```
% This script borrows heavily from the examples included in the Spinach
% documentation.


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% This is a Spinach script that computes chemically weighted observables
% as described in the accompanying article: (((DOI-URL)))
% The spin system in this script is a 14-spin system which includes two
% 3-monofluoro pyridine ligands in the SABRE complex. Both coherent and
% incoherent interactions, including SRSK, are accounted for. The basis
% set used is the approximate IK-0.
% The script was run with Spinach 2.8.6280 on MATLAB R2023b using MATLAB
% Parallel Server.
% It may require approximately 125 GB memory when running in serial.



function [output] = Code_example()

% Paths that need to be defined when running on a computer cluster:
% spinach_root='/path/to/Spinach/root';
% addpath(genpath(strcat(spinach_root,'/kernel')));
% addpath(genpath(strcat(spinach_root,'/etc')));
% addpath(genpath(strcat(spinach_root,'/experiments')));
% addpath(genpath(strcat(spinach_root,'/interfaces')));
% sys.scratch='/path/to/scratch/directory';

% Spin system
sys.isotopes= ...
    {'1H','1H','19F','19F','1H','1H','1H','1H','1H','1H','1H','1H','14N','14N'};

% External magnetic field
sys.magnet=8e-3;%T

% Isotropic chemical shifts in ppm
% Hydride 1H have an empirical correction of -15 ppm, to mimic spin-orbit
% interactions.
inter.zeeman.scalar={ ...
```

```
    31.8-38.76-15, ...
    31.8-38.39-15, ...
    0-299.18, ...
    0-295.30, ...
    31.8-23.52, ...
    31.8-23.92, ...
    31.8-23.96, ...
    31.8-23.74, ...
    31.8-24.26, ...
    31.8-23.73, ...
    31.8-22.79, ...
    31.8-22.62, ...
    0-(-50.40), ...
    0-(-46.65)
};

% Quadrupolar couplings in Hz
quadrupole_interaction_matrix_N13= ...
    [-1.17768258856086 -0.393220967215213 -0.998512389249073; ...
    -0.393220967215213 0.702950919489465 0.140209033602540; ...
    -0.998512389249073 0.140209033602540 0.474731669071391]*1000000;
quadrupole_interaction_matrix_N14= ...
    [0.515532213218896 0.691522149831549 0.012066997811812; ...
    0.691522149831549 -1.04842609086094 0.900862905381405; ...
    0.012066997811812 0.900862905381405 0.532893877642048]*1000000;
quadrupole_interaction_matrix_N13=quadrupole_interaction_matrix_N13 ...
    -diag((1/3)*trace(quadrupole_interaction_matrix_N13)*ones(1,3));
quadrupole_interaction_matrix_N14=quadrupole_interaction_matrix_N14 ...
    -diag((1/3)*trace(quadrupole_interaction_matrix_N14)*ones(1,3));
inter.coupling.matrix{13,13}=quadrupole_interaction_matrix_N13;
inter.coupling.matrix{14,14}=quadrupole_interaction_matrix_N14;

% J-couplings in Hz
inter.coupling.scalar=cell(14);
inter.coupling.scalar{1,2}=-7.67;
inter.coupling.scalar{1,3}=-0.05;
inter.coupling.scalar{1,4}=1.87;
inter.coupling.scalar{1,5}=-0.03;
inter.coupling.scalar{1,6}=1.65;
inter.coupling.scalar{1,7}=0.02;
inter.coupling.scalar{1,8}=0.02;
inter.coupling.scalar{1,9}=-0.02;
inter.coupling.scalar{1,10}=0.41;
inter.coupling.scalar{1,11}=-0.10;
inter.coupling.scalar{1,12}=1.42;
inter.coupling.scalar{1,13}=-0.23;
