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Vibrational Spectra , Normal Coordinate And Molecular Calculations For 1-Hexyne

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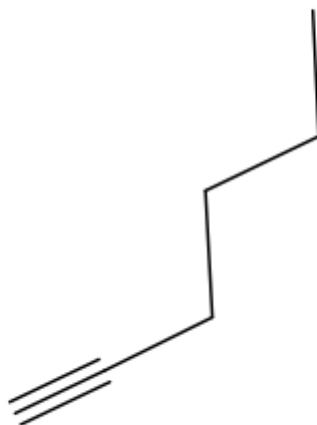
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ABSTRACT: IR and Raman spectra were obtained for 3-methyl-1-hexyne and 5-methyl-1-hexyne. The spectra were interpreted with the aid of normal coordinate calculations. Molecular mechanics calculations were made for all possible conformers of each compound. 3-Methyl-1-hexyne existed mainly in one stable conformation (C7-C3-C4-C5-C6 coplanar), but smaller amounts of several other conformers were present. 5-Methyl-1-hexyne existed mainly as two conformers, but smaller amounts of three others were probably present.

KEYWORDS- vibrational, spectra, coordinate, i-hexyne, molecular, calculations

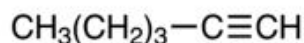
I.INTRODUCTION

A chemical structure of a molecule includes the arrangement of atoms and the chemical bonds that hold the atoms together. The 1-HEXYNE molecule contains a total of 15 bond(s). There are 5 non-H bond(s), 1 multiple bond(s), 2 rotatable bond(s), and 1 triple bond(s). Images of the chemical structure of 1-HEXYNE are given below:



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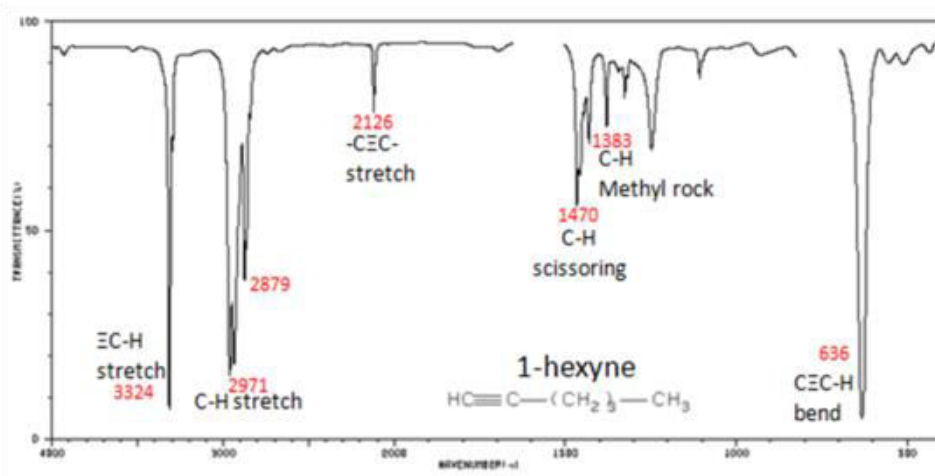
The 2D chemical structure image of 1-HEXYNE is also called skeletal formula, which is the standard notation for organic molecules. The carbon atoms in the chemical structure of 1-HEXYNE are implied to be located at the corner(s) and hydrogen atoms attached to carbon atoms are not indicated – each carbon atom is considered to be associated with enough hydrogen atoms to provide the carbon atom with four bonds.[1]



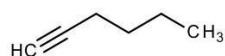
The 3D chemical structure image of 1-HEXYNE is based on the ball-and-stick model which displays both the three-dimensional position of the atoms and the bonds between them. The radius of the spheres is therefore smaller than the rod lengths in order to provide a clearer view of the atoms and bonds throughout the chemical structure model of 1-HEXYNE.

II.DISCUSSION

The spectrum of 1-hexyne, a terminal alkyne, is shown below

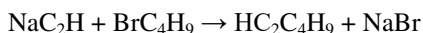


1-Hexyne is a hydrocarbon consisting of a straight six-carbon chain having a terminal alkyne. Its molecular formula is $\text{HC}_2\text{C}_4\text{H}_9$. A colorless liquid, it is one of three isomers of hexyne.^[1] It is used as a reagent in organic synthesis.^[2]



Synthesis and reactions

1-Hexyne can be prepared by the reaction of monosodium acetylide with butyl bromide:^[1]



Its reactivity illustrates the behavior of terminal alkyacetylenes. The hexyl derivative is common test substrate because it is conveniently volatile. It undergoes deprotonation at C-3 and C-1 with butyl lithium:



