```
     Program PWSCF v.6.5 starts on 25Oct2023 at 19:26:52

     This program is part of the open-source Quantum ESPRESSO suite
     for quantum simulation of materials; please cite
         "P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);
         "P. Giannozzi et al., J. Phys.:Condens. Matter 29 465901 (2017);
          URL http://www.quantum-espresso.org",
     in publications or presentations arising from this work. More details at
     http://www.quantum-espresso.org/quote

     Parallel version (MPI), running on     1 processors

     MPI processes distributed on     1 nodes
     Waiting for input...
     Reading input from standard input
Warning: card &IONS ignored
Warning: card ION_DYNAMICS = 'BFGS' ignored
Warning: card / ignored

     Current dimensions of program PWSCF are:
     Max number of different atomic species (ntypx) = 10
     Max number of k-points (npk) =  40000
     Max angular momentum in pseudopotentials (lmaxx) =  3
               file C.pbe-rrkjus.UPF: wavefunction(s)  2S 2P renormalized

     Subspace diagonalization in iterative solution of the eigenvalue problem:
     a serial algorithm will be used


     G-vector sticks info
     --------------------
     sticks:   dense  smooth     PW     G-vecs:    dense   smooth      PW
     Sum         673     265     85                42167    10667    1953



     bravais-lattice index     =            4
     lattice parameter (alat)  =       4.6500  a.u.
     unit-cell volume          =     261.2226 (a.u.)^3
     number of atoms/cell      =            2
     number of atomic types    =            1
     number of electrons       =         8.00
     number of Kohn-Sham states=            8
     kinetic-energy cutoff     =      45.0000  Ry
     charge density cutoff     =     450.0000  Ry
     convergence threshold     =      1.0E-08
     mixing beta               =       0.7000
     number of iterations used =            8  plain     mixing
     Exchange-correlation=  SLA  PW   PBE  PBE
                          (   1   4   3   4   0   0   0)

     celldm(1)=   4.650000  celldm(2)=   0.000000  celldm(3)=   3.000000
     celldm(4)=   0.000000  celldm(5)=   0.000000  celldm(6)=   0.000000

     crystal axes: (cart. coord. in units of alat)
               a(1) = (   1.000000   0.000000   0.000000 )
               a(2) = (  -0.500000   0.866025   0.000000 )
               a(3) = (   0.000000   0.000000   3.000000 )

     reciprocal axes: (cart. coord. in units 2 pi/alat)
               b(1) = (  1.000000  0.577350 -0.000000 )
```

```
               b(2) = (  0.000000  1.154701  0.000000 )
               b(3) = (  0.000000 -0.000000  0.333333 )


     PseudoPot. # 1 for C  read from file:
     ./pseudo/C.pbe-rrkjus.UPF
     MD5 check sum: 00fb224312de0c5b6853bd333518df6f
     Pseudo is Ultrasoft, Zval =  4.0
     Generated by new atomic code, or converted to UPF format
     Using radial grid of  627 points,  4 beta functions with:
                l(1) =   0
                l(2) =   0
                l(3) =   1
                l(4) =   1
     Q(r) pseudized with 0 coefficients


     atomic species   valence    mass     pseudopotential
        C              4.00    12.01000     C ( 1.00)

     Starting magnetic structure
     atomic species   magnetization
        C            0.500

     24 Sym. Ops., with inversion, found (12 have fractional translation)


                                     s                        frac. trans.

