

November 12 – 13, 2015

*Ultrahigh Field NMR and MRI: Science at the
Crossroads*

*Biotechnology Resource Center for NMR Molecular
Imaging of Proteins*

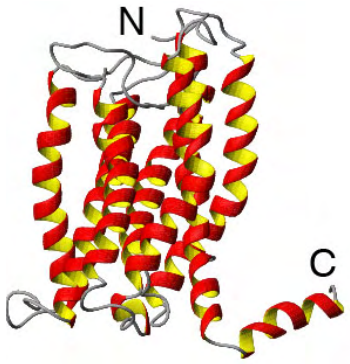
P41 EB002031

*Department of Chemistry and Biochemistry
University of California, San Diego*

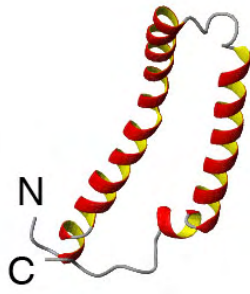


Membrane protein structures determined in phospholipid bilayers.

CXCR1



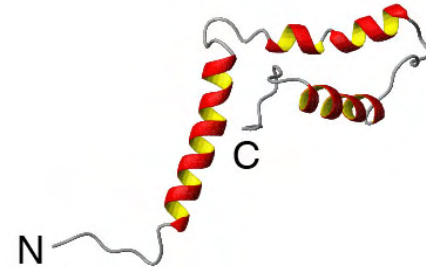
MerF



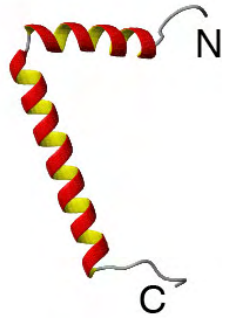
p7



Vpu

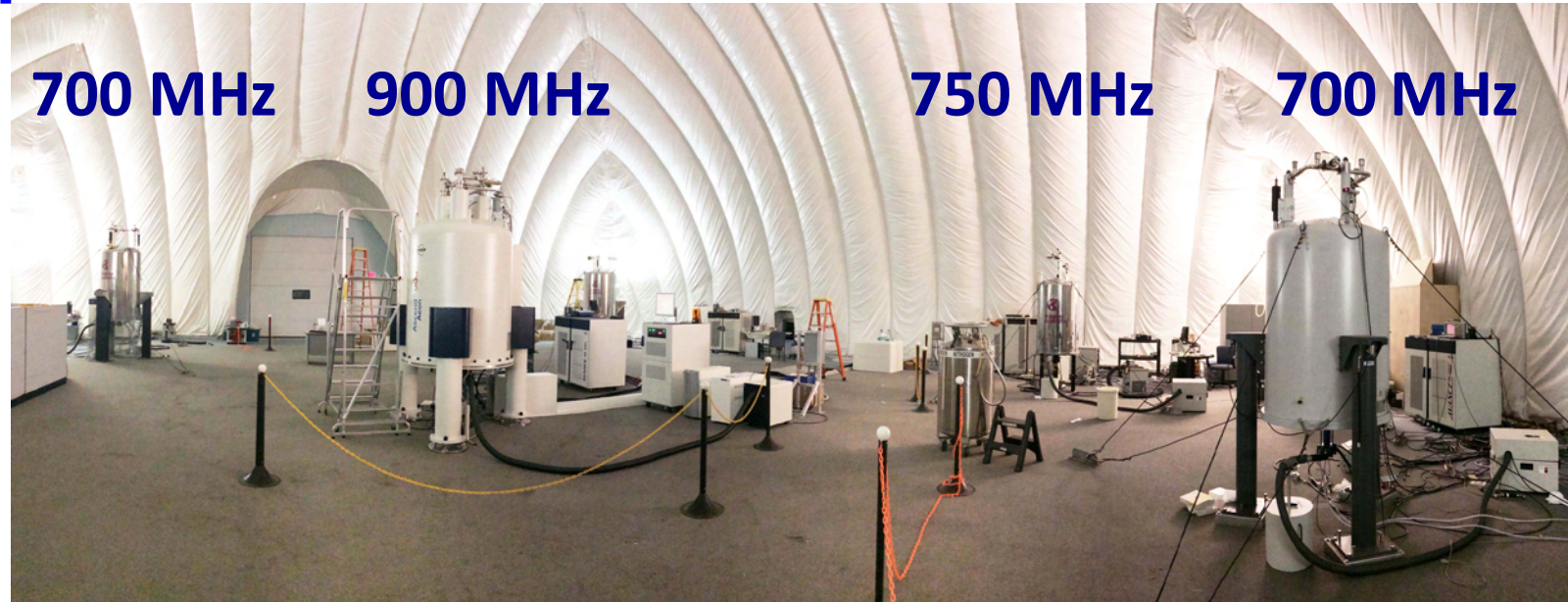


fd coat



NMR and biochemistry laboratories.

