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Get["QUADRUPOLE"];

(*
One-dimensional phase-modulated shifted-antiecho MQMAS of a spin I = 5/2,
Three-pulse sequence,
-3Q antiecho amplitude optimization with the second pulse,
Coherence transfer pathway 0Q → -3Q → 1Q → -1Q,
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 = 100; (* strong RF pulse strength in kHz unit *)
ωRF3kHz = 10; (* weak RF pulse strength in kHz unit *)
spinRatekHz = 15;
powderFile = "rep100_simp";
numberOfGammaAngles = 10;
t1 = 4; (* the first-pulse duration in microsecond unit *)
t2 = 4; (* the second-pulse duration in microsecond unit *)
t3 = 15; (* 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}; (* 1Q coherences *)
detectelt = {{4, 3}}; (* central-transition matrix element of a spin 5/2 *)

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

  acq0;
  For [p = 1, p ≤ np, p++, {
    pulse[Δt, ωRFkHz]; (* second pulse *)
    store[2];
    filterCoh[coherence2]; (* 1Q coherence pathway selection *)
    pulse[t3, ωRF3kHz]; (* third pulse *)
    acq[p];
    recall[2];
  }];
);

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(*--- Execute, plot, and save simulation
  in "shifted_antiecho_P2" file -----*)
run;
tabgraph["shifted_antiecho_P2"];
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(* ----- *)
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Rang	t (μ s)	intensity
0	0	0.
1	0.25	0.0003433263073
2	0.5	0.004638760487
3	0.75	0.01800421293
4	1.	0.03985612632
5	1.25	0.06248075627
6	1.5	0.07641097253
7	1.75	0.07664773228
8	2.	0.06459537187
9	2.25	0.04600087734
10	2.5	0.02795125851
11	2.75	0.01640695275
12	3.	0.01427933791
13	3.25	0.02081799072
14	3.5	0.03259516022
15	3.75	0.04510367501
16	4.	0.0543645275

Intensity (A.U.)

