applied sciences

MDPI

Supplementary Materials: Chemical Analysis of Fluorobenzenes via Multinuclear Detection in the Strong Heteronuclear *J*-Coupling Regime

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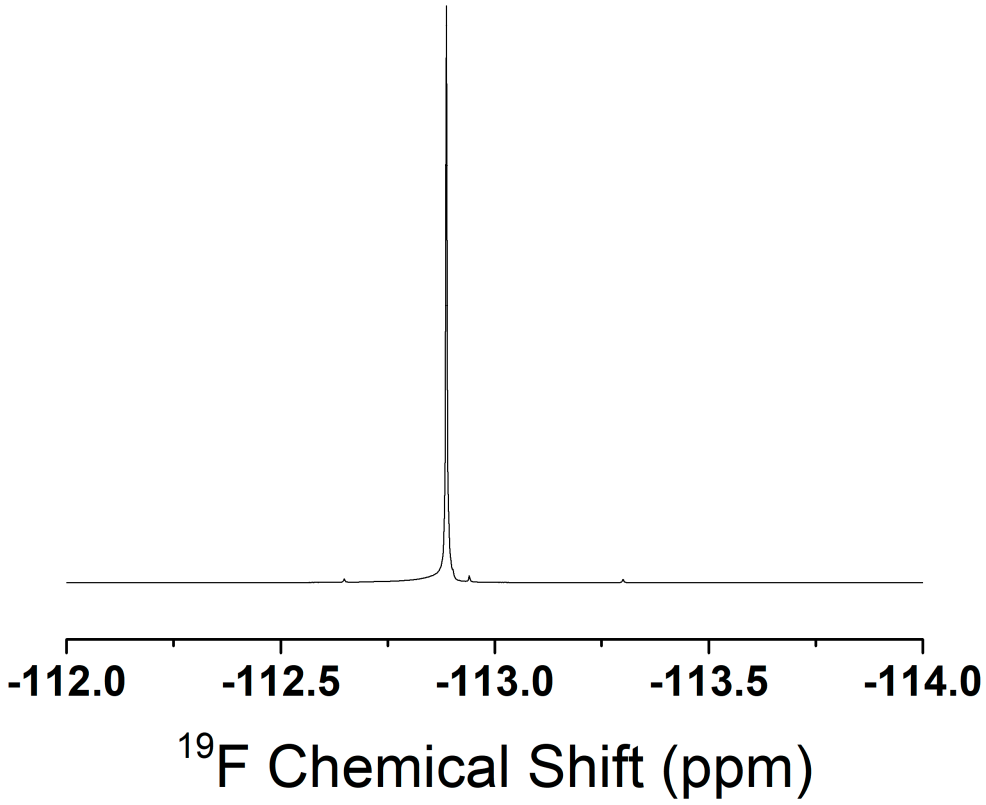

Figure S1. ^{19}F spectrum of monofluorobenzene collected at 9.4 T with ^{1}H decoupling.

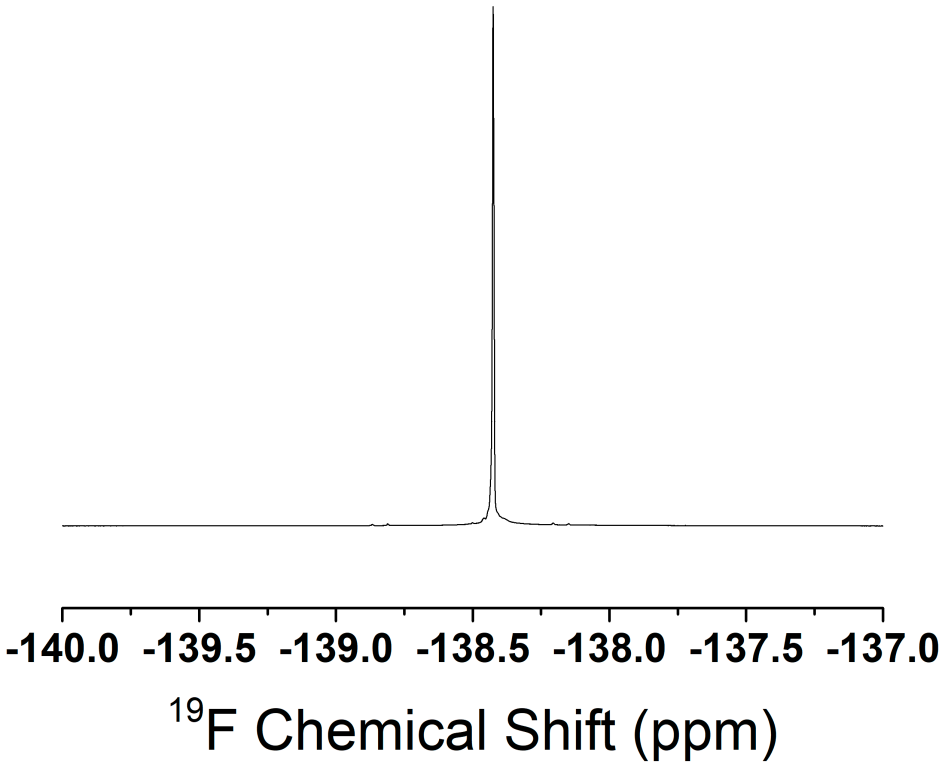

Figure S2. ^{19}F spectrum of 1,2-difluorobenzene collected at 9.4 T with ^{1}H decoupling.

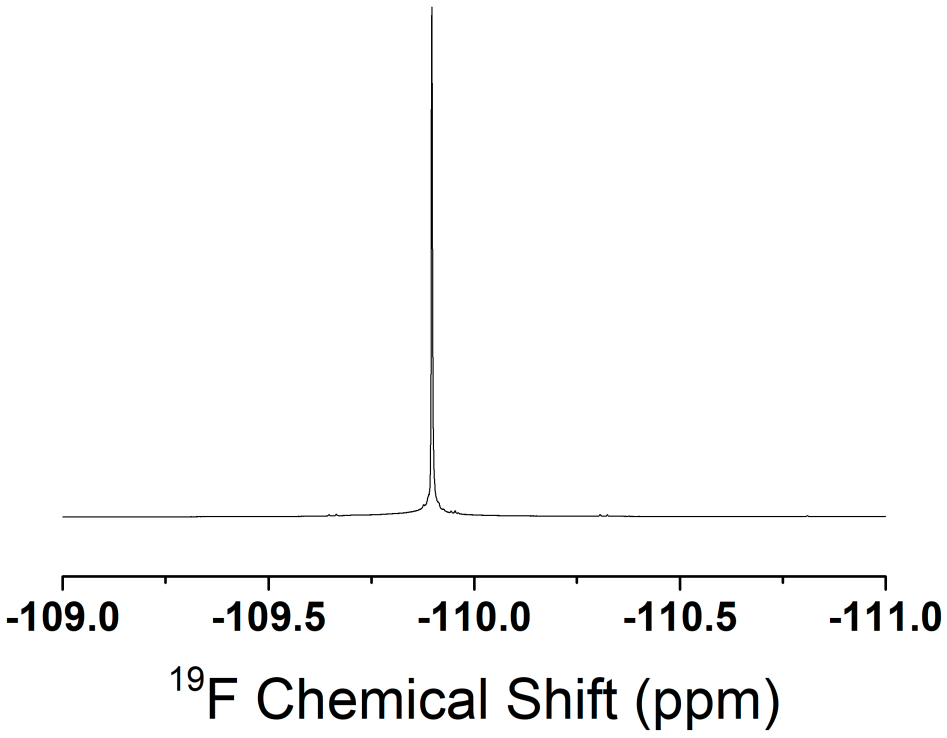

Figure S3. ^{19}F spectrum of 1,3-difluorobenzene collected at 9.4 T with ^{1}H decoupling.

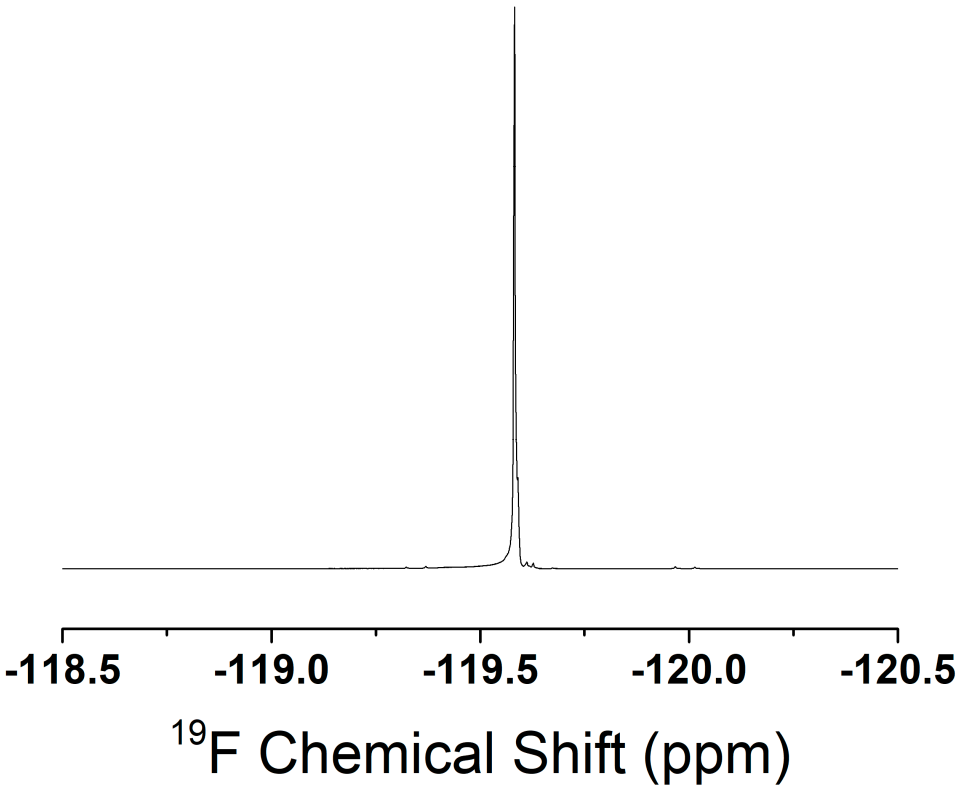

Figure S4. ^{19}F spectrum of 1,4-difluorobenzene collected at 9.4 T with ^{1}H decoupling.

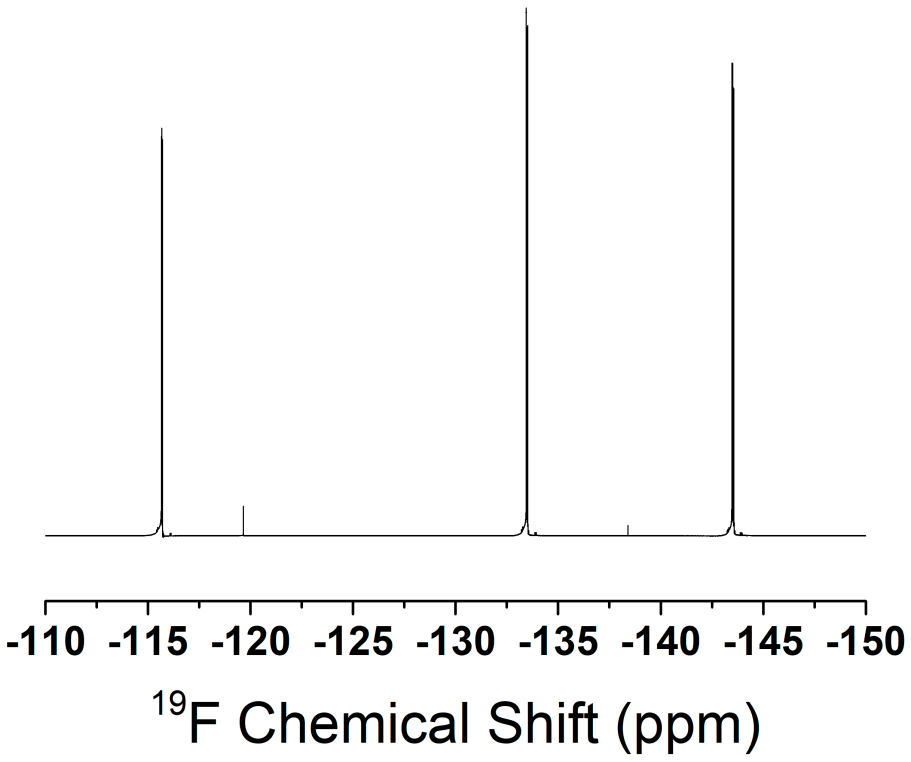

Figure S5. ^{19}F spectrum of 1,2,4-trifluorobenzene collected at 9.4 T with ^{1}H decoupling.

