Study of Chemical Exchange by NMR

Product used : Nuclear Magnetic Resonance (NMR)

NMR is a powerful tool for the study of chemical exchange.
When a spin exchanges between two sites with different chemical shifts then the NMR signal for that spin is largely determined by the time scale of the exchange event.
If the chemical shift difference between the two sites is larger than the exchange rate then the exchange is described as slow exchange on the NMR time scale. Hallmark of slow exchange is the appearance of two separate NMR signals representing the two states.
Slow exchange can be verified and quantitatively analyzed by a simple 1D NMR experiment.

Selective Inversion Recovery Experiment

In the Selective Inversion Recovery experiment (double_pulse_shape.jxp), one of the two signals under exchange is selectively inverted. Due to exchange, the perturbation of one signal is propagated to the second signal. The magnetization recovery of both signals can be monitored and analyzed in order to extract information about the exchange event.
In order to facilitate fitting, supplementary experiments can be conducted. For instance, the above experiment can be repeated with selective inversion of the second signal or an experiment can be conducted where one of the two signals is selectively saturated.

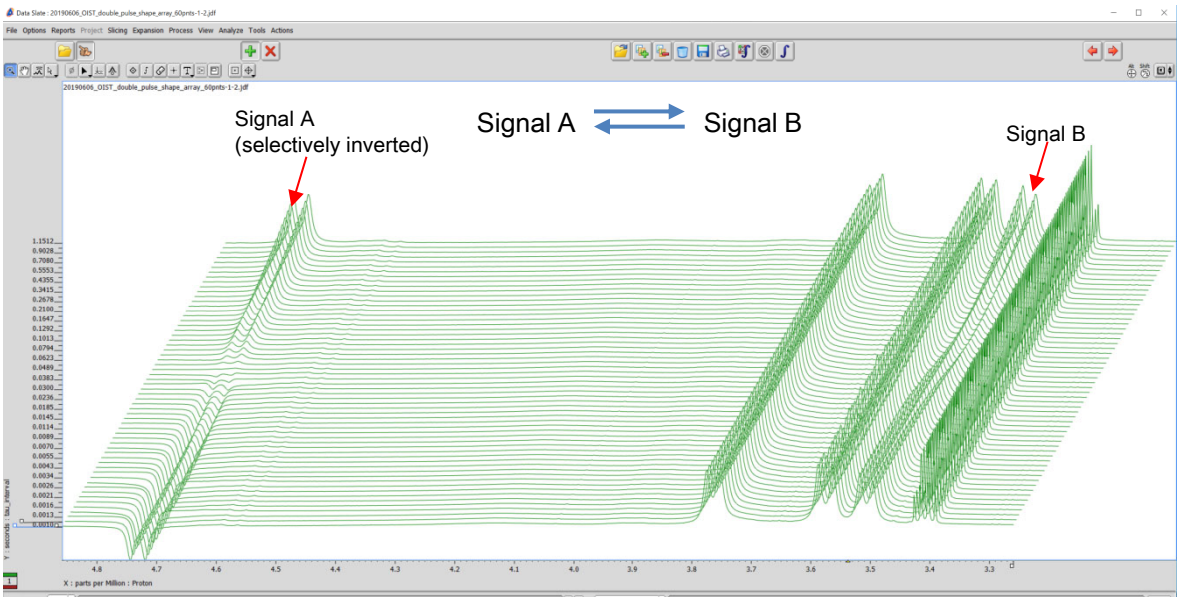

Fig 1: Selective inversion recovery. Data analyzed with Data Slate.

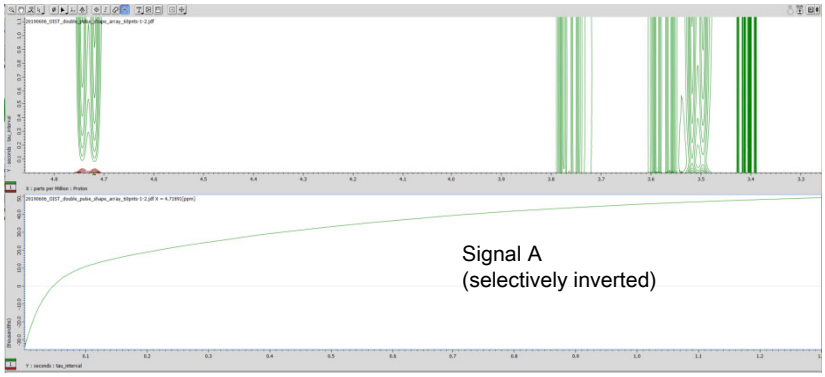

Fig 2: Magnetization Recovery of signal A. Data analyzed with Curve Analysis using peak heights

