Supporting Information for:

Fast magic angle spinning solid state 1H NMR reveals structural relationships in the high explosive 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105)

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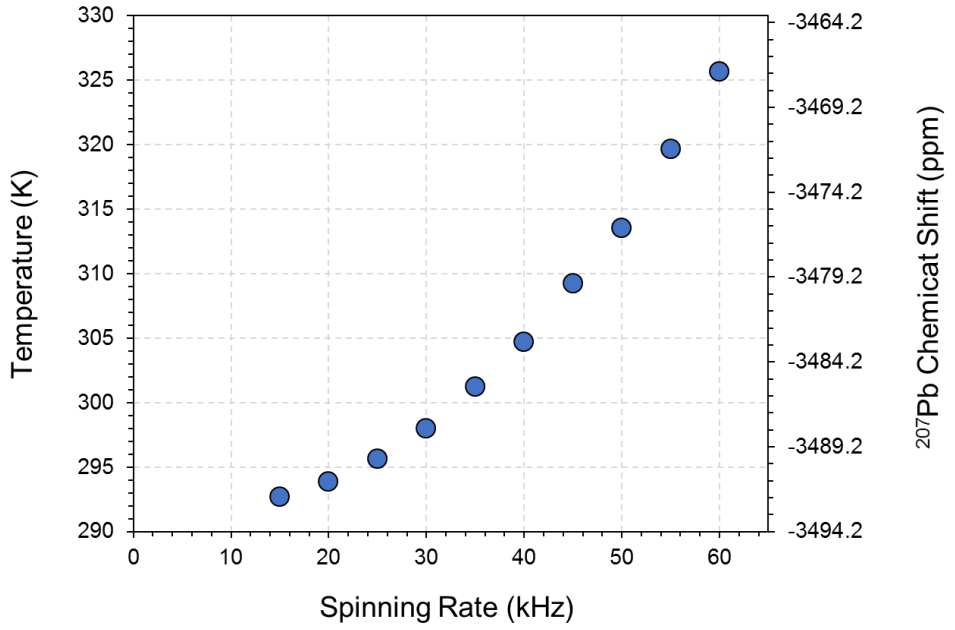

Figure S1. Sample temperature and corresponding chemical shift of $Pb(NO_3)_2$ in the 1.3 mm rotor plotted as a function of the sample spinning speed.

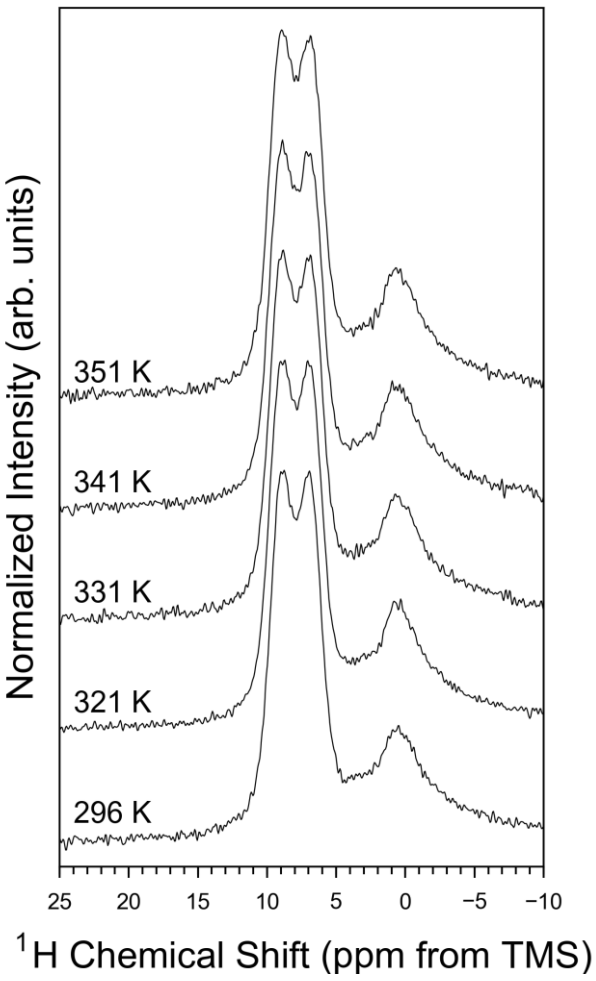

Figure S2. ^{1}H SP/MAS NMR spectra collected of LLM-105 at 50 kHz spinning speed and the indicated temperature. A 30 s recycle delay was used to collect the data.

