

```

&CONTROL
  calculation = 'bands',
  restart_mode = 'from_scratch'
  prefix = 'A',
  outdir = './tmp-hetero/'
  pseudo_dir = './pseudo'
  tstress = .true.
  tprnfor = .true.
  verbosity = 'high'
  etot_conv_thr = 1.0D-4,
  forc_conv_thr = 1.0D-3,
/
&SYSTEM
 ibrav = 4,
nat = 2, ntyp = 2,
celldm(1) = 4.75,
celldm(3) = 3,
ecutwfc = 40,
ecutrho = 400,
starting_magnetization(1)=0.5,
starting_magnetization(2)=-0.5,
occupations = 'smearing',
nspin = 2,
degauss = 0.001 ,
smearing = 'm-v'
/
&ELECTRONS
diagonalization='david',
mixing_mode = 'plain',
mixing_beta = 0.7,
electron_maxstep = 200,
conv_thr = 1.0D-8,
/
&IONS
ion_dynamics = 'bfgs'
/
ATOMIC_SPECIES
  B 10.8100 B.pbe-n-rrkjus_psl.0.1.UPF
  N 14.0100 N.pbe-n-rrkjus_psl.0.1.UPF

ATOMIC_POSITIONS (crystal)
N      0.0000000000      0.0000000000      0.5000000000
B      0.333333300      0.6666666667      0.5000000000

K_POINTS crystal
  400
    0.0000000000      0.0000000000      0.0000000000      1.0
    0.0034246575      0.0000000000      0.0000000000      1.0
    0.0068493151      0.0000000000      0.0000000000      1.0
    0.0102739726      0.0000000000      0.0000000000      1.0
    0.0136986301      0.0000000000      0.0000000000      1.0
    0.0171232877      0.0000000000      0.0000000000      1.0
    0.0205479452      0.0000000000      0.0000000000      1.0
    0.0239726027      0.0000000000      0.0000000000      1.0
    0.0273972603      0.0000000000      0.0000000000      1.0
    0.0308219178      0.0000000000      0.0000000000      1.0
    0.0342465753      0.0000000000      0.0000000000      1.0
    0.0376712329      0.0000000000      0.0000000000      1.0
    0.0410958904      0.0000000000      0.0000000000      1.0
    0.0445205479      0.0000000000      0.0000000000      1.0
    0.0479452055      0.0000000000      0.0000000000      1.0
    0.0513698630      0.0000000000      0.0000000000      1.0

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0.0650684932	0.0000000000	0.0000000000	1.0
0.0684931507	0.0000000000	0.0000000000	1.0
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0.1438356164	0.0000000000	0.0000000000	1.0
0.1472602740	0.0000000000	0.0000000000	1.0
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0.1678082192	0.0000000000	0.0000000000	1.0
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0.1746575342	0.0000000000	0.0000000000	1.0
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0.0138065680	0.0138065680	0.0000000000	1.0
0.0118342012	0.0118342012	0.0000000000	1.0
0.0098618343	0.0098618343	0.0000000000	1.0
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0.0059171006	0.0059171006	0.0000000000	1.0
0.0039447337	0.0039447337	0.0000000000	1.0
0.0019723669	0.0019723669	0.0000000000	1.0
0.0000000000	0.0000000000	0.0000000000	1.0