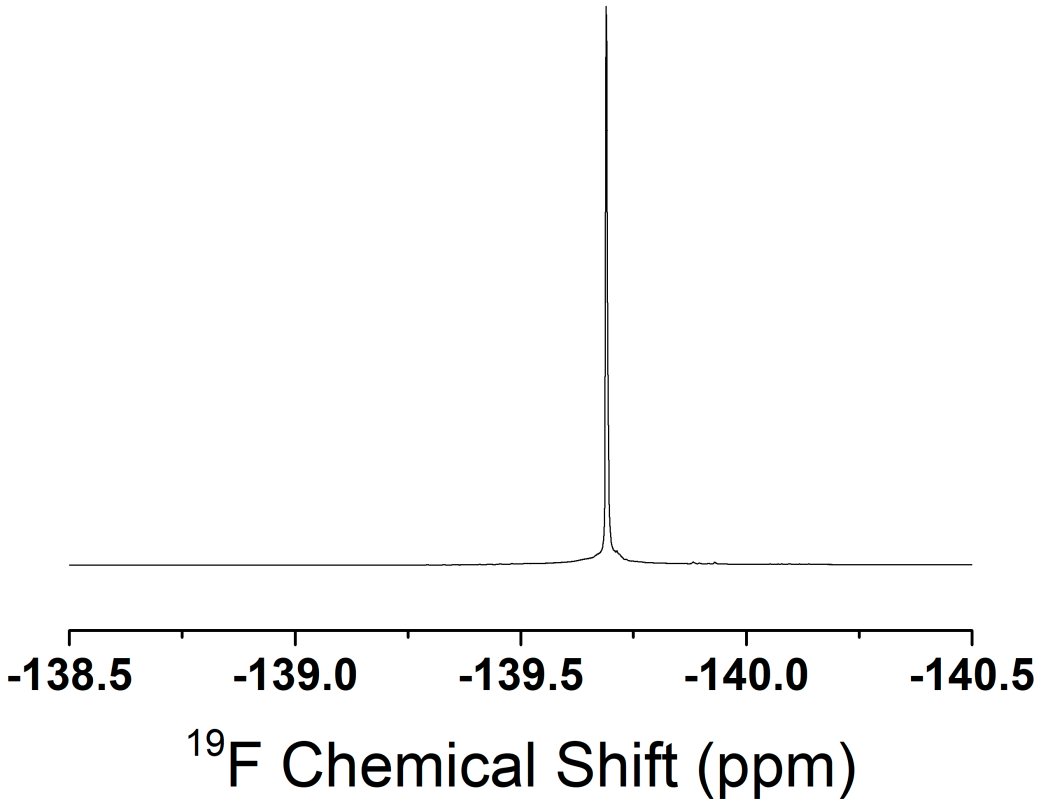

Figure S6. ^{19}F spectrum of 1,2,4,5-tetrafluorobenzene collected at 9.4 T with ^{1}H decoupling.

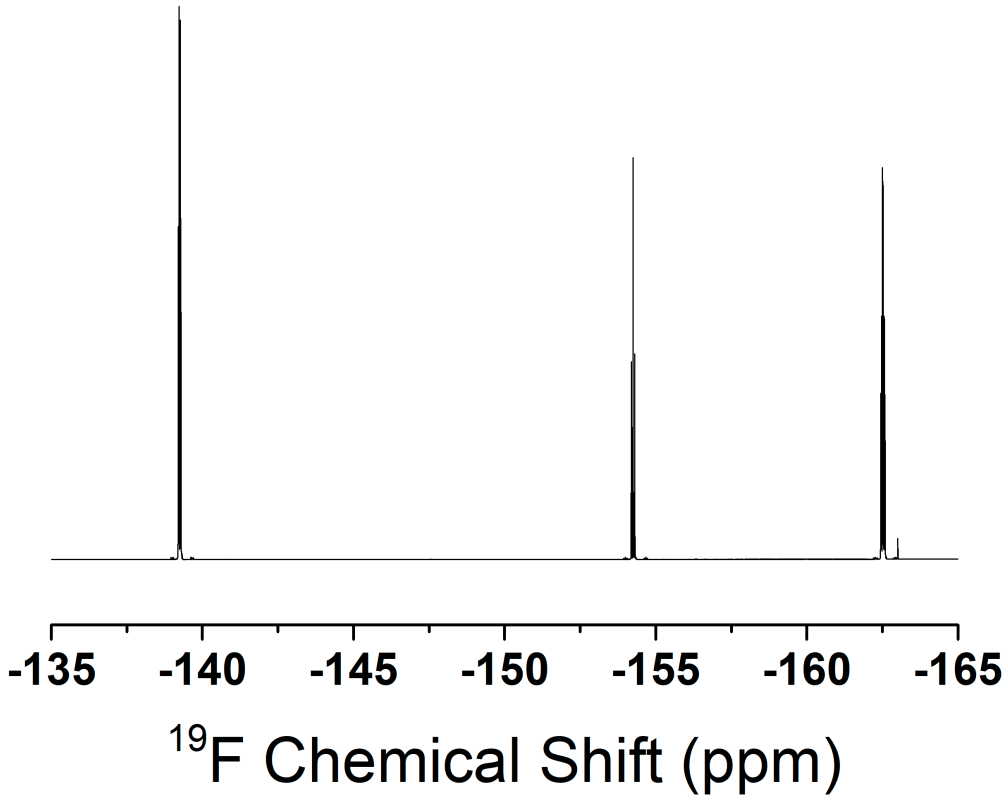

Figure S7. ^{19}F spectrum of pentafluorobenzene collected at 9.4 T with ^{1}H decoupling.

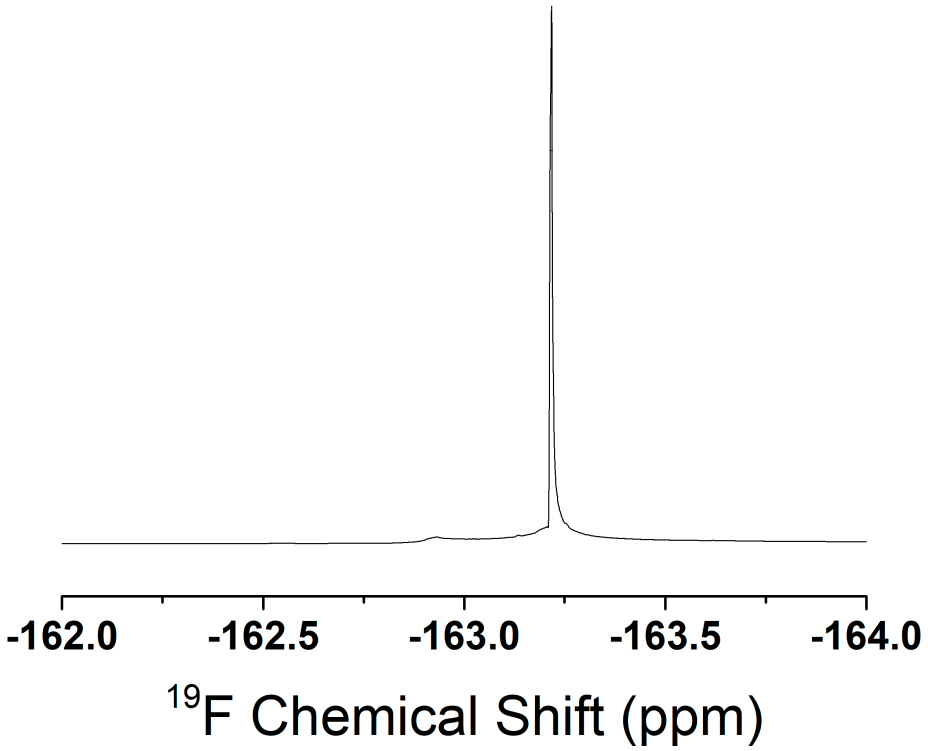

Figure S8. ^{19}F spectrum of hexafluorobenzene collected at 9.4 T with ^{1}H decoupling.

MATLAB Function for Optimizing monofluorobenzene

```
function Rfactors=MFBf(J)
sys.enable={'greedy','gpu','caching'};
sys.output='hush';
sys.isotopes={'19Fr','1H','1H','1H','1H','1H'};
J=round(J,2); % Round all parameters to 2 decimal places
Fz=-112.9; % Flourine Chemical Shift
H1z=6.8; % Proton Chemical Shifts
H2z=6.89; % Proton Chemical Shifts
H3z=6.75; % Proton Chemical Shifts

inter.zeeman.scalar={ Fz H1z H2z H3z H2z H1z};
inter.coupling.scalar={0 J(1) J(2) J(3) J(2) J(1);
                       0 0 J(4) J(5) J(6) J(7);
                       0 0 0 J(8) J(9) J(6) ;
                       0 0 0 0 J(8) J(5);
                       0 0 0 0 0 J(4);
                       0 0 0 0 0 0};

sys.enable={'greedy','gpu','caching'};
   g=spin('1H')/(2*pi);
   sys.magnet=J(12)/g;

   %Relaxation
   FWHMF=J(10); % Fluorine Relaxation Rate
   FWHMH=J(11); % Hydrogen Relaxation Rate
   inter.r2_rates=[FWHMF FWHMH FWHMH FWHMH FWHMH FWHMH];
   inter.relaxation={'t1_t2'};
   inter.r1_rates=inter.r2_rates;
   inter.rlx_keep='diagonal';
   inter.equilibrium='zero';

   % Basis set
   bas.connectivity='scalar_couplings';
   bas.space_level=4;
   bas.level=4;
   bas.formalism='sphten-liouv';
   bas.approximation='IK-2';

    % Sequence parameters
   parameters.sweep=1/1E-4;
   parameters.npoints=50000;
   parameters.zerofill=300*1024;
   parameters.spins={'1H'};
   parameters.offset=0;
   parameters.axis_units='Hz';
   parameters.invert_axis=0;

   % Spinach housekeeping
   spin_system=create(sys,inter);
   spin_system=basis(spin_system,bas);
```

```
% Simulation
fid=liquid(spin_system,@zerofield,parameters,'labframe');

% Fourier transform
spectrum=fftshift(fft(fid,parameters.zerofill));
spectrum1=real(spectrum);

spectrum2=sum(spectrum1,2);
spectrum3=spectrum2./max(real(spectrum2));
 %
% Frequency
inc=parameters.sweep/parameters.zerofill;
hz=[-(parameters.sweep/2)+inc:inc:(parameters.sweep/2)];
hz=hz';

%Experimenatal Parameters
offset=2120;

%Read in 19F
a=dlmread('MFB_19F.txt');
b=dlmread('MFB_1H.txt');
hzFe=a(:,2)+offset;
hzHe=b(:,2)+offset;

ExpspectrumF=a(:,3)./1.52; %Scaling factor for instrument response
ExpspectrumH=b(:,3);


%Combine Spectra
Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
Expspecsum=Expspecsum./max(Expspecsum);
hze=vertcat(hzFe,hzHe);

%Normalize simulated spectrum to exp
spectrum3n=spectrum3;

%Round Hz
dp=1; %decimal places to round
hzr=round(hz,dp);
hzer=round(hze,dp);

%1H Residuals
lower=66.00+2120;
upper=85.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzh=hz(idxhl(1,1):idxhu(1,1));
hspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlhe=find(hzer==lower);
idxuhe=find(hzer==upper);
hzhe=hze(idxlhe(1,1):idxuhe(1,1));
```

```
hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
residhs=((hspece-hspec));
%
%19F Residuals
lower=-69.00+2120;
upper=-30.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzf=hz(idxhl(1,1):idxhu(1,1));
fspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlfe=find(hzer==lower);
idxufe=find(hzer==upper);
hzfe=hze(idxlfe(1,1):idxufe(1,1));
fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
residfs=((fspece-fspec));

%Combine Residuals
resids=vertcat(residfs,residhs);
expspec=vertcat(fspece,hspece);
RSS=sum(resids.^2);
Rfactor=100*(RSS/sum(expspec.^2))^.5
%
for i=1:size(J,2)
   Rfactors(i)=Rfactor;
end
J
end
```

