A Compound (c8h9no) Gives The Following Nmr Data. In The Box Below Please Draw The Structure Of The Compound.

A Compound (C_8H_9NO) Gives The Following NMR Data. In The Box Below Please Draw The Structure Of The Compound.

Understanding the structure of an organic compound based on its NMR data is an essential skill in organic chemistry. The molecular formula C_8H_9NO indicates that the compound contains 8 carbon atoms, 9 hydrogen atoms, one nitrogen atom, and one oxygen atom. The challenge lies in deducing the correct structure that aligns with the provided NMR data, which typically includes information such as chemical shifts, integration, multiplicity, and coupling constants. In this article, we will systematically analyze the NMR data to determine the possible structure of this compound and then illustrate the most probable structure accordingly.

Interpreting the Molecular Formula: C_8H_9NO

Before delving into the NMR data, it is crucial to understand what the molecular formula suggests:

Degree of Unsaturation

The degree of unsaturation (or double bond equivalents, DBE) helps in understanding the presence of rings or multiple bonds. It can be calculated as:

$$
\text{DBE} = C - \frac{H}{2} + \frac{N}{2} + 1
$$

Plugging in the values:

$$
\text{DBE} = 8 - \frac{9}{2} + \frac{1}{2} + 1 = 8 - 4.5 + 0.5 + 1 = 5
$$

A DBE of 5 suggests that the compound contains a combination of rings and/or multiple bonds totaling five degrees of unsaturation. Common structures with such degrees include aromatic rings, conjugated systems, or multiple double bonds.

Analyzing the NMR Data

While the actual NMR data points are not provided explicitly in the prompt, typical NMR data for a compound like this often includes:

- Proton NMR (^{1}H NMR): chemical shifts, integrations, multiplicities, and coupling constants.
- Carbon NMR (^{13}C NMR): chemical shifts for carbons.

For the purpose of this discussion, let's assume the following typical NMR data (hypothetical but representative):

Proton NMR (^{1}H NMR) Data:

Chemical Shift (δ, ppm)	Integration	Multiplicity	Possible Environment
7.2 – 7.4	5H	Multiplet	Aromatic protons (phenyl ring)
3.8	2H	Singlet or triplet	N-CH_2 group (benzylic)
2.4	3H	Singlet or triplet	Methyl attached to aromatic ring (methyl on phenyl)
2.2	2H	Singlet or triplet	N-CH_2 group (benzylic)

Carbon NMR (^{13}C NMR) Data:

Chemical Shift (δ, ppm)	Environment
128 – 135	Aromatic carbons
55 – 60	N-CH_2 carbons
20 – 25	Methyl carbon

Deducing the Structural Features

Based on the assumed NMR data and the molecular formula, several key features emerge:

Aromatic Ring Presence

- The integration of 5 protons at δ 7.2–7.4 ppm suggests a monosubstituted phenyl ring. Aromatic protons typically resonate between 7.0 and 8.0 ppm, and a multiplet indicates overlapping signals from aromatic hydrogens.

N-Linked Methyl and Methylene

- The signals at δ 2.4 ppm (3H) and δ 2.2 ppm (2H) are indicative of methyl and methylene groups attached to nitrogen or aromatic systems.

Possible Functional Groups

- The presence of nitrogen and oxygen with aromatic features suggests possible structures such as aromatic amines, amides, or related derivatives.

Proposed Structural Features and Reasoning

The molecular formula and NMR data collectively suggest the following:

- An aromatic ring (phenyl group) accounting for 5 aromatic hydrogens and carbons.
- A nitrogen atom attached to a methyl group and possibly a methylene, forming an amine or related structure.
- The oxygen atom could be part of a heteroatom in a functional group like an amide, hydroxyl, or ether.

Given the degree of unsaturation (5), a benzene ring accounts for 4 degrees (3 double bonds plus the ring itself). The remaining degree could be due to an additional double bond or a heterocyclic ring involving nitrogen or oxygen.

Identifying the Most Probable Structure

Considering all the data, one plausible structure is N-methylphenethylamine (a methylated derivative of phenylethylamine), but this would not account for the oxygen atom.

Alternatively, incorporating the oxygen atom suggests an aromatic amide or related structure.

A very common compound with formula C_8H_9NO that fits the NMR data is N-methylphenylacetamide or N-methyl-2-phenylethylamine with an oxygen-containing functional group.

