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&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 = 63, 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      0.085108451    0.914690073    0.523931479
C      0.168336408    0.831454760    0.520778666
C      0.084854952    0.664648148    0.520343744
C      0.168225798    0.581277875    0.518141077
C      0.085004069    0.414709489    0.520827060
C      0.168405944    0.331383982    0.522348811
C      0.335143234    0.414766852    0.522631809
C      0.418320462    0.331498431    0.526256076
C      0.418459825    0.581267387    0.519525845
C      0.335081067    0.664605263    0.516551095
C      0.418481047    0.831568032    0.517221896
C      0.335117560    0.914946894    0.519677638
C      0.585149595    0.914850683    0.519470181
C      0.668460122    0.831392813    0.521167648
C      0.585074174    0.664628427    0.521940479
C      0.668280774    0.581495385    0.526013882
C      0.585003289    0.414792046    0.527557200
C      0.668425944    0.331307986    0.527446570
C      0.834966724    0.914701191    0.523813563
C      0.918395350    0.831395247    0.524758562
C      0.835098696    0.664764769    0.525768452

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C	0.918580121	0.581464836	0.524479572
C	0.835138204	0.414755532	0.525571850
C	0.918452399	0.331471167	0.523512106
C	0.835033970	0.164721797	0.523591954
C	0.918387899	0.081392740	0.523860123
C	0.668327725	0.081359809	0.522575635
C	0.585039065	0.164664264	0.524891009
C	0.418343486	0.081250877	0.523784978
C	0.335040061	0.164660699	0.525786034
C	0.168395103	0.081376264	0.525008961
C	0.085066935	0.164799545	0.524516297
B	0.085063997	0.914730181	0.250010315
N	0.169141602	0.830652580	0.249987977
B	0.088921605	0.663585502	0.250013076
N	0.177336742	0.581282653	0.249991611
B	0.085638768	0.415022756	0.250018176
N	0.177350096	0.340469768	0.249991895
B	0.348452317	0.441519465	0.249996916
N	0.418516615	0.340470753	0.249992037
B	0.348424440	0.651369932	0.249996989
N	0.418507241	0.822453926	0.249991509
B	0.336206908	0.910867141	0.250013096
B	0.584767666	0.914151255	0.250018244
N	0.659324654	0.822442903	0.249991816
B	0.558271618	0.651340562	0.249996917
N	0.659323458	0.581274917	0.249992017
B	0.584774666	0.415016140	0.250017864
N	0.668085966	0.331706699	0.249988243
B	0.830041197	0.910853394	0.250012830
N	0.916897151	0.830648325	0.249988212
B	0.830026910	0.663588624	0.250012833
N	0.918796349	0.582218519	0.249991140
B	0.835299417	0.415200987	0.250011024
N	0.919015168	0.331702985	0.249988209
B	0.835306645	0.164487011	0.250011459
N	0.918811365	0.080983385	0.249991034
N	0.668089510	0.080774502	0.249988175
B	0.584591394	0.164493469	0.250011123
N	0.417571063	0.080995000	0.249991132
B	0.336205879	0.169768507	0.250012865
N	0.169145335	0.082897386	0.249988236
B	0.088939802	0.169752509	0.250012780
K_POINTS crystal			
100			
	0.0000000000	0.0000000000	0.0000000000 1.0
	0.0000000000	-0.0138888889	0.0000000000 1.0
	0.0000000000	-0.0277777778	0.0000000000 1.0
	0.0000000000	-0.0416666667	0.0000000000 1.0
	0.0000000000	-0.0555555556	0.0000000000 1.0
	0.0000000000	-0.0694444444	0.0000000000 1.0
	0.0000000000	-0.0833333333	0.0000000000 1.0
	0.0000000000	-0.0972222222	0.0000000000 1.0
	0.0000000000	-0.1111111111	0.0000000000 1.0
	0.0000000000	-0.1250000000	0.0000000000 1.0
	0.0000000000	-0.1388888889	0.0000000000 1.0
	0.0000000000	-0.1527777778	0.0000000000 1.0
	0.0000000000	-0.1666666667	0.0000000000 1.0
	0.0000000000	-0.1805555556	0.0000000000 1.0
	0.0000000000	-0.1944444444	0.0000000000 1.0
	0.0000000000	-0.2083333333	0.0000000000 1.0
	0.0000000000	-0.2222222222	0.0000000000 1.0
	0.0000000000	-0.2361111111	0.0000000000 1.0