MATLAB Script for Optimizing monofluorobenzene

```
%Initial Parameters
J1=9.1;
J2=5.72;
J3=0.12;
J4=8.38;
J5=1.13;
J6=0.54;
J7=2.91;
J8=7.57;
J9=1.9031;
J10=.2;
J11=.2;
J12=2191.9
J0=[J1 J2 J3 J4 J5 J6 J7 J8 J9 J10 J11 J12];
% Constrain bounds
lb=J0-.5;
ub=lb+1;
lb(10)=.15;
lb(11)=.15;
ub(10)=.25;
ub(11)=.25;
%Fitting OPtions
options=optimoptions('lsqnonlin','FiniteDifferenceStepSize', 0.01,....
   'FiniteDifferenceType','forward','MaxFunctionEvaluations',2000,....
   'StepTolerance',.01, 'OptimalityTolerance', .01, 'FunctionTolerance', .01);
options.Algorithm='trust-region-reflective';
%Fitting
[x,fval]=lsqnonlin(@MFBf, J0,  lb, ub,options)
```

MATLAB Script for Calculating R-factors for Experimental, Literature and Calculated J-couplings in monofluorobenzene

```
clear all

sys.enable={'greedy','gpu','caching'};

%Monofluorobenzene
sys.isotopes={'19Fr','1H','1H','1H','1H','1H'};
J1=9.12;
J2=5.77;
J3=0.15;
J4=8.38;
J5=1.13;
J6=0.53;
J7=2.90;
J8=7.56;
J9=1.90;
Fz=-112.9;
H1z=6.8;
H2z=6.89;
H3z=6.75;
inter.zeeman.scalar={ Fz H1z H2z H3z H2z H1z};
inter.coupling.scalar={0 J1 J2 J3 J2 J1;
                       0 0 J4 J5 J6 J7;
                       0 0 0 J8 J9 J6 ;
                       0 0 0 0 J8 J5;
                       0 0 0 0 0 J4;
                       0 0 0 0 0 0};

sys.enable={'greedy','gpu','caching'};
   H=2194.9 ;
   g=spin('1H')/(2*pi);
   sys.magnet=H/g;

   %Relaxation
   FWHMF=0.2;
   FWHMH=0.2;
   inter.r2_rates=[FWHMF FWHMH FWHMH FWHMH FWHMH FWHMH]
   inter.relaxation={'t1_t2'};
   inter.r1_rates=inter.r2_rates;
   inter.rlx_keep='diagonal';
   inter.equilibrium='zero';

   % Basis set
   bas.connectivity='scalar_couplings';
   bas.space_level=4;
   bas.level=4;
   bas.formalism='sphten-liouv';
   bas.approximation='IK-2';

    % Sequence parameters
```

```
parameters.sweep=1/1E-4;
parameters.npoints=50000;
parameters.zerofill=300*1024;
parameters.spins={'1H'};
parameters.offset=0;
parameters.axis_units='Hz';
parameters.invert_axis=0;

% Spinach housekeeping
spin_system=create(sys,inter);
spin_system=basis(spin_system,bas);

% Simulation
fid=liquid(spin_system,@zerofield,parameters,'labframe');

% Fourier transform
spectrum=fftshift(fft(fid,parameters.zerofill));
spectrum1=real(spectrum);

spectrum2=sum(spectrum1,2);
spectrum3=spectrum2./max(real(spectrum2));
plot(spectrum3)
%
% Frequency
inc=parameters.sweep/parameters.zerofill;
hz=[-(parameters.sweep/2)+inc:inc:(parameters.sweep/2)];
hz=hz';

%Experimenatal Parameters
offset=2120;

%Read in 19F
a=dlmread('MFB_19F.txt');
b=dlmread('MFB_1H.txt');
hzFe=a(:,2)+offset;
hzHe=b(:,2)+offset;

ExpspectrumF=a(:,3)./1.52;
ExpspectrumH=b(:,3);


%Combine Spectra
Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
Expspecsum=Expspecsum./max(Expspecsum);
hze=vertcat(hzFe,hzHe);

%Normalize simulated spectrum to exp
spectrum3n=spectrum3;%.*max(Expspecsum);
plot(hz, spectrum3n)
xlim([2100 2300]);
%
%Round Hz
```

```
dp=1; %decimal places to round
hzr=round(hz,dp);
hzer=round(hze,dp);

%1H Residuals
lower=66.00+2120;
upper=85.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzh=hz(idxhl(1,1):idxhu(1,1));
hspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlhe=find(hzer==lower);
idxuhe=find(hzer==upper);
hzhe=hze(idxlhe(1,1):idxuhe(1,1));
hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
residhs=((hspece-hspec));
%
%19F Residuals
lower=-69.00+2120;
upper=-30.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzf=hz(idxhl(1,1):idxhu(1,1));
fspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlfe=find(hzer==lower);
idxufe=find(hzer==upper);
hzfe=hze(idxlfe(1,1):idxufe(1,1));
fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
residfs=((fspece-fspec));

%Combine Residuals
resids=vertcat(residfs,residhs);
spec=vertcat(fspec,hspec);
specexp=vertcat(fspece,hspece);
hzexp=vertcat(hzfe,hzhe);
%R Factor
RSS=sum(resids.^2)
Rfactor=100*(RSS/sum(specexp.^2))^.5

RSSh=sum(residhs.^2);
Rfactorh=100*(RSSh/sum(hspece.^2))^.5;
y=num2str(Rfactorh);

RSSf=sum(residfs.^2);
Rfactorf=100*(RSSf/sum(fspece.^2))^.5;
z=num2str(Rfactorf);
%Plotting
subplot(2,1,1)
plot(hzfe,fspec,'color','r')
hold on
```

```
plot(hzfe,fspece,'color','k')
plot(hzfe,(residfs),'color','g')
title(z)
hold off

subplot(2,1,2)
plot(hzhe,hspec,'color','r')
hold on
plot(hzhe,hspece,'color','k')
plot(hzhe,residhs,'color','g')
hold off
title(y)
```

MATLAB Function for Optimization of 1,2 Difluorobenzene

```
function Rfactors=DFB_12f(J)
% Chemical Shifts
Fz=-138.4;
H1z=6.67;
H2z=6.5;
J=round(J,2);
inter.zeeman.scalar={ Fz Fz H1z H2z H2z H1z};
sys.isotopes={ '19Fr','19Fr','1H','1H','1H','1H'};
sys.output='hush';
inter.coupling.scalar={0 J(1) J(2) J(3) J(4) J(5);
                       0 0 J(5) J(4) J(3) J(2);
                       0 0 0 J(6) J(7) J(8) ;
                       0 0 0 0 J(9) J(7);
                       0 0 0 0 0 J(6);
                       0 0 0 0 0 0};


sys.enable={'greedy','gpu','caching'};
   g=spin('1H')/(2*pi);
   sys.magnet=J(10)/g;

   %Relaxation
   [a spinsize]=size(sys.isotopes);
   Fr=J(11);
   Hr=J(12);
   inter.r2_rates=[Fr Fr Hr Hr Hr Hr];
   inter.relaxation={'t1_t2'};
   inter.r1_rates=inter.r2_rates;
   inter.rlx_keep='diagonal';
   inter.equilibrium='zero';

   % Basis set
   bas.connectivity='scalar_couplings';
   bas.space_level=4;
   bas.level=4;
   bas.formalism='sphten-liouv';
   bas.approximation='IK-2';

    % Sequence parameters
   parameters.sweep=1/1E-4;
   parameters.npoints=50000;
   parameters.zerofill=300*1024;
   parameters.spins={'1H'};
   parameters.offset=0;
   parameters.axis_units='Hz';
   parameters.invert_axis=0;

   % Spinach housekeeping
   spin_system=create(sys,inter);
   spin_system=basis(spin_system,bas);
```

```
% Simulation
fid=liquid(spin_system,@zerofield,parameters,'labframe');

% Fourier transform
spectrum=fftshift(fft(fid,parameters.zerofill));
spectrum3=real(spectrum)./max(real(spectrum));

% Frequency
inc=parameters.sweep/parameters.zerofill;
hz=[-(parameters.sweep/2)+inc:inc:(parameters.sweep/2)];
hz=hz';

%Experimenatal Parameters
offset=2120;

%Read in 19F
a=dlmread('12DFB_19F.txt');
b=dlmread('12DFB_1H.txt');
hzFe=a(:,2)+offset;
hzHe=b(:,2)+offset;

ExpspectrumF=a(:,3)./1.52;
ExpspectrumH=b(:,3);


%Combine Spectra
Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
Expspecsum=Expspecsum./max(Expspecsum);
hze=vertcat(hzFe,hzHe);

%Normalize simulated spectrum to exp
spectrum3n=spectrum3;

%Round Hz
dp=1; %decimal places to round
hzr=round(hz,dp);
hzer=round(hze,dp);

%1H Residuals
lower=53.00+2120;
upper=95.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzh=hz(idxhl(1,1):idxhu(1,1));
hspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlhe=find(hzer==lower);
idxuhe=find(hzer==upper);
hzhe=hze(idxlhe(1,1):idxuhe(1,1));
hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
residhs=((hspece-hspec));
```

```
    %19F Residuals
    lower=-80.00+2120;
    upper=-31.00+2120;
    idxhl=find(hzr==lower);
    idxhu=find(hzr==upper);
    hzf=hz(idxhl(1,1):idxhu(1,1));
    fspec=spectrum3n(idxhl(1,1):idxhu(1,1));

    idxlfe=find(hzer==lower);
    idxufe=find(hzer==upper);
    hzfe=hze(idxlfe(1,1):idxufe(1,1));
    fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
    residfs=((fspece-fspec));

    %Combine Residuals
    resids=vertcat(residfs,residhs);
    expspec=vertcat(fspece,hspece);
    RSS=sum(resids.^2);
    Rfactor=100*(RSS/sum(expspec.^2))^.5
    for i=1:size(J,2)
       Rfactors(i)=Rfactor;
    end
    J

end
```

MATLAB Script for Optimizing 1,2-difluorobenzene

```
%Inital Parameters
J1=-20.82; %F-F Coupling
J2=8.1; %F-H Coupling
J3=-1.4; %F-H Coupling
J4=4.53; %F-H Coupling
J5=10.70; %F-H Coupling
J6=8.30; %H-H Coupling
J7=1.61; %H-H Coupling
J8=0.26; %H-H Coupling
J9=7.61; %7.61 %H-H Coupling
J10=2195.5;
J11=.15;
J12=.15;
J0=[J1 J2 J3 J4 J5 J6 J7 J8 J9 J10 J11 J12];
%Parameter Bounds
lbJ=J0-.5;
lbJ(10)=2195.4;
ubJ=lbJ+1;
ubJ(10)=2195.6;
ubJ(11)=.2;
ubJ(12)=.2;
%Fitting Options
options=optimoptions('lsqnonlin','FiniteDifferenceStepSize', 0.01,....
   'FiniteDifferenceType','forward','MaxFunctionEvaluations',2000,....
   'StepTolerance',.01, 'OptimalityTolerance', .01, 'FunctionTolerance', .01);
options.Algorithm='trust-region-reflective';
%Fitting
[x,fval]=lsqnonlin(@DFB_12f, J0,  lbJ, ubJ,options)
```