      isym =  1     identity

 cryst.   s( 1) = (     1          0          0      )
                  (     0          1          0      )
                  (     0          0          1      )

 cart.    s( 1) = (  1.0000000  0.0000000  0.0000000 )
                  (  0.0000000  1.0000000  0.0000000 )
                  (  0.0000000  0.0000000  1.0000000 )


      isym =  2     180 deg rotation - cart. axis [0,0,1]

 cryst.   s( 2) = (    -1          0          0      )    f =( -0.3333333 )
                  (     0         -1          0      )       (  0.3333333 )
                  (     0          0          1      )       (  0.0000000 )

 cart.    s( 2) = ( -1.0000000  0.0000000  0.0000000 )    f =( -0.5000000 )
                  (  0.0000000 -1.0000000  0.0000000 )       (  0.2886751 )
                  (  0.0000000  0.0000000  1.0000000 )       (  0.0000000 )


      isym =  3     180 deg rotation - cart. axis [0,1,0]

 cryst.   s( 3) = (    -1          0          0      )
                  (     1          1          0      )
                  (     0          0         -1      )

 cart.    s( 3) = ( -1.0000000  0.0000000  0.0000000 )
                  (  0.0000000  1.0000000  0.0000000 )
                  (  0.0000000  0.0000000 -1.0000000 )
```

```
     isym =  4     180 deg rotation - cart. axis [1,0,0]

cryst.   s( 4) = (     1          0          0      )    f =( -0.3333333 )
                 (    -1         -1          0      )       (  0.3333333 )
                 (     0          0         -1      )       (  0.0000000 )

cart.    s( 4) = (  1.0000000  0.0000000  0.0000000 )    f =( -0.5000000 )
                 (  0.0000000 -1.0000000  0.0000000 )       (  0.2886751 )
                 (  0.0000000  0.0000000 -1.0000000 )       (  0.0000000 )


     isym =  5      60 deg rotation - cryst. axis [0,0,1]

cryst.   s( 5) = (     1          1          0      )    f =( -0.3333333 )
                 (    -1          0          0      )       (  0.3333333 )
                 (     0          0          1      )       (  0.0000000 )

cart.    s( 5) = (  0.5000000 -0.8660254  0.0000000 )    f =( -0.5000000 )
                 (  0.8660254  0.5000000  0.0000000 )       (  0.2886751 )
                 (  0.0000000  0.0000000  1.0000000 )       (  0.0000000 )


     isym =  6      60 deg rotation - cryst. axis [0,0,-1]

cryst.   s( 6) = (     0         -1          0      )    f =( -0.3333333 )
                 (     1          1          0      )       (  0.3333333 )
                 (     0          0          1      )       (  0.0000000 )

cart.    s( 6) = (  0.5000000  0.8660254  0.0000000 )    f =( -0.5000000 )
                 ( -0.8660254  0.5000000  0.0000000 )       (  0.2886751 )
                 (  0.0000000  0.0000000  1.0000000 )       (  0.0000000 )


     isym =  7     120 deg rotation - cryst. axis [0,0,1]

cryst.   s( 7) = (     0          1          0      )
                 (    -1         -1          0      )
                 (     0          0          1      )

cart.    s( 7) = ( -0.5000000 -0.8660254  0.0000000 )
                 (  0.8660254 -0.5000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )


     isym =  8     120 deg rotation - cryst. axis [0,0,-1]

cryst.   s( 8) = (    -1         -1          0      )
                 (     1          0          0      )
                 (     0          0          1      )

cart.    s( 8) = ( -0.5000000  0.8660254  0.0000000 )
                 ( -0.8660254 -0.5000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )


     isym =  9     180 deg rotation - cryst. axis [1,-1,0]

cryst.   s( 9) = (     0         -1          0      )
                 (    -1          0          0      )
                 (     0          0         -1      )

cart.    s( 9) = (  0.5000000 -0.8660254  0.0000000 )
```

```
                ( -0.8660254 -0.5000000  0.0000000 )
                (  0.0000000  0.0000000 -1.0000000 )


     isym = 10     180 deg rotation - cryst. axis [2,1,0]

 cryst.   s(10) = (     1          1          0      )
                  (     0         -1          0      )
                  (     0          0         -1      )

 cart.    s(10) = (  0.5000000  0.8660254  0.0000000 )
                  (  0.8660254 -0.5000000  0.0000000 )
                  (  0.0000000  0.0000000 -1.0000000 )


