```
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 third pulse,
 Coherence pathway 0 Q → ±3 Q → 0 Q → -1 Q,
 Coherences belonging to the same pathway are considered,
 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 = t3 / Δt;  (* number increment of the third-pulse duration *)

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

fsimulation := (
  pulse[t1, ωRFkHz];     (* first pulse *)
     filterCoh[coherence1];      (* ±3 Q coherence pathway selection *)
  pulse[t2, ωRFkHz];     (* second pulse *)
     filterCoh[coherence2];      (* 0 Q coherence pathway selection *)
     acq0;

  For [p = 1, p ≤ np, p++, {
    pulse[Δt, ωRF3kHz]; (* third pulse *)
       acq[p];
   }];
 );
```

```
(*--- Execute, plot, and save simulation
   in "zfilter_P3S" file ---------------*)
run;
tabgraph["zfilter_P3S"];

(* ------------------------------------- *)
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Rang	t(μs)	intensity
0	0	0.
1	0.25	−0.001045665134
2	0.5	−0.002098261919
3	0.75	−0.003160254396
4	1.	−0.004228062739
5	1.25	−0.005293911967
6	1.5	−0.006349072309
7	1.75	−0.007386010546
8	2.	−0.008398747219
9	2.25	−0.00938263411
10	2.5	−0.01033484698
11	2.75	−0.01125531682
12	3.	−0.01214662314
13	3.25	−0.01301207896
14	3.5	−0.01385316237
15	3.75	−0.01466842756
16	4.	−0.0154548445
17	4.25	−0.01621028591
18	4.5	−0.01693486998
19	4.75	−0.01763014524
20	5.	−0.01829730867
21	5.25	−0.01893644443
22	5.5	−0.01954738406
23	5.75	−0.02013084673
24	6.	−0.02068820626
25	6.25	−0.02121986376
26	6.5	−0.02172396856
27	6.75	−0.02219710582
28	7.	−0.02263657673
29	7.25	−0.02304219399
30	7.5	−0.0234159587
31	7.75	−0.02376001332
32	8.	−0.02407478195
33	8.25	−0.02435881294
34	8.5	−0.02461008796
35	8.75	−0.02482745194
36	9.	−0.02501123257