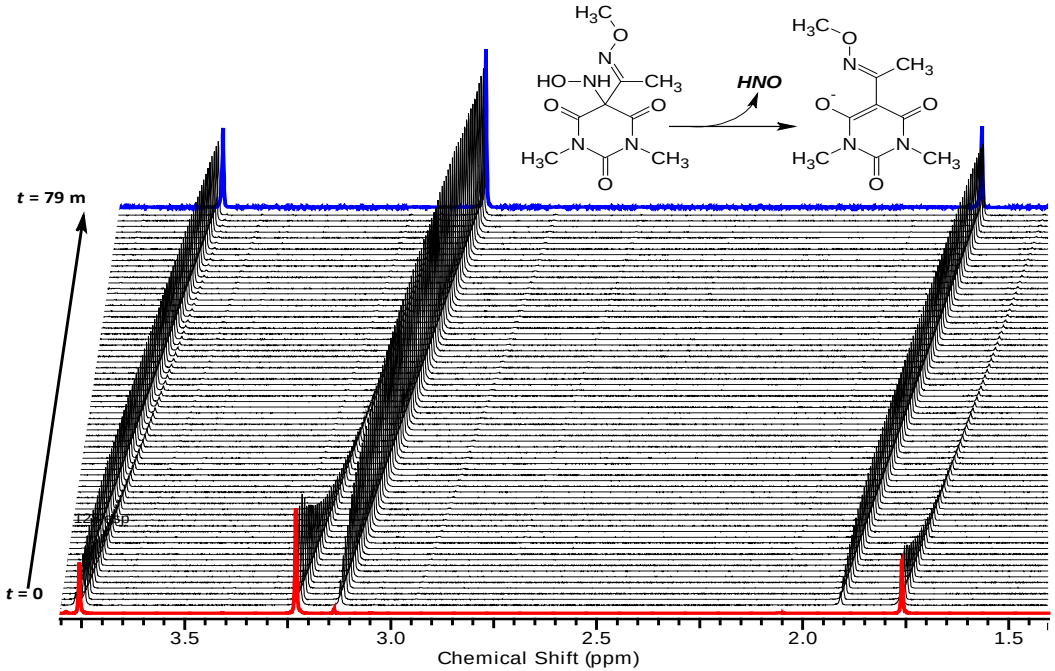
Monitoring Reactions by NMR



This experiment requires some knowledge of the reaction before actually acquiring the data:

- Does it have an induction period?
- How long does it take to complete?
- Is it exothermic? (please don't run it in the NMR if it is very exothermic)

This information can be obtained by other methods, like UV-vis or TLC time points. Once the timeframe for the reaction has been determined, then the specifics of the NMR scale reaction can occur.

NMR reaction monitoring

- Run a 1D of the reactants and products in the deuterated version of the reaction solvent
- Have a good idea of the reaction half life to enable reasonable estimation of parameters **d20** and **td1**
- Use Pulse sequence **zg2d** (to the right)
- With **td1** set to 1, use the experiment time command, expt, to determine how long the 1D takes to acquire
  - **d20** is the time between the start of the two experiments
  - **d20** must be longer than the time required to acquire the 1D experiment so that DELTA is not a negative number
  - the number of time points to be taken is defined by **td1**
  - total reaction time/d20 = **td1**
- Acquire the data using zg
- Process the data with either xf2, xau splitser, or rser x

```
;zg2d
;avance-version (04/01/15)
;pseudo 2D sequence

#include <Avance.incl>
#include <Delay.incl>
"DELTA=d20-((d1+aq)*(ns+ds))-30m"
"acqt0=-p1*2/3.1416"

1 ze
  30m
2 DELTA
3 d1
  p1 ph1
  go=3 ph31
  30 m wr #0 if #0 ze
  lo to 2 times td1
exit

ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1

;pl1 : f1 channel - power level for pulse (default)
;p1 : f1 channel -  90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1
;d20: delay between start of different 1D spectra
;NS: 1 * n
;td1: number of experiments
;FnMODE: QF
```