# syml.foobar

Symmetry line for the band plot.
We can generate `syml.foobar` by `getsyml`.

## Get symmetry lines for band plot and Brillouwin zone plot.

`syml.*` is generated from `ctrl.*`. `syml.*` is needed for band plot.
After generated, you can easily edit `syml.*` for `job_band`.

At ecalj/GetSyml, we have getsyml.py, which is based on the
seekpath at https://github.com/giovannipizzi/seekpath/
and spglib at https://anaconda.org/conda-forge/spglib

### Usage:

We have softlink getsyml.py as getsyml during InstallAll.py.
Run

```
getsyml nio
(or)
getsyml ctrls.nio
```

. This show 3D Brillouin zone together with symmetry lines for band plot.
See BZsamples here.
The symmetry lines are written into the `syml.*` file for ecalj.
The number of divisions for `syml` is give by a crude algorism, so edit it if necessary.

### Needed citations

PROF

In addition to usual ecalj acknowledgement, following citations are required when you make a publication.

1.Y. Hinuma, G. Pizzi, Y. Kumagai, F. Oba, I. Tanaka,
Band structure diagram paths based on crystallography,
Comp. Mat. Sci. 128, 140 (2017)

2.You should also cite spglib that is an essential library used in the implementation.
https://github.com/atztogo/spglib.git

- See Lincence.txt for spglib and seekpath.

### (memo for developer)

a.Modify lmchk to write required information to supply reasonable.
For example, ndiv (mesh size along lines).

b.Numerical accuracy of calculations.

np.set_printoptions(precision=16) is not meaningful since we read output of lmchk