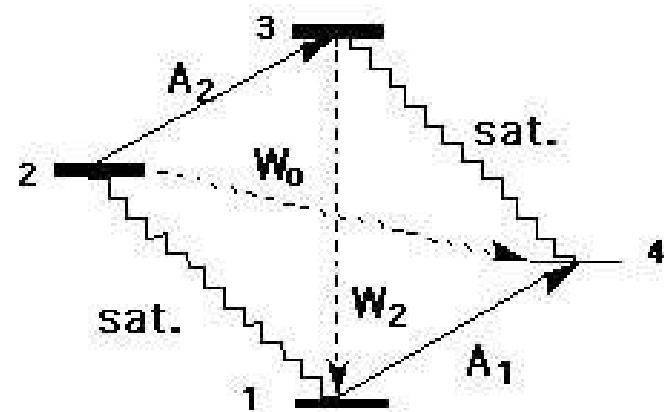
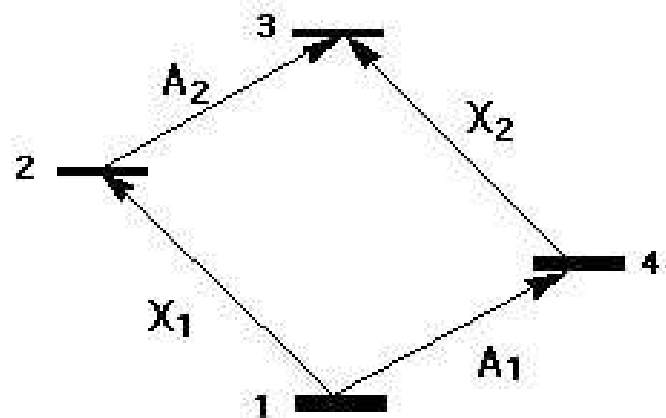


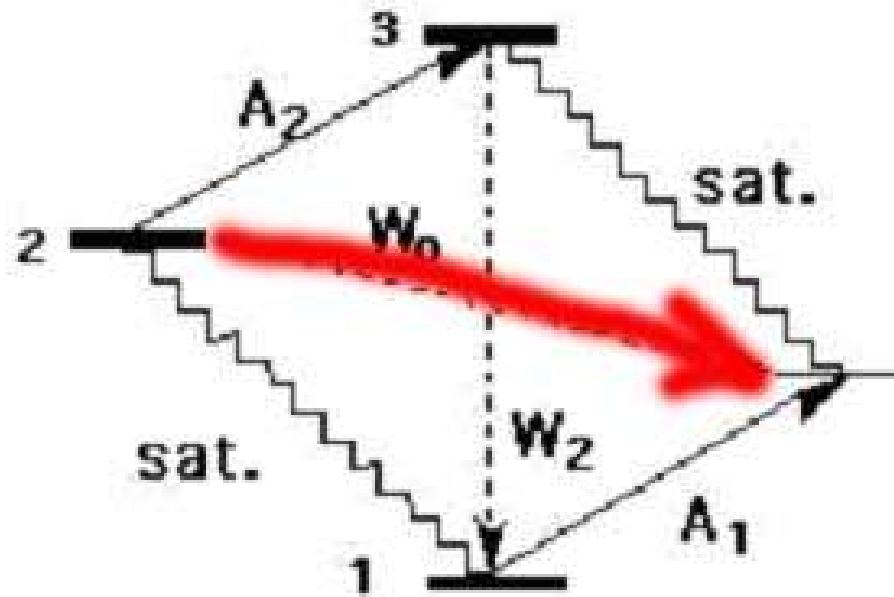
Effetto Overhauser

n.O.e.