Matlab Script for Calculating R-factors for Experimental, Literature and Calculated J-couplings in 1,2-difluorobenzene

```
clear all
tic
    sys.output='hush';
    %12difluorobenzene
    J1=-13.98; %F-F Coupling
    J2=8.39; %F-H Coupling
    J3=-3.42; %F-H Coupling
    J4=4.12; %F-H Coupling
    J5=13.03; %F-H Coupling
    J6=
    10.70;% Coupling
    J7=.35; %H-H Coupling
    J8=1.00; %H-H Coupling
    J9=10.12; %7.61 %H-H Coupling
    Fz=-138.4;
    H1z=6.67;
    H2z=6.5;

    inter.zeeman.scalar={ Fz Fz H1z H2z H2z H1z};
    sys.isotopes={ '19Fr','19Fr','1H','1H','1H','1H'};
    inter.coupling.scalar={0 J1 J2 J3 J4 J5;
                           0 0 J5 J4 J3 J2;
                           0 0 0 J6 J7 J8 ;
                           0 0 0 0 J9 J7;
                           0 0 0 0 0 J6;
                           0 0 0 0 0 0};


sys.enable={'greedy','gpu','caching'};
  H=2195.57 ;
  g=spin('1H')/(2*pi);
  sys.magnet=H/g;

  %Relaxation
  [a spinsize]=size(sys.isotopes);
  Fr=.15;
  Hr=.14;
  inter.r2_rates=[Fr Fr Hr Hr Hr Hr];
  inter.relaxation={'t1_t2'};
  inter.r1_rates=inter.r2_rates;
  inter.rlx_keep='diagonal';
  inter.equilibrium='zero';

  % Basis set
  bas.connectivity='scalar_couplings';
  bas.space_level=4;
  bas.level=4;
  bas.formalism='sphten-liouv';
  bas.approximation='IK-2';
```

```
 % Sequence parameters
parameters.sweep=1/1E-4;
parameters.npoints=50000;
parameters.zerofill=300*1024;
parameters.spins={'1H'};
parameters.offset=0;
parameters.axis_units='Hz';
parameters.invert_axis=0;

% Spinach housekeeping
spin_system=create(sys,inter);
spin_system=basis(spin_system,bas);

% Simulation
fid=liquid(spin_system,@zerofield,parameters,'labframe');

% Fourier transform
spectrum=fftshift(fft(fid,parameters.zerofill));
spectrum1=real(spectrum);

spectrum2=sum(spectrum1,2);
spectrum3=spectrum2./max(real(spectrum2));
plot(spectrum3)
%
% Frequency
inc=parameters.sweep/parameters.zerofill;
hz=[-(parameters.sweep/2)+inc:inc:(parameters.sweep/2)];
hz=hz';
%save('hz.mat','hz')
%save(name,'spectrum')
%Experimenatal Parameters
offset=2120;

%Read in 19F
a=dlmread('12DFB_19F.txt');
b=dlmread('12DFB_1H.txt');
hzFe=a(:,2)+offset;
hzHe=b(:,2)+offset;

ExpspectrumF=a(:,3)./1.52;
ExpspectrumH=b(:,3);


%Combine Spectra
Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
Expspecsum=(Expspecsum./max(Expspecsum));
hze=vertcat(hzFe,hzHe);

%Normalize simulated spectrum to exp
spectrum3n=spectrum3;%.*max(Expspecsum);

%Round Hz
```

```
dp=1; %decimal places to round
hzr=round(hz,dp);
hzer=round(hze,dp);

%1H Residuals
lower=53.00+2120;
upper=95.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzh=hz(idxhl(1,1):idxhu(1,1));
hspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlhe=find(hzer==lower);
idxuhe=find(hzer==upper);
hzhe=hze(idxlhe(1,1):idxuhe(1,1));
hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
residhs=((hspece-hspec));
%
%19F Residuals
lower=-80.00+2120;
upper=-31.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzf=hz(idxhl(1,1):idxhu(1,1));
fspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlfe=find(hzer==lower);
idxufe=find(hzer==upper);
hzfe=hze(idxlfe(1,1):idxufe(1,1));
fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
residfs=((fspece-fspec));

%Combine Residuals
resids=vertcat(residfs,residhs);
spec=vertcat(fspec,hspec);
specexp=vertcat(fspece,hspece);
hzexp=vertcat(hzfe,hzhe);
%R Factor
RSS=sum(resids.^2)
Rfactor=100*(RSS/sum(specexp.^2))^.5

RSSh=sum(residhs.^2);
Rfactorh=100*(RSSh/sum(hspece.^2))^.5;
y=num2str(Rfactorh);

RSSf=sum(residfs.^2);
Rfactorf=100*(RSSf/sum(fspece.^2))^.5;
z=num2str(Rfactorf);
%Plotting
subplot(2,1,1)
plot(hzfe,fspec,'color','r')
hold on
```

```
plot(hzfe,fspece,'color','k')
plot(hzfe,(residfs),'color','g')
title(z)
hold off

subplot(2,1,2)
plot(hzhe,hspec,'color','r')
hold on
plot(hzhe,hspece,'color','k')
plot(hzhe,residhs,'color','g')
hold off
title(y)
```

MATLAB Function for Optimizing 1,3-difluorobenzene

```
function Rfactors=DFB_13f(J)
% Isotopes
sys.isotopes={'19Fr','1H','19Fr','1H','1H','1H'};
sys.output='hush';
% Magnetic Field
sys.magnet=J(10)/(spin('1H')/(2*pi));
% Chemical shifts
inter.zeeman.scalar={-109.9  6.62 -109.9  6.45  6.44 6.45};

J=round(J,2);

inter.coupling.scalar={0 J(1) J(2) J(3) J(4) J(5);
                       0 0 J(1) J(6) J(7) J(6);
                      0 0 0 J(5) J(4) J(3) ;
                       0 0 0 0 J(9) J(8);
                       0 0 0 0 0 J(9);
                       0 0 0 0 0 0};
% Relaxation model
inter.relaxation={'t1_t2'};
inter.rlx_keep='diagonal';
inter.r1_rates=[J(11) J(12) J(11) J(12) J(12) J(12)];
inter.r2_rates=inter.r1_rates;
inter.equilibrium='zero';

% Basis set
bas.formalism='sphten-liouv';
bas.approximation='IK-2';
bas.connectivity='scalar_couplings';
bas.space_level=4;

% Spinach housekeeping
spin_system=create(sys,inter);
spin_system=basis(spin_system,bas);

% Sequence parameters
parameters.sweep=1/1E-4;
   parameters.npoints=50000;
   parameters.zerofill=300*1024;
   parameters.spins={'1H'};
   parameters.offset=0;
   parameters.axis_units='Hz';
   parameters.invert_axis=0;


   % Simulation
   fid=liquid(spin_system,@zerofield,parameters,'labframe');


   % Fourier transform
   spectrum=fftshift(fft(fid,parameters.zerofill));
   spectrum1=real(spectrum);
```

```
spectrum2=sum(spectrum1,2);
spectrum3=spectrum2./max(real(spectrum2));

%
% Frequency
inc=parameters.sweep/parameters.zerofill;
hz=[-(parameters.sweep/2)+inc:inc:(parameters.sweep/2)];
hz=hz';
%save('hz.mat','hz')
%save(name,'spectrum')
%Experimenatal Parameters
offset=2120;

%Read in 19F
a=dlmread('13DFB_19F.txt');
b=dlmread('13DFB_1H.txt');
hzFe=a(:,2)+offset;
hzHe=b(:,2)+offset;

ExpspectrumF=a(:,3)./1.52;
ExpspectrumH=b(:,3);


%Combine Spectra
Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
Expspecsum=Expspecsum./max(Expspecsum);
hze=vertcat(hzFe,hzHe);

%Normalize simulated spectrum to exp
spectrum3n=spectrum3;

%Round Hz
dp=1; %decimal places to round
hzr=round(hz,dp);
hzer=round(hze,dp);

%1H Residuals
lower=63.00+2120;
upper=95.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzh=hz(idxhl(1,1):idxhu(1,1));
hspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlhe=find(hzer==lower);
idxuhe=find(hzer==upper);
hzhe=hze(idxlhe(1,1):idxuhe(1,1));
hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
residhs=((hspece-hspec));
%
%19F Residuals
```

```
    lower=-70.00+2120;
    upper=-35.00+2120;
    idxhl=find(hzr==lower);
    idxhu=find(hzr==upper);
    hzf=hz(idxhl(1,1):idxhu(1,1));
    fspec=spectrum3n(idxhl(1,1):idxhu(1,1));

    idxlfe=find(hzer==lower);
    idxufe=find(hzer==upper);
    hzfe=hze(idxlfe(1,1):idxufe(1,1));
    fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
    residfs=((fspece-fspec));

    %Combine Residuals
    resids=vertcat(residfs,residhs);
    expspec=vertcat(fspece,hspece);
    RSS=sum(resids.^2);
    Rfactor=100*(RSS/sum(expspec.^2))^.5
    for i=1:size(J,2)
       Rfactors(i)=Rfactor;
    end
    J

end
```

MATLAB Script for Optimization of 1,3-difluorobenzene

```
%Initial Parameters
J1=9.42; %H-F Coupling
J2=6.52; %F-F Coupling
J3=-.81; %F-H Coupling
J4=6.63; %F-H Coupling
J5=8.43; %F-H Coupling
J6=2.44; %H-H Coupling
J7=0.32; %H-H Coupling
J8=0.87; %H-H Coupling
J9=8.43; %H-H Coupling
J10=2196.52 ;
J11=.15;
J12=.15;
J0=[J1 J2 J3 J4 J5 J6 J7 J8 J9 J10 J11 J12];
%Parameter Bounds
lb(10)=2196.62;
lb=J0-.5
ub(10)=2196.4;
ub=lb+1;
ubJ(11)=.2;
ubJ(12)=.2;
%Fitting Options
options=optimoptions('lsqnonlin','FiniteDifferenceStepSize', 0.01,....
   'FiniteDifferenceType','forward','MaxFunctionEvaluations',2000,....
   'StepTolerance',.01, 'OptimalityTolerance', .01, 'FunctionTolerance', .01);
options.Algorithm='trust-region-reflective';
%Fitting
[x,fval]=lsqnonlin(@DFB_13f, J0,  lb, ub,options)
```

MATLAB Script for Calculating R-factors for Experimental, Literature and Calculated J-couplings in 1,3-difluorobenzene

```
clear all
sys.output='hush';
sys.enable={'greedy','gpu','caching'};
% Isotopes
sys.isotopes={'19Fr','1H','19Fr','1H','1H','1H'};

% Magnetic Field
   H=2196.52 ;
   g=spin('1H')/(2*pi);
   sys.magnet=H/g;

% Chemical shifts0.14
Fz=-109.9;
H1z=6.44;
H2z=6.45;
H3z=6.62;
inter.zeeman.scalar={Fz  H1z Fz  H2z  H3z H2z};

J1=11.5; %F-H Coupling
J5=10.38; %F-H Coupling
J4=6.63; %F-H Coupling
J3=-2.81; %F-H Coupling
J2=5.14; %F-F Coupling
J9=10.38; %H-H Coupling
J6=1.44; %H-H Coupling
J7=1.06; %H-H Coupling
J8=-.22; %H-H Coupling

inter.coupling.scalar={0 J1 J2 J3 J4 J5;
                       0 0 J1 J6 J7 J6;
                       0 0 0 J5 J4 J3 ;
                       0 0 0 0 J9 J8;
                       0 0 0 0 0 J9;
                       0 0 0 0 0 0};
% Relaxation model
inter.relaxation={'t1_t2'};
inter.rlx_keep='diagonal';
FWHMF=.14;
FWHMH=.14;
inter.r1_rates=[FWHMF FWHMH FWHMF FWHMH FWHMH FWHMH];
inter.r2_rates=inter.r1_rates;
inter.equilibrium='zero';

% Basis set
bas.formalism='sphten-liouv';
bas.approximation='IK-2';
bas.connectivity='scalar_couplings';
bas.space_level=4;
% Sequence parameters
   parameters.sweep=1/1E-4;
```

```
parameters.npoints=50000;
parameters.zerofill=300*1024;
parameters.spins={'1H'};
parameters.offset=0;
parameters.axis_units='Hz';
parameters.invert_axis=0;

% Spinach housekeeping
spin_system=create(sys,inter);
spin_system=basis(spin_system,bas);

% Simulation
fid=liquid(spin_system,@zerofield,parameters,'labframe');

% Fourier transform
spectrum=fftshift(fft(fid,parameters.zerofill));
spectrum1=real(spectrum);

spectrum2=sum(spectrum1,2);
spectrum3=spectrum2./max(real(spectrum2));
plot(spectrum3)
%
% Frequency
inc=parameters.sweep/parameters.zerofill;
hz=[-(parameters.sweep/2)+inc:inc:(parameters.sweep/2)];
hz=hz';
%save('hz.mat','hz')
%save(name,'spectrum')
%Experimenatal Parameters
offset=2120;

%Read in 19F
a=dlmread('13DFB_19F.txt');
b=dlmread('13DFB_1H.txt');
hzFe=a(:,2)+offset;
hzHe=b(:,2)+offset;

ExpspectrumF=a(:,3)./1.52;
ExpspectrumH=b(:,3);


%Combine Spectra
Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
Expspecsum=Expspecsum./max(Expspecsum);
hze=vertcat(hzFe,hzHe);

%Normalize simulated spectrum to exp
spectrum3n=spectrum3;%.*max(Expspecsum);

%Round Hz
dp=1; %decimal places to round
hzr=round(hz,dp);
```

```
hzer=round(hze,dp);

%1H Residuals
lower=63.00+2120;
upper=95.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzh=hz(idxhl(1,1):idxhu(1,1));
hspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlhe=find(hzer==lower);
idxuhe=find(hzer==upper);
hzhe=hze(idxlhe(1,1):idxuhe(1,1));
hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
residhs=((hspece-hspec));
%
%19F Residuals
lower=-70.00+2120;
upper=-35.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzf=hz(idxhl(1,1):idxhu(1,1));
fspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlfe=find(hzer==lower);
idxufe=find(hzer==upper);
hzfe=hze(idxlfe(1,1):idxufe(1,1));
fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
residfs=((fspece-fspec));

%Combine Residuals
resids=vertcat(residfs,residhs);
spec=vertcat(fspec,hspec);
specexp=vertcat(fspece,hspece);
hzexp=vertcat(hzfe,hzhe);
%R Factor
RSS=sum(resids.^2)
Rfactor=100*(RSS/sum(specexp.^2))^.5

RSSh=sum(residhs.^2);
Rfactorh=100*(RSSh/sum(hspece.^2))^.5;
y=num2str(Rfactorh);

RSSf=sum(residfs.^2);
Rfactorf=100*(RSSf/sum(fspece.^2))^.5;
z=num2str(Rfactorf);
%Plotting
subplot(2,1,1)
plot(hzfe,fspec,'color','r')
hold on
plot(hzfe,fspece,'color','k')
plot(hzfe,(residfs),'color','g')
```

```
title(z)
hold off

subplot(2,1,2)
plot(hzhe,hspec,'color','r')
hold on
plot(hzhe,hspece,'color','k')
plot(hzhe,residhs,'color','g')
hold off
title(y)
```