This reaction allows alkylation at the 3-position.^[2]

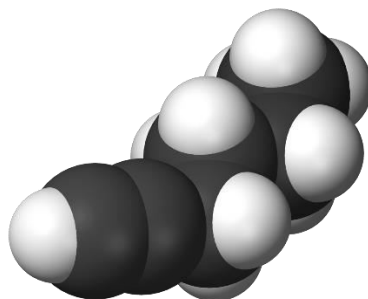
Catechol borane adds to 1-hexyne to give the 1-hexenyl borane.^[3]

1-Hexyne reacts with diethyl fumarate to produce n-hexylsuccinic acid.^[4]

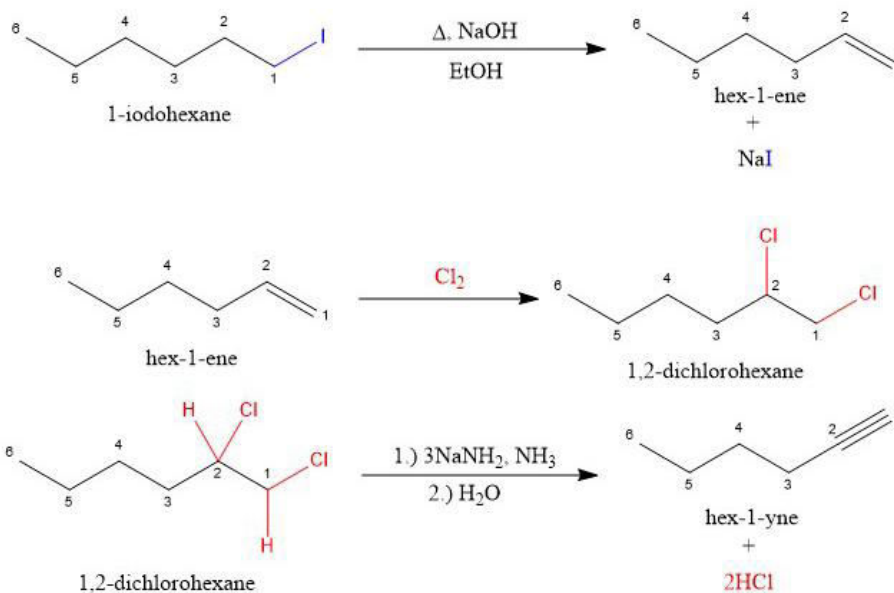
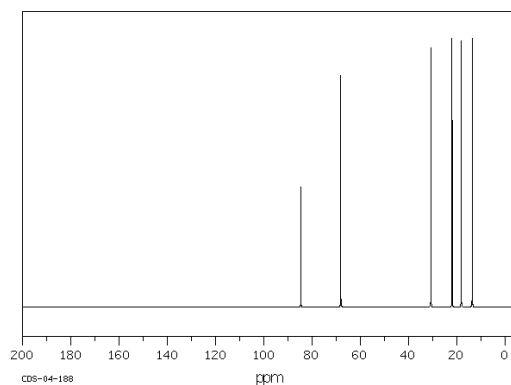
III.RESULTS

The 1-HEXYNE molecule consists of 10 Hydrogen atom(s) and 6 Carbon atom(s) - a total of 16 atom(s). The molecular weight of 1-HEXYNE is determined by the sum of the atomic weights of each constituent element multiplied by the number of atoms.

The exact term of the above molecular weight is “molar mass”, which is based on the atomic mass of each element. Molecular weight is actually an older term of “relative molar mass” or “molecular mass”, which is a dimensionless quantity equal to the molar mass divided by the molar mass constant defined by 1 g/mol.^[3]



Molecular masses are calculated from the standard atomic weights of each nuclide, while molar masses are calculated from the atomic mass of each element. The atomic mass takes into account the isotopic distribution of the element in a given sample.



IV.CONCLUSION

PRODUCT : 1-HEXYNE

CAS No. : 693-02-7

Synonym : Butylacetylene - Hex-1-yne - Hexyne

Molecular Formula : C_6H_{10}

Molecular weight : 82.14

PRODUCT SPECIFICATIONS OF 1-HEXYNE

Appearance : Clear, colourless to pale yellow liquid

GC Purity : 90.0% minimum

APPLICATIONS OF 1-HEXYNE

1-Hexyne is a basic building block for the synthesis of complex acetylenic molecules in perfumery, agrochemical, and pharmaceutical industry. It is specifically known to take part in cycloadditions to provide substituted isoindolinones and azides.[4]

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