

```

&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 = 64, ntyp = 3,
celldm(1)= 18.006,
celldm(3)= 3.00,
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-6,
/
&IONS
ion_dynamics = 'bfgs'
/
ATOMIC_SPECIES
  C 12.01 C.pbe-rrkjus.UPF
  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)
C      0.085107644    0.914690268    0.523924967
C      0.168334303    0.831456094    0.520777078
C      0.084852501    0.664639460    0.520350109
C      0.168232763    0.581285666    0.518175746
C      0.085006906    0.414711119    0.520835117
C      0.168398786    0.331389737    0.522379636
C      0.335146151    0.414766160    0.522624493
C      0.418320694    0.331505360    0.526281481
C      0.418459616    0.581266394    0.519459015
C      0.335075404    0.664608142    0.516548321
C      0.418474669    0.831562343    0.517258491
C      0.335124833    0.914948754    0.519685540
C      0.585146952    0.914845516    0.519480347
C      0.668454254    0.831399519    0.521200277
C      0.585073148    0.664623048    0.521933356
C      0.668273005    0.581496873    0.526039236
C      0.585003913    0.414789956    0.527557621
C      0.668420578    0.331313492    0.527438544
C      0.834971553    0.914697484    0.523817573
C      0.918389519    0.831394187    0.524751449
C      0.835087800    0.664759226    0.525766498

```

C	0.918566263	0.581465548	0.524465180
C	0.835134440	0.414749492	0.525566812
C	0.918450615	0.331471787	0.523506134
C	0.835040018	0.164714794	0.523586343
C	0.918392669	0.081392019	0.523846967
C	0.668327897	0.081362727	0.522570000
C	0.585042578	0.164665876	0.524886077
C	0.418343202	0.081266238	0.523771460
C	0.335042470	0.164668834	0.525783658
C	0.168396812	0.081383127	0.525001178
C	0.085070349	0.164794109	0.524518623
B	0.085067611	0.914721273	0.349999512
N	0.168400129	0.831388037	0.349999559
B	0.085046599	0.664730088	0.349999552
N	0.168373501	0.581393364	0.349999241
B	0.085054338	0.414715885	0.349999546
N	0.168402845	0.331402120	0.349999547
B	0.335064030	0.414742508	0.349999533
N	0.418372432	0.331399275	0.349999606
N	0.418403414	0.581390480	0.349999315
B	0.335064600	0.664715180	0.349999686
N	0.418396419	0.831415135	0.349999188
B	0.335059575	0.914753322	0.349999572
B	0.585088300	0.914745706	0.349999547
N	0.668389610	0.831386366	0.349999403
B	0.585050632	0.664727056	0.349999549
N	0.668387831	0.581416257	0.349999605
B	0.585061144	0.414737504	0.349999280
N	0.668397684	0.331385888	0.349999595
B	0.835053018	0.914719925	0.349999346
N	0.918404756	0.831407039	0.349999529
B	0.835051621	0.664703669	0.349999286
N	0.918406321	0.581396753	0.349999489
B	0.835073205	0.414739504	0.349999311
N	0.918403992	0.331397213	0.349999470
B	0.835055210	0.164729538	0.349999386
N	0.918403645	0.081386777	0.349999526
N	0.668393080	0.081394086	0.349999445
B	0.585051806	0.164713303	0.349999366
N	0.418400557	0.081389440	0.349999457
B	0.335086561	0.164732183	0.349999314
N	0.168386632	0.081386633	0.349999555
B	0.085070600	0.164737139	0.349999354
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	0.0000000000	-0.0068493151	0.0000000000 1.0
	0.0000000000	-0.0136986301	0.0000000000 1.0
	0.0000000000	-0.0205479452	0.0000000000 1.0
	0.0000000000	-0.0273972603	0.0000000000 1.0
	0.0000000000	-0.0342465753	0.0000000000 1.0
	0.0000000000	-0.0410958904	0.0000000000 1.0
	0.0000000000	-0.0479452055	0.0000000000 1.0
	0.0000000000	-0.0547945205	0.0000000000 1.0
	0.0000000000	-0.0616438356	0.0000000000 1.0
	0.0000000000	-0.0684931507	0.0000000000 1.0
	0.0000000000	-0.0753424658	0.0000000000 1.0
	0.0000000000	-0.0821917808	0.0000000000 1.0
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	0.0000000000	-0.0958904110	0.0000000000 1.0
	0.0000000000	-0.1027397260	0.0000000000 1.0
	0.0000000000	-0.1095890411	0.0000000000 1.0

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0.0555550000	-0.5277783333	0.0000000000	1.0
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0.0714278571	-0.5357150000	0.0000000000	1.0
0.0793642857	-0.5396833333	0.0000000000	1.0
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0.1031735714	-0.5515883333	0.0000000000	1.0
0.1111100000	-0.5555566667	0.0000000000	1.0
0.1190464286	-0.5595250000	0.0000000000	1.0
0.1269828571	-0.5634933333	0.0000000000	1.0
0.1349192857	-0.5674616667	0.0000000000	1.0
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0.1746014286	-0.5873033333	0.0000000000	1.0
0.1825378571	-0.5912716667	0.0000000000	1.0
0.1904742857	-0.5952400000	0.0000000000	1.0
0.1984107143	-0.5992083333	0.0000000000	1.0
0.2063471429	-0.6031766667	0.0000000000	1.0
0.2142835714	-0.6071450000	0.0000000000	1.0
0.2222200000	-0.6111133333	0.0000000000	1.0
0.2301564286	-0.6150816667	0.0000000000	1.0
0.2380928571	-0.6190500000	0.0000000000	1.0
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0.3015842857	-0.6031776190	0.0000000000	1.0
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0.2698385714	-0.5396852381	0.0000000000	1.0
0.2658703571	-0.5317486905	0.0000000000	1.0
0.2619021429	-0.5238121429	0.0000000000	1.0
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0.0952371429	-0.1904771429	0.0000000000	1.0
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