Solid-state NMR spectroscopy



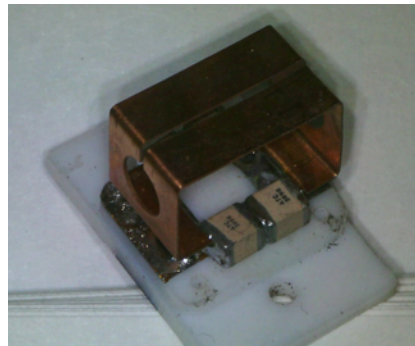
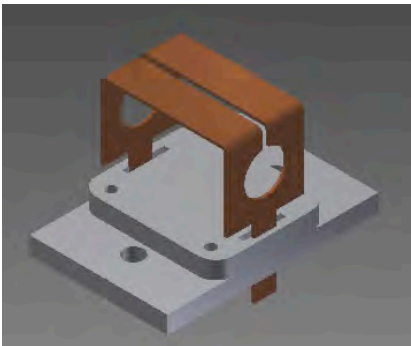
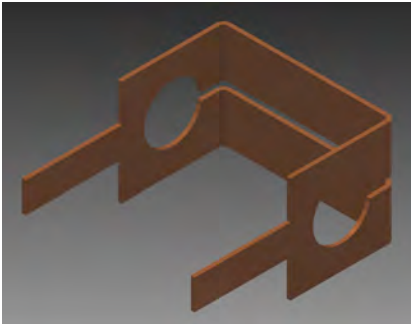
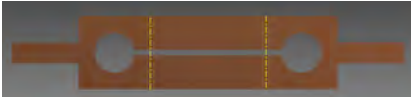
Molecular biology and biochemistry



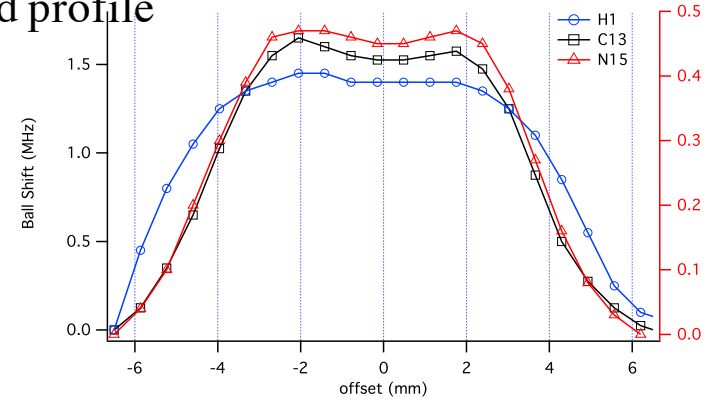
Coil Design from Concept to Implementation