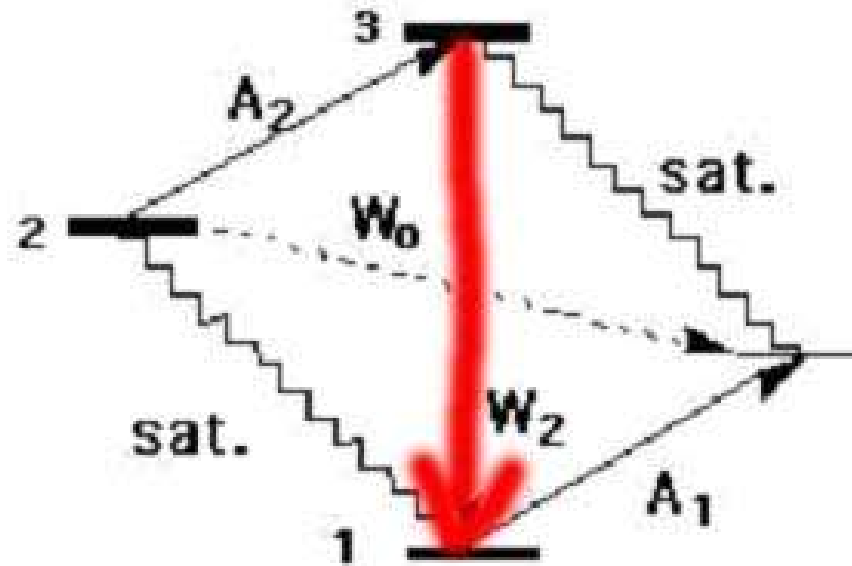
NOE Stazionario



Transizione a zero quanto W_0



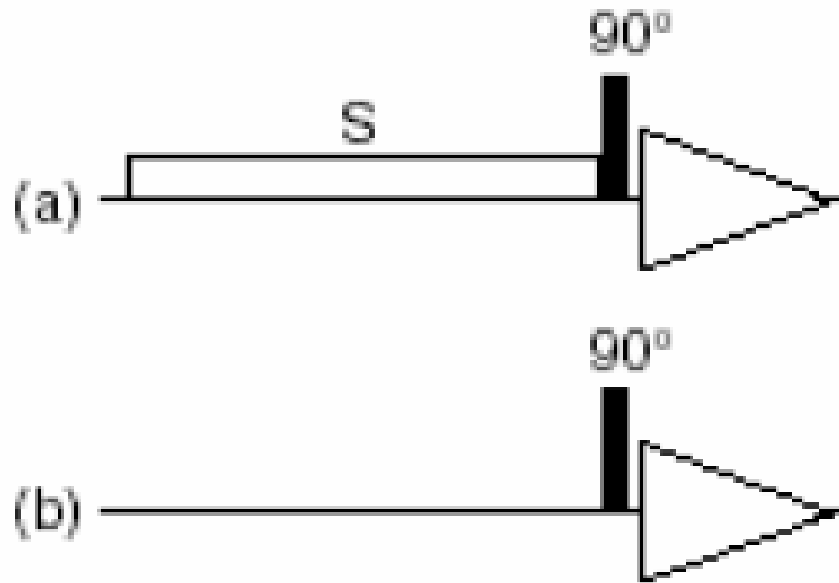
Transizione a doppio quanto W_2



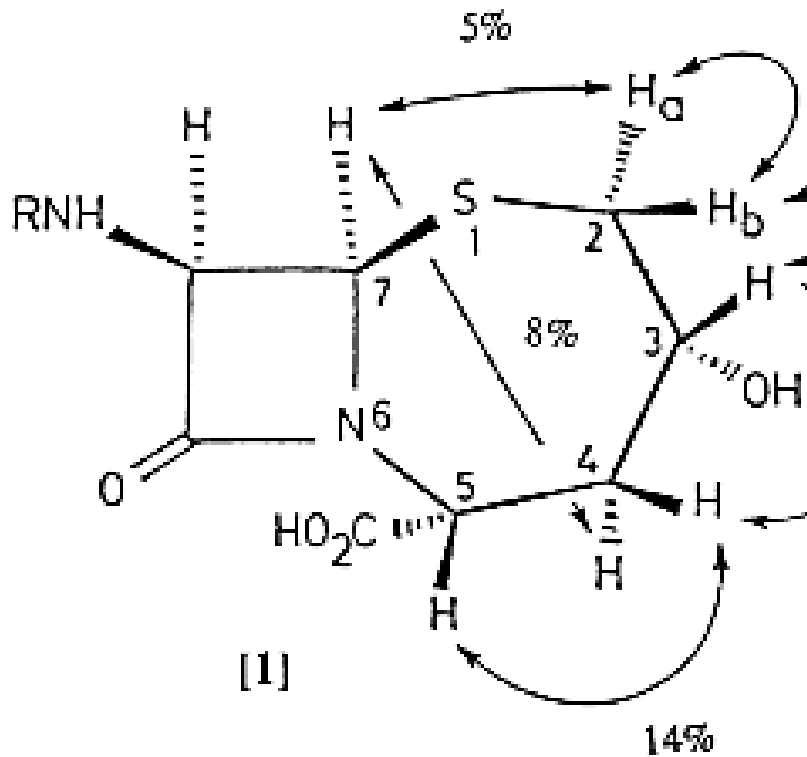
Segno del NOE

$$\xi = \frac{\sigma_{IS}}{\rho_I} \cdot \frac{S_z^0}{I_z^0} = \frac{\gamma_S}{\gamma_I} \cdot \frac{W_2 - W_0}{W_0 + 2W_1^I + W_2}$$

