SYNTHESIS OF ACETYLENE AMINO ALCOHOLS AND THEIR QUATERNARY AMMONIUM SALTS

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ANNOTATION: This article focuses on the structure and properties of acetylene amino alcohols, their synthesis methods, physicochemical parameters, and the synthesis of their quaternary ammonium salts. Additionally, the chemical and biological properties of quaternary ammonium salts, as well as their applications in cosmetics, pharmaceuticals, and industry, are discussed.

KEYWORDS: acetylene, alcohol, catalyst, ammonium salts, organic synthesis, halogen.

Introduction

Acetylene amino alcohols and their quaternary ammonium salts play a vital role in organic chemistry due to their unique physicochemical and biological properties. These compounds find applications in pharmaceuticals, materials science, and the chemical industry. This article explores their chemical structures, synthetic methods, and practical significance.

Structure and Properties of Acetylene Amino Alcohols

Acetylene amino alcohols are compounds formed by the combination of acetylene (C_2H_2) and amine ($–NH_2$) groups, generally classified as alkylamines or alkanolamines. Acetylene is a highly reactive two-carbon aliphatic compound, while the amine group modifies its chemical properties and extends its application across different systems.

Structurally, they typically include a triple-bonded carbon-carbon (C≡C) linkage attached to an amine group. These compounds can be classified as primary or secondary amines, with modifications to form quaternary ammonium salts being particularly significant.

Synthesis of Acetylene Amino Alcohols

Nitrogen-containing acetylene compounds and their halogen derivatives have broad applications, including use as physiologically active substances and corrosion inhibitors. The study synthesized previously unknown chlorine and bromine derivatives of acetylene amino alcohols.

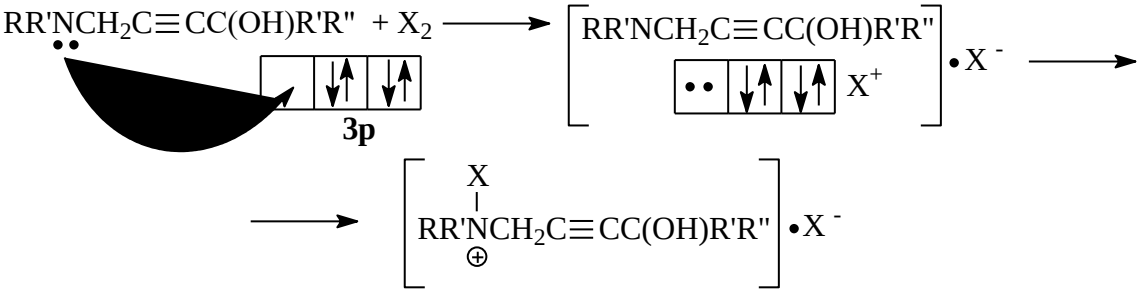
Acetylene alcohols were converted to amino alcohols via the Mannich reaction and purified using vacuum distillation. Chlorination and bromination of the synthesized compounds were performed in chloroform at 0°C, producing quaternary ammonium salts through controlled conditions.

$$\underset{1\text{-}6}{(R)_2NCH_2C{\equiv}CC(OH)R`R``} + X_2 \longrightarrow \underset{7\text{-}16}{[(R)_2N^+XCH_2C{\equiv}CC(OH)R`R`]\cdot X^-},$$

When the reactant acetylenic amino alcohol [9] and halogens are taken in equimolar amounts, their addition to the C≡C bond does not occur, but instead, as a result of the sp^3 hybridization of the nitrogen

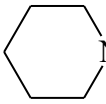
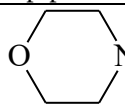
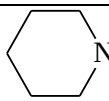
atom, a spatial overlap of two electron clouds occurs. In the halogen molecule, an additional σ-bond also appears between the unshared electron pair of one atom and the free 3d and 4d orbitals of the other atom. As a result, the unshared electron pair of the nitrogen atom interacts with the halogen.

