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Get["QUADRUPOLE"];

(*
 One-dimensional SPAM MQMAS of a spin I = 5/2,
 Three pulse sequence with three x phases,
 -3 Q antiecho amplitude optimization with the second pulse,
 Coherence pathway 0 Q → -3 Q → -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};    (* -1 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 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_-3Q-1Qxxx" file ----------*)
run;
tabgraph["spam_P2_-3Q-1Qxxx"];

(* ------------------------------------- *)
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Rang	t (μs)	intensity
0	0	0.
1	0.25	0.009973014993
2	0.5	0.03360737868
3	0.75	0.05727307073
4	1.	0.0701488871
5	1.25	0.06989126369
6	1.5	0.06083860859
7	1.75	0.04889124548
8	2.	0.03845232406
9	2.25	0.03191567336
10	2.5	0.02982008506
11	2.75	0.03085927877
12	3.	0.03256653199
13	3.25	0.03299324108
14	3.5	0.03200225921
15	3.75	0.03099541345
16	4.	0.0315392104