MATLAB Function for Optimizing 1,4-difluorobenzene

```
function Rfactors=DFB_14(J)

    sys.isotopes={'19Fr','1H','1H','19Fr','1H','1H'};
    sys.output='hush';
    J=round(J,2);
    %Chemical Shifts
    Fz=-119.6;
    Hz=6.50;
    inter.zeeman.scalar={ Fz Hz Hz Fz Hz Hz};

    inter.coupling.scalar={0 J(1) J(2) J(3) J(2) J(1);
                           0 0 J(4) J(2) J(5) J(6);
                           0 0 0 J(1) J(6) J(5) ;
                           0 0 0 0 J(1) J(2);
                           0 0 0 0 0 J(4);
                           0 0 0 0 0 0};


sys.enable={'greedy','gpu','caching'};
  g=spin('1H')/(2*pi);
  sys.magnet=J(9)/g;

  %Relaxation
  inter.r2_rates=[J(7) J(8) J(8) J(7) J(8) J(8)];
  inter.relaxation={'t1_t2'};
  inter.r1_rates=inter.r2_rates;
  inter.rlx_keep='diagonal';
  inter.equilibrium='zero';

  % Basis set
  bas.connectivity='scalar_couplings';
  bas.space_level=4;
  bas.level=4;
  bas.formalism='sphten-liouv';
  bas.approximation='IK-2';


  % Sequence parameters
  parameters.sweep=1/1E-4;
  parameters.npoints=50000;
  parameters.zerofill=300*1000;
  parameters.spins={'1H'};
  parameters.offset=0;
  parameters.axis_units='Hz';
  parameters.invert_axis=0;

  % Spinach housekeeping
  spin_system=create(sys,inter);
  spin_system=basis(spin_system,bas);
```

```
% Simulation
   fid=liquid(spin_system,@zerofield,parameters,'labframe');

% Fourier transform
   spectrum=fftshift(fft(fid,parameters.zerofill));
   spectrum3=real(spectrum)./max(real(spectrum));
%
% Frequency
   hz=axis_1d(spin_system, parameters);
   hz=hz';

%Experimenatal Parameters
   offset=2120;

%Read in Experimental Parameters
   a=dlmread('14DFB_19F.txt');
   b=dlmread('14DFB_1H.txt');
   hzFe=a(:,2)+offset;
   hzHe=b(:,2)+offset;

% Normalize to Q-factor
   ExpspectrumF=a(:,3)./1.52;
   ExpspectrumH=b(:,3);

%Combine Spectra
   Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
   Expspecsum=Expspecsum./max(Expspecsum);
   hze=vertcat(hzFe,hzHe);

%Round Hz
   dp=1; %decimal places to round
   hzr=round(hz,dp);
   hzer=round(hze,dp);

%1H Residuals
   lower=65.00+2120;
   upper=85.00+2120;
   idxhl=find(hzr==lower);
   idxhu=find(hzr==upper);
   hzh=hz(idxhl(1,1):idxhu(1,1));
   hspec=spectrum3(idxhl(1,1):idxhu(1,1));

   idxlhe=find(hzer==lower);
   idxuhe=find(hzer==upper);
   hzhe=hze(idxlhe(1,1):idxuhe(1,1));
   hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
   residhs=((hspece-hspec));

%19F Residuals
   lower=-70.00+2120;
   upper=-40.00+2120;
   idxhl=find(hzr==lower);
```

```
    idxhu=find(hzr==upper);
    hzf=hz(idxhl(1,1):idxhu(1,1));
    fspec=spectrum3(idxhl(1,1):idxhu(1,1));

    idxlfe=find(hzer==lower);
    idxufe=find(hzer==upper);
    hzfe=hze(idxlfe(1,1):idxufe(1,1));
    fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
    residfs=((fspece-fspec));

%Combine Residuals
    resids=vertcat(residfs,residhs);
    spec=vertcat(fspec,hspec);
    specexp=vertcat(fspece,hspece);
    hzexp=vertcat(hzfe,hzhe);
%R Factor
    RSS=sum(resids.^2)
    Rfactor=100*(RSS/sum(specexp.^2))^.5

%Hydrogen Residuals
    RSSh=sum(residhs.^2);
    Rfactorh=100*(RSSh/sum(hspece.^2))^.5;
    y=num2str(Rfactorh);

%Fluorine Residuals
    RSSf=sum(residfs.^2);
    Rfactorf=100*(RSSf/sum(fspece.^2))^.5;
    z=num2str(Rfactorf);
    for i=1:size(J,2)
        Rfactors(i)=Rfactor;
    end
    J
    end
```

MATLAB Script for Optimization of 1,4-difluorobenzene

```
%Initial Parameters
J0(1)=8.09;
J0(2)=4.16;
J0(3)=17.65;
J0(4)=9.09;
J0(5)=0;
J0(6)=3.15;
J0(7)=.13;
J0(8)=.12;
J0(9)=2195.45;
%Constraints
lb=J0-.5;
lb(7)=.08;
lb(8)=.08;

ub=lb+1;
ub(7)=.16;
ub(8)=.16;
%Fitting Options
options=optimoptions('lsqnonlin','FiniteDifferenceStepSize', 0.01,....
   'FiniteDifferenceType','forward','MaxFunctionEvaluations',2000,....
   'StepTolerance',.01, 'OptimalityTolerance', .01, 'FunctionTolerance', .01);
options.Algorithm='trust-region-reflective';
%Fitting Function
[x,fval]=lsqnonlin(@DFB_14f, J0,  lb, ub,options)
```

Matlab Script for Calculating R-factors for Experimental, Literature and Calculated J-couplings in 1,4-difluorobenzene

```
clear all
tic

    sys.isotopes={'19Fr','1H','1H','19Fr','1H','1H'};
    J1=9.89;
    J2=3.99;
    J3=21.95;
    J4=11.64;
    J5=1.12;
    J6=2.11;
    Fz=-119.6;
    Hz=6.50;
    inter.zeeman.scalar={ Fz Hz Hz Fz Hz Hz};

    inter.coupling.scalar={0 J1 J2 J3 J2 J1;
                           0 0 J4 J2 J5 J6;
                           0 0 0 J1 J6 J5 ;
                           0 0 0 0 J1 J2;
                           0 0 0 0 0 J4;
                           0 0 0 0 0 0};


sys.enable={'greedy','gpu','caching'};
  H=2195.435;
  g=spin('1H')/(2*pi);
  sys.magnet=H/g;

  %Relaxation
  FWHM_H=.12;
  FWHM_F=.13;
  inter.r2_rates=[ FWHM_F FWHM_H FWHM_H  FWHM_F FWHM_H FWHM_H];
  inter.relaxation={'t1_t2'};
  inter.r1_rates=inter.r2_rates;
  inter.rlx_keep='diagonal';
  inter.equilibrium='zero';

  % Basis set
  bas.connectivity='scalar_couplings';
  bas.space_level=4;
  bas.level=4;
  bas.formalism='sphten-liouv';
  bas.approximation='IK-2';


  % Sequence parameters
  parameters.sweep=1/1E-4;
  parameters.npoints=50000;
  parameters.zerofill= 300*1000;
  parameters.spins={'1H'};
  parameters.offset=0;
```

```
parameters.axis_units='Hz';
parameters.invert_axis=0;

% Spinach housekeeping
spin_system=create(sys,inter);
spin_system=basis(spin_system,bas);

% Simulation
fid=liquid(spin_system,@zerofield,parameters,'labframe');

% Fourier transform
spectrum=fftshift(fft(fid,parameters.zerofill));
spectrum1=real(spectrum);

spectrum2=sum(spectrum1,2);
spectrum3=spectrum2./max(real(spectrum2));

%
% Frequency
inc=parameters.sweep/parameters.zerofill;
hz=[-(parameters.sweep/2)+inc:inc:(parameters.sweep/2)];
hz=hz';
plot(hz,spectrum3)
%
%save('hz.mat','hz')
%save(name,'spectrum')
%Experimenatal Parameters
offset=2120;

%Read in 19F
a=dlmread('14DFB_19F.txt');
b=dlmread('14DFB_1H.txt');
hzFe=a(:,2)+offset;
hzHe=b(:,2)+offset;

ExpspectrumF=a(:,3)./1.52;
ExpspectrumH=b(:,3);


%Sum Spectrum
ExpspecsumH=sum(ExpspectrumH,2);
ExpspecsumF=sum(ExpspectrumF,2);
%
%Combine Spectra
Expspecsum=vertcat(ExpspecsumF,ExpspecsumH);
Expspecsum=Expspecsum./max(Expspecsum);
hze=vertcat(hzFe,hzHe);

%Normalize simulated spectrum to exp
spectrum3n=spectrum3./max(spectrum3);
%Round Hz
dp=1; %decimal places to round
```

```
hzr=round(hz,dp);
hzer=round(hze,dp);

%1H Residuals
lower=65.00+2120;
upper=85.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzh=hz(idxhl(1,1):idxhu(1,1));
hspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlhe=find(hzer==lower);
idxuhe=find(hzer==upper);
hzhe=hze(idxlhe(1,1):idxuhe(1,1));
hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
residhs=((hspece-hspec));

%19F Residuals

lower=-70.00+2120;
upper=-40.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzf=hz(idxhl(1,1):idxhu(1,1));
fspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlfe=find(hzer==lower);
idxufe=find(hzer==upper);
hzfe=hze(idxlfe(1,1):idxufe(1,1));
fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
residfs=((fspece-fspec));

%Combine Residuals
resids=vertcat(residfs,residhs);
spec=vertcat(fspec,hspec);
specexp=vertcat(fspece,hspece);
hzexp=vertcat(hzfe,hzhe);
%R Factor
RSS=sum(resids.^2)
Rfactor=100*(RSS/sum(specexp.^2))^.5
%Chi Squared
chi2=(resids.^2)./abs(spec);
ch2s=sum(chi2);
x=num2str(ch2s);
%Hydrogen Residuals
chi2h=(residhs.^2)./abs(hspec);
ch2sh=sum(chi2h);
RSSh=sum(residhs.^2);
Rfactorh=100*(RSSh/sum(hspece.^2))^.5;
y=num2str(Rfactorh);

%Fluorine Residuals
```

```
chi2f=(residfs.^2)./abs(fspec);
ch2sf=sum(chi2f);
RSSf=sum(residfs.^2);
Rfactorf=100*(RSSf/sum(fspece.^2))^.5;
z=num2str(Rfactorf);
%Plotting
subplot(2,1,1)

plot(hzfe,fspec,'color','r')
hold on
plot(hzfe,fspece,'color','k')
plot(hzfe,(residfs),'color','g')
title(z)
hold off

subplot(2,1,2)
plot(hzhe,hspec,'color','r')
hold on
plot(hzhe,hspece,'color','k')
plot(hzhe,residhs,'color','g')
hold off
title(y)
%sgtitle(x)
%}
```