The results of this study show that acetylenic amino alcohols can be efficiently converted to quaternary ammonium salts under controlled conditions, which opens up possibilities for the synthesis of compounds containing new functional groups in the fields of chemistry and medicine.



Physicochemical Properties

Table 1 Provides the physicochemical properties of synthesized acetylene amino alcohols, including boiling points, refractive indices, and densities.

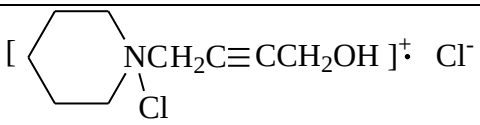
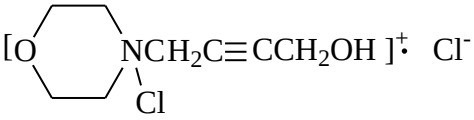
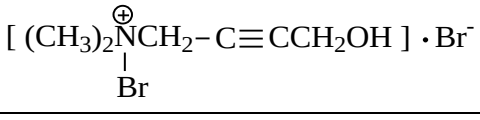
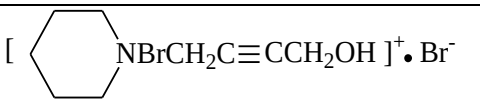
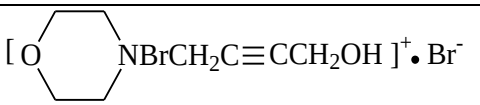
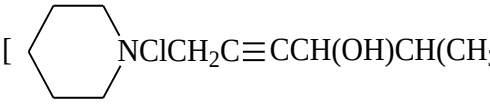
№	Structural formula and name	Boiling point, °C mm.s.ust.	n_D^{20}	d_4^{20}
1	$(H_3C)_2NCH_2C{\equiv}CCH_2OH$ 1-dimetilaminobut-2-in-4-ol	77-78/3	1,5140	0,856
2	$(CH_3CH_2)_2NCH_2{-}C{\equiv}CCH_2OH$ 1-dietilaminobut-2-in-4-ol	88-90/3	1,5218	-
3	$(H_3C)_2NCH_2C{\equiv}CC(OH)(CH_3$ 1-dimetilamino-4-metilpent-2-in-4-ol	110-111/3	1,5018	-
4	 $NCH_2C{\equiv}CCH_2OH$ 1-piperidinobutin-2-ol-4	101-102/3	1,5068	-
5	 $NCH_2C{\equiv}CCH_2OH$ 1-morfolinobutin-2-ol-4	110-111/3	1,5118	-
6	 $NCH_2C{\equiv}CC(OH)(CH_3)_2$ 1-piperidino-4-mtilpentin-2-ol-4	92-93/4	1,4614	0,9011

The constants of halogen ammonium salts of some synthesized acetylenic amino alcohols are given in Table 2.

Table - 2

Halogenated ammonium salts of acetylenic amino alcohols

№	Ammonium salt	Brutto formula	Melting temperature ^{0}C.
7	$[(H_3C)_2\overset{\oplus}{N}ClCH_2CCH_2OH]\cdot Cl^-$	$C_6H_{11}NOCl_2$	68-69
8	$[(H_3CCH_2)_2\overset{\oplus}{N}ClCH_2C{\equiv}CCH_2OH]\cdot Cl$	$C_8H_{15}NOCl_2$	70-71

9		$C_9H_{15}NOCl_2$	73-74
10		$C_8H_{13}NO_2Cl_2$	72-73
11		$C_6H_{11}NOBr_2$	78-79
12	$[(H_5C_2)_2NBrCH_2C{\equiv}CCH_2OH]^+ \cdot Br^-$	$C_8H_{15}NOBr_2$	88-89
13		$C_9H_{15}NO_2Br_2$	90-92
14		$C_8H_{13}NO_2Br_2$	102-104
15	$[(H_3C)_2NClCH_2C{\equiv}CC(OH)(CH_3)_2]^+ \cdot Cl^-$	$C_8H_{15}NOCl_2$	106-108
16		$C_{11}H_{21}NOCl$	110-112

Subsequent chlorination and bromination processes failed to yield halide derivatives due to the presence of steric hindrance through the C≡C bond. This conclusion is also confirmed by the results of IR spectroscopy and elemental analysis. The halide ammonium salts of all synthesized amino alcohols (7-16) are well soluble in water, ethanol, and chloroform, but poorly soluble in acetone, ether, and carbon tetrachloride.

