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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 echo amplitude optimization with the second pulse,
 Coherence pathway 0 Q → 3 Q → 0 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 = {{2, 5}}; (* 3 Q matrix element *)
coherence2 = {0};     (* 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]; (* 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_3Q0Qxx-x" file -----------*)
run;
tabgraph["spam_P2_3Q0Qxx-x"];

(* ------------------------------------ *)
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Rang	t (μs)	intensity
0	0	0.
1	0.25	0.00214081286
2	0.5	0.01446315658
3	0.75	0.03723841517
4	1.	0.06106300445
5	1.25	0.07504249991
6	1.5	0.07406941544
7	1.75	0.05985291197
8	2.	0.03793931695
9	2.25	0.01479822295
10	2.5	−0.003672435923
11	2.75	−0.01343538655
12	3.	−0.01389012914
13	3.25	−0.008062134187
14	3.5	−0.0005058142115
15	3.75	0.005434209101
16	4.	0.008959828674