MATLAB Function for Optimizing 1,2,4-trifluorobenzene

```
function Rfactors=TFB_124f(J)
J=round(J,2);
sys.magnet  = J(18)/(spin('1H')/(2*pi));
sys.enable={'greedy','gpu','caching'};
sys.isotopes={'19Fr','19Fr','1H','19Fr','1H','1H'};
sys.output='hush';
inter.r2_rates=[J(16) J(16) J(17) J(16) J(17) J(17)];
inter.zeeman.scalar={-143.5 -133.5 6.14  -115.7  6.326 6.38};
inter.coupling.scalar={0 J(1) J(2) J(3) J(4) J(5);
                       0 0 J(6) J(7) (J8) J(9);
                       0 0 0 J(10) J(11) J(12) ;
                       0 0 0 0 J(13) J(14);
                       0 0 0 0 0 J(15);
                       0 0 0 0 0 0};


%
%Relaxation
inter.relaxation={'t1_t2'};
inter.r1_rates=inter.r2_rates;
inter.rlx_keep='diagonal';
inter.equilibrium='zero';

%% Basis set
tic
bas.connectivity='scalar_couplings';
bas.space_level=4;
bas.level=4;
bas.formalism='sphten-liouv';
bas.approximation='IK-2';

% Sequence parameters
parameters.sweep=1/1E-4;
   parameters.npoints=50000;
   parameters.zerofill=300*1024;
   parameters.spins={'1H'};
   parameters.offset=0;
   parameters.axis_units='Hz';
   parameters.invert_axis=0;


% Spinach housekeeping
spin_system=create(sys,inter);
spin_system=basis(spin_system,bas);

% Simulation
fid=liquid(spin_system,@zerofield,parameters,'labframe');


% Fourier transform
   spectrum=fftshift(fft(fid,parameters.zerofill));
```

```
spectrum1=real(spectrum);

spectrum2=sum(spectrum1,2);
spectrum3=spectrum2./max(real(spectrum2));

%
% Frequency
inc=parameters.sweep/parameters.zerofill;
hz=[-(parameters.sweep/2)+inc:inc:(parameters.sweep/2)];
hz=hz';
%save('hz.mat','hz')
%save(name,'spectrum')
%Experimenatal Parameters
offset=2120;

%Read in 19F
a=dlmread('124TFB_19F_LS.txt');
b=dlmread('124TFB_1H_LS.txt');
hzFe=a(:,2)+offset;
hzHe=b(:,2)+offset;

ExpspectrumF=a(:,3)./1.52;
ExpspectrumH=b(:,3)-4E-5;


%Combine Spectra
Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
Expspecsum=Expspecsum./max(Expspecsum);
hze=vertcat(hzFe,hzHe);

%Normalize simulated spectrum to exp
spectrum3n=spectrum3;

%Round Hz
dp=1; %decimal places to round
hzr=round(hz,dp);
hzer=round(hze,dp);

%1H Residuals
lower=53.00+2120;
upper=95.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzh=hz(idxhl(1,1):idxhu(1,1));
hspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlhe=find(hzer==lower);
idxuhe=find(hzer==upper);
hzhe=hze(idxlhe(1,1):idxuhe(1,1));
hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
residhs=((hspece-hspec));
%
```

```
    %19F Residuals
    lower=-79.00+2120;
    upper=-30.00+2120;
    idxhl=find(hzr==lower);
    idxhu=find(hzr==upper);
    hzf=hz(idxhl(2,1):idxhu(1,1));
    fspec=spectrum3n(idxhl(2,1):idxhu(1,1));

    idxlfe=find(hzer==lower);
    idxufe=find(hzer==upper);
    hzfe=hze(idxlfe(1,1):idxufe(1,1));
    fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
    residfs=((fspece-fspec));

    %Combine Residuals
    resids=vertcat(residfs,residhs);
    expspec=vertcat(fspece,hspece);
    RSS=sum(resids.^2);
    Rfactor=100*(RSS/sum(expspec.^2))^.5
    for i=1:size(J,2)
       Rfactors(i)=Rfactor;
    end
    J

end
```

MATLAB Script for Optimization of 1,2,4-trifluorobenzene

```
%Initial Parameters
J1=-20.01;
J2=6.31;
J3=15.03;
J4=3.28;
J5=10.06;
J6= 10.72;
J7=3.14;
J8=-2.03;
J9=8.87;
J10=8.34;
J11=3.07;
J12=0.36;
J13=7.8;
J14=5.07;
J15=9.19;
J16=.11;
J17=.11;
J18 = 2195.92;
J0=[J1 J2 J3 J4 J5 J6 J7 J8 J9 J10 J11 J12 J13 J14 J15 J16 J17 J18];
%Bounds
lb=J0-.5;
lb(17)=.05;
lb(16)=.05;
lb(18)=-2195.7;
ub=lb+1;
ub(17)=.20;
ub(16)=.20;
ub(18)=2196.20;
%Options
options=optimoptions('lsqnonlin','FiniteDifferenceStepSize', 0.01,....
   'FiniteDifferenceType','forward','MaxFunctionEvaluations',2000,....
   'StepTolerance',.01, 'OptimalityTolerance', .01, 'FunctionTolerance', .01);
options.Algorithm='trust-region-reflective';
%Fitting
[x,fval]=lsqnonlin(@TFB_124f, J0,  lb, ub,options)
```

Matlab Script for Calculating R-factors for Experimental, Literature and Calculated J-couplings in 1,2,4-trifluorobenzene

```
clear all
sys.output='hush';
    H1z=6.14;
    H2z=6.326;
    H3z=6.38;
    F1z=-143.5;
    F2z=-133.5;
    F3z=-115.7;
     sys.isotopes={'19Fr','19Fr','1H','19Fr','1H','1H'};
     inter.zeeman.scalar={ F1z F2z H1z F3z H2z H3z};
     inter.coupling.scalar={0 -14.67 6.87 19.87 3.05 12.47;
                0 0 13.34 2.14 -3.871 9.34;
                0 0 0 10.55 2.14 1.09 ;
                0 0 0 0 9.64 4.94;
                0 0 0 0 0 11.80;
                0 0 0 0 0 0};


sys.enable={'greedy','gpu','caching'};
   H=2195.92 ;
   g=spin('1H')/(2*pi);
   sys.magnet=H/g;

   %Relaxation
   FWHMF=0.11;
   FHWMH=.11;
   inter.r2_rates= [FWHMF FWHMF FHWMH FWHMF FHWMH FHWMH] ;
   inter.relaxation={'t1_t2'};
   inter.r1_rates=inter.r2_rates;
   inter.rlx_keep='diagonal';
   inter.equilibrium='zero';

   % Basis set
   bas.connectivity='scalar_couplings';
   bas.space_level=4;
   bas.level=4;
   bas.formalism='sphten-liouv';
   bas.approximation='IK-2';

   % Sequence parameters
   parameters.sweep=1/1E-4;
   parameters.npoints=50000;
   parameters.zerofill=300*1024;
   parameters.offset=0;
   parameters.spins={'1H'};
   parameters.axis_units='Hz';
   parameters.invert_axis=0;

   % Spinach housekeeping
   spin_system=create(sys,inter);
```

```
spin_system=basis(spin_system,bas);

% Simulation
fid=liquid(spin_system,@zerofield,parameters,'labframe');
% Fourier transform
spectrum=fftshift(fft(fid,parameters.zerofill));
spectrum1=real(spectrum);

spectrum2=sum(spectrum1,2);
spectrum3=spectrum2./max(real(spectrum2));
plot(spectrum3)
%
% Frequency
inc=parameters.sweep/parameters.zerofill;
hz=[-(parameters.sweep/2)+inc:inc:(parameters.sweep/2)];
hz=hz';
%save('hz.mat','hz')
%save(name,'spectrum')
%Experimenatal Parameters
offset=2120;

%Read in 19F
a=dlmread('124TFB_19F_LS.txt');
b=dlmread('124TFB_1H_LS.txt');
hzFe=a(:,2)+offset;
hzHe=b(:,2)+offset;

ExpspectrumF=a(:,3)/1.52;
ExpspectrumH=b(:,3)-4E-5;


%Combine Spectra
Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
Expspecsum=Expspecsum./max(Expspecsum);
hze=vertcat(hzFe,hzHe);

%Normalize simulated spectrum to exp
spectrum3n=spectrum3;%.*max(Expspecsum);

%Round Hz
dp=1; %decimal places to round
hzr=round(hz,dp);
hzer=round(hze,dp);

%1H Residuals
lower=53.00+2120;
upper=95.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzh=hz(idxhl(1,1):idxhu(1,1));
hspec=spectrum3n(idxhl(1,1):idxhu(1,1));
```

```
idxlhe=find(hzer==lower);
idxuhe=find(hzer==upper);
hzhe=hze(idxlhe(1,1):idxuhe(1,1));
hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
residhs=((hspece-hspec));
%
%19F Residuals
lower=-79.00+2120;
upper=-30.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzf=hz(idxhl(2,1):idxhu(1,1));
fspec=spectrum3n(idxhl(2,1):idxhu(1,1));

idxlfe=find(hzer==lower);
idxufe=find(hzer==upper);
hzfe=hze(idxlfe(1,1):idxufe(1,1));
fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
residfs=((fspece-fspec));

%Combine Residuals
resids=vertcat(residfs,residhs);
spec=vertcat(fspec,hspec);
specexp=vertcat(fspece,hspece);
hzexp=vertcat(hzfe,hzhe);
%R Factor
RSS=sum(resids.^2)
Rfactor=100*(RSS/sum(specexp.^2))^.5

RSSh=sum(residhs.^2);
Rfactorh=100*(RSSh/sum(hspece.^2))^.5;
y=num2str(Rfactorh);

RSSf=sum(residfs.^2);
Rfactorf=100*(RSSf/sum(fspece.^2))^.5;
z=num2str(Rfactorf);
%Plotting
subplot(2,1,1)
plot(hzfe,fspec,'color','r')
hold on
plot(hzfe,fspece,'color','k')
plot(hzfe,(residfs),'color','g')
title(z)
hold off

subplot(2,1,2)
plot(hzhe,hspec,'color','r')
hold on
plot(hzhe,hspece,'color','k')
plot(hzhe,residhs,'color','g')
hold off
title(y)
```

