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1 4 di t butyl 2 5 dimethoxybenzene nmr

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Understanding the NMR Spectrum of 1,4 Di tert butyl 2,5 Dimethoxybenzene

When chemists set out to characterize a newly synthesized aromatic compound, one of the first tools they turn to is nuclear magnetic resonance (NMR) spectroscopy. NMR offers a window into the electronic environment of each nucleus, allowing researchers to confirm structure, purity, and even subtle conformational details. In this article we dive deep into the NMR analysis of a particularly interesting substrate: **1,4 di tert butyl 2,5 dimethoxybenzene**. This molecule combines two bulky tert butyl groups with two methoxy substituents, creating a unique pattern of chemical shifts and coupling constants that make it an excellent teaching example for both proton and carbon NMR.

Why Study 1,4 Di tert butyl 2,5 Dimethoxybenzene?

From a synthetic standpoint, 1,4 di tert butyl 2,5 dimethoxybenzene is a versatile intermediate. Its symmetry and electron rich aromatic ring make it a good candidate for electrophilic aromatic substitution, cross coupling reactions, and as a protecting group scaffold. Moreover, the tert butyl groups provide steric shielding that can influence reactivity and selectivity. When a chemist wants to confirm that the desired substitution pattern has been achieved, the NMR fingerprint becomes the gold standard.

Structural Overview

The structure of 1,4 di tert butyl 2,5 dimethoxybenzene can be broken down into three main components:

- Aromatic Core: A benzene ring with four positions substituted.
- Tert butyl Groups: Two bulky, electron donating tert butyl groups occupy the para positions (1 and 4).
- Methoxy Groups: Two methoxy (-OCH3) substituents occupy the meta positions (2 and 5).

This arrangement gives the molecule D2H symmetry, meaning that the ring has a two fold rotational axis and a mirror plane. As a result, the NMR spectrum displays fewer distinct signals than one would expect for a random substitution pattern.

Synthesis Pathways

Although several routes exist, a common laboratory synthesis involves the following steps:

1. Preparation of 2,5 Dimethoxy 1,4 dihydroxybenzene (also known as 2,5 bis(benzyloxy)resorcinol). This can be achieved via methylation of resorcinol using methyl iodide and a base.
2. Protection of the Phenolic Hydroxyls as benzyl ethers to prevent side reactions during tert butylation.
3. Introduction of Tert butyl Groups via Friedel–Crafts alkylation using tert butyl chloride and a Lewis acid such as AlCl3. The reaction is directed to the 1 and 4 positions due to the directing effects of the methoxy groups.
4. Deprotection of the Benzyl Ethers using hydrogenolysis (H2/Pd–C) to reveal the final 1,4 di tert butyl 2,5 dimethoxybenzene.

After purification by column chromatography, the product is typically obtained as a pale yellow solid with a melting point around 120 /°C.

Proton (^{1}H) NMR Fundamentals

Proton NMR measures the environment of hydrogen atoms in a molecule. Key parameters include:

- Chemical Shift (;B“ Indicates the electronic shielding of a proton.

- Multiplicity (Splitting Pattern): Reflects coupling with neighboring protons.
- Integration: Proportional to the number of protons contributing to a signal.
- Coupling Constant (J): Expressed in hertz (Hz), describes the interaction strength between coupled protons.

For aromatic compounds, typical chemical shifts for protons range from 6.0 to 8.5 ppm, while aliphatic protons appear between 0.5 and 3.0 /ppm. Methoxy protons usually resonate around 3.5–4.0 /ppm.

