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1 4 Di T Butyl 2 5 Dimethoxybenzene Msds

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Unlocking the Secrets of 1,4-Di-tert-butyl-2,5-dimethoxybenzene: A Comprehensive NMR Analysis

The world of organic chemistry is built upon the precise identification and characterization of molecular structures. Among the myriad of analytical techniques available to the modern chemist, Nuclear Magnetic Resonance (NMR) spectroscopy stands as an indispensable tool. When faced with a symmetrically substituted aromatic compound like 1,4-di-tert-butyl-2,5-dimethoxybenzene, the NMR spectrum offers a fascinating window into its electronic environment, symmetry, and dynamic behavior. Understanding the **1 4 di t butyl 2 5 dimethoxybenzene nmr**spectrum is not merely an academic exercise; it is a practical lesson in how molecular symmetry simplifies spectral data and how substituent effects dictate chemical shifts. This article provides a detailed, step-by-step guide to interpreting the proton and carbon NMR spectra of this compound, making the complex accessible to students, researchers, and seasoned chemists alike.

Molecular Structure and Symmetry: The Foundation of the NMR Spectrum

Before delving into the specific peaks and coupling patterns, it is crucial to establish the molecular architecture of the compound. 1,4-Di-tert-butyl-2,5-dimethoxybenzene is a derivative of benzene, the quintessential aromatic ring. Its structure is defined by a central benzene ring bearing four substituents. At the 1 and 4 positions (the *para*positions relative to each other), there are two bulky tert-butyl groups (-C(CH ƒ) ƒ). At the 2 and 5 positions, there are two methoxy groups (-OCH ƒ).

The key to understanding the **1 4 di t butyl 2 5 dimethoxybenzene nmr**lies in the molecule's exceptional symmetry. The molecule possesses a center of inversion. This means that if you rotate the molecule by 180 degrees, it looks exactly the same. This symmetry has profound consequences for the NMR spectrum. Chemically equivalent nuclei will resonate at the same frequency. In this case, the two tert-butyl groups are chemically identical, and the two methoxy groups are also chemically identical. This symmetry drastically reduces the number of signals we expect to see in both the proton (^{1}H) and carbon (^{13}C) NMR spectra.

Proton NMR (^{1}H NMR) Spectrum Analysis

The ^{1}H NMR spectrum of 1,4-di-tert-butyl-2,5-dimethoxybenzene is remarkably simple, a direct result of its high symmetry. Let us break down the expected signals.

The Aromatic Proton Signal: A Lone Sentinel

The most striking feature of the aromatic region is the presence of only one signal. With two tert-butyl groups occupying the 1 and 4 positions, and two methoxy groups occupying the 2 and 5 positions, the only remaining

positions on the ring are the 3 and 6 positions. These two positions are occupied by hydrogen atoms. Crucially, due to the molecule's symmetry, these two aromatic protons are chemically equivalent. They experience exactly the same magnetic environment.

This single aromatic proton appears as a sharp singlet. There is no splitting because the two protons are magnetically equivalent; they do not couple with each other in a way that produces a multiplet. The presence of this one singlet in the aromatic region is the most immediate and powerful piece of evidence confirming the 1,2,4,5-tetrasubstitution pattern. The chemical shift for this proton is typically observed around **;B bã, Đ** This value is slightly upfield from a typical benzene proton (;@ 7.27 ppm) because the electron-donating methoxy groups increase the electron density in the aromatic ring, shielding the proton and moving its resonance to a lower frequency.

The Methoxy Proton Signal: A Clear Triplet of Singlets

Moving upfield into the region where aliphatic protons resonate, we encounter the signal from the methoxy groups (-OCH ƒ). As established, the two methoxy groups are chemically equivalent. Each group contains three identical hydrogen atoms. These nine protons (3 from each of the two groups, but they are magnetically equivalent and yield one signal) appear as a sharp, intense singlet. The chemical shift for the methoxy protons in this compound is typically found near **;B 2ã, Đ** This is a very characteristic region for methoxy groups attached to an aromatic ring. The signal is a singlet because there are no adjacent non-equivalent protons to cause splitting.

The Tert-Butyl Proton Signal: A Massive Upfield Peak

The most upfield signal, and often the most intense in the spectrum, belongs to the tert-butyl groups. Each tert-butyl group contains nine equivalent methyl protons. With two equivalent tert-butyl groups, a total of 18 protons contribute to this single signal. This signal appears as a very tall, sharp singlet. Its chemical shift is typically around **;B ã2 Đ** This is a classic position for tert-butyl groups, which are highly branched and have their protons well-shielded from the anisotropic effects of the aromatic ring due to the sp^3 hybridized carbon attached directly to the ring. The sheer intensity of this peak relative to the others (an 18:6:2 ratio for tert-butyl:methoxy:aromatic protons) is a clear indicator of the molecular composition.

Summary of ^{1}H NMR Spectrum:

- ;B ã ã2 Ó Singlet, 18H, two equivalent tert-butyl groups (-C(CH ƒ) ƒ).
- ;B ã2ã, Ó Singlet, 6H, two equivalent methoxy groups (-OCH ƒ).
- ;B ãbã, Ó Singlet, 2H, two equivalent aromatic protons (H-3 and H-6).