MATLAB Function for Optimizing 1,2,4,5-tetrafluorobenzene

```
function Rfactors=TFB_1245f(J)
    J=round(J,2);
    sys.output='hush';
    sys.isotopes={'19Fr','19Fr','1H','19Fr','19Fr','1H'};
    Fz=-139.7;
    Hz=6.2;
    inter.zeeman.scalar={ Fz Fz Hz Fz Fz Hz};
    inter.coupling.scalar={0 J(1) J(2) J(3) J(4) J(5);
                0 0 J(5) J(4) J(3) J(2);
                0 0 0 J(5) J(2) J(6) ;
                0 0 0 0 J(1) J(2);
                0 0 0 0 0 J(5);
                0 0 0 0 0 0};


sys.enable={'greedy','gpu','caching'};

  g=spin('1H')/(2*pi);
  sys.magnet=J(7)/g;

  %Relaxation

  inter.r2_rates=[J(8) J(8) J(9) J(8) J(8) J(9)];
  inter.relaxation={'t1_t2'};
  inter.r1_rates=inter.r2_rates;
  inter.rlx_keep='diagonal';
  inter.equilibrium='zero';

  % Basis set
  bas.connectivity='scalar_couplings';
  bas.space_level=4;
  bas.level=4;
  bas.formalism='sphten-liouv';
  bas.approximation='IK-2';

   % Sequence parameters
  parameters.sweep=1/1E-4;
  parameters.npoints=50000;
  parameters.zerofill=300*1024;
  parameters.spins={'1H'};
  parameters.offset=0;
  parameters.axis_units='Hz';
  parameters.invert_axis=0;

  % Spinach housekeeping
  spin_system=create(sys,inter);
  spin_system=basis(spin_system,bas);

  % Simulation
  fid=liquid(spin_system,@zerofield,parameters,'labframe');
```

```
% Fourier transform
spectrum=fftshift(fft(fid,parameters.zerofill));
spectrum1=real(spectrum);

spectrum2=sum(spectrum1,2);
spectrum3=spectrum2./max(real(spectrum2));
%plot(spectrum3)
%
% Frequency
inc=parameters.sweep/parameters.zerofill;
hz=[-(parameters.sweep/2)+inc:inc:(parameters.sweep/2)];
hz=hz';
%save('hz.mat','hz')
%save(name,'spectrum')
%Experimenatal Parameters
offset=2120;

%Read in 19F
a=dlmread('1245_TFB_19F.txt');
b=dlmread('1245_TFB_1H.txt');
hzFe=a(:,2)+offset;
hzHe=b(:,2)+offset;

ExpspectrumF=(a(:,3)-.25E-4)./1.52;
ExpspectrumH=b(:,3);


%Combine Spectra
Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
Expspecsum=Expspecsum./max(Expspecsum);
hze=vertcat(hzFe,hzHe);

%Normalize simulated spectrum to exp
spectrum3n=spectrum3;%.*max(Expspecsum);

%Round Hz
dp=1; %decimal places to round
hzr=round(hz,dp);
hzer=round(hze,dp);

%1H Residuals
lower=50.00+2120;
upper=97.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzh=hz(idxhl(1,1):idxhu(1,1));
hspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlhe=find(hzer==lower);
idxuhe=find(hzer==upper);
hzhe=hze(idxlhe(1,1):idxuhe(1,1));
```

```
    hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
    residhs=((hspece-hspec));
   %
    %19F Residuals
    lower=-70.00+2120;
    upper=-39.00+2120;
    idxhl=find(hzr==lower);
    idxhu=find(hzr==upper);
    hzf=hz(idxhl(1,1):idxhu(1,1));
    fspec=spectrum3n(idxhl(1,1):idxhu(1,1));

    idxlfe=find(hzer==lower);
    idxufe=find(hzer==upper);
    hzfe=hze(idxlfe(1,1):idxufe(1,1));
    fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
    residfs=((fspece-fspec));

    %Combine Residuals
    resids=vertcat(residfs,residhs);
    spec=vertcat(fspec,hspec);
    specexp=vertcat(fspece,hspece);
    hzexp=vertcat(hzfe,hzhe);
    %R Factor
    RSS=sum(resids.^2)
    Rfactor=100*(RSS/sum(specexp.^2))^.5

    RSSh=sum(residhs.^2);
    Rfactorh=100*(RSSh/sum(hspece.^2))^.5;
    y=num2str(Rfactorh);

    RSSf=sum(residfs.^2);
    Rfactorf=100*(RSSf/sum(fspece.^2))^.5;
    z=num2str(Rfactorf);
    for i=1:size(J,2)
       Rfactors(i)=Rfactor;
    end
    J

end
```

MATLAB Script for Optimization of 1,2,4,5-tetrafluorobenzene

```
%Parameters
J1=-20.74; % F-F
J2=7.45; %F-H
J3=13.22; %F-F
J4=-0.5; %F-F
J5=10.03; %F-H
J6=.53;
J7=2196.03 ;
J8=0.11;
J9=.11;
J0=[J1 J2 J3 J4 J5 J6 J7 J8 J9];
%Bounds
lb(7)=2195.8;
lb=J0-.5
ub(8)=.08;
ub(9)=.08;
ub(7)=2196.2;
ub=lb+1;
ub(8)=.2;
ub(9)=.2;
%Fitting Options
options=optimoptions('lsqnonlin','FiniteDifferenceStepSize', 0.01,....
   'FiniteDifferenceType','forward','MaxFunctionEvaluations',2000,....
   'StepTolerance',.1, 'OptimalityTolerance', .01, 'FunctionTolerance', .01);
options.Algorithm='trust-region-reflective';
%Fitting
[x,fval]=lsqnonlin(@TFB_1245f, J0,  lb, ub,options)
```

Matlab Script for Calculating R-factors for Experimental, Literature and Calculated J-couplings in 1,2,4,5-tetrafluorobenzene

```
clear all

    sys.output='hush';
    sys.isotopes={'19Fr','19Fr','1H','19Fr','19Fr','1H'};
    J1=-14.67; % F-F
    J2=8; %F-H
    J3=18.54; %F-F
    J4=-4.65; %F-F
    J5=12.98; %F-H
    J6=1.35;
    Fz=-139.7;
    Hz=6.2;
    inter.zeeman.scalar={ Fz Fz Hz Fz Fz Hz};
    inter.coupling.scalar={0 J1 J2 J3 J4 J5;
                           0 0 J5 J4 J3 J2;
                           0 0 0 J5 J2 J6 ;
                           0 0 0 0 J1 J2;
                           0 0 0 0 0 J5;
                           0 0 0 0 0 0};


sys.enable={'greedy','gpu','caching'};
  H=2196.03 ;
  g=spin('1H')/(2*pi);
  sys.magnet=H/g;

  %Relaxation
  FWHMF=0.11;
  FWHMH=.11;
  inter.r2_rates=[FWHMF FWHMF FWHMH FWHMF FWHMF FWHMH];
  inter.relaxation={'t1_t2'};
  inter.r1_rates=inter.r2_rates;
  inter.rlx_keep='diagonal';
  inter.equilibrium='zero';

  % Basis set
  bas.connectivity='scalar_couplings';
  bas.space_level=4;
  bas.level=4;
  bas.formalism='sphten-liouv';
  bas.approximation='IK-2';

   % Sequence parameters
  parameters.sweep=1/1E-4;
  parameters.npoints=50000;
  parameters.zerofill=300*1024;
  parameters.spins={'1H'};
  parameters.offset=0;
  parameters.axis_units='Hz';
  parameters.invert_axis=0;
```

```
% Spinach housekeeping
spin_system=create(sys,inter);
spin_system=basis(spin_system,bas);

% Simulation
fid=liquid(spin_system,@zerofield,parameters,'labframe');

% Fourier transform
spectrum=fftshift(fft(fid,parameters.zerofill));
spectrum1=real(spectrum);

spectrum2=sum(spectrum1,2);
spectrum3=spectrum2./max(real(spectrum2));
%plot(spectrum3)
%
% Frequency
inc=parameters.sweep/parameters.zerofill;
hz=[-(parameters.sweep/2)+inc:inc:(parameters.sweep/2)];
hz=hz';
%save('hz.mat','hz')
%save(name,'spectrum')
%Experimenatal Parameters
offset=2120;

%Read in 19F
a=dlmread('1245_TFB_19F.txt');
b=dlmread('1245_TFB_1H.txt');
hzFe=a(:,2)+offset;
hzHe=b(:,2)+offset;

ExpspectrumF=(a(:,3)-.25E-4)./1.52;
ExpspectrumH=b(:,3);


%Combine Spectra
Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
Expspecsum=Expspecsum./max(Expspecsum);
hze=vertcat(hzFe,hzHe);

%Normalize simulated spectrum to exp
spectrum3n=spectrum3;%.*max(Expspecsum);

%Round Hz
dp=1; %decimal places to round
hzr=round(hz,dp);
hzer=round(hze,dp);

%1H Residuals
lower=50.00+2120;
upper=97.00+2120;
idxhl=find(hzr==lower);
```

```
idxhu=find(hzr==upper);
hzh=hz(idxhl(1,1):idxhu(1,1));
hspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlhe=find(hzer==lower);
idxuhe=find(hzer==upper);
hzhe=hze(idxlhe(1,1):idxuhe(1,1));
hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
residhs=((hspece-hspec));
%
%19F Residuals
lower=-70.00+2120;
upper=-39.00+2120;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzf=hz(idxhl(1,1):idxhu(1,1));
fspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlfe=find(hzer==lower);
idxufe=find(hzer==upper);
hzfe=hze(idxlfe(1,1):idxufe(1,1));
fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
residfs=((fspece-fspec));

%Combine Residuals
resids=vertcat(residfs,residhs);
spec=vertcat(fspec,hspec);
specexp=vertcat(fspece,hspece);
hzexp=vertcat(hzfe,hzhe);
%R Factor
RSS=sum(resids.^2)
Rfactor=100*(RSS/sum(specexp.^2))^.5

RSSh=sum(residhs.^2);
Rfactorh=100*(RSSh/sum(hspece.^2))^.5;
y=num2str(Rfactorh);

RSSf=sum(residfs.^2);
Rfactorf=100*(RSSf/sum(fspece.^2))^.5;
z=num2str(Rfactorf);
%Plotting
subplot(2,1,1)
plot(hzfe,fspec,'color','r')
hold on
plot(hzfe,fspece,'color','k')
plot(hzfe,(residfs),'color','g')
title(z)
hold off

subplot(2,1,2)
plot(hzhe,hspec,'color','r')
hold on
```

```
plot(hzhe,hspece,'color','k')
plot(hzhe,residhs,'color','g')
hold off
title(y)
```

MATLAB Function for Optimizing pentafluorobenzene

```
function Rfactors=PFBf(P)
%Parameters
   Fz1=-139.2;
   Fz2=-162.5;
   Fz3=-154.2;
   Hz=5.8;
   FWHMH=.11;
   FWHMF=.11;
   P=round(P,2);
%Setting  up System Parameters
sys.enable={'greedy','gpu','caching'};
sys.output='hush';
g=spin('1H')/(2*pi);
sys.magnet=P(1)/g;
sys.isotopes={'1H','19Fr','19Fr','19Fr','19Fr','19Fr'};
%J-couplings and Chemical Shifts
inter.zeeman.scalar={ Hz Fz1 Fz2 Fz3 Fz2 Fz1};
inter.coupling.scalar={0 P(2) P(3) P(4) P(3) P(2);
            0 0 P(5) P(6) P(7) P(10);
            0 0 0 P(9) P(8) P(7) ;
            0 0 0 0 P(9) P(6);
            0 0 0 0 0 P(5);
            0 0 0 0 0 0};
%Relaxation
   inter.r2_rates=[P(11) P(12) P(12) P(12) P(12) P(12)];
   inter.relaxation={'t1_t2'};
   inter.r1_rates=inter.r2_rates;
   inter.rlx_keep='diagonal';
   inter.equilibrium='zero';

% Basis set
   bas.connectivity='scalar_couplings';
   bas.space_level=4;
   bas.level=4;
   bas.formalism='sphten-liouv';
   bas.approximation='IK-2';

% Sequence parameters
   parameters.sweep=1/1E-4;
   parameters.npoints=50000;
   parameters.zerofill=300*1024;
   parameters.spins={'1H'};
   parameters.offset=0;
   parameters.axis_units='Hz';
   parameters.invert_axis=0;

% Spinach housekeeping
   spin_system=create(sys,inter);
   spin_system=basis(spin_system,bas);

% Simulation
```

```
   fid=liquid(spin_system,@zerofield,parameters,'labframe');

% Fourier transform
   spectrum=fftshift(fft(fid,parameters.zerofill));
   spectrum3=real(spectrum)./max(real(spectrum));
%
% Frequency (Reads same as Python Script)
   hz=axis_1d(spin_system, parameters);
   hz=hz';

%Experimenatal Parameters
   offset=2120;

%Read in Experimental Parameters
   a=dlmread('PFB_19F.txt');
   b=dlmread('PFB_1H.txt');
   hzFe=a(:,2)+offset;
   hzHe=b(:,2)+offset;

% Normalize to Q-factor
   ExpspectrumF=a(:,3)./1.52;
   ExpspectrumH=b(:,3);

%Combine Spectra
   Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
   Expspecsum=Expspecsum./max(Expspecsum);
   hze=vertcat(hzFe,hzHe);

%Round Hz
   dp=1; %decimal places to round
   hzr=round(hz,dp);
   hzer=round(hze,dp);

%1H Residuals
   lower=53.00+2120;
   upper=95.00+2120;
   idxhl=find(hzr==lower);
   idxhu=find(hzr==upper);
   hzh=hz(idxhl(1,1):idxhu(1,1));
   hspec=spectrum3(idxhl(1,1):idxhu(1,1));

   idxlhe=find(hzer==lower);
   idxuhe=find(hzer==upper);
   hzhe=hze(idxlhe(1,1):idxuhe(1,1));
   hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
   residhs=((hspece-hspec));

%19F Residuals
   lower=-70.00+2120;
   upper=-41.00+2120;
   idxhl=find(hzr==lower);
   idxhu=find(hzr==upper);
```

```
    hzf=hz(idxhl(2,1):idxhu(1,1));
    fspec=spectrum3(idxhl(2,1):idxhu(1,1));

    idxlfe=find(hzer==lower);
    idxufe=find(hzer==upper);
    hzfe=hze(idxlfe(1,1):idxufe(1,1));
    fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
    residfs=((fspece-fspec));

%Combine Residuals
    resids=vertcat(residfs,residhs);
    spec=vertcat(fspec,hspec);
    specexp=vertcat(fspece,hspece);
    hzexp=vertcat(hzfe,hzhe);
%R Factor
    RSS=sum(resids.^2)
    Rfactor=100*(RSS/sum(specexp.^2))^.5

%Hydrogen Residuals
    RSSh=sum(residhs.^2);
    Rfactorh=100*(RSSh/sum(hspece.^2))^.5;
    y=num2str(Rfactorh);

%Fluorine Residuals
    RSSf=sum(residfs.^2);
    Rfactorf=100*(RSSf/sum(fspece.^2))^.5;
    z=num2str(Rfactorf);
    for i=1:size(P,2)
        Rfactors(i)=Rfactor;
    end
    P
    end
%}
```