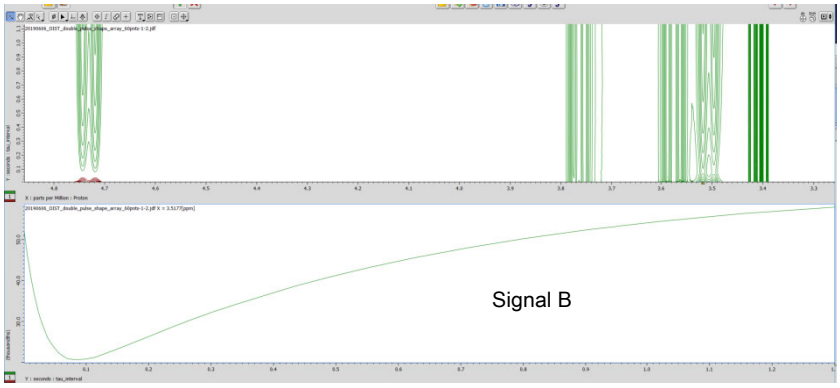

Fig 3: Magnetization Recovery of signal B. Data analyzed with Curve Analysis using peak heights

Data can be exported as txt, csv or excel file for analysis with a third party software. Exported files can easily be prepared with 'Curve Analysis' or 'Kinetics Analysis' tool.

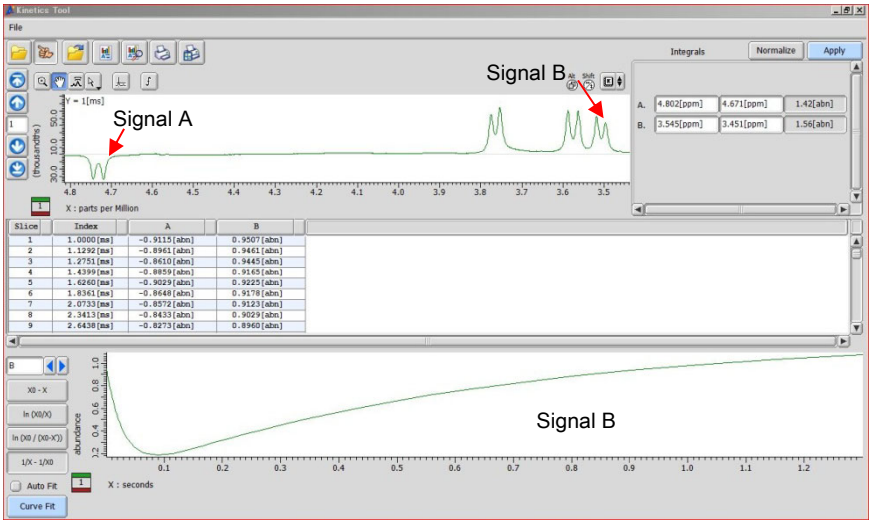

Fig 4: Selective inversion recovery. Data analyzed with 'Kinetics Analysis' tool using peak integrals

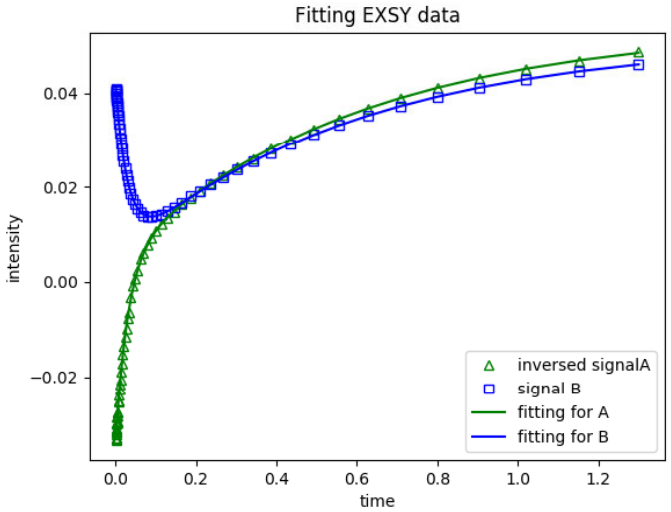

Fig 5: EXSY data analysis. Exported data were analyzed with a in-house prepared python script

Sample , a conformationally flexible cationic Cu(I) complex, courtesy of Assist. Prof. Julia Khusnutdinova , Coordination Chemistry and Catalysis Unit, OIST, Japan

Reference: *J. Magnetic Resonance. 1977, 27, 137-141.*

console: JNM-ECZ600R+ROYALPROBE™ HFX

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