inter.coupling.scalar{1,14}=15.32;
inter.coupling.scalar{2,3}=2.08;
inter.coupling.scalar{2,4}=-0.02;
inter.coupling.scalar{2,5}=1.77;
inter.coupling.scalar{2,6}=0.39;
inter.coupling.scalar{2,7}=0.01;
inter.coupling.scalar{2,8}=-0.02;
inter.coupling.scalar{2,9}=0.45;
inter.coupling.scalar{2,10}=-0.10;
inter.coupling.scalar{2,11}=1.49;
inter.coupling.scalar{2,12}=0.08;
inter.coupling.scalar{2,13}=16.49;
inter.coupling.scalar{2,14}=-0.41;
inter.coupling.scalar{3,4}=-0.07;
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```
inter.coupling.scalar{3,5}=1.34;
inter.coupling.scalar{3,6}=-0.07;
inter.coupling.scalar{3,7}=5.69;
inter.coupling.scalar{3,8}=-0.04;
inter.coupling.scalar{3,9}=5.07;
%inter.coupling.scalar{3,10}=0.00;
inter.coupling.scalar{3,11}=-0.12;
inter.coupling.scalar{3,12}=-0.05;
inter.coupling.scalar{3,13}=-3.56;
%inter.coupling.scalar{3,14}=0.00;
inter.coupling.scalar{4,5}=-0.21;
inter.coupling.scalar{4,6}=1.56;
inter.coupling.scalar{4,7}=-0.05;
inter.coupling.scalar{4,8}=5.34;
inter.coupling.scalar{4,9}=-0.06;
inter.coupling.scalar{4,10}=4.80;
inter.coupling.scalar{4,11}=-0.07;
inter.coupling.scalar{4,12}=-0.23;
inter.coupling.scalar{4,13}=-0.02;
inter.coupling.scalar{4,14}=-2.85;
inter.coupling.scalar{5,6}=0.01;
inter.coupling.scalar{5,7}=2.32;
inter.coupling.scalar{5,8}=-0.03;
inter.coupling.scalar{5,9}=0.62;
inter.coupling.scalar{5,10}=0.11;
inter.coupling.scalar{5,11}=-0.31;
inter.coupling.scalar{5,12}=-0.11;
inter.coupling.scalar{5,13}=4.42;
inter.coupling.scalar{5,14}=0.07;
inter.coupling.scalar{6,7}=-0.05;
inter.coupling.scalar{6,8}=2.38;
inter.coupling.scalar{6,9}=-0.04;
inter.coupling.scalar{6,10}=0.63;
inter.coupling.scalar{6,11}=0.02;
inter.coupling.scalar{6,12}=-0.31;
%inter.coupling.scalar{6,13}=0.00;
inter.coupling.scalar{6,14}=3.77;
inter.coupling.scalar{7,8}=-0.04;
inter.coupling.scalar{7,9}=8.76;
inter.coupling.scalar{7,10}=-0.04;
inter.coupling.scalar{7,11}=0.70;
inter.coupling.scalar{7,12}=-0.02;
inter.coupling.scalar{7,13}=-0.32;
%inter.coupling.scalar{7,14}=0.00;
inter.coupling.scalar{8,9}=-0.05;
inter.coupling.scalar{8,10}=8.77;
inter.coupling.scalar{8,11}=-0.06;
inter.coupling.scalar{8,12}=0.68;
%inter.coupling.scalar{8,13}=0.00;
inter.coupling.scalar{8,14}=-0.32;
inter.coupling.scalar{9,10}=-0.05;
inter.coupling.scalar{9,11}=5.80;
inter.coupling.scalar{9,12}=-0.05;
inter.coupling.scalar{9,13}=2.11;
%inter.coupling.scalar{9,14}=0.00;
inter.coupling.scalar{10,11}=-0.06;
inter.coupling.scalar{10,12}=5.66;
%inter.coupling.scalar{10,13}=0.00;
inter.coupling.scalar{10,14}=2.13;
inter.coupling.scalar{11,12}=-0.02;
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```
inter.coupling.scalar{11,13}=4.76;
inter.coupling.scalar{11,14}=-0.03;
inter.coupling.scalar{12,13}=-0.09;
inter.coupling.scalar{12,14}=4.96;
%inter.coupling.scalar{13,14}=0.00;

% Coordinates in Å
inter.coordinates={ ...
    [0.139824 1.6439053 -1.3060737], ...
    [1.8274179 0.4353038 -0.6527717], ...
    [-4.5494695 -2.4608498 -1.0762939], ...
    [3.3929648 -4.1979363 -0.6198634], ...
