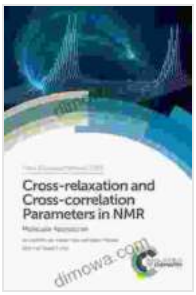
Cross Relaxation and Cross Correlation Parameters in NMR: A Comprehensive Guide



Cross-relaxation and Cross-correlation Parameters in NMR: Molecular Approaches (ISSN) by Sunil Tanna

★★★★★ 5 out of 5

Language	: English
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Text-to-Speech	: Enabled
Screen Reader	: Supported
Enhanced typesetting	: Enabled
Print length	: 383 pages

Nuclear magnetic resonance (NMR) spectroscopy is a powerful tool for studying the structure and dynamics of molecules. Cross relaxation and cross correlation parameters are two important types of NMR parameters that can provide valuable information about the interactions between different atoms in a molecule.

Cross Relaxation

Cross relaxation is a process in which the magnetization of one atom is transferred to another atom through a dipole-dipole interaction. This process can occur between any two atoms that are close enough together, but it is most efficient between atoms that have similar chemical shifts.

The rate of cross relaxation is determined by the strength of the dipole-dipole interaction between the two atoms and the correlation time of the

motion that is responsible for the interaction. The correlation time is the average time that it takes for the two atoms to move relative to each other.

Cross relaxation can be used to measure the distance between two atoms. The distance between two atoms can be determined by measuring the rate of cross relaxation between the two atoms and then using the following equation:

r = (1/d^3) * (kT/h) * (6J(0) / J(\omega_0))

where:

* r is the distance between the two atoms * d is the dipole-dipole coupling constant * k is the Boltzmann constant * T is the temperature * h is the Planck constant * J(0) is the spectral density at zero frequency * J(\omega_0) is the spectral density at the Larmor frequency

Cross Correlation

Cross correlation is a process in which the magnetization of one atom is modulated by the magnetization of another atom. This process can occur between any two atoms that are close enough together, but it is most efficient between atoms that have similar chemical shifts.

The rate of cross correlation is determined by the strength of the dipole-dipole interaction between the two atoms and the correlation time of the motion that is responsible for the interaction.

Cross correlation can be used to measure the distance between two atoms. The distance between two atoms can be determined by measuring the rate

of cross correlation between the two atoms and then using the following equation:

r = (1/d^3) * (kT/h) * (2J(0) / J(\omega_0))

where:

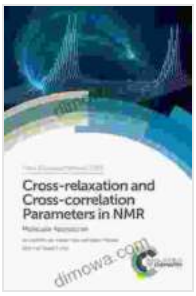
* r is the distance between the two atoms * d is the dipole-dipole coupling constant * k is the Boltzmann constant * T is the temperature * h is the Planck constant * J(0) is the spectral density at zero frequency * J(\omega_0) is the spectral density at the Larmor frequency

Applications of Cross Relaxation and Cross Correlation Parameters

Cross relaxation and cross correlation parameters are used in a wide variety of applications, including:

- **Structural biology:** Cross relaxation and cross correlation parameters can be used to determine the structure of proteins and other macromolecules.
- **Drug discovery:** Cross relaxation and cross correlation parameters can be used to study the interactions between drugs and their targets.
- **Materials science:** Cross relaxation and cross correlation parameters can be used to study the structure and dynamics of materials.

Cross relaxation and cross correlation parameters are two important types of NMR parameters that can provide valuable information about the interactions between different atoms in a molecule. These parameters are used in a wide variety of applications, including structural biology, drug discovery, and materials science.



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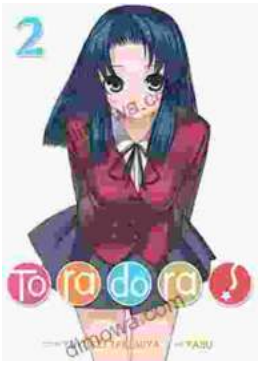

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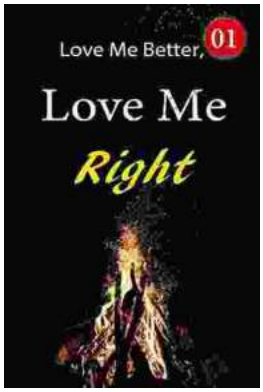

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