The structure of the synthesized compounds was assessed based on their IR spectra. The spectra of the studied substances contain broad absorption bands associated with hydroxyl groups in the range of 3400–3255 cm^{-1}, as well as peaks of moderate intensity corresponding to the valence vibrations of the amino group and methyl and methylene groups in the range of 2955–2810 cm^{-1}. Absorption bands in the range of 785–715 cm^{-1} indicate the presence of chlorine, and at 630 cm^{-1} correspond to bromine. In the range of 1365–1340 cm^{-1} there is a doublet characteristic of the antisymmetry vibrations of the methyl group.

It should be noted that the spectra of the obtained halide derivatives do not contain absorption bands characteristic of the valence vibrations of the acetylene bond. However, they all have an absorption band corresponding to the acetylene carbon-carbon triple bond in the range of 1665–1655 cm^{-1}. Substances with quaternary nitrogen (7–16) show strong deformation vibrations in the range of 1585–1580 cm^{-1}.

Experimental part

Synthesis of the dichloroammonium salt of 1-dimethylamino-4-methylpentyn-2-ol-4. 4 g of 1-dimethylamino-4-methylpentyn-2-ol-4 and 80 ml of carbon tetrachloride were added to a flask equipped with a stirrer, reflux condenser, and a tube for introducing chlorine. The reaction flask was cooled with ice water and purified gaseous chlorine was passed through until the formation of crystals ceased. The completion of chlorination was determined by a change in the color of the reaction mass to green. The precipitate was separated by suction, washed in acetone, and dried over anhydrous calcium chloride to constant weight. The dichloroammonium salt of 1-dimethylamino-4-methylpentyn-2-ol-4 obtained was obtained as slightly brown crystals with a faint halogen odor. Other chlorine derivatives were synthesized in a similar manner.

Bromination of amino alcohols differs from their chlorination, since instead of gaseous chlorine, the required amount of liquid bromine is added to the reaction mass.

The results obtained are used in Organic Chemistry lessons at the Faculty of Natural Sciences of the Nizami State Technical University.

Chemical and biological properties of quaternary ammonium salts of acetylenic amino alcohols

Quaternary ammonium salts of acetylenic amino alcohols are widely used in various fields due to their chemical and biological activity. The following properties make them suitable for scientific research and practical application:

Antimicrobial properties

Quaternary ammonium salts have effective antibacterial, antifungal and antiviral activity against many microorganisms. Quaternary ammonium salts of acetylenic amino alcohols are used as antiseptics and disinfectants. They affect the cell membranes of bacteria and fungi, stopping their growth. Therefore, quaternary ammonium salts are widely used in medicine as antiseptics and antibiotics.

High solubility and biological activity

Quaternary ammonium salts of acetylenic amino alcohols have high solubility, which allows them to be effectively used in biological systems. Their cationic nature also increases their ability to penetrate cell membranes and helps in delivering active ingredients to the desired locations in the body.

Cosmetic and industrial applications

Quaternary ammonium salts of acetylenic amino alcohols are used in the cosmetic industry, especially as shampoos, conditioners and emulsifiers. Their effect on emulsion formation and high solubility help improve the quality of cosmetic products.

Pharmaceutical applications

Quaternary ammonium salts can be used as drug carriers. They effectively penetrate biological systems and ensure that drugs reach cells and sites of inflammation.

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