

# Step 1:

```
$ phonopy --tolerance 0.01 --symmetry -c POSCAR
$ vim PPOSCAR
$ cp PPOSCAR POSCAR
```

```
/anaconda3/bin/phonopy --tolerance 0.01 --symmetry -c POSCAR
phonopy_version: '1.13.2'
space_group_type: 'R-3m'
space_group_number: 166
point_group_type: '-3m'
space_group_operations:
- rotation: # 1
  - [ 1, 0, 0]
  - [ 0, 1, 0]
  - [ 0, 0, 1]
  translation: [ 0.00000, 0.00000, 0.00000 ]
- rotation: # 2
  - [-1, 0, 0]
  - [ 0, -1, 0]
  - [ 0, 0, -1]
  translation: [ 0.00000, 0.00000, 0.00000 ]
```

## “POSCAR”

```
1 generated by phonopy
2 1.0
3 2.0690000000000000 1.1945377069533354 9.5466666571200012
4 -2.0690000000000000 1.1945377069533354 9.5466666571200012
5 0.0000000000000000 -2.3890754139066708 9.5466666571200012
6 Bi Se
7 2 3
8 Direct
9 0.6009999996010008 0.6009999996010008 0.6009999996010009
10 0.3990000003989990 0.3990000003989991 0.3990000003989989
11 0.7939999997940036 0.7939999997940036 0.7939999997940036
12 0.2060000002059964 0.2060000002059964 0.2060000002059964
13 0.0000000000000000 0.0000000000000000 0.0000000000000000
~
"PPOSCAR" 13L, 560C
```