MATLAB Script for Optimization of pentafluorobenzene

```
%Inital Parameters
H=2195.25 ;
J1=10.31; % F-H
J2=6.93; %F-H
J3=-2.70; %F-H
J4=-21.10; %F-F
J8=-18.95;
J6=9.10;
J9=-2.3;
J5=1.3; %F-H
J7=-.65;
FWHMH=.11;
FWHMF=.11;
P=[ H J1 J2 J3 J4 J5 J6 J7 J8 J9 FWHMH FWHMF];
%Bounds
lb=P0-.5;
ub=lb+1;
lb(1)=H-.04;
ub(1)=H+.04;
lb(12)=.08;
lb(13)=.08;
ub(12)=.16;
ub(13)=.16;
%Fitting Options
options=optimoptions('lsqnonlin','FiniteDifferenceStepSize', 0.1,....
'FiniteDifferenceType','forward','MaxFunctionEvaluations',2000,....
'StepTolerance',.1, 'OptimalityTolerance', .1, 'FunctionTolerance', .1);
options.Algorithm='trust-region-reflective';
%Fitting
[x,fval]=lsqnonlin(@PFBf, P0,  lb, ub,options)
```

Matlab Script for Calculating R-factors for Experimental, Literature and Calculated J-couplings in pentafluorobenzene

```
% Pentafluorobenzene Simulation
clear all

%Parameters
   H=2195.25 ;
   J1=10.31; % F-H
   J2=6.93; %F-H
   J3=-2.70; %F-H
   J4=-21.10; %F-F
   J8=-18.95;
   J6=9.10;
   J9=-2.3;
   J5=1.3; %F-H
   J7=-.65;
   Fz1=-139.2;
   Fz2=-162.5;
   Fz3=-154.2;
   Hz=5.8;
   FWHMH=.11;
   FWHMF=.11;
P=[ H J1 J2 J3 J4 J5 J6 J7 J8 J9 FWHMH FWHMF];
%Setting  up System Parameters
sys.enable={'greedy','gpu','caching'};
sys.output='hush';
g=spin('1H')/(2*pi);
sys.magnet=P(1)/g;
sys.isotopes={'1H','19Fr','19Fr','19Fr','19Fr','19Fr'};
%J-couplings and Chemical Shifts
inter.zeeman.scalar={ Hz Fz1 Fz2 Fz3 Fz2 Fz1};
inter.coupling.scalar={0 P(2) P(3) P(4) P(3) P(2);
            0 0 P(5) P(6) P(7) P(10);
            0 0 0 P(9) P(8) P(7) ;
            0 0 0 0 P(9) P(6);
            0 0 0 0 0 P(5);
            0 0 0 0 0 0};
%Relaxation
   inter.r2_rates=[P(11) P(12) P(12) P(12) P(12) P(12)];
   inter.relaxation={'t1_t2'};
   inter.r1_rates=inter.r2_rates;
   inter.rlx_keep='diagonal';
   inter.equilibrium='zero';

% Basis set
   bas.connectivity='scalar_couplings';
   bas.space_level=4;
   bas.level=4;
   bas.formalism='sphten-liouv';
   bas.approximation='IK-2';

% Sequence parameters
```

```
    parameters.sweep=1/1E-4;
    parameters.npoints=50000;
    parameters.zerofill=300*1024;
    parameters.spins={'1H'};
    parameters.offset=0;
    parameters.axis_units='Hz';
    parameters.invert_axis=0;

% Spinach housekeeping
    spin_system=create(sys,inter);
    spin_system=basis(spin_system,bas);

% Simulation
    fid=liquid(spin_system,@zerofield,parameters,'labframe');

% Fourier transform
    spectrum=fftshift(fft(fid,parameters.zerofill));
    spectrum3=real(spectrum)./max(real(spectrum));
%
% Frequency (Reads same as Python Script)
    hz=axis_1d(spin_system, parameters);
    hz=hz';

%Experimenatal Parameters
    offset=2120;

%Read in Experimental Parameters
    a=dlmread('PFB_19F.txt');
    b=dlmread('PFB_1H.txt');
    hzFe=a(:,2)+offset;
    hzHe=b(:,2)+offset;

% Normalize to Q-factor
    ExpspectrumF=a(:,3)./1.52;
    ExpspectrumH=b(:,3);

%Combine Spectra
    Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
    Expspecsum=Expspecsum./max(Expspecsum);
    hze=vertcat(hzFe,hzHe);

%Round Hz
    dp=1; %decimal places to round
    hzr=round(hz,dp);
    hzer=round(hze,dp);

%1H Residuals
    lower=53.00+2120;
    upper=95.00+2120;
    idxhl=find(hzr==lower);
    idxhu=find(hzr==upper);
    hzh=hz(idxhl(1,1):idxhu(1,1));
```

```
    hspec=spectrum3(idxhl(1,1):idxhu(1,1));

    idxlhe=find(hzer==lower);
    idxuhe=find(hzer==upper);
    hzhe=hze(idxlhe(1,1):idxuhe(1,1));
    hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
    residhs=((hspece-hspec));

%19F Residuals
    lower=-70.00+2120;
    upper=-41.00+2120;
    idxhl=find(hzr==lower);
    idxhu=find(hzr==upper);
    hzf=hz(idxhl(2,1):idxhu(1,1));
    fspec=spectrum3(idxhl(2,1):idxhu(1,1));

    idxlfe=find(hzer==lower);
    idxufe=find(hzer==upper);
    hzfe=hze(idxlfe(1,1):idxufe(1,1));
    fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
    residfs=((fspece-fspec));

%Combine Residuals
    resids=vertcat(residfs,residhs);
    spec=vertcat(fspec,hspec);
    specexp=vertcat(fspece,hspece);
    hzexp=vertcat(hzfe,hzhe);
%R Factor
    RSS=sum(resids.^2)
    Rfactor=100*(RSS/sum(specexp.^2))^.5

%Hydrogen Residuals
    RSSh=sum(residhs.^2);
    Rfactorh=100*(RSSh/sum(hspece.^2))^.5;
    y=num2str(Rfactorh);

%Fluorine Residuals
    RSSf=sum(residfs.^2);
    Rfactorf=100*(RSSf/sum(fspece.^2))^.5;
    z=num2str(Rfactorf);
%Plotting
subplot(2,1,1)
plot(hzfe,fspec,'color','r')
hold on
plot(hzfe,fspece,'color','k')
plot(hzfe,(residfs),'color','g')
title(z)
hold off

subplot(2,1,2)
plot(hzhe,hspec,'color','r')
hold on
```

```
plot(hzhe,hspece,'color','k')
plot(hzhe,residhs,'color','g')
hold off
title(y)
%}
```

MATLAB Script for simulating hexafluorobenzene

```
clear all

    sys.isotopes={ '19F','1H','19F','1H'};
    inter.coupling.scalar{4,4}=0;

sys.enable={'greedy','gpu','caching'};
  H=2198.74;
  sys.magnet=H/(spin('1H')/(2*pi));
  H1=7.3;
  Fz=-163.2;
  inter.zeeman.scalar={ Fz H1 Fz H1};
  %Relaxation
  FWHM=0.31;
  [a spinsize]=size(sys.isotopes)
  for I=1:spinsize
    inter.r2_rates(I)=FWHM;
  end
  inter.relaxation={'t1_t2'};
  inter.r1_rates=inter.r2_rates;
  inter.rlx_keep='diagonal';
  inter.equilibrium='zero';

  % Basis set
  bas.connectivity='scalar_couplings';
  bas.space_level=4;
  bas.level=4;
  bas.formalism='sphten-liouv';
  bas.approximation='IK-2';

  % Sequence parameters
  parameters.sweep=1/1E-4;
  parameters.npoints=100000;
  parameters.zerofill=900*1024;
  parameters.offset=0;
  parameters.spins={'1H'};
  parameters.axis_units='Hz';
  parameters.invert_axis=0;

% Spinach housekeeping
  spin_system=create(sys,inter);
  spin_system=basis(spin_system,bas);

  % Simulation
  fid=liquid(spin_system,@zerofield,parameters,'labframe');

  % Fourier transform
  spectrum=fftshift(fft(fid,parameters.zerofill));
  spectrum1=real(spectrum);

  spectrum2=sum(spectrum1,2);
  spectrum3=spectrum2./max(real(spectrum2));
```

```
plot(spectrum3)
%
% Frequency
inc=parameters.sweep/parameters.zerofill;
hz=[-(parameters.sweep/2)+inc:inc:(parameters.sweep/2)];
hz=hz';
%save('hz.mat','hz')
%save(name,'spectrum')
%Experimenatal Parameters
offset=0;

%Read in 19F
a=dlmread('HFB_19F.txt');
b=dlmread('HFB_1H.txt');
hzFe=a(:,2)+offset;
hzHe=b(:,2)+offset;

ExpspectrumF=a(:,3);
ExpspectrumH=b(:,3);


%Combine Spectra
Expspecsum=vertcat(ExpspectrumF,ExpspectrumH);
Expspecsum=(Expspecsum./max(Expspecsum));
hze=vertcat(hzFe,hzHe);

%Normalize simulated spectrum to exp
spectrum3n=spectrum3;%.*max(Expspecsum);
%
%Round Hz
dp=1; %decimal places to round
hzr=round(hz,dp);
hzer=round(hze,dp);

%1H Residuals
lower=2196.00;
upper=2202.00;
idxhl=find(hzr==lower);
idxhu=find(hzr==upper);
hzh=hz(idxhl(1,1):idxhu(1,1));
hspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlhe=find(hzer==lower);
idxuhe=find(hzer==upper);
hzhe=hze(idxlhe(1,1):idxuhe(1,1));
hspece=Expspecsum(idxlhe(1,1):idxuhe(1,1));
residhs=((hspece-hspec));
%
%19F Residuals
lower=2065.00;
upper=2072.00;
idxhl=find(hzr==lower);
```

```
idxhu=find(hzr==upper);
hzf=hz(idxhl(1,1):idxhu(1,1));
fspec=spectrum3n(idxhl(1,1):idxhu(1,1));

idxlfe=find(hzer==lower);
idxufe=find(hzer==upper);
hzfe=hze(idxlfe(1,1):idxufe(1,1));
fspece=Expspecsum(idxlfe(1,1):idxufe(1,1)) ;
residfs=((fspece-fspec));

%Combine Residuals
resids=vertcat(residfs,residhs);
spec=vertcat(fspec,hspec);
specexp=vertcat(fspece,hspece);
hzexp=vertcat(hzfe,hzhe);
%R Factor
RSS=sum(resids.^2)
Rfactor=100*(RSS/sum(specexp.^2))^.5

RSSh=sum(residhs.^2);
Rfactorh=100*(RSSh/sum(hspece.^2))^.5;
y=num2str(Rfactorh);

RSSf=sum(residfs.^2);
Rfactorf=100*(RSSf/sum(fspece.^2))^.5;
z=num2str(Rfactorf);
%Plotting
subplot(2,1,1)
plot(hzfe,fspec,'color','r')
hold on
plot(hzfe,fspece,'color','k')
plot(hzfe,(residfs),'color','g')
title(z)
hold off

subplot(2,1,2)
plot(hzhe,hspec,'color','r')
hold on
plot(hzhe,hspece,'color','k')
plot(hzhe,residhs,'color','g')
hold off
title(y)
```