```
Get["QUADRUPOLE"];

(*
 One-dimensional z-filtered MQMAS of a spin I = 5/2,
 Three pulse sequence,
 3Q echo and -3Q antiecho amplitude optimization with the first pulse,
 Coherence pathway 0Q → ±3Q → 0Q → -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 ---------*)
elements1 = {{2, 5}, {5, 2}}; (* ±3Q matrix elements *)
coherence2 = {0};            (* 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 *)
        store[2];
        filterElt[elements1]; (* ±3Q coherence pathway selection *)
     pulse[t2, ωRFkHz]; (* second pulse *)
        filterCoh[coherence2]; (* 0Q coherence pathway selection *)
     pulse[t3, ωRF3kHz]; (* third pulse *)
       acq[p];
       recall[2];
   }];
 );
```

```
(*--- Execute, plot, and save simulation
  in "zfilter_P1" file -----------------*)
run;
tabgraph["zfilter_P1"];

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

Rang	t (μs)	intensity
0	0	0.
1	0.25	$-2.73100612 \times 10^{-6}$
2	0.5	−0.00007729068524
3	0.75	−0.0004733416269
4	1.	−0.001488256011
5	1.25	−0.003181145906
6	1.5	−0.005308446136
7	1.75	−0.007492761079
8	2.	−0.009441186671
9	2.25	−0.0110348856
10	2.5	−0.01226156018
11	2.75	−0.01317927604
12	3.	−0.01391518774
13	3.25	−0.01458832845
14	3.5	−0.01527667174
15	3.75	−0.01605772532
16	4.	−0.01702925149