PURE SHIFT IMPLEMENTATION

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Basics

\[ H \psi = E \psi \]
Experiment submission

1. Experiment submission

2. Automated acquisition and processing

3. Job parameters and scheduling
Proton vs Pure shift (ZS)
Processing
Typical processing of single pulse
1D from 2D interferogram (old)
1D from 2D interferogram (new)

Next Delta release: 2D from 3D interferograms
Covariance processing
Pulse sequence coding
header
  process  = "pureshift.list";
  include "header";
end header;

instrument
  include "instrument";
end instrument;

acquisition
  x_domain  => "Proton";
  x_offset  => 5[ppm];
  x_sweep   => 10[ppm];
  x_points  => 2000;
  scans     => 8;
  [...]
end acquisition;

pulse
  collect COMPLEX, OBS REAL;

  x_pulse   => x90, help "90deg pulse width";
  x_atn     => xatn;
  relaxation_delay => 2[s], help "inter-pulse delay";
  [...]

  phase_1   = {0, 180, 180, 0, 90, 270, 270, 90};
  phase_2   = {0, 0, 180, 180};
  phase_3   = {0};
  phase_4   = {90};
  phase_slice = {0, 0, 180, 180};
  phase_acq = {0, 180, 180, 0, 90, 270, 270, 90};
  [...]

Basics (ZS)
begin

relaxation_delay;

x_pulse, (obs.gate, obs.phs.phase_1, obs.atn.x_atn);

t1 ystep 1/(2*y_sweep);

grad_1, (fgz.gate, fgz.shape.grad_1_shape, fgz.amp.grad_1_amp);

tau_a - grad_1;

obs_sel_180, (obs.gate, obs.phs.phase_slice, obs.atn.obs_sel_atn180, obs.shape.obs_sel_shape, fgz.gate, fgz.shape.grad_slice_shape, fgz.amp.grad_slice_amp);

parallel

begin

(tau_a + tau_b);

justify center

grad_2, (fgz.gate, fgz.shape.grad_2_shape, fgz.amp.grad_2_amp);

end parallel;

x_pulse * 2, (obs.gate, obs.phs.phase_2, obs.atn.x_atn);

grad_3, (fgz.gate, fgz.shape.grad_3_shape, fgz.amp.grad_3_amp);

tau_b - grad_3;

t1 ystep 1/(2*y_sweep);

acq( dead_time, delay, phase_acq );

end pulse;
Pulse shape calculations (PSYCHE)

\[
b_{1\_attn} = 20[\text{dB}] \times \log (\sqrt{0.5 \times \text{band\_width/\text{chirp\_pulse}} \times q}) \times 4 \times \text{chirp\_pulse};
\]

\[
\text{chirp\_atn\_calc} = \text{hard\_square\_atn} - b_{1\_attn}, \quad \text{help } "\text{attenuator for 180 chirp pulse}";
\]

\[
\text{chirp\_atn} \Rightarrow \text{chirp\_atn\_calc} + 24[\text{dB}], \quad \text{help } "20\text{deg pulse (chirp +24dB)}";
\]
NUS with pure shift

Setup as in any other 2D experiment
Real time pure shift

module_config = "continuous_fid";  
(concatenate acquisitions in one file instead of separate files)

loop n times
  [...] 
  x_pulse*2,(obs.gate,obs.phs.phase_y,obs.atn.x_atn);

  when irr_decoupling do 
    on (irr.gate, irr.noise.irr_noise, irr.atn.irr_atn_dec);
  end when;

  acquire begin 
  [...] 
  end acquire;

  when irr_decoupling do 
    off (irr.gate, irr.noise.irr_noise, irr.atn.irr_atn_dec);
  end when;

  [...] 
end loop;
Thank you

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  - Description of our products
  - Free processing software
  - Free natural products database
  - Application notes
  - Events
  - And more

- http://nmrsupport.jeol.com/ (for our users)