```
Get["QUADRUPOLE"];

(*
 One-dimensional phase-modulated shifted-echo MQMAS of a spin I = 5/2,
 Three-pulse sequence,
 3 Q echo amplitude optimization with the first pulse,
 Coherence transfer pathway 0 Q → 3 Q → 1 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 = 100;  (* strong RF pulse strength in kHz unit *)
ωRF3kHz = 10;  (* weak RF pulse strength in kHz unit *)
spinRatekHz = 15;
powderFile = "rep100_simp";
numberOfGammaAngles = 10;
t1 = 4;    (* the first-pulse duration in microsecond unit *)
t2 = 1;    (* the second-pulse duration in microsecond unit *)
t3 = 15;   (* 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};    (* 3 Q coherences *)
coherence2 = {1};    (* 1 Q 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];
       filterCoh[coherence1];  (* 3 Q coherence pathway selection *)
     pulse[t2, ωRFkHz]; (* second pulse *)
        filterCoh[coherence2];  (* 1 Q coherence pathway selection *)
     pulse[t3, ωRF3kHz]; (* third pulse *)
       acq[p];
       recall[2];
   }];
 );
```

```
(*--- Execute, plot, and save simulation
  in "shifted_echo_P1" file ----------------*)
run;
tabgraph["shifted_echo_P1"];

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

powderFile: rep100_simp

Rang	t (μs)	intensity
0	0	0.
1	0.25	−0.00001932936026
2	0.5	−0.0005256680406
3	0.75	−0.003327063063
4	1.	−0.0108029139
5	1.25	−0.02380561379
6	1.5	−0.04057912798
7	1.75	−0.05810827717
8	2.	−0.07392078898
9	2.25	−0.08693360057
10	2.5	−0.09696353803
11	2.75	−0.1043371026
12	3.	−0.1097288136
13	3.25	−0.1138299293
14	3.5	−0.1171477694
15	3.75	−0.1198566192
16	4.	−0.1216860303