Computer Aided design

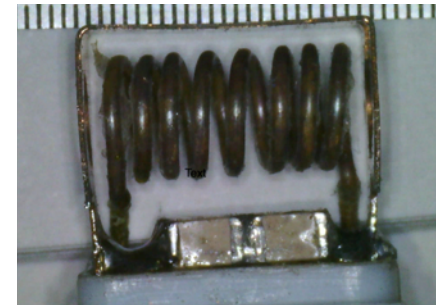
Implementation



B1 field profile

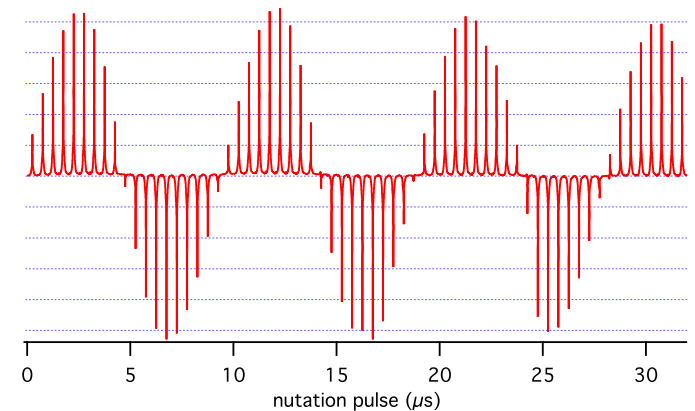


Cross coil



^1H channel:
200 Watts

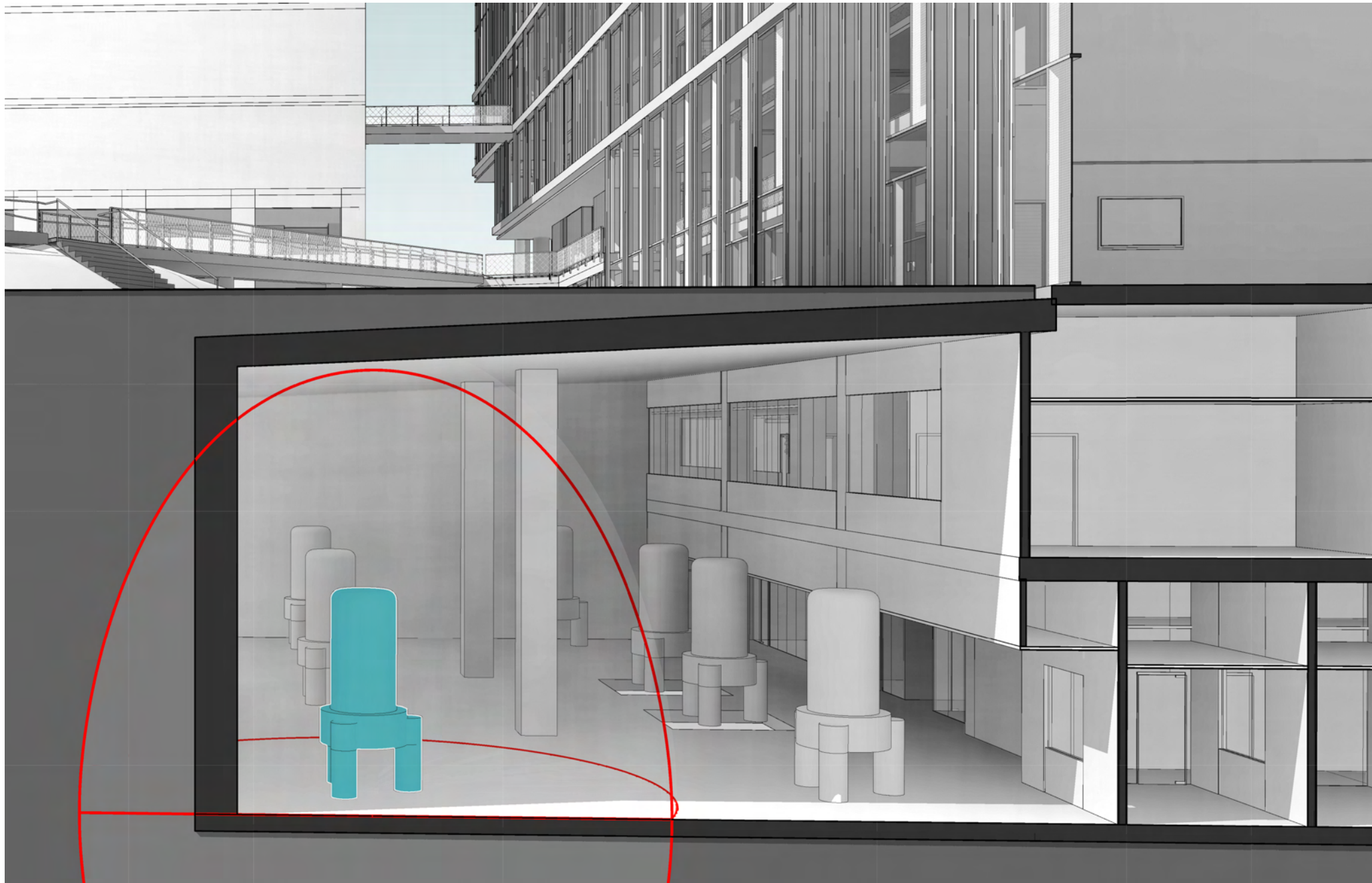
810/90: 95%
 B_1 : 106 kHz



New Biological and Physical Sciences building with NMR pavilion.