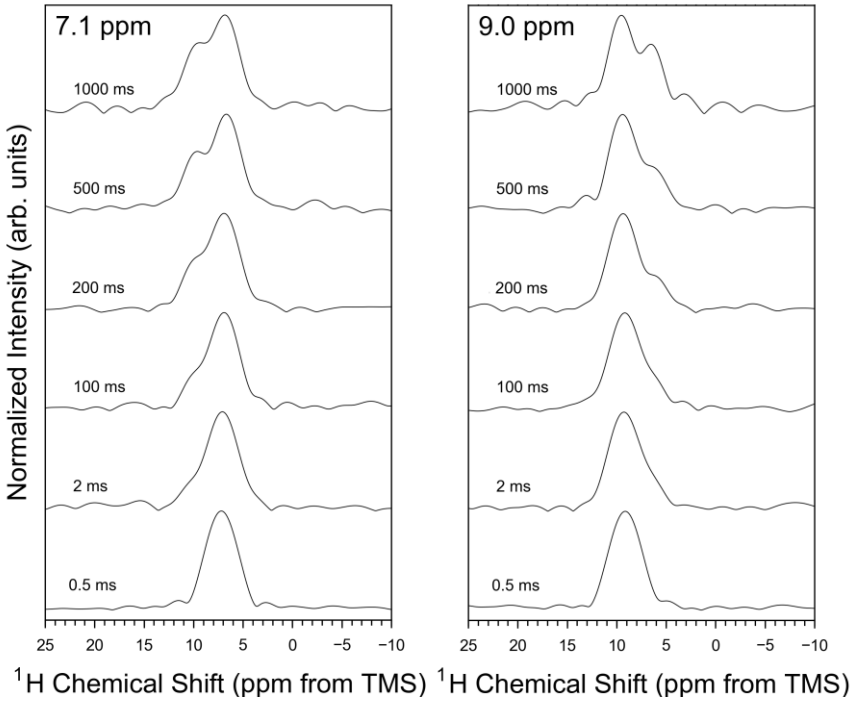

Figure S3. Indirect dimension (F1) slices taken at given positions from the ^{1}H EXSY NMR spectra collected of LLM-105 at the indicated mixing times.

Pulse sequence for Bruker Avance III spectrometer running Topspin 3.x

```
;csarec
;avance-version (12/01/11)
;
;2D gamma encoded R-based 1H CSA recoupling sequence
;Uses rotor synchronized echo prior to acquisition to remove probe
background
;R sequence is coded into a seperate decoupling sequence
;
;Harris E Mason
;Lawrence Livermore National Laboratory
;Avance II+/III Verson
;Topspin 3.x
:
;$CLASS=Solids
;$DIM=1D
;$TYPE=
;$SUBTYPE=
;$COMMENT=
;
;referncees
;(1) Pandey, M. K.; Malon, M.; Ramamoorthy, A.; Nishiyama, Y., J. Mag.
Res. 2015, 250, 45-55
;(2) Pandey, M. K.; Nishiyama, Y. J. Mag. Res. 2015, 261, 133 - 140

#include <Avance.incl>


"p2=p1*3"
define delay del25          ;calculate sync. delays
"del25=(2s*(cnst29/cnst30)/cnst31)" ;modifies tau, duration of R
sequence.  d12 is the variable

1 ze
2 30m
  d1 do:f1
3 (del25 cpds1 ph4):f1  ; R sequence
lo to 3 times c
  2u do:f1
  (p1 ph1):f1
  d6
  (p2 ph2):f1
  d7
  go=2 ph31
  d11 wr #0 if #0 ivc
  lo to 1 times td1
exit


ph1=0 0 2 2 1 1 3 3
```

```
ph2=1 3 1 3 0 2 0 2
ph4=0 2 0 2
ph31=0 0 2 2 1 1 3 3


;pl1 : f1 channel - power level for pulse (default)
;p1 : f1 channel -  90 degree high power pulse
;p2 : f1 channel - 180 degree high power pulse
;d1 : recycle delay
;d6 : echo delay
;d7 : d6 - de
;del25 : delay period for R sequence
;cnst29 : small n
;cnst30 : large N
;cnst31 : = MAS spin rate
;cpds1 : R sequence used
;pl13 : power level for R sequence
;
;For a particular R sequence pl13 need setting so rf=(N*wr/2*n)
;
;ns:  16 * n, total number of scans: NS * TD0
;
;$Id: csarec,v 1.4 2012/01/31 17:49:31 ber Exp $
```

CPD Program for the $R12_5^4$ sequence

```
  0.5u pl=pl12
1 p31:60
  p32:240
  p31:300
  p32:120
jump to 1
```