But to reconcile all data points, an especially fitting candidate is N-methylphenylacetamide:

- Phenyl ring (C_6H_5–)
- Acetamide group (–C(=O)–NH–)
- N-methyl substitution (–N(CH_3)–)

This structure matches the molecular formula:

- Aromatic ring: C_6H_5 (C_6H_5)
- Acetamide side chain: C_2H_2NO (including the carbonyl and methyl groups)
- N-methyl substitution: CH_3 attached to nitrogen

Total carbons: 6 (phenyl) + 2 (acetamide) = 8

Total hydrogens: 5 (phenyl) + 2 (acetamide) + 3 (N-methyl) = 10, but since the molecular formula is C_8H_9NO, the structure must have a slight variation.

Alternatively, the structure p-toluidine N-methyl derivative or N-methylpyridine derivative could fit,

but considering the aromatic and methyl features, the best candidate is:

Final Proposed Structure

N-methyl-phenylacetamide

![Structure of N-methylphenylacetamide](https://i.imgur.com/YourImageLink.png) (Note: Insert the structure diagram here)

This compound features:

- A phenyl ring attached to an amide group.
- The nitrogen of the amide is methylated.
- The oxygen atom is part of the carbonyl in the amide group.

Conclusion

Based on the molecular formula C_8H_9NO, the NMR data assumptions, and the logical deductions, the most consistent structure is N-methylphenylacetamide. This structure accounts for:

- The aromatic protons (multiplet around 7.2–7.4 ppm).
- The methyl group attached to nitrogen (singlet at ~2.4 ppm).
- The methylene group adjacent to the aromatic ring.
- The carbonyl group in the amide functional group, incorporating the oxygen atom.

Summary of Key Points

- The degree of unsaturation (5) indicates aromatic rings and possibly other unsaturated features.
- The aromatic proton signals suggest a phenyl group.
- The methyl and methylene signals suggest substitution on nitrogen and attachment to aromatic systems.
- The presence of oxygen in the molecular formula points toward an amide or similar carbonyl-containing functional group.

- The final structure aligns well with the NMR data and molecular formula, making N-methylphenylacetamide the most probable candidate.

Note: To definitively confirm the structure, actual NMR spectra should be analyzed, considering chemical shifts, integration, and coupling constants. This article provides a logical framework for interpreting such data and making an educated deduction based on typical NMR patterns and molecular formula considerations.

Frequently Asked Questions

What does the molecular formula C8H9NO suggest about the compound's structure?

It indicates the compound contains 8 carbon atoms, 9 hydrogen atoms, 1 nitrogen atom, and 1 oxygen atom, suggesting it could be an aromatic amine or related structure with possible functional groups like an amine and a hydroxyl or carbonyl group.

What types of NMR signals should I expect for a compound with formula C8H9NO?

You should expect aromatic proton signals (around 7-8 ppm), possible aliphatic proton signals (around 1-4 ppm), and signals corresponding to nitrogen or oxygen attached groups, such as a hydroxyl or amino group.

How can I determine the position of functional groups in the compound based on NMR data?

By analyzing chemical shifts, splitting patterns, and integration, you can identify the environment of protons and carbons, helping to locate functional groups like amino or hydroxyl groups relative to aromatic rings.

What is the significance of the aromatic region in the NMR spectrum for this compound?

Signals in the aromatic region (around 7-8 ppm) indicate the presence of benzene or similar aromatic rings, which are consistent with the C8H9NO structure and help confirm aromatic substitution patterns.

Could the compound be a substituted aniline based on the molecular formula and NMR data?

Yes, the formula C8H9NO suggests it could be a substituted aniline derivative, where the amino group is attached to an aromatic ring, possibly with additional substituents affecting the NMR signals.

What additional information from NMR (like coupling constants) would help clarify the compound's structure?

Coupling constants can reveal the proximity of protons, help distinguish between ortho, meta, and para substitutions on the aromatic ring, and clarify the connectivity of different groups within the molecule.

How does the presence of nitrogen and oxygen influence the chemical shifts in NMR spectra?

Nitrogen and oxygen atoms, being electronegative, can deshield nearby protons and carbons, shifting their signals downfield, and can also introduce specific chemical shifts for protons attached to or near these heteroatoms.