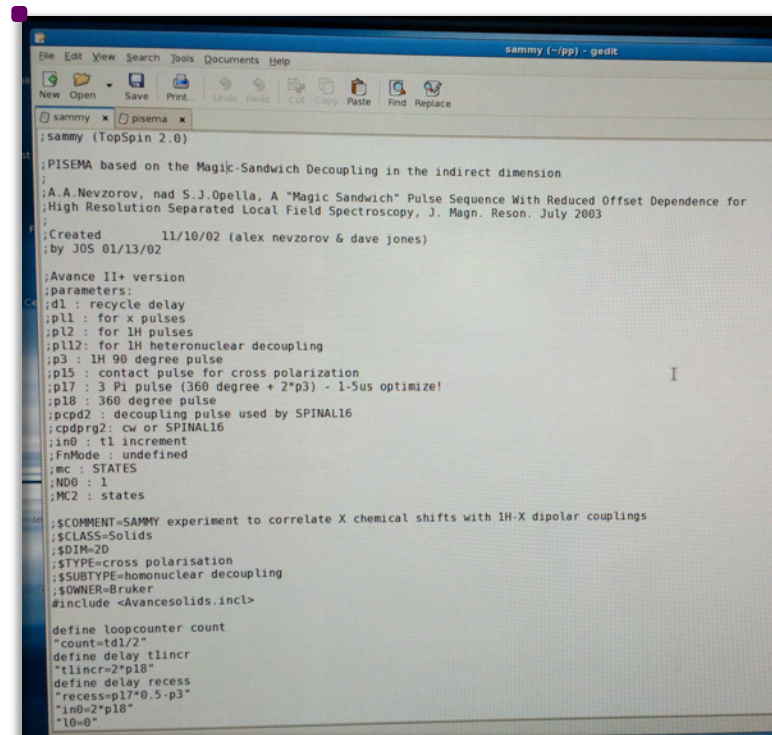


Placement of a UHF magnet in the new Biological and Physical Sciences building.



Dissemination of pulse sequences: NMR vendors.

- Advantages:
 - Polished and tested programs.
 - Instructions to calibrate.
 - Different software versions available.
- Disadvantages:
 - May take a while to be listed.



```
File Edit View Search Tools Documents Help
New Open Save Print Link Undo Cut Copy Paste Find Replace

sammy x piseema x
;sammy (TopSpin 2.0)
;PISEMA based on the Magic-Sandwich Decoupling in the indirect dimension
;A. A. Nevzorov, nad S. J. Opella, A "Magic Sandwich" Pulse Sequence With Reduced Offset Dependence for
;High Resolution Separated Local Field Spectroscopy, J. Magn. Reson. July 2003
;Created 11/10/02 (alex nevzorov & dave jones)
;by JOS 01/13/02

;Advance II+ version
;parameters:
;d1 : recycle delay
;p11 : for x pulses
;p12 : for 1H pulses
;p112: for 1H heteronuclear decoupling
;p3 : 1H 90 degree pulse
;p15 : contact pulse for cross polarization
;p17 : 3 Pi pulse (360 degree + 2*p3) - 1.5us optimize!
;p18 : 360 degree pulse
;pcpd2 : decoupling pulse used by SPINAL16
;cpdprg2: cw or SPINAL16
;in0 : t1 increment
;FnMode : undefined
;mc : STATES
;ND0 : 1
;MC2 : states

; $COMMENT=SAMMY experiment to correlate X chemical shifts with 1H-X dipolar couplings
; $CLASS=Solids
; $DIM=2D
; $TYPE=cross polarisation
; $SUBTYPE=homonuclear decoupling
; $OWNER=Bruker
; #include <Avancesolids.incl>

define loopcounter count
"count=td1/2"
define delay t1incr
"t1incr=2*p18"
define delay recess
"recess=p17*0.5-p3"
"in0=2*p18"
"l0=0"
```

*SAMPI-4 sequence from
the Opella Laboratory,
available in Bruker
Topspin*

Dissemination of pulse sequences: Individual Groups.

- Common methods.
 - One-to-one communication is the most widely used by small groups
 - Request through a website.
 - Direct download.
 - Download with registration.
- Advantages.
 - Rapid dissemination of the latest pulse sequences.
 - Interact directly with the originators.
- Disadvantages.
 - Generally less polished sequences.
 - Only one or a few software versions available.
 - May require personal communications.

