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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,
 All the -3 Q coherences are considered,
 Coherence pathway 0 Q → -3 Q → (1 Q, 0 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 = t3 / Δt;  (* number increment of the third-pulse duration*)

(*--------- Pulse sequence ---------*)
coherence1 = {-3};       (* -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 *)
     filterCoh[coherence1];  (* -3 Q coherence pathway selection *)
  pulse[t2, ωRFkHz];      (* second pulse with x phase *)
     filterCoh[coherence2];  (* ±1 Q and 0 Q coherence pathway selection *)
  acq0;

  For [p = 1, p ≤ np, p++, {
     pulse[Δt, -ωRF3kHz]; (* third pulse with -x phase *)
        store[2];
        acq[p];
        recall[2];
   }];
```

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 );

(*--- Execute, plot, and save simulation
  in "spam_P3_-3Qxx-xS" file -----------*)
run;
tabgraph["spam_P3_-3Qxx-xS"];

(* ------------------------------------ *)
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Rang	t(μs)	intensity
0	0	0.05885419924
1	0.25	0.0593526513
2	0.5	0.0598773793
3	0.75	0.06047625958
4	1.	0.06115628327
5	1.25	0.06189511963
6	1.5	0.06265588175
7	1.75	0.06339592627
8	2.	0.0640743792
9	2.25	0.06466508934
10	2.5	0.06517015703
11	2.75	0.0656200672
12	3.	0.06605388547
13	3.25	0.06649176268
14	3.5	0.06692196835
15	3.75	0.0673132116
16	4.	0.06764011863
17	4.25	0.06789834243
18	4.5	0.06809725835
19	4.75	0.06824145734
20	5.	0.06832294355
21	5.25	0.06833291824
22	5.5	0.06827934357
23	5.75	0.06818862843
24	6.	0.06808585778
25	6.25	0.06797138343
26	6.5	0.06781759958
27	6.75	0.0675913926
28	7.	0.06728286456
29	7.25	0.06691483492
30	7.5	0.06652654968
31	7.75	0.06614795817
32	8.	0.06578502329
33	8.25	0.06542204298
34	8.5	0.06503208916
35	8.75	0.06458687897
36	9.	0.06406590064