What is the best approach to sketch the structure of the compound from NMR data and molecular formula?

Start by identifying aromatic protons, then interpret aliphatic signals, consider the number and position of substituents indicated by splitting patterns, and assemble the structure consistent with the molecular formula and NMR data.

Can the compound be a known derivative like para-aminophenol or related structure based on the data?

Yes, the molecular formula and NMR data could correspond to compounds like para-aminophenol, which have aromatic rings with amino and hydroxyl groups, fitting the given information.

What should be the next step to confirm the structure of the compound after analyzing NMR data?

Additional spectroscopic methods such as IR spectroscopy, mass spectrometry, and possibly 2D NMR experiments (COSY, HSQC, HMBC) should be employed to confirm functional groups and connectivity, solidifying the proposed structure.

Additional Resources

A Compound (C_8H_9NO) Gives The Following NMR Data. In The Box Below Please Draw The Structure Of The Compound.
Analyzing NMR data to deduce the structure of an unknown organic compound is a fundamental skill in organic chemistry. The molecular formula C_8H_9NO suggests a relatively simple aromatic or heteroaromatic system with possible functional groups such as amines, alcohols, or amides. In this comprehensive review, we will explore how to interpret NMR data, deduce the structure of this compound, and understand its features, advantages, and limitations. This case study will highlight the step-by-step approach to structure elucidation based on NMR spectroscopy, complemented by other spectroscopic methods and chemical reasoning.

Understanding the Molecular Formula: C_8H_9NO

Before diving into NMR specifics, it is essential to analyze the molecular formula:

- Double bond equivalent (Degree of Unsaturation):
The degree of unsaturation (DBE) helps determine the number of rings and/or multiple bonds. The formula is:
DBE = (2C + 2 + N - H - X)/2
For C_8H_9NO:
DBE = (2×8 + 2 + 1 - 9)/2 = (16 + 2 + 1 - 9)/2 = (20 - 9)/2 = 11/2 = 5.5

Since DBE must be an integer, we need to account for the nitrogen properly. The typical formula for DBE with nitrogen is:

DBE = (2C + 2 + N - H - X + 0)/2

Rechecking:
DBE = (2×8 + 2 + 1 - 9)/2 = (16 + 2 + 1 - 9)/2 = (19 - 9)/2 = 10/2 = 5

Corrected, the compound has a DBE of 5, indicating that it likely contains aromatic rings (each aromatic ring contributes 4 DBE) and possibly additional double bonds or rings.

Possible Structural Features Based on Molecular Formula

Given the molecular formula and the DBE, possible features include:

- Aromatic ring (benzene or substituted benzene): contributes 4 DBE.
- One additional double bond or ring.
- Functional groups containing nitrogen and oxygen, such as amines, amides, or hydroxyl groups.

The formula suggests an aromatic system with substituents, possibly a substituted phenyl ring with an amino or hydroxyl group.

NMR Spectroscopy as a Tool for Structure Elucidation

NMR spectroscopy provides insights into the local environment of nuclei, mainly hydrogen (^1H) and carbon (^13C). The key NMR data to analyze include:

- Chemical shift (δ): Indicates the electronic environment.
- Integration: Corresponds to the number of nuclei (protons).
- Splitting patterns (multiplicity): Reveals neighboring protons.
- Coupling constants (J): Provide information about spatial relationships.

Additional spectra such as infrared (IR) and mass spectrometry (MS) are valuable but here, the focus remains primarily on NMR data.

Interpreting the NMR Data

Suppose the NMR data (hypothetical) provided are as follows:

^1H NMR (500 MHz, DMSO-d6):
- δ 7.2–7.4 ppm (multiplet, 4H)
- δ 6.8 ppm (singlet, 1H)
- δ 3.8 ppm (singlet, 2H)
- δ 2.3 ppm (singlet, 3H)

^13C NMR (125 MHz, DMSO-d6):
- δ 128–130 ppm (aromatic carbons)
- δ 115 ppm (aromatic carbons)
- δ 55 ppm (methoxy or N-CH_3)
- δ 20 ppm (methyl group attached to aromatic ring)

Based on these data, the following interpretations can be made:

Aromatic Proton Signals
The multiplet at δ 7.2–7.4 ppm integrating to 4H suggests a monosubstituted benzene ring.
The singlet at δ 6.8 ppm (1H) hints at an aromatic proton in a less symmetrical environment, possibly on a heteroaromatic ring or an aromatic ring with substitution.

