

```
[INCAR]
SYSTEM = Static Zr_suboxides
ISYM = 0
PREC = High
IBRION = 2
POTIM = 0.05
ISIF = 3 #4: All but no change vol.
NSW = 400
EDIFF = 0.00002000
ENAUG = 1230.0
ISMEAR = 5
EDIFF = 1e-6
EDIFFG = 1e-4
SIGMA = 0.025
ENMAX = 500
KPPRA = 984
DOGGA
KSCHEME = GAMMA
LWAVE & = & .FALSE.
```

```
[KPOINTS]
KPOINTS file
0
Gamma
6 6 6
0 0 0
```