

```
Get["QUADRUPOLE"];
(*----- Nucleus -----*)
quadrupoleSpin = 1.5;
larmorFrequencyMhz = 105.8731007;

(*----- Quadrupole interaction -----*)
quadrupoleOrder = 2; QCCMhz = 8;  $\eta$  = -1;

(*---- Rotor Euler angles in PAS ----*)
 $\alpha_{PR}$  = 30;  $\beta_{PR}$  = 30;  $\gamma_{PR}$  = 30;

(*----- Parameters -----*)
startOperator = 0.4 * Iz;
 $\omega_{RF}$ kHz = 100;
spinRatekHz = 15;
powderFile = "rep100_simp";
numberOfGammaAngles = 1;
t1 = 20;
 $\Delta t$  = 1;
np = t1 /  $\Delta t$ ;

(*----- Pulse sequence -----*)
detectelt = {{3, 2}};

fsimulation := (
  acq0;
  For [p = 1, p <= np, p++, {
    pulse[ $\Delta t$ ,  $\omega_{RF}$ kHz];
    acq[p];
  }];
);

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

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

Rang	t (μ s)	intensity
0	0	0.
1	1	0.1909263462
2	2	0.1179498378
3	3	-0.1095760968
4	4	-0.1748410673
5	5	0.05933795078
6	6	0.349769756
7	7	0.3342515848
8	8	-0.2783335973
9	9	-0.4104664941
10	10	-0.04702774168
11	11	0.4073285563
12	12	0.3241038495
13	13	-0.1948624526
14	14	-0.4306262691
15	15	-0.05748909539
16	16	0.4018103486
17	17	0.3128637066
18	18	-0.1999188914
19	19	-0.4520927211
20	20	-0.01315623676