```
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 → 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 = {{5, 2}}; (* -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];
   }];
 );
```

```
(*--- Execute, plot, and save simulation
  in "spam_P2_-3Q0Qxxx" file -----------*)
run;
tabgraph["spam_P2_-3Q0Qxxx"];

(* ------------------------------------ *)
```

Rang	t (μs)	intensity
0	0	0.
1	0.25	−0.002132692381
2	0.5	−0.01441526456
3	0.75	−0.03713431734
4	1.	−0.06093435764
5	1.25	−0.07497399494
6	1.5	−0.07418021984
7	1.75	−0.06025814104
8	2.	−0.03870094472
9	2.25	−0.01588209845
10	2.5	0.002414608402
11	2.75	0.01224072967
12	3.	0.01301674735
13	3.25	0.007703450752
14	3.5	0.0007189206386
15	3.75	−0.004758815163
16	4.	−0.008069422819