```
Get["QUADRUPOLE"];

(*
 One-dimensional SPAM MQMAS of a spin I = 5/2,
 Three pulse sequence with three x phases,
 3Q echo amplitude optimization with the second pulse,
 All the 3Q coherences are considered,
 Coherence pathway 0Q → 3Q → (1Q, 0Q, and -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 = 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 = t1 / Δt;   (* number increment of the first-pulse duration *)

(*--------- Pulse sequence ---------*)
coherence1 = {3};        (* 3Q matrix coherences *)
coherence2 = {1, 0, -1}; (* ±1Q and 0Q coherences *)
detectelt = {{4, 3}}; (* central-transition matrix element of a spin 5/2 *)

fsimulation := (
  acq0;

  For [p = 1, p ≤ np, p++, {
    pulse[Δt, ωRFkHz];  (* first pulse with x phase *)
       store[2];
       filterCoh[coherence1];  (* 3Q coherence pathway selection *)
    pulse[t2, ωRFkHz];  (* second pulse with x phase *)
       filterCoh[coherence2]; (* ±1Q and 0Q coherence pathway selection *)
    pulse[t3, ωRF3kHz]; (* third pulse with x phase *)
       acq[p];
       recall[2];
   }];
```

```
);

(*--- Execute, plot, and save simulation
  in "spam_P1_3QxxxS" file -----------*)
run;
tabgraph["spam_P1_3QxxxS"];

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

Rang	t(μs)	intensity
0	0	0.
1	0.25	$-7.728113561\times 10^{-6}$
2	0.5	−0.0001986398211
3	0.75	−0.001225558043
4	1.	−0.003934339857
5	1.25	−0.008539199067
6	1.5	−0.01446774881
7	1.75	−0.02067686011
8	2.	−0.02625969242
9	2.25	−0.03097334929
10	2.5	−0.03489380385
11	2.75	−0.0382617157
12	3.	−0.04136267586
13	3.25	−0.04433824389
14	3.5	−0.04708942785
15	3.75	−0.04952877402
16	4.	−0.0516873895