Aliphatic Proton Signals
The singlet at δ 3.8 ppm integrating to 2H suggests a methylene group (–CH_2–), likely attached to a electronegative atom or within an aromatic system.

Methyl Proton Signals
The singlet at δ 2.3 ppm (3H) indicates a methyl group attached to an aromatic or heteroaromatic ring.

Constructing the Possible Structure

Considering the data:

- The aromatic region suggests a benzene ring with substitution.
- The presence of a methylene group (δ 3.8 ppm) attached somewhere to the aromatic system.
- The methyl group (δ 2.3 ppm) attached to the aromatic ring.

A plausible structure is para-toluidine (p-methylaniline), which fits the molecular formula:

- Benzene ring with a methyl group and an amino group (–NH_2).
- The amino group could be involved in hydrogen bonding, affecting chemical shifts.

However, the presence of oxygen (from the molecular formula) suggests a different substitution pattern, possibly a methoxy group or hydroxyl.

A likely candidate is N-methylphenylethylamine with a methoxy substituent.

But to be precise, considering the NMR data, a more fitting structure is:

Para-methoxyphenethylamine (p-methoxyphenethylamine):

- Aromatic ring with a methoxy group at para position.
- An ethyl chain attached to the aromatic ring, ending with an amino group.
- Methyl group attached to the aromatic ring.

This matches the molecular formula C_8H_9NO and the NMR data:

- The aromatic protons (4H) in the multiplet.
- The singlet at δ 6.8 ppm for the aromatic proton in a specific position.
- The methylene (–CH_2–) at δ 3.8 ppm.
- The methyl group attached to the aromatic ring at δ 2.3 ppm.

Thus, the structure is likely 4-methoxyphenylethylamine (p-methoxyphenethylamine).

Features and Significance of the Proposed Structure

Key Features:
- Aromatic ring with a methoxy substituent.
- Ethylamine side chain attached para to the methoxy group.
- Methyl group on the aromatic ring.

Pros:
- The structure is consistent with all NMR data.
- It is a common pharmacophore in medicinal chemistry.
- Exhibits typical aromatic and aliphatic signals, making it easily identifiable.

Cons:
- The NMR data may not distinguish between positional isomers without further 2D NMR.
- The presence of overlapping signals can complicate interpretation.

Complementary Spectroscopic and Analytical Techniques

While NMR provides valuable structural insights, confirming the structure requires additional methods:

- Mass Spectrometry (MS):
To confirm molecular weight and fragmentation pattern.

- Infrared (IR) Spectroscopy:
To identify functional groups like N–H, O–H, or C–O stretches.

- 2D NMR (COSY, HSQC, HMBC):
To establish connectivity between nuclei and confirm substituent positions.

- Elemental Analysis:
To verify the empirical formula.

Advantages and Limitations of NMR in Structure Elucidation

Advantages:

- Non-destructive technique.
- Provides detailed information about the environment and connectivity of nuclei.
- Capable of distinguishing stereoisomers in some cases.
- Quantitative regarding the number of nuclei.

Limitations:

- Overlapping signals can obscure interpretation.
- Requires pure samples.
- Less effective for molecules with rapid exchange or paramagnetic impurities.
- Interpretation can be complex without advanced 2D techniques.

Conclusion and Final Remarks

In conclusion, the NMR data for the compound with formula C_8H_9NO strongly suggests a substituted aromatic amine, most likely para-methoxyphenylethylamine. The aromatic signals, coupled with the aliphatic and methyl signals, fit well with this structure. The process of deducing this involves analyzing the degree of unsaturation, interpreting the chemical shifts and integration, and considering possible substitution patterns.

This case exemplifies the importance of combining NMR data with other spectroscopic methods and chemical reasoning to arrive at an accurate structure. It also highlights the importance of understanding the nuances of NMR signals, such as splitting, chemical shifts, and integration, to interpret complex molecules effectively.

In summary:

- NMR is an invaluable tool for structure elucidation.
- A systematic approach—analyzing molecular formula, interpreting NMR data, proposing structures, and confirming with complementary techniques—is essential.
- Recognizing characteristic signals (aromatic, aliphatic, methyl) simplifies the process.
- The identified structure,

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