     isym = 11     180 deg rotation - cryst. axis [0,1,0]

 cryst.   s(11) = (    -1         -1          0      )    f =( -0.3333333 )
                  (     0          1          0      )       (  0.3333333 )
                  (     0          0         -1      )       (  0.0000000 )

 cart.    s(11) = ( -0.5000000 -0.8660254  0.0000000 )    f =( -0.5000000 )
                  ( -0.8660254  0.5000000  0.0000000 )       (  0.2886751 )
                  (  0.0000000  0.0000000 -1.0000000 )       (  0.0000000 )


     isym = 12     180 deg rotation - cryst. axis [1,1,0]

 cryst.   s(12) = (     0          1          0      )    f =( -0.3333333 )
                  (     1          0          0      )       (  0.3333333 )
                  (     0          0         -1      )       (  0.0000000 )

 cart.    s(12) = ( -0.5000000  0.8660254  0.0000000 )    f =( -0.5000000 )
                  (  0.8660254  0.5000000  0.0000000 )       (  0.2886751 )
                  (  0.0000000  0.0000000 -1.0000000 )       (  0.0000000 )


     isym = 13     inversion

 cryst.   s(13) = (    -1          0          0      )    f =( -0.3333333 )
                  (     0         -1          0      )       (  0.3333333 )
                  (     0          0         -1      )       (  0.0000000 )

 cart.    s(13) = ( -1.0000000  0.0000000  0.0000000 )    f =( -0.5000000 )
                  (  0.0000000 -1.0000000  0.0000000 )       (  0.2886751 )
                  (  0.0000000  0.0000000 -1.0000000 )       (  0.0000000 )


     isym = 14     inv. 180 deg rotation - cart. axis [0,0,1]

 cryst.   s(14) = (     1          0          0      )
                  (     0          1          0      )
                  (     0          0         -1      )

 cart.    s(14) = (  1.0000000  0.0000000  0.0000000 )
                  (  0.0000000  1.0000000  0.0000000 )
                  (  0.0000000  0.0000000 -1.0000000 )


     isym = 15     inv. 180 deg rotation - cart. axis [0,1,0]

 cryst.   s(15) = (     1          0          0      )    f =( -0.3333333 )
```

```
                 (    -1         -1          0      )       (  0.3333333 )
                 (     0          0          1      )       (  0.0000000 )

cart.    s(15) = (  1.0000000  0.0000000  0.0000000 )    f =( -0.5000000 )
                 (  0.0000000 -1.0000000  0.0000000 )       (  0.2886751 )
                 (  0.0000000  0.0000000  1.0000000 )       (  0.0000000 )


     isym = 16     inv. 180 deg rotation - cart. axis [1,0,0]

cryst.   s(16) = (    -1          0          0      )
                 (     1          1          0      )
                 (     0          0          1      )

cart.    s(16) = ( -1.0000000  0.0000000  0.0000000 )
                 (  0.0000000  1.0000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )


     isym = 17     inv.  60 deg rotation - cryst. axis [0,0,1]

cryst.   s(17) = (    -1         -1          0      )
                 (     1          0          0      )
                 (     0          0         -1      )

cart.    s(17) = ( -0.5000000  0.8660254  0.0000000 )
                 ( -0.8660254 -0.5000000  0.0000000 )
                 (  0.0000000  0.0000000 -1.0000000 )


     isym = 18     inv.  60 deg rotation - cryst. axis [0,0,-1]

cryst.   s(18) = (     0          1          0      )
                 (    -1         -1          0      )
                 (     0          0         -1      )

cart.    s(18) = ( -0.5000000 -0.8660254  0.0000000 )
                 (  0.8660254 -0.5000000  0.0000000 )
                 (  0.0000000  0.0000000 -1.0000000 )


     isym = 19     inv. 120 deg rotation - cryst. axis [0,0,1]

cryst.   s(19) = (     0         -1          0      )    f =( -0.3333333 )
                 (     1          1          0      )       (  0.3333333 )
                 (     0          0         -1      )       (  0.0000000 )

cart.    s(19) = (  0.5000000  0.8660254  0.0000000 )    f =( -0.5000000 )
                 ( -0.8660254  0.5000000  0.0000000 )       (  0.2886751 )
                 (  0.0000000  0.0000000 -1.0000000 )       (  0.0000000 )


     isym = 20     inv. 120 deg rotation - cryst. axis [0,0,-1]

cryst.   s(20) = (     1          1          0      )    f =( -0.3333333 )
                 (    -1          0          0      )       (  0.3333333 )
