylpropene

Acid-catalyzed hydration of 2-methylpropene follows Markovnikov addition. Protonation occurs in the direction that forms the more stable tertiary carbocation, and water then attacks the carbocation. After deprotonation, the product is 2-methylpropan-2-ol, the tertiary alcohol designated as compound O in the original discussion.

This reaction is the reverse conceptual relationship of dehydration, although practical equilibrium conditions and rearrangements must be considered. The hydroxyl group ends up on the more substituted carbon. The reaction illustrates how alkene structure and carbocation stability control product orientation.

Ether Isomers of $C_4H_{10}O$

Three ethers have the molecular formula $C_4H_{10}O$. Ethoxyethane has two ethyl groups: $CH_3CH_2OCH_2CH_3$. 1-Methoxypropane contains a methyl group and an n-propyl group: $CH_3OCH_2CH_2CH_3$. 2-Methoxypropane contains a methyl group and an isopropyl group: $CH_3OCH(CH_3)_2$.

The original essay refers simply to methoxypropane. Because two positional forms are possible, the name should specify 1-methoxypropane or 2-methoxypropane. The listed reaction between n-propyl iodide and sodium methoxide would produce 1-methoxypropane. The synthesis strategy must be selected according to the exact target.

Williamson Synthesis of 1-Methoxypropane

Williamson ether synthesis involves reaction of an alkoxide ion with an alkyl halide through an S_N2 mechanism. To prepare 1-methoxypropane, one possible pair is sodium methoxide and 1-iodopropane:

$CH_3O^-Na^+ + CH_3CH_2CH_2I \rightarrow CH_3OCH_2CH_2CH_3 + NaI$

A second and usually more favorable pair is sodium propoxide and iodomethane or bromomethane:

$CH_3CH_2CH_2O^-Na^+ + CH_3I \rightarrow CH_3CH_2CH_2OCH_3 + NaI$

The original essay lists sodium ethoxide and chloromethane, but that pair would produce methoxyethane, C_3H_8O, not a four-carbon ether. The carbon atoms of both reactants must be counted before predicting the product.

Which Williamson Pair Gives the Higher Yield?

The S_N2 mechanism is fastest when the alkyl halide is least hindered and carries a good leaving group. Methyl halides are especially reactive because the nucleophile can approach the carbon easily. Therefore, sodium propoxide with iodomethane is generally expected to give a higher substitution yield than sodium methoxide with 1-iodopropane, assuming suitable conditions. Both methyl and primary halides can react effectively, but the methyl halide provides minimal steric hindrance.

The original essay states that chloride in 1-propyl chloride is easily lost. This is incorrect because iodide and bromide are generally better leaving groups than chloride in S_N2 reactions. A primary iodide would usually react faster than the corresponding primary chloride. The higher-yield design should place the less hindered group, preferably methyl, on the halide and use the larger group as the alkoxide.

Mechanism of Williamson Ether Synthesis

The reaction occurs in one concerted step. The alkoxide oxygen attacks the electrophilic carbon from the side opposite the leaving group. As the carbon–oxygen bond forms, the carbon–halogen bond breaks. There is no stable carbocation intermediate. The backside attack produces inversion of configuration when the reacting carbon is chiral.

Because elimination can compete with substitution, tertiary alkyl halides are unsuitable for Williamson synthesis. A strong alkoxide reacting with a tertiary halide is more likely to remove a proton and form an alkene. Methyl and primary halides are preferred, while some secondary halides may give mixtures.

Grignard Reagents and Alcohol Synthesis

A Grignard reagent has the general formula RMgX, where R is an organic group and X is a halogen. The carbon bonded to magnesium behaves as a strong nucleophile and attacks the carbonyl carbon of aldehydes or ketones. After acidic workup, formaldehyde produces a primary alcohol, other aldehydes produce secondary alcohols, and ketones produce tertiary alcohols.

The original essay proposes methylmagnesium bromide and propanal for preparation of compound E. That pair would form butan-2-ol after workup, not 2-methylpropan-1-ol. Methylmagnesium bromide adds a methyl group to propanal’s carbonyl carbon, creating a four-carbon secondary alcohol.

Grignard Preparation of 2-Methylpropan-1-ol

To prepare 2-methylpropan-1-ol, a suitable Grignard reagent is isopropylmagnesium bromide reacting with formaldehyde, followed by acidic workup:

$(CH_3)_2CHMgBr + HCHO \rightarrow (CH_3)_2CHCH_2OMgBr \rightarrow H_3O^+ \rightarrow (CH_3)_2CHCH_2OH$

Formaldehyde contributes the carbon that becomes CH_2OH, while the isopropyl group provides the other three carbons. The final product is the required primary alcohol. The reaction must be performed under dry conditions because water, alcohols, and other proton sources destroy Grignard reagents before they can attack the carbonyl compound.

Grignard Preparation of Butan-2-ol

The original pair of methylmagnesium bromide and propanal is still chemically useful, but its correct product is butan-2-ol:

$CH_3MgBr + CH_3CH_2CHO \rightarrow CH_3CH_2CH(OMgBr)CH_3 \rightarrow H_3O^+ \rightarrow CH_3CH_2CH(OH)CH_3$

This example demonstrates the rule that addition of a Grignard reagent to an aldehyde other than formaldehyde produces a secondary alcohol. Carbon counting provides a quick check: one carbon from the methyl reagent plus three carbons from propanal gives the four-carbon product.

Safety and Green Chemistry Considerations

Several reagents in these reactions require careful handling. Chromium(VI) compounds are toxic, carcinogenic, and environmentally hazardous. Modern laboratories often prefer less hazardous oxidation methods when possible. Grignard reagents are moisture sensitive and commonly prepared in flammable ether solvents. Strong acids used for dehydration can cause severe burns, and alkenes and ethers may be volatile and flammable.

Green chemistry encourages selection of safer oxidants, reduced solvent use, efficient atom economy, and proper waste treatment. Understanding traditional reagents remains educationally important, but reaction design should include hazard assessment rather than focusing only on yield.

Conclusion

The molecular formula $C_4H_{10}O$ represents four alcohols and three ethers. Butan-1-ol and 2-methylpropan-1-ol are primary alcohols, butan-2-ol is secondary, and 2-methylpropan-2-ol is tertiary. Collins-type oxidation converts the primary alcohols to butanal and 2-methylpropanal and converts

butan-2-ol to butanone. Further oxidation of the aldehydes produces butanoic acid and 2-methylpropanoic acid.

Dehydration of butan-1-ol produces but-1-ene as the direct product, while butan-2-ol can form but-1-ene and the cis and trans forms of but-2-ene. 2-Methylpropan-1-ol produces 2-methylpropene, which can be hydrated to 2-methylpropan-2-ol. Williamson ether synthesis is most efficient when the alkyl halide is methyl or primary, and 1-methoxypropane can be prepared effectively from sodium propoxide and iodomethane. Finally, 2-methylpropan-1-ol can be synthesized through reaction of isopropylmagnesium bromide with formaldehyde followed by acidic workup. Correct naming, carbon counting, alcohol classification, and mechanism analysis provide reliable checks for every stage of the assignment.

References

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Solomons, T. W. G., Fryhle, C. B., & Snyder, S. A. (2016). *Organic chemistry* (12th ed.). Wiley.