```
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 second 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 = 4;  (* 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 = t2 / Δt;  (* number increment of the second-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 := (
  pulse[t1, ωRFkHz];       (* first pulse *)
  filterCoh[coherence1];       (* 3 Q coherence pathway selection *)

  acq0;
  For [p = 1, p ≤ np, p++, {
     pulse[Δt, ωRFkHz];    (* second pulse *)
       store[2];
        filterCoh[coherence2];  (* 1 Q coherence pathway selection *)
     pulse[t3, ωRF3kHz];   (* third pulse *)
       acq[p];
       recall[2];
   }];
 );
```

```
(*--- Execute, plot, and save simulation
  in "shifted_echo_P2" file ----------------*)
run;
tabgraph["shifted_echo_P2"];

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

powderFile: rep100_simp

| Rang | t (μs) | intensity |
|---|---|---|
| 0 | 0 | 0. |
| 1 | 0.25 | −0.02339826479 |
| 2 | 0.5 | −0.07313803379 |
| 3 | 0.75 | −0.1126102397 |
| 4 | 1. | −0.1216860303 |
| 5 | 1.25 | −0.1051434335 |
| 6 | 1.5 | −0.07982738163 |
| 7 | 1.75 | −0.05936013207 |
| 8 | 2. | −0.04865253492 |
| 9 | 2.25 | −0.046880573 |
| 10 | 2.5 | −0.05042026715 |
| 11 | 2.75 | −0.05448935861 |
| 12 | 3. | −0.05626589898 |
| 13 | 3.25 | −0.05649185758 |
| 14 | 3.5 | −0.05735787659 |
| 15 | 3.75 | −0.05929103329 |
| 16 | 4. | −0.06023638259 |