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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,
 -3 Q antiecho amplitude optimization with the second-pulse duration,
 Coherence pathway 0 Q → -3 Q → (1 Q, 0 Q, and -1 Q) → -1 Q,
 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 = {{5, 2}};    (* -3 Q matrix element *)
coherence2 = {1, 0, -1}; (* ±1 Q and 0 Q coherences *)
detectelt = {{4, 3}}; (* central-transition matrix element of a spin 5/2 *)

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

  For [p = 1, p ≤ np, p++, {
     pulse[Δt, ωRFkHz];  (* second pulse with x phase *)
        store[2];
        filterCoh[coherence2]; (* ±1 Q and 0 Q 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-x" file -----------*)
run;
tabgraph["spam_P2_-3Qxx-x"];

(* ------------------------------------ *)
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Rang	t (μs)	intensity
0	0	0.
1	0.25	0.01222420901
2	0.5	0.04969639989
3	0.75	0.1013497758
4	1.	0.1478570295
5	1.25	0.1742297455
6	1.5	0.176172828
7	1.75	0.1578524538
8	2.	0.1272671782
9	2.25	0.09330936941
10	2.5	0.06420767631
11	2.75	0.04557880755
12	3.	0.03849772938
13	3.25	0.0398928951
14	3.5	0.0453871532
15	3.75	0.0520645784
16	4.	0.0592659267