Dissemination of pulse sequences: Individual group: Pascal M. Man website.

www.pascal-man.com

About P. Man | FAQ | Periodic Table | Related site | Site map | What's new

pascal-man.com

Quadrupole coupling in NMR

四極偶合

Search

Download source code	Phase cycling as Cogwheel	Pulse program	Pulse sequence	Quadrupole interaction	Search or Submit NMR reference
<ul style="list-style-type: none"> Running Java applet in Windows 7 			<p>Knowing the quadrupole coupling in NMR (nuclear magnetic resonance) of a nucleus in solids allows us to determine the local symmetry of a crystallographic site.</p> <p>With a featureless NMR lineshape, lineshape analysis is not suitable for determining the quadrupole coupling. Since the variation of the line intensity versus the RF (radio-frequency) pulse length depends on the quadrupole coupling, the one-dimensional nutation method, which records a series of spectra for increasing RF pulse length, allows us to extract the quadrupole coupling by fitting the experimental line intensities to the theoretical curve.</p> <p>Java applets are provided for calculating the nutation NMR line intensity of half-integer quadrupole spins, excited by various RF pulse sequences, in order to determine the quadrupole coupling in a single crystal and powder by fitting a series of experimental line intensities with the Simplex procedure.</p> <p>The applets have been written with SUN's JDK1.0.2, JDK1.1.8, and JDK1.3. The fastest execution of an applet is provided by:</p> <ul style="list-style-type: none"> Firefox, Internet Explorer, Google Chrome, Opera. 		
<p>GPU, JAVA 7 APPLICATION for denoising an FID with SVD</p> <ul style="list-style-type: none"> GPU_2012 SVD Java 7 application 					
<p>JDK1.4 JAVA APPLICATION</p> <ul style="list-style-type: none"> harmonic inversion harmonic inversion for improving spectrum resolution harmonic inversion for dead time correction 					
<p>JDK1.4 JAVA APPLET or APPLICATION for denoising an FID with SVD</p> <ul style="list-style-type: none"> with web browser or with Java Web Start and JCAMP-DX file SVD Java application New SVD Java application 2012 SVD Java application 					
<p>JDK1.3 JAVA APPLET</p>					

Recent NMR books, encyclopedia, reviews, and theses

Cours de DEA sur les symétries (PDF)
Franck Laloë

The Feynman Lectures on Physics

Solid-state NMR bibliography for

- Aluminum-27 (鋁)
- Antimony-121/123 (銻)
- Arsenic-75 (砷)
- Barium-135/137 (鋇)
- Beryllium-9 (鈹)
- Bismuth-209 (鉍)
- Boron-10/11 (硼)
- Bromine-79/81 (溴)
- Calcium-43 (鈣)
- Cesium-133 (銫)
- Chlorine-35/37 (氯)
- Chromium-53 (鉻)
- Cobalt-59 (鈷)
- Copper-63/65 (銅)
- Deuterium-2 (氘)
- Gallium-69/71 (鎵)
- Germanium-73 (鍬)
- Gold-197 (金)
- Hafnium-177/179 (鈦)
- Indium-113-115 (銻)
- Iodine-127 (碘)
- Iridium-191/193 (銦)
- Krypton-83 (氪)
- Lanthanum-139 (釷)
- Lithium-6/7 (鋰)
- Magnesium-25 (鎂)
- Manganese-55 (錳)
- Mercury-201 (汞)
- Molybdenum-95/97 (鉬)
- Neon-21 (氖)

Below NMR pulse program describes the **z-filter** approach for (1D and 2D) +3Q-MAS experiment applied to half-integer spin.

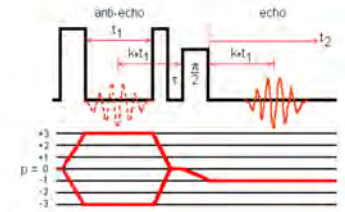


Fig. 1: Z-filter 3QMAS NMR pulse sequence and coherence transfer pathway. The echo amplitude and the antiecho amplitude have the same sign. The phase cycling for 3 strong pulses is discussed.