    [-2.2138624 -1.867503 -0.2265224], ...
    [2.441178 -1.9091981 -1.3226375], ...
    [-5.3610375 -0.751848 -2.876061], ...
    [1.8928928 -5.3271308 1.1896737], ...
    [-3.9361017 1.2008714 -3.5904467], ...
    [-0.1943524 -4.2212801 2.0681563], ...
    [-1.7070923 1.4960972 -2.552751], ...
    [-0.8211581 -1.9967074 1.1897339], ...
    [-1.8489176 -0.1574955 -1.3461032], ...
    [0.7487676 -1.8700346 -0.1273093]
};

% Basis set
bas.formalism='sphten-liouv';
bas.approximation='IK-0';
bas.level=4;

% Relaxation theory
inter.relaxation={'redfield','SRSK'};
inter.tau_c={30e-12};%s (rotational correlation time of SABRE complex)
inter.rlx_keep='labframe';
inter.rlx_dfs='keep';
inter.srsk_sources=[13 14];
inter.equilibrium='dibari';
inter.temperature=298;%K

% Numerical settings
sys.disable={'krylov'};
sys.tols.inter_cutoff=1e-12;
sys.tols.liouv_zero=1e-12;
sys.tols.prop_chop=1e-12;
sys.tols.subs_drop=1e-12;
sys.tols.irrep_drop=1e-12;
sys.tols.rlx_integration=1e-6;
sys.tols.zte_tol=1e-30;
sys.tols.zte_nsteps=64;

% Start computations
spin_system=create(sys,inter);
spin_system=basis(spin_system,bas);

% Get the Hamiltonian superoperator
H=hamiltonian(assume(spin_system,'labframe'));

% Get the relaxation superoperator
R=relaxation(spin_system);

% Calculate total Liouvillian
```

```
L=H+1i*R;

% Define initial state as singlet of hydride
rho=singlet(spin_system,1,2);
init_norm = norm(rho,'inf'); % Initial state norm

%Propagation in time
timeduration_of_polarization = 5;%s
number_of_averagingsteps = 10000;
timestep=timeduration_of_polarization/number_of_averagingsteps;
rhos=evolution(spin_system,L,[],rho,timestep,number_of_averagingsteps,'trajectory');

% Weighted average to account for chemical exchange
% including correction of lifetime of complex to account for length of timestep
lifetime_of_complex=1/19.6;%s
lifetime_of_complex=lifetime_of_complex*exp(timestep/(2*lifetime_of_complex));
normalization_factor=1;
for j = 2:(number_of_averagingsteps+1)
    rho = rho + rhos(:,j)*exp(-timestep*(j-1)/lifetime_of_complex);
    normalization_factor= ...
        normalization_factor+exp(-timestep*(j-1)/lifetime_of_complex);
end
rho = rho/normalization_factor;
clear rhos;

% Creating "coil" state for measurement of polarizations and
% antiphasecoefficient
coil_ligand_1=[ ...
    state(spin_system,{'Lz'},{3}) state(spin_system,{'Lz'},{5}) ...
    state(spin_system,{'Lz'},{7}) state(spin_system,{'Lz'},{9}) ...
    state(spin_system,{'Lz'},{11}) state(spin_system,{'Lz'},{13}) ...
    state(spin_system,{'Lz','Lz'},{3,5}) state(spin_system,{'Lz','Lz'},{3,7}) ...
    state(spin_system,{'Lz','Lz'},{3,9}) state(spin_system,{'Lz','Lz'},{3,11}) ...
    state(spin_system,{'Lz','Lz'},{5,7}) state(spin_system,{'Lz','Lz'},{5,9}) ...
    state(spin_system,{'Lz','Lz'},{5,11}) state(spin_system,{'Lz','Lz'},{7,9}) ...
    state(spin_system,{'Lz','Lz'},{7,11}) state(spin_system,{'Lz','Lz'},{9,11})
];
coil_ligand_2=[ ...
    state(spin_system,{'Lz'},{4}) state(spin_system,{'Lz'},{6}) ...
    state(spin_system,{'Lz'},{8}) state(spin_system,{'Lz'},{10}) ...
    state(spin_system,{'Lz'},{12}) state(spin_system,{'Lz'},{14}) ...
