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Get["QUADRUPOLE"];

(*
One-dimensional SPAM MQMAS of a spin I = 5/2,
Three pulse sequence with x, x, and -x phases,
-3Q antiecho amplitude optimization with the second-pulse duration,
All the -3Q coherences are considered,
Coherence pathway 0Q → -3Q → (1Q, 0Q, and -1Q) → -1Q,
Wolfram Mathematica 5.0,
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*)

(*----- 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 -----*)
coherence1 = {-3}; (* -3Q coherences *)
coherence2 = {1, 0, -1}; (* ±1Q and 0Q coherences *)
detectelt = {{4, 3}}; (* central-transition matrix element of a spin 5/2 *)

fsimulation := (
  pulse[t1, ωRFkHz]; (* first pulse with x phase *)
  filterCoh[coherence1]; (* -3Q coherence pathway selection *)
  acq0;

  For[p = 1, p ≤ np, p++, {
    pulse[Δt, ωRFkHz]; (* second pulse with x phase *)
    store[2];
    filterCoh[coherence2]; (* ±1Q and 0Q 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_-3Qxx-xS" file -----*)  
run;  
tabgraph["spam_P2_-3Qxx-xS"];  
  
(* ----- *)
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Rang	t (μ s)	intensity
0	0	0.
1	0.25	0.01316905455
2	0.5	0.05303970706
3	0.75	0.1067343492
4	1.	0.1532255262
5	1.25	0.1772216003
6	1.5	0.1754669263
7	1.75	0.1535346984
8	2.	0.1207914806
9	2.25	0.0868415758
10	2.5	0.05970776502
11	2.75	0.04414098095
12	3.	0.04015875963
13	3.25	0.04388559139
14	3.5	0.05067092103
15	3.75	0.05756496864
16	4.	0.06406590064