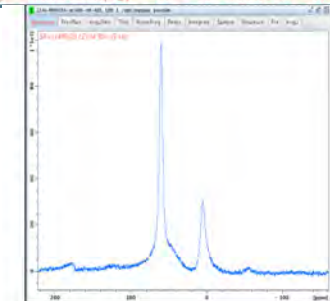
This NMR pulse program is for **Bruker Avance spectrometers**.

A pure absorption 2D spectrum is obtained with the **shearing transformation**.

Code for Avance III spectrometers

```

; mp3qzqf
; 3Q MAS pulse program for half-integer spin nuclei
; 3-pulse experiment with zero quantum filter:
; excitation(13Q) - conversion(9Q) - tau - 90° selective - ACQ(-10);
    
```



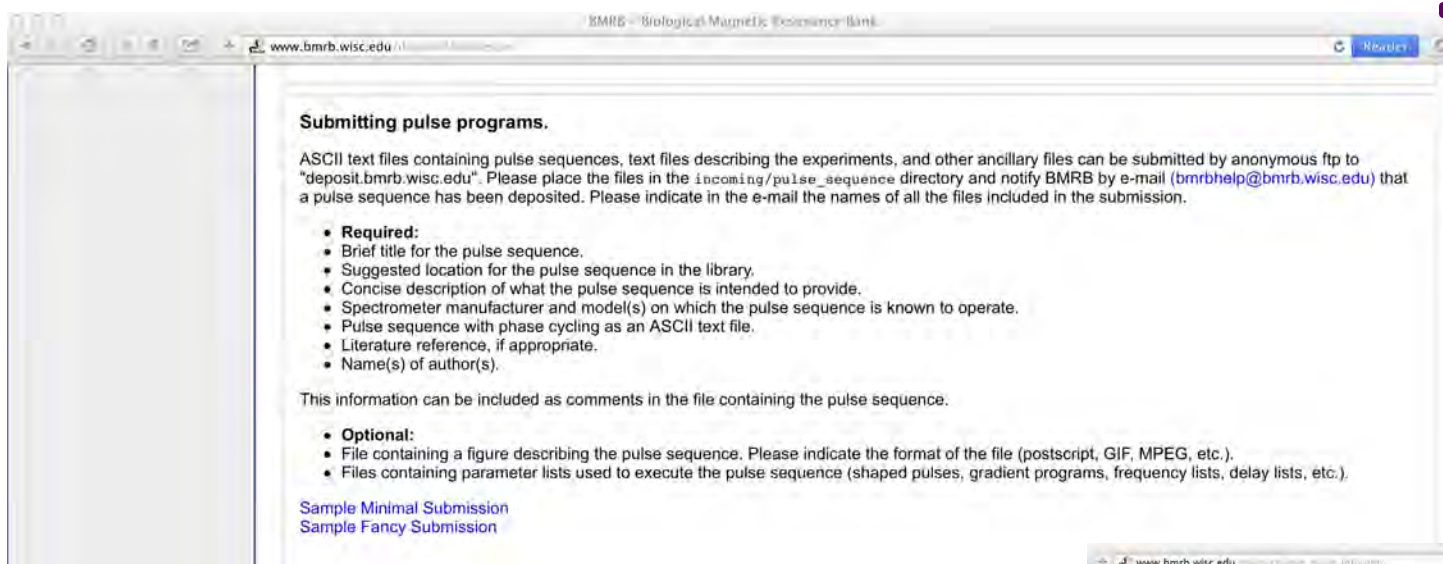
29Si zeolite, acquired with a 4-mm diameter rotor spinning at 15 kHz, D1 recorded with Bruker Avance III, 500 MHz.

Pulseprogram parameters for zg:

General

- code
- diagrams
- detailed settings
- example data

Dissemination of pulse sequences: Large center: redistributes pulse sequences.



Submitting pulse programs.

ASCII text files containing pulse sequences, text files describing the experiments, and other ancillary files can be submitted by anonymous ftp to "deposit.bmrw.wisc.edu". Please place the files in the `incoming/pulse_sequence` directory and notify BMRB by e-mail (bmrhelp@bmrw.wisc.edu) that a pulse sequence has been deposited. Please indicate in the e-mail the names of all the files included in the submission.

- **Required:**
 - Brief title for the pulse sequence.
 - Suggested location for the pulse sequence in the library.
 - Concise description of what the pulse sequence is intended to provide.
 - Spectrometer manufacturer and model(s) on which the pulse sequence is known to operate.
 - Pulse sequence with phase cycling as an ASCII text file.
 - Literature reference, if appropriate.
 - Name(s) of author(s).