^{1}H NMR of 1,4 Di tert butyl 2,5 Dimethoxybenzene

Because of the molecule's symmetry, the aromatic protons are equivalent in pairs. The expected proton spectrum in deuterated chloroform (CDCl3) at 400 /MHz is summarized below:

- Aromatic Protons (H 3 & H 6): Two equivalent protons appear as a doublet of doublets (dd) or a doublet (d) depending on the coupling network. Typical ;B `alues are 7.30–7.40 /ppm with J "H 8 /Hz.
- Methoxy Protons (OCH3): Two equivalent singlets at ;B $, 2ãs, ÷ ÒÂ –çFVprating to 6 /H.
- Tert butyl Methyl Groups: Six equivalent methyl protons (two tert butyl groups each contributing three methyls) produce a singlet at ;B $, ã#R ÷ ÒÂ –çFVprating to 18 /H.

Because the tert butyl groups are electronically donating, they shift the aromatic protons slightly upfield compared to unsubstituted anisole. The methoxy groups also contribute to electron donation, further influencing the chemical shifts.

Carbon (^{13}C) NMR Basics

Carbon NMR provides information on the different carbon environments in a molecule. Key points include:

- Chemical Shift (;B“ Typically ranges from 0 to 220 /ppm.
- Multiplicity (DEPT, HSQC): Distinguishes between CH, CH2, CH3, and quaternary carbons.
- Integration: Not commonly used because ^{13}C signals are inherently weak and often measured with full relaxation delays.

^{13}C NMR of 1,4 Di tert butyl 2,5 Dimethoxybenzene

In a typical 100 /MHz ^{13}C spectrum (CDCl3), the following peaks are expected:

- Quaternary Aromatic Carbons (C 1, C 4): ;B $, C c CR ÷ Òà
- Aromatic Carbons Attached to Methoxy (C 2, C 5): ;B $, # c #R ÷ Òà
- Aromatic Carbons Attached to tert butyl (C 3, C 6): ;B $, Yc , ÷ Òà
- Methoxy Carbons: ;B $, SYcc ÷ Òà
- Tert butyl Quaternary Carbons: ;B $, 3Yc3, ÷ Òà
- Tert butyl Methyl Carbons: ;B $, #Yc#r ÷ Òà

The DEPT 135 experiment will show all CH and CH3 signals as positive, while quaternary carbons will appear as negative or absent, confirming the presence of the tert butyl groups.

Advanced 2D NMR Techniques

While 1D spectra are sufficient for basic identification, 2D NMR provides deeper insights, especially when dealing with complex mixtures or overlapping signals.

Shows scalar (through bond) coupling between protons. In 1,4 di tert butyl 2,5 dimethoxybenzene, the COSY will display cross peaks between the aromatic protons (H 3 !” H 6) confirming their adjacency.

Correlates each proton with the directly attached carbon. This allows unambiguous assignment of the methoxy and tert butyl signals, ensuring that the ^{1}H and ^{13}C data match.

Provides long range (2–3 bond) correlations. Useful for confirming the connectivity between the methoxy groups and the aromatic ring, especially when the ^{13}C signals overlap.

Comparing to Analogous Compounds

By studying related molecules—such as 1,4 di tert butylbenzene or 1,4 dimethoxybenzene—we can see how substituents influence NMR parameters.

- 1,4 Di tert butylbenzene: Lacks methoxy groups; aromatic protons appear slightly downfield (;B $, rã# crã3 ÷ Ò’ due to reduced electron donation.
- 1,4 Dimethoxybenzene: Lacks tert butyl groups; aromatic protons shift upfield (;B $, bã“ crã ÷ Ò’ &V6 W6R methoxy groups donate more electron density.
- 1,4 Di tert butyl 2,5 dimethoxybenzene: Shows a balanced shift (;B $, rã3 crãC ÷ Ò’ GVR Fò 6öÖ&–æVB Vf`ects.

These comparisons illustrate how NMR can serve as a diagnostic tool for subtle electronic changes.

Practical Considerations for Accurate NMR Measurement

Achieving reliable spectra requires attention to several experimental details:

- Solvent Choice: CDCl3 is standard, but for highly polar compounds DMSO d6 or CD3OD may be preferable.
- Concentration: 5–10 /mg/mL is typical; too dilute and signals become weak, too concentrated and peak broadening can occur.

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