    state(spin_system,{'Lz','Lz'},{4,6}) state(spin_system,{'Lz','Lz'},{4,8}) ...
    state(spin_system,{'Lz','Lz'},{4,10}) state(spin_system,{'Lz','Lz'},{4,12}) ...
    state(spin_system,{'Lz','Lz'},{6,8}) state(spin_system,{'Lz','Lz'},{6,10}) ...
    state(spin_system,{'Lz','Lz'},{6,12}) state(spin_system,{'Lz','Lz'},{8,10}) ...
    state(spin_system,{'Lz','Lz'},{8,12}) state(spin_system,{'Lz','Lz'},{10,12})
];

% Normalisation of the results
% In-phase terms have a maximum eigenvalue equal to spin
for j=1:6
    [~,mult]=spin(sys.isotopes{2*j+1});
    coil_ligand_1(:,j)=coil_ligand_1(:,j) ...
        *((mult-1)/2)/(init_norm*norm(coil_ligand_1(:,j),"inf"));
end
for j=1:6
    [~,mult]=spin(sys.isotopes{2*j+2});
    coil_ligand_2(:,j)=coil_ligand_2(:,j) ...
        *((mult-1)/2)/(init_norm*norm(coil_ligand_2(:,j),"inf"));
end
```

```
% Anti-phase terms between spin-1/2 nuclei have a max eigenvalue of 1/4
for j=7:16
    coil_ligand_1(:,j)=coil_ligand_1(:,j) ...
        *0.25/(init_norm*norm(coil_ligand_1(:,j),"inf"));
    coil_ligand_2(:,j)=coil_ligand_2(:,j) ...
        *0.25/(init_norm*norm(coil_ligand_2(:,j),"inf"));
end
coil=0.5*(coil_ligand_1+coil_ligand_2);

% "Measuring" polarization (and antiphasecoefficents) in weighted average
% state
polarization=zeros(16,1);
for j=1:16
    polarization(j)=coil(:,j)'*rho;
end

% Output
polarization_F=polarization(1);
polarization_H=sum(polarization(2:5));
polarization_N=polarization(6);
antiphasecoeff_FzHz=sum(polarization(7:10));
antiphasecoeff_HzHz=sum(polarization(11:16));
polarization_total=polarization_F+polarization_H+polarization_N;

output.polarization = polarization;
output.polarization_total = polarization_total;
output.polarizationF = polarization_F;
output.polarizationH = polarization_H;
output.polarizationN = polarization_N;
output.antiphasecoeffFzHz = antiphasecoeff_FzHz;
output.antiphasecoeffHzHz = antiphasecoeff_HzHz;

format longG;

disp('Polarization:');
disp('F, sum');
disp(real(polarization_F));
disp('H, sum');
disp(real(polarization_H));
disp('N, sum');
disp(real(polarization_N));

disp('H5 + H6');
disp(real(polarization(2)));
disp('H7 + H8');
disp(real(polarization(3)));
disp('H9 + H10');
disp(real(polarization(4)));
disp('H11 + H12');
disp(real(polarization(5)));

disp('Antiphasecoefficients:');
disp('Fz-Hz, sum');
disp(real(antiphasecoeff_FzHz));
disp('Hz-Hz, sum');
disp(real(antiphasecoeff_HzHz));

disp('F3z-H5z + F4z-H6z');
disp(real(polarization(7)));
disp('F3z-H7z + F4z-H8z');
```

```
disp(real(polarization(8)));
disp('F3z-H9z + F4z-H10z');
disp(real(polarization(9)));
disp('F3z-H11z + F4z-H12z');
disp(real(polarization(10)));

disp('H5z-H7z + H6z-H8z');
disp(real(polarization(11)));
disp('H5z-H9z + H6z-H10z');
disp(real(polarization(12)));
disp('H5z-H11z + H6z-H12z');
disp(real(polarization(13)));
disp('H7z-H9z + H8z-H10z');
disp(real(polarization(14)));
disp('H7z-H11z + H8z-H12z');
disp(real(polarization(15)));
disp('H9z-H11z + H10z-H12z');
disp(real(polarization(16)));

end
```