

Some notes for the installation and use of critic

Quick installation guide for VASP:

1) Compilation

```
cd src/  
make mrproper
```

**** modify the Makefile.inc for changing compiler ****

```
make grid
```

2) Routes

Remember to add the critic route to your .bashrc

```
export CRITIC_HOME=/home/user1/critic2/
```

3) Common problems with the VASP compilation : Problems when compiling the library which reads the cifs (ciftbx)?

a)Recompile it directly :

```
cd ciftbx  
make clean  
make  
cd ..
```

b)Recompile the whole

```
make grid
```

What to know when making your own input

What is ZCORE?

ZCORE is what you obtain for the variable ZVAL when you make

```
grep ZVAL POTCAR
```

****Note that, unlike in the POTCAR, they should be input as natural numbers****

****Both typat ant zcore should respect the order in which they appear in the POTCAR****