0.0000000000	-0.2500000000	0.0000000000	1.0
0.0000000000	-0.2638888889	0.0000000000	1.0
0.0000000000	-0.2777777778	0.0000000000	1.0
0.0000000000	-0.2916666667	0.0000000000	1.0
0.0000000000	-0.3055555556	0.0000000000	1.0
0.0000000000	-0.3194444444	0.0000000000	1.0
0.0000000000	-0.3333333333	0.0000000000	1.0
0.0000000000	-0.3472222222	0.0000000000	1.0
0.0000000000	-0.3611111111	0.0000000000	1.0
0.0000000000	-0.3750000000	0.0000000000	1.0
0.0000000000	-0.3888888889	0.0000000000	1.0
0.0000000000	-0.4027777778	0.0000000000	1.0
0.0000000000	-0.4166666667	0.0000000000	1.0
0.0000000000	-0.4305555556	0.0000000000	1.0
0.0000000000	-0.4444444444	0.0000000000	1.0
0.0000000000	-0.4583333333	0.0000000000	1.0
0.0000000000	-0.4722222222	0.0000000000	1.0
0.0000000000	-0.4861111111	0.0000000000	1.0
0.0000000000	-0.5000000000	0.0000000000	1.0
0.0158728571	-0.5079366667	0.0000000000	1.0
0.0317457143	-0.5158733333	0.0000000000	1.0
0.0476185714	-0.5238100000	0.0000000000	1.0
0.0634914286	-0.5317466667	0.0000000000	1.0
0.0793642857	-0.5396833333	0.0000000000	1.0
0.0952371429	-0.5476200000	0.0000000000	1.0
0.1111100000	-0.5555566667	0.0000000000	1.0
0.1269828571	-0.5634933333	0.0000000000	1.0
0.1428557143	-0.5714300000	0.0000000000	1.0
0.1587285714	-0.5793666667	0.0000000000	1.0
0.1746014286	-0.5873033333	0.0000000000	1.0
0.1904742857	-0.5952400000	0.0000000000	1.0
0.2063471429	-0.6031766667	0.0000000000	1.0
0.2222200000	-0.6111133333	0.0000000000	1.0
0.2380928571	-0.6190500000	0.0000000000	1.0
0.2539657143	-0.6269866667	0.0000000000	1.0
0.2698385714	-0.6349233333	0.0000000000	1.0
0.2857114286	-0.6428600000	0.0000000000	1.0
0.3015842857	-0.6507966667	0.0000000000	1.0
0.3174571429	-0.6587333333	0.0000000000	1.0
0.3333300000	-0.6666700000	0.0000000000	1.0
0.3253935714	-0.6507969048	0.0000000000	1.0
0.3174571429	-0.6349238095	0.0000000000	1.0
0.3095207143	-0.6190507143	0.0000000000	1.0
0.3015842857	-0.6031776190	0.0000000000	1.0
0.2936478571	-0.5873045238	0.0000000000	1.0
0.2857114286	-0.5714314286	0.0000000000	1.0
0.2777500000	-0.5555583333	0.0000000000	1.0
0.2698385714	-0.5396852381	0.0000000000	1.0
0.2619021429	-0.5238121429	0.0000000000	1.0
0.2539657143	-0.5079390476	0.0000000000	1.0
0.2460292857	-0.4920659524	0.0000000000	1.0
0.2380928571	-0.4761928571	0.0000000000	1.0
0.2301564286	-0.4603197619	0.0000000000	1.0
0.2222200000	-0.4444466667	0.0000000000	1.0
0.2142835714	-0.4285735714	0.0000000000	1.0
0.2063471429	-0.4127004762	0.0000000000	1.0
0.1984107143	-0.3968273810	0.0000000000	1.0
0.1904742857	-0.3809542857	0.0000000000	1.0
0.1825378571	-0.3650811905	0.0000000000	1.0
0.1746014286	-0.3492080952	0.0000000000	1.0
0.1666650000	-0.3333350000	0.0000000000	1.0
0.1587285714	-0.3174619048	0.0000000000	1.0

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0.1507921429	-0.3015888095	0.0000000000	1.0
0.1428557143	-0.2857157143	0.0000000000	1.0
0.1349192857	-0.2698426190	0.0000000000	1.0
0.1269828571	-0.2539695238	0.0000000000	1.0
0.1190464286	-0.2380964286	0.0000000000	1.0
0.1111100000	-0.2222233333	0.0000000000	1.0
0.1031735714	-0.2063502381	0.0000000000	1.0
0.0952371429	-0.1904771429	0.0000000000	1.0
0.0873007143	-0.1746040476	0.0000000000	1.0
0.0793642857	-0.1587309524	0.0000000000	1.0
0.0714278571	-0.1428578571	0.0000000000	1.0
0.0634914286	-0.1269847619	0.0000000000	1.0
0.0555550000	-0.1111116667	0.0000000000	1.0
0.0476185714	-0.0952385714	0.0000000000	1.0
0.0396821429	-0.0793654762	0.0000000000	1.0
0.0317457143	-0.0634923810	0.0000000000	1.0
0.0238092857	-0.0476192857	0.0000000000	1.0
0.0158728571	-0.0317461905	0.0000000000	1.0
0.0079364286	-0.0158730952	0.0000000000	1.0
0.0000000000	0.0000000000	0.0000000000	1.0