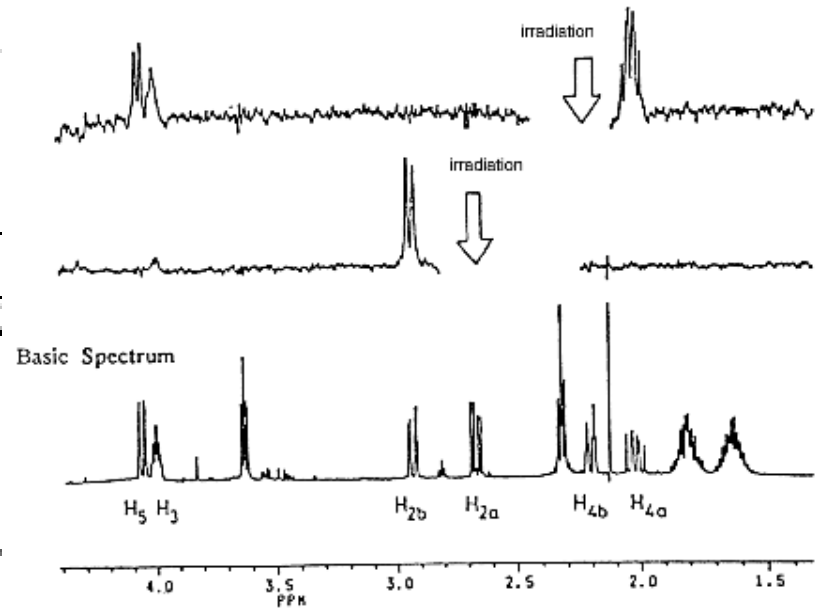
NOE differenza



Esempio



NOE Difference spectra.



Indicazioni Bruker

Introduction

The NOE difference experiment is useful for detecting NOE signals in small molecules. The main advantage over a 2D NOESY experiment is the time required for this experiment. If you are only concerned with a small number of NOE relationships and the compound under investigation yields a fairly well resolved ^1H spectrum, you can perform a NOE-DIFF experiment in about one tenth the time it takes for the 2D experiment.

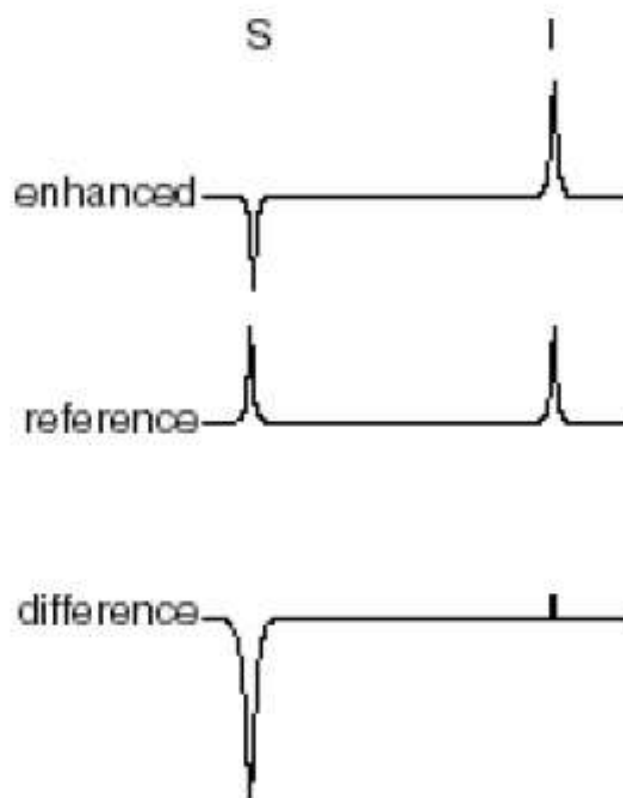
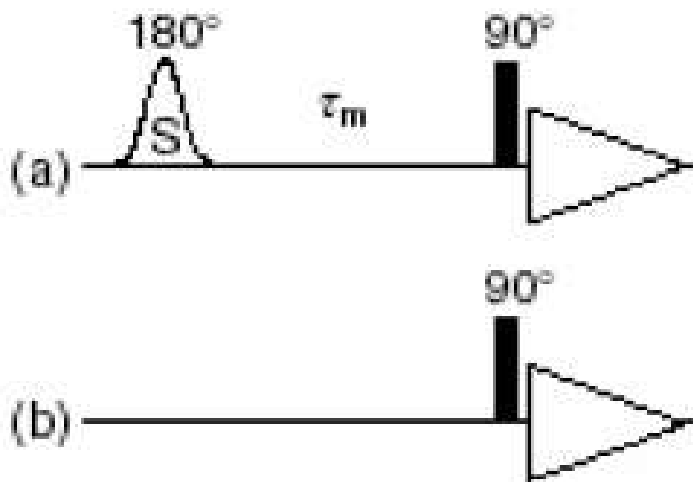
Sample Preparation

