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Get["QUADRUPOLE"];

(*
One-dimensional SPAM MQMAS of a spin I = 5/2,
Three pulse sequence with three x phases,
3Q echo amplitude optimization with the second pulse,
Coherence pathway 0Q → 3Q → 1Q → -1Q,
Wolfram Mathematica 5.0,
Author: R. HAJJAR
*)

(*----- Nucleus -----*)
quadrupoleSpin = 2.5;
larmorFrequencyMhz = 208.61889974; (* Al-27 with 800 MHz NMR spectrometer *)

(*----- Quadrupole interaction -----*)
quadrupoleOrder = 2;
QCCMHz = 5;      η = -1;

(*--- Rotor Euler angles in PAS ---*)
αPR = 0;      βPR = 0;      γPR = 0;

(*----- Parameters -----*)
startOperator = Iz;
ωRFkHz = 90;      (* strong RF pulse strength in kHz unit *)
ωRF3kHz = 9.3;   (* weak RF pulse strength in kHz unit *)
spinRatekHz = 5;
powderFile = "rep100_simp";
numberOfGammaAngles = 10;
t1 = 4;          (* the first-pulse duration in microsecond unit *)
t2 = 4;          (* the second-pulse duration in microsecond unit *)
t3 = 9;          (* the third-pulse duration in microsecond unit *)
Δt = 0.25;      (* pulse duration increment in microsecond unit *)
np = t2 / Δt;   (* number increment of the second-pulse duration *)

(*----- Pulse sequence -----*)
elements1 = {{2, 5}}; (* 3Q matrix element *)
coherence2 = {1};     (* 1Q coherences *)
detectelt = {{4, 3}}; (* central-transition matrix element of a spin 5/2 *)

fsimulation := (
  pulse[t1, ωRFkHz]; (* first pulse with x phase *)
  filterElt[elements1]; (* 3Q coherence pathway selection *)
  acq0;

  For[p = 1, p ≤ np, p++, {
    pulse[Δt, ωRFkHz]; (* second pulse with x phase *)
    store[2];
    filterCoh[coherence2]; (* 1Q coherence pathway selection *)
    pulse[t3, ωRF3kHz]; (* third pulse with x phase *)
    acq[p];
    recall[2];
  }];
);

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(*--- Execute, plot, and save simulation
  in "spam_P2_3Q1Qxxx" file -----*)
run;
tabgraph["spam_P2_3Q1Qxxx"];
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(* ----- *)
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Rang	t ( $\mu$ s)	intensity
0	0	0.
1	0.25	-0.01016186424
2	0.5	-0.03344502775
3	0.75	-0.05580253887
4	1.	-0.06708181602
5	1.25	-0.06576040399
6	1.5	-0.05648729702
7	1.75	-0.04509269277
8	2.	-0.03578318001
9	2.25	-0.03071872648
10	2.5	-0.03007906989
11	2.75	-0.03204512492
12	3.	-0.03373227048
13	3.25	-0.03313401346
14	3.5	-0.0303861447
15	3.75	-0.02731115577
16	4.	-0.02586355565