This information can be included as comments in the file containing the pulse sequence.

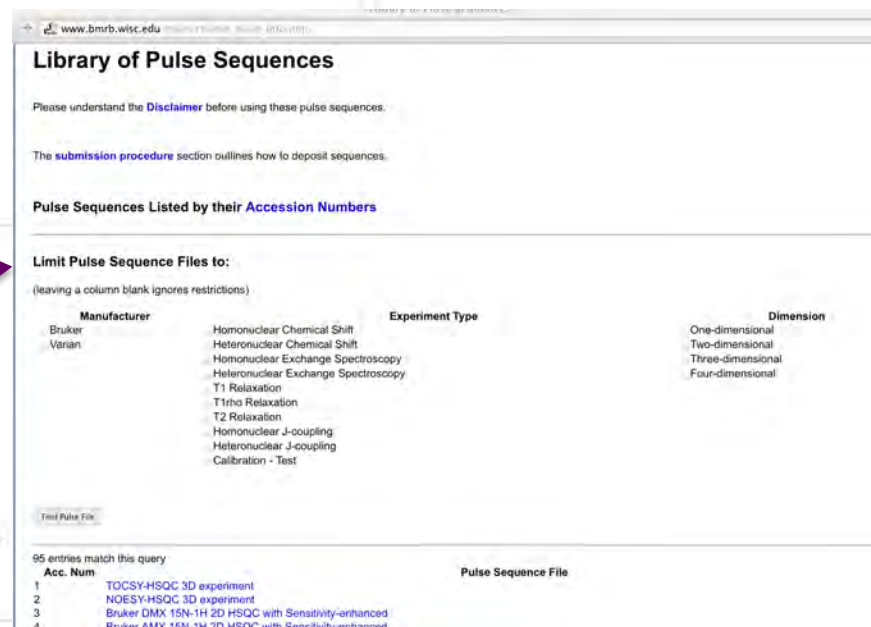
- **Optional:**
 - File containing a figure describing the pulse sequence. Please indicate the format of the file (postscript, GIF, MPEG, etc.).
 - Files containing parameter lists used to execute the pulse sequence (shaped pulses, gradient programs, frequency lists, delay lists, etc.).

[Sample Minimal Submission](#)
[Sample Fancy Submission](#)

Biological Magnetic Resonance Data Bank

NMR experiments and pulse programs

- [Ad Bax Group Pulse Sequence Library](#)
- [BMRB Library of NMR Pulse Sequences](#)
- [GFT NMR Package](#) - G-matrix Fourier Transform Package
- [Lewis Kay Lab Pulse Sequence Request Form](#)
- [NESG Wiki](#) - for sharing experimental protocols as well as training and educational materials
- [NMR Pulse Programs](#) from BMRB Time Domain Data Sets
- [Art Palmer Group](#) - Bruker AMX Pulse Programs
- [Software and Pulse Sequences](#) hosted by NMRFAM
- [NMR Pulse Sequence Library](#) of Carlsberg Laboratory
- [CABM NMR Pulse Sequence Library](#) at the Center for Advanced Biotechnology and Medicine - Rutgers
- [Eric Zuiderweg Group](#) University of Michigan



Library of Pulse Sequences

Please understand the [Disclaimer](#) before using these pulse sequences.

The [submission procedure](#) section outlines how to deposit sequences.

Pulse Sequences Listed by their Accession Numbers

Limit Pulse Sequence Files to:
(leaving a column blank ignores restrictions)

Manufacturer	Experiment Type	Dimension
Bruker	Homonuclear Chemical Shift	One-dimensional
Varian	Heteronuclear Chemical Shift	Two-dimensional
	Homonuclear Exchange Spectroscopy	Three-dimensional
	Heteronuclear Exchange Spectroscopy	Four-dimensional
	T1 Relaxation	
	T1rho Relaxation	
	T2 Relaxation	
	Homonuclear J-coupling	
	Heteronuclear J-coupling	
	Calibration - Test	

55 entries match this query

Acc. Num	Pulse Sequence File
1	TQCSY-HSQC 3D experiment
2	NOESY-HSQC 3D experiment
3	Bruker DMX 15N-1H 2D HSQC with Sensitivity-enhanced
4	Bruker AMX 15N-1H 2D HSQC with Sensitivity-enhanced