It is essential that you start with a dilute, degassed sample. It is recommended that you use a concentration of about 1% (v/v) or roughly 5mg of sample per 700 μL of deuterated solvent. You should degas your sample by freezing it in liquid nitrogen and pulling a vacuum on the frozen solid for 5-10 minutes and the sample thawed. This procedure should be repeated three times. Use caution when performing the freeze-pump-thaw cycles.

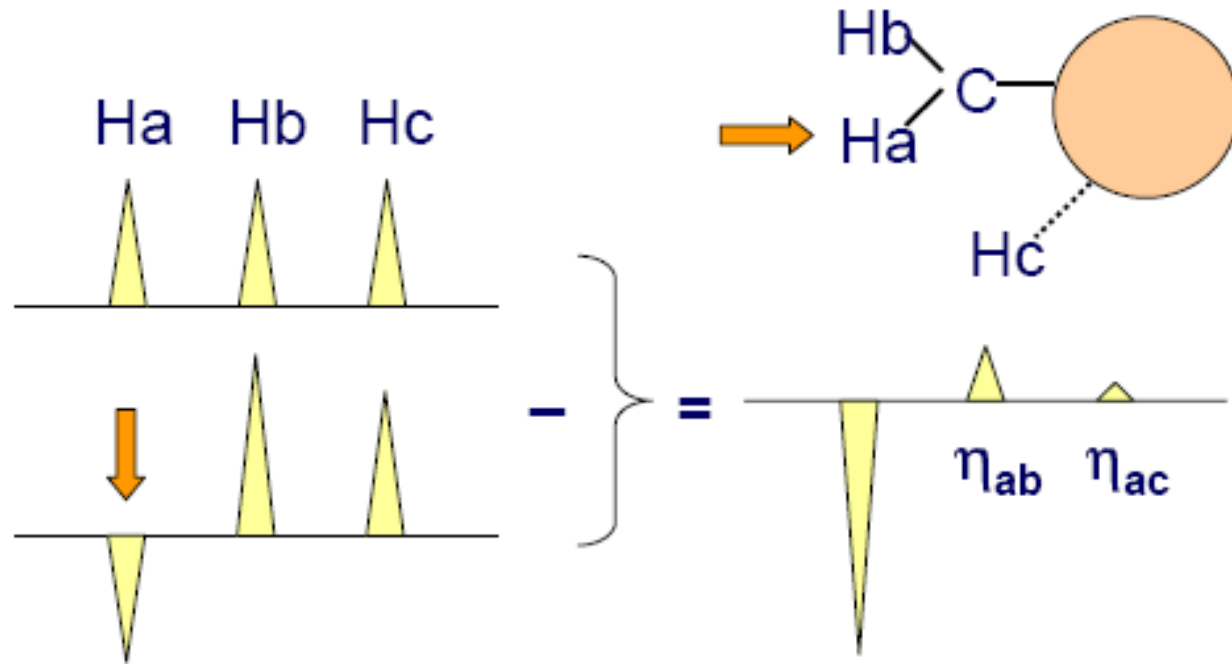
Acquire standard spectrum

- Lock and shim your sample as you would normally do. Once this is completed, turn off the spinning. This experiment detects small changes in signals and even a slight wobble in sample spinning can mask NOE.

