

```

(*_____Main Program _____*)
ClearAll["Global`*"]
SetDirectory["write here the working directory path"];
<< group_ops.txt
irnum = 3;(* irnum is the irrep number in the character table *)
<< generaCharacter.txt
<< nPot.txt (* Code corresponding the n-th power *)
<< descompNoSquare.txt

(*_____Example "group_ops": C3v _____*)

m = Table[0, {i, 1, 6}];
m[[1]] = {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}};
m[[2]] = {{0, -1, 0}, {1, -1, 0}, {0, 0, 1}};
m[[3]] = {{-1, 1, 0}, {-1, 0, 0}, {0, 0, 1}};
m[[4]] = {{0, -1, 0}, {-1, 0, 0}, {0, 0, 1}};
m[[5]] = {{-1, 1, 0}, {0, 1, 0}, {0, 0, 1}};
m[[6]] = {{1, 0, 0}, {1, -1, 0}, {0, 0, 1}};
irreps = {A1, A2, "E"}; degen = {1, 2, 3}; dimclass = {1, 2, 3};
CharTab = {{1, 1, 1}, {1, 1, -1}, {2, -1, -0}};
(* In this case irnum=3 points irrep E of the group*)

(*_____ generaCharacter.txt _____*)

caract = Table[0, {i, 1, Length[m]}];
cont = 0;
For[i = 1, i ≤ Length[dimclass], i++,
  For[j = 1, j ≤ dimclass[[i]], j++,
    cont = cont + 1;
    caract[[cont]] = CharTab[[irnum]][[i]]
  ]
];

```

```

(*_____ Example n=3 (third power) of nPot.txt _____*)

(***** S3 *****)
S3Sym = {"[3]", "[2 1]", "[1^3]"}; S3dim = {1, 2, 1};
(* ----- *)
rep3tot = {}; rep21tot = {}; rep13tot = {};
For[i = 1, i ≤ Length[m], i++,
  xx = m[[i]];
  rep3 =  $\frac{1}{6}$  (caract[[Position[m, xx][[1, 1]]]]3 +
    3 caract[[Position[m, xx.xx][[1, 1]]]] caract[[Position[m, xx][[1, 1]]]] +
    2 caract[[Position[m, xx.xx.xx][[1, 1]]]]);
  rep21 =  $\frac{2}{3}$  (caract[[Position[m, xx][[1, 1]]]]3 -
    caract[[Position[m, xx.xx.xx][[1, 1]]]]);
  rep13 =  $\frac{1}{6}$  (caract[[Position[m, xx][[1, 1]]]]3 -
    3 caract[[Position[m, xx.xx][[1, 1]]]] caract[[Position[m, xx][[1, 1]]]] +
    2 caract[[Position[m, xx.xx.xx][[1, 1]]]]);
  rep3tot = AppendTo[rep3tot, rep3]; rep21tot = AppendTo[rep21tot, rep21];
  rep13tot = AppendTo[rep13tot, rep13];];
(* selecting just one operation per class and dividing
  by permutation S3 class dimension (Boyle) *)
rep3b = {rep3tot[[1]] / S3dim[[1]]}; rep21b = {rep21tot[[1]] / S3dim[[2]]};
rep13b = {rep13tot[[1]] / S3dim[[3]]};
index = 1;
For[i = 2, i ≤ Length[dimclass], i++,
  index = index + dimclass[[i - 1]];
  rep3b = AppendTo[rep3b, rep3tot[[index]] / S3dim[[1]]];
  rep21b = AppendTo[rep21b, rep21tot[[index]] / S3dim[[2]]];
  rep13b = AppendTo[rep13b, rep13tot[[index]] / S3dim[[3]]];
];
reductibletot = rep3b * S3dim[[1]] + rep21b * S3dim[[2]] + rep13b * S3dim[[3]];
reductible = {rep3b, rep21b, rep13b};
symbolsIR = {irreps[[irnum]]3, {irreps[[irnum]]3, "[3]"},
  {irreps[[irnum]]3, "[2 1]"}, {irreps[[irnum]]3, "[1^3]"};
nombreSnirreps = Length[reductible];

(*_____ descompNoSquare.txt _____*)

output0 = "----- irrep Decomposition -----";
output1 = {symbolsIR[[1]],
  "|" Inverse[CharTab.Transpose[CharTab]].CharTab.reductibletot.irreps};
output2 = "----- irrep Decomposition - Sn adapted -----";
output3 = {};
For[i = 1, i ≤ nombreSnirreps, i++,
  output3 = AppendTo[output3, {symbolsIR[[i + 1]],
    Inverse[CharTab.Transpose[CharTab]].CharTab.reductible[[i]].irreps}];];
output = {output0, "", output1, "", output2, "", output3 // MatrixForm} // MatrixForm;
Export["output.pdf", output];

```