GENERAL

# nmr chemical shifts of common laboratory solvents as trace impurities

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## Introduction

When working in a chemical laboratory, the quality of your NMR data can be the difference between a successful experiment and a frustrating dead end. Even the most carefully prepared samples can be compromised by tiny amounts of unwanted species that appear as unexpected peaks in the spectrum. These trace impurities often come from the solvents themselves – the very liquids that dissolve your analytes and provide a reference frame for the chemical shift scale.

In this article we will explore the **nmr chemical shifts of common laboratory solvents as trace impurities**, detailing how they appear, why they matter, and how to identify and mitigate them. We'll cover the fundamentals of NMR chemical shifts, discuss the most frequently used solvents, and provide a practical guide to recognizing solvent derived impurities in your spectra. Whether you're a student learning the basics of NMR or a seasoned researcher troubleshooting a problematic spectrum, this comprehensive resource will give you the knowledge you need to maintain data integrity.

## 1. Understanding NMR Chemical Shifts

### 1.1 Basic Principles of NMR

Nuclear Magnetic Resonance (NMR) spectroscopy exploits the magnetic properties of atomic nuclei. When placed in a strong magnetic field, nuclei such as 1H or 13C precess at characteristic frequencies. By applying radiofrequency pulses, we perturb these spins and detect the resulting free induction decay (FID), which is then transformed into a spectrum. The position of each resonance peak is expressed in parts per million (ppm) relative to a reference compound, typically tetramethylsilane (TMS) for 1H and 13C NMR.

### 1.2 Why Chemical Shift Matters

The chemical shift reflects the electronic environment surrounding a nucleus. Electrons shield the nucleus from the external magnetic field; the more shielding, the lower the resonance frequency (upfield). Conversely, deshielding shifts the resonance downfield (higher ppm). Because chemical shifts are highly sensitive to subtle changes in electronic structure, they provide a fingerprint that can identify functional groups, confirm molecular structure, and detect impurities.

### 1.3 The Role of Solvent in Chemical Shift Referencing

Solvents not only dissolve the analyte but also contribute a set of resonances that serve as internal references. For deuterated solvents, the non-deuterated hydrogen atoms produce a small but measurable signal (often called the "solvent peak") that appears at a well defined ppm. For example, deuterated chloroform (CDCl3) shows a singlet at 7.26 ppm in 1H NMR. These solvent peaks are routinely used for calibration, but when trace impurities are present, additional peaks can appear near or overlapping the solvent signal, complicating interpretation.

## 2. Common Laboratory Solvents

### 2.1 Solvent Categories

- Non deuterated solvents – used for sample preparation and extraction.
- Deuterated solvents – essential for NMR because deuterium ($^2H$) is NMR silent for 1H and 13C, reducing background signals.
- Polar aprotic solvents – e.g., DMSO, DMF, acetonitrile; often used for challenging substrates.
- Non polar solvents – e.g., hexane, toluene; useful for hydrophobic compounds.

### 2.2 Typical Purity and Availability

High purity solvents are available from major suppliers, but even “anhydrous” or “spectroscopic” grades can contain trace amounts of contaminants such as residual water, dissolved gases, or solvent decomposition products. Deuterated solvents are usually labeled as “99.9 % D” or “99.99 % D”, but the remaining fraction can contain non deuterated species that contribute to impurity peaks.

### 2.3 List of Frequently Used Deuterated Solvents

1. CDCl3 – deuterated chloroform
2. C6D6 – deuterated benzene
3. CD3OD – deuterated methanol
4. CD3CN – deuterated acetonitrile
5. DMSO d6 – deuterated dimethyl sulfoxide
6. CD3COOD – deuterated acetic acid
7. CD3CO2CH3 – deuterated ethyl acetate
8. CD3CH3 – deuterated acetone
9. CD3CO2D – deuterated formic acid

## 3. Trace Impurities in Solvents

### 3.1 Sources of Impurities

Impurities can arise from several stages:

- Manufacturing residues – incomplete deuteration, contaminants introduced during synthesis.
- Storage conditions – exposure to moisture, air, or temperature fluctuations.
- Sample handling – transfer through glassware that may leach silicates or other species.
- Decomposition – solvents can degrade over time, especially under light or heat.

### 3.2 Impact on NMR Data

Even trace levels (ppm or sub ppm) of impurities can produce distinct peaks that interfere with the interpretation of a spectrum. For instance, residual water in CDCl3 appears as a broad singlet at ~1.5 ppm, potentially overlapping with aliphatic methylene signals. Similarly, small amounts of residual 1H in DMSO d6 can produce a peak at 2.50 ppm, which might be mistaken for a methyl group. Recognizing these impurity signatures is essential to avoid misassignments.

## 4. NMR Chemical Shifts of Common Solvents as Trace Impurities

### 4.1 Reference Table of Solvent Impurity Peaks

Below is a concise table summarizing the most common solvent impurities and their typical chemical shift positions in 1H NMR. These values are averages and may vary slightly depending on temperature and instrument calibration.

| Solvent | Impurity | Typical ppm (1H) |
|---|---|---|
| CDCl3 | Residual CHCl3 | 7.26 |
| CDCl3 | Water (H2O) | 1.5 |
| CDCl3 | CH2Cl2 | 5.25 |
| C6D6 | Residual C6H6 | 7.26 |
| C6D6 | Water | 3.4 |
| CD3OD | Residual CD3OD | 3.31 |
| CD3OD | Water | 3.5 |
| CD3CN | Residual CD3CN | 2.05 |
| CD3CN | Water | 4.7 |
| DMSO d6 | Residual DMSO | 2.50 |
| DMSO d6 | Water | 3.3 |
| CD3COOD | Residual CD3COOD | 2.0 |
| CD3COOD | Water | 3.3 |
| CD3CO2CH3 | Residual CD3CO2CH3 | 2.04 |
| CD3CO2CH3 | Water | 3.3 |
| CD3CH3 | Residual CD3CH3 | 1.20 |
| CD3CH3 | Water | 3.3 |

### 4.2 Detailed Discussion of Each Solvent

CDCl3 is the most widely used solvent for 1H NMR because of its excellent solvating ability and low boiling point. Its residual CHCl3 peak at 7.26 ppm is a convenient reference but can also mask signals in the aromatic region. Water in CDCl3 appears as a broad singlet near 1.5 ppm; it is usually suppressed by drying the solvent over molecular sieves or by adding a small amount of dry benzene.

In aromatic chemistry, C6D6 is preferred because it does not interfere with the aromatic region of the sample. The residual C6H6 peak at 7.26 ppm is useful for referencing. However, water in C6D6 appears at 3.4 ppm, potentially overlapping with aliphatic methine protons.

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