NOE transiente



Misura di distanze internucleari

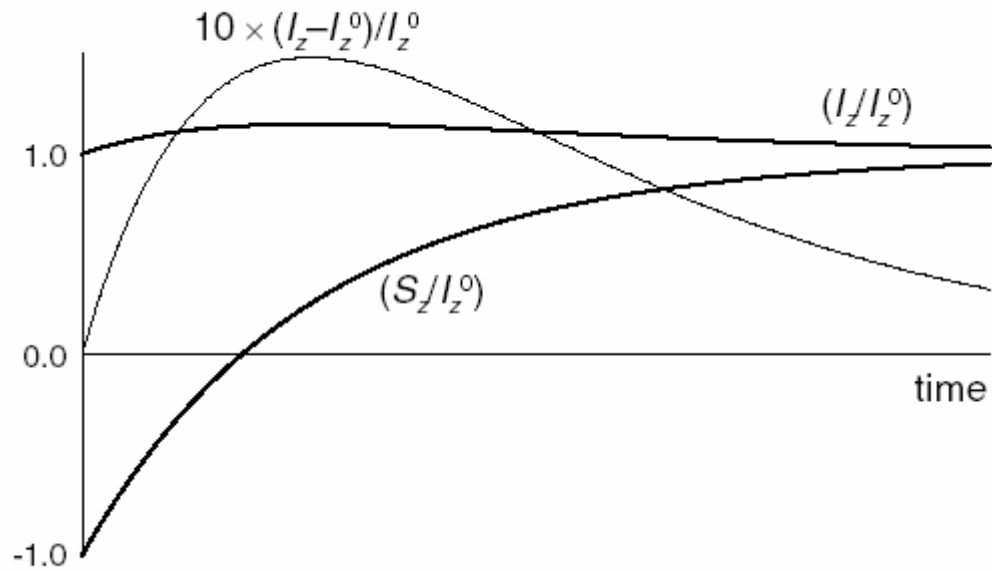


$$\eta_{ab} \propto r_{ab}^{-6}$$

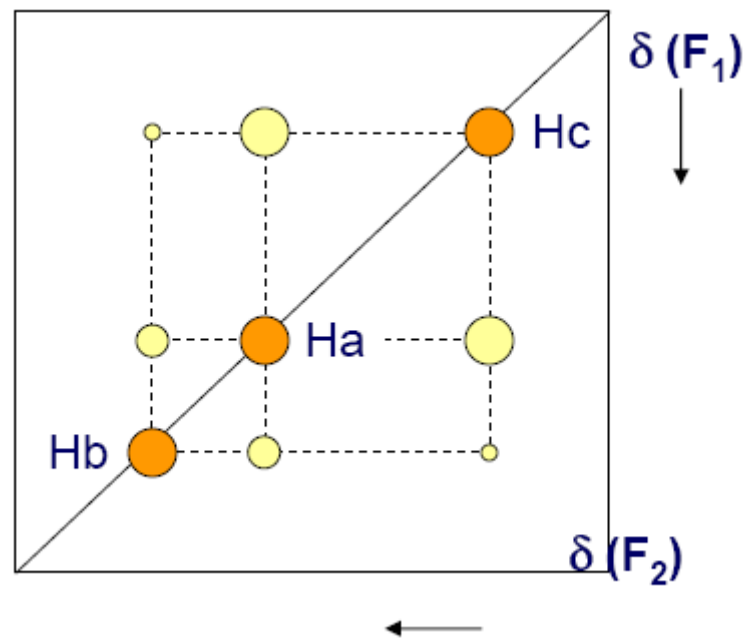
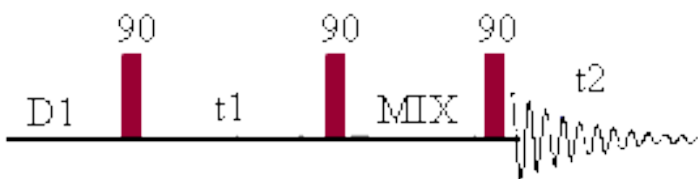
$$\eta_{ac} \propto r_{ac}^{-6}$$

$$r_{ac} = r_{ab} * (\eta_{ab} / \eta_{ac})^{-1/6}$$

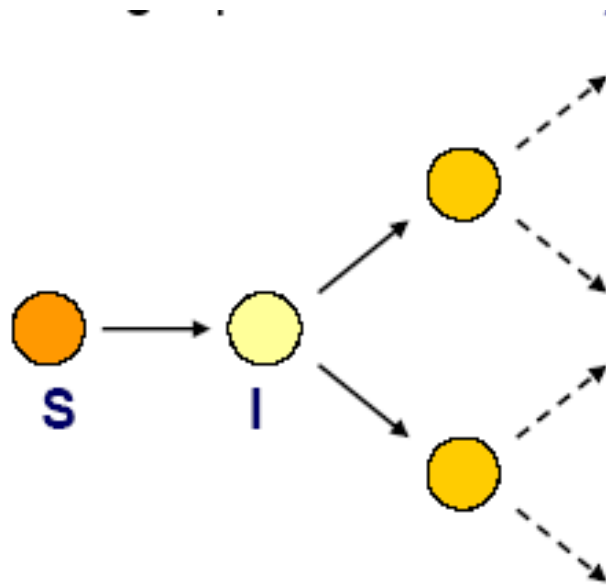
Crescita del n.O.e.



NOESY



Spin Diffusion



ROESY