Carbon-13 NMR (^{13}C NMR) Spectrum Analysis

The ^{13}C NMR spectrum, while showing more signals than the proton spectrum, is still elegantly simple due to the molecule's symmetry. For a molecule with 10 carbon atoms in its structure, symmetry dictates that we will observe exactly **5 distinct carbon resonances**.

Aromatic Carbons: A Tale of Four Signals

The aromatic ring contains four unique types of carbon atoms. Because of the symmetry, the two carbons bearing the tert-butyl groups (C-1 and C-4) are equivalent and produce one signal. The two carbons bearing the methoxy groups (C-2 and C-5) are also equivalent, producing a second signal. Finally, the two carbon atoms that are bonded to hydrogen (C-3 and C-6) are equivalent, giving a third signal. The ring itself, having four distinct environments, contributes four signals in total, but the ipso carbons (those directly attached to substituents) are often quaternary and have lower intensity.

1. C-1 and C-4 (Ipso to tert-butyl): These carbons are highly substituted and deshielded. Their chemical shift is typically observed around ;B C Ó CR Òà

2. C-2 and C-5 (Ipso to methoxy): The oxygen atom is strongly electron-withdrawing by induction but strongly electron-donating by resonance. This results in a significant downfield shift for these carbons, typically appearing around ;B S Ó SR Òà

3. C-3 and C-6 (Aromatic CH): These are the protonated aromatic carbons. They appear further upfield in the aromatic region, usually around ;B Ó R Òà This is significantly upfield compared to benzene (;B #, Ò' due to the electron-donating effects of the substituents.

Aliphatic Carbons: Two Distinct Signals

1. The Methoxy Carbon (-OCH ƒ): The carbon atom in the methoxy group is directly attached to oxygen, which deshields it strongly. It appears as a single, relatively intense peak around ;B SRÓc Òà

2. The Tert-Butyl Carbons: The tert-butyl group shows two distinct carbon signals. The central, quaternary carbon (the one directly attached to the ring) is deshielded and appears around ;B 3BÓ3R Òà The three equivalent methyl carbons of the tert-butyl group are highly shielded and appear as an intense, sharp peak around ;B 3 Ó3 Òà

Summary of ^{13}C NMR Spectrum (5 signals total):

- ;B ã3 Ó3 Ó CH ƒ carbons of tert-butyl groups.
- ;B ã3BÓ3R Ó Quaternary carbon of tert-butyl groups.
- ;B ãSRÓc Ó Methoxy carbon (-OCH ƒ).
- ;B ã Ó R Ó Aromatic CH carbons (C-3, C-6).
- ;B ã C Ó CR Ó Aromatic C-N (C-1, C-4, ipso to tert-butyl).
- ;B ã S Ó SR Ó Aromatic C-O (C-2, C-5, ipso to methoxy).

Factors Influencing the NMR Chemical Shifts

The observed chemical shifts in the **1 4 di t butyl 2 5 dimethoxybenzene nmr**spectrum are not arbitrary; they are the result of several fundamental electronic and steric effects.

The Electron-Donating Effect of Methoxy Groups

The methoxy group is a classic electron-donating group through resonance. The lone pairs on the oxygen atom can be delocalized into the < ×7—7FVÐ of the aromatic ring. This increases the electron density at the ortho and para positions (relative to the methoxy group). In this specific molecule, the methoxy groups are at the 2 and 5 positions. Their ortho positions would be C-1/C-3 and C-4/C-6, and their para positions would be C-4 and C-1. This electron donation shields the aromatic protons at C-3 and C-6, shifting their resonance upfield (to a lower ppm value) compared to a typical aromatic proton.

The Bulky Tert-Butyl Group: Steric and Inductive Effects

The tert-butyl group is a large, sterically demanding substituent. While it is a weak electron-donating group through hyperconjugation (the sigma-pi conjugation), its primary effect in this molecule is steric. The bulky tert-butyl groups force the methoxy groups to adopt a preferred conformation. They likely lie slightly out of the plane of the aromatic ring to minimize steric clash. This can slightly influence the degree of resonance donation from the oxygen. Furthermore, the tert-butyl groups themselves have a well-defined chemical shift (;B ã ã2 Ò' F† B —2 remarkably consistent across different molecules, making them a reliable fingerprint in the **1 4 di t butyl 2 5 dimethoxybenzene nmr** spectrum.

Practical Applications and Relevance of the NMR Data

Understanding the NMR spectrum of this compound is not just an intellectual curiosity; it has practical applications in organic synthesis and materials science.

Purity Assessment

The simplicity and intensity of the **1 4 di t butyl 2 5 dimethoxybenzene nmr**spectrum make it an excellent

tool for assessing purity. The presence of any extra peaks in the aliphatic or aromatic region would immediately indicate the presence of impurities, such as unreacted starting materials or side products. The sharp, well-resolved singlets are a hallmare of a pure, symmetrical compound.

Monitoring Reactions

This compound is often used as a building block in organic synthesis, particularly in the preparation of electron-rich aromatic systems or as a precursor to quinones and other oxidized derivatives. By taking NMR spectra at various time points, chemists can monitor the disappearance of the characteristic signals of 1,4-di-tert-butyl-2,5-dimethoxybenzene and the appearance of signals from the product. The unique "signature" of this molecule makes it easy to track

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