

**a)**

```
&CONTROL
  calculation = 'vc-relax',
  prefix = 'Si',
  pseudo_dir = './',
  outdir = './',
  etot_conv_thr=1.D-7,
  forc_conv_thr=2.D-6,
  nstep=150,
```

**b)**

```
/
&SYSTEM
 ibrav = 2,
celldm(1) = 10.26221 ,
nat = 8,
ntyp = 1,
ecutwfc = 40,
ecutrho = 320,
occupations = 'smearing',
smearing = 'gaussian',
degauss = 0.02,
input_dft = 'WC',
```

**c)**

```
/
&ELECTRONS
  electron_maxstep = 150,
  diagonalization = 'david',
  conv_thr = 1.0d-7,
  mixing_beta = 0.20,
```

**d)**

```
/
&IONS
/
&CELL
  press = 0.0,
/
```

**e)**

```
ATOMIC_SPECIES
Si 28.0855 si_pbe_v1.uspp.F.UPF
```

ATOMIC\_POSITIONS (crystal)

Si	0.125	0.125	0.125
Si	0.125	0.625	0.625
Si	0.625	0.125	0.625
Si	0.625	0.625	0.125
Si	0.875	0.375	0.375
Si	0.875	0.875	0.875
Si	0.375	0.375	0.875
Si	0.375	0.875	0.375

**f)**

```
K_POINTS {automatic}
10 10 10 0 0 0
```