

ROSY: The answer to mixture analysis in solid state NMR

The ROSY method facilitates easier and faster analysis of samples mixed with more than two components (crystals).

Mixture analysis by ROSY(Relaxation Ordered Spectroscopy) method

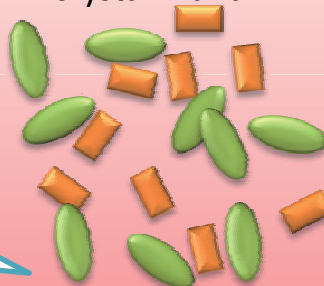
Due to the fast spin-diffusion among ^1H spins, the longitudinal relaxation time (T_1) of ^1H spins is governed by the fast relaxing fractions and is uniform within each crystal. Thus we can separate ^{13}C CPMAS spectra of each crystal by sorting spectra of the mixture into order of ^1H T_1 time. The procedure is numerically done by inverse Laplace transformation.

^{13}C CPMAS spectrum of physical mixture of crystal A and B



^{13}C CPMAS spectra shows signals both crystal A and crystal B overlapped each other.

physical mixture of crystal A and B



T_1 relaxation measurement of ^1H nuclei via ^{13}C CPMAS observation + inverse Laplace transformation

^{13}C CPMAS spectrum of crystal A



only A is visible



only B is visible

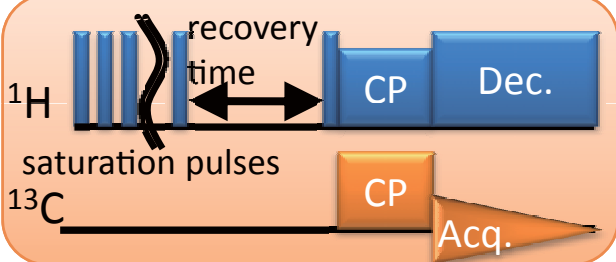


Obtain separated ^{13}C spectra!

^{13}C CPMAS spectrum of crystal B

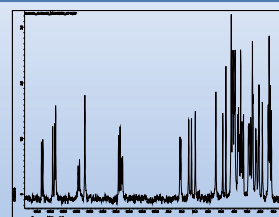
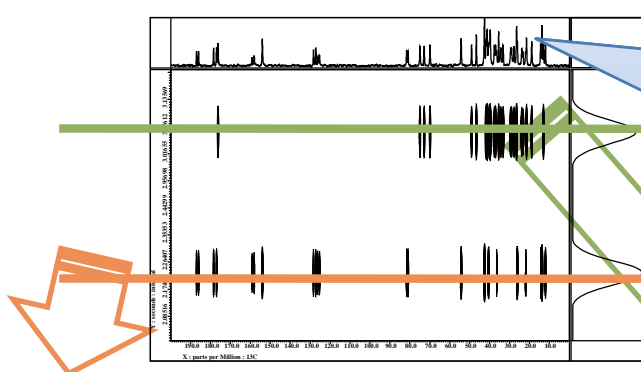


Experiments and processes



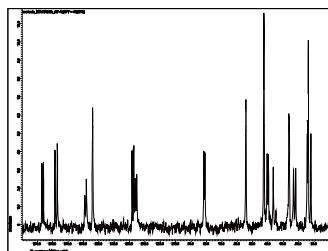
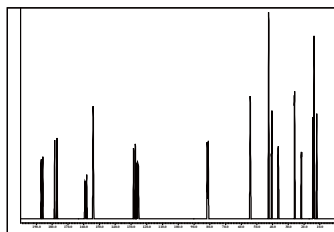
inverse Laplace transformation

Results: the mixture of santonin and cholic acid



¹³C CPMAS spectrum shows overlapped signals of santonin and cholic acid.

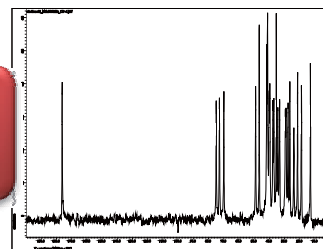
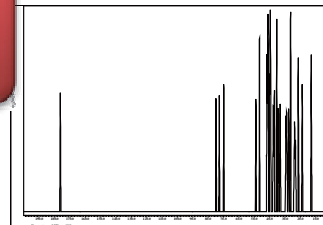
santonin



slices of ROSY spectrum of the mixture

CPMAS spectra of pure materials for each sample

cholic acid



ROSY method provides a separate ¹³C CPMAS spectra from the mixture

※Inverse Laplace Transforms for ROSY will be available in Delta V 5.0.