```
Get["QUADRUPOLE"];

(*
 One-dimensional z-filtered MQMAS of a spin I = 5/2,
 Three pulse sequence,
 3 Q echo and -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 = {{2, 5}, {5, 2}};  (* ±3 Q matrix elements *)
coherence2 = {0};             (* 0 Q coherences *)
detectElt = {{4, 3}}; (* central-transition matrix element of a spin 5/2 *)

fsimulation := (
  pulse[t1, ωRFkHz];     (* first pulse *)
  filterElt[elements1];       (* ±3 Q coherence pathway selection *)
  acq0;

  For [p = 1, p ≤ np, p++, {
     pulse[Δt, ωRFkHz];  (* second pulse *)
        store[2];
        filterCoh[coherence2]; (* 0 Q coherence pathway selection *)
     pulse[t3, ωRF3kHz]; (* third pulse *)
       acq[p];
       recall[2];
   }];
 );
```

```
(*--- Execute, plot, and save simulation
  in "zfilter_P2" file -----------*)
run;
tabgraph["zfilter_P2"];

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

Rang	t(μs)	intensity
0	0	0.
1	0.25	−0.004273505241
2	0.5	−0.02887842114
3	0.75	−0.07437273251
4	1.	−0.1219973621
5	1.25	−0.1500164949
6	1.5	−0.1482496353
7	1.75	−0.120111053
8	2.	−0.07664026167
9	2.25	−0.0306803214
10	2.5	0.006087044325
11	2.75	0.02567611622
12	3.	0.02690687649
13	3.25	0.01576558494
14	3.5	0.00122473485
15	3.75	−0.01019302426
16	4.	−0.01702925149