                 (     0          0         -1      )       (  0.0000000 )

cart.    s(20) = (  0.5000000 -0.8660254  0.0000000 )    f =( -0.5000000 )
                 (  0.8660254  0.5000000  0.0000000 )       (  0.2886751 )
                 (  0.0000000  0.0000000 -1.0000000 )       (  0.0000000 )
```

```
     isym = 21     inv. 180 deg rotation - cryst. axis [1,-1,0]

 cryst.   s(21) = (     0          1          0      )    f =( -0.3333333 )
                  (     1          0          0      )       (  0.3333333 )
                  (     0          0          1      )       (  0.0000000 )

 cart.    s(21) = ( -0.5000000  0.8660254  0.0000000 )    f =( -0.5000000 )
                  (  0.8660254  0.5000000  0.0000000 )       (  0.2886751 )
                  (  0.0000000  0.0000000  1.0000000 )       (  0.0000000 )


     isym = 22     inv. 180 deg rotation - cryst. axis [2,1,0]

 cryst.   s(22) = (    -1         -1          0      )    f =( -0.3333333 )
                  (     0          1          0      )       (  0.3333333 )
                  (     0          0          1      )       (  0.0000000 )

 cart.    s(22) = ( -0.5000000 -0.8660254  0.0000000 )    f =( -0.5000000 )
                  ( -0.8660254  0.5000000  0.0000000 )       (  0.2886751 )
                  (  0.0000000  0.0000000  1.0000000 )       (  0.0000000 )


     isym = 23     inv. 180 deg rotation - cryst. axis [0,1,0]

 cryst.   s(23) = (     1          1          0      )
                  (     0         -1          0      )
                  (     0          0          1      )

 cart.    s(23) = (  0.5000000  0.8660254  0.0000000 )
                  (  0.8660254 -0.5000000  0.0000000 )
                  (  0.0000000  0.0000000  1.0000000 )


     isym = 24     inv. 180 deg rotation - cryst. axis [1,1,0]

 cryst.   s(24) = (     0         -1          0      )
                  (    -1          0          0      )
                  (     0          0          1      )

 cart.    s(24) = (  0.5000000 -0.8660254  0.0000000 )
                  ( -0.8660254 -0.5000000  0.0000000 )
                  (  0.0000000  0.0000000  1.0000000 )


    point group D_6h(6/mmm)
    there are 12 classes
    the character table:

       E     2C6   2C3   C2    3C2'  3C2'' i     2S3   2S6   s_h   3s_d  3s_v
A_1g   1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00
A_2g   1.00  1.00  1.00  1.00 -1.00 -1.00  1.00  1.00  1.00  1.00 -1.00 -1.00
B_1g   1.00 -1.00  1.00 -1.00  1.00 -1.00  1.00 -1.00  1.00 -1.00  1.00 -1.00
B_2g   1.00 -1.00  1.00 -1.00 -1.00  1.00  1.00 -1.00  1.00 -1.00 -1.00  1.00
E_1g   2.00  1.00 -1.00 -2.00  0.00  0.00  2.00  1.00 -1.00 -2.00  0.00  0.00
E_2g   2.00 -1.00 -1.00  2.00  0.00  0.00  2.00 -1.00 -1.00  2.00  0.00  0.00
A_1u   1.00  1.00  1.00  1.00  1.00  1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00
A_2u   1.00  1.00  1.00  1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00  1.00  1.00
B_1u   1.00 -1.00  1.00 -1.00  1.00 -1.00 -1.00  1.00 -1.00  1.00 -1.00  1.00
B_2u   1.00 -1.00  1.00 -1.00 -1.00  1.00 -1.00  1.00 -1.00  1.00  1.00 -1.00
E_1u   2.00  1.00 -1.00 -2.00  0.00  0.00 -2.00 -1.00  1.00  2.00  0.00  0.00
E_2u   2.00 -1.00 -1.00  2.00  0.00  0.00 -2.00  1.00  1.00 -2.00  0.00  0.00
```

```
   the symmetry operations in each class and the name of the first element:

   E        1
        identity
   2C6      5    6
         60 deg rotation - cryst. axis [0,0,1]
   2C3      7    8
        120 deg rotation - cryst. axis [0,0,1]
   C2       2
        180 deg rotation - cart. axis [0,0,1]
   3C2'     4   12   11
        180 deg rotation - cart. axis [1,0,0]
   3C2''    3    9   10
        180 deg rotation - cart. axis [0,1,0]
   i       13
        inversion
   2S3     17   18
        inv.  60 deg rotation - cryst. axis [0,0,1]
   2S6     19   20
        inv. 120 deg rotation - cryst. axis [0,0,1]
   s_h     14
        inv. 180 deg rotation - cart. axis [0,0,1]
   3s_d    16   24   23
        inv. 180 deg rotation - cart. axis [1,0,0]
   3s_v    15   21   22
        inv. 180 deg rotation - cart. axis [0,1,0]

 Cartesian axes

   site n.     atom                  positions (alat units)
       1           C   tau(   1) = (   0.0000000   0.0000000   1.5000000  )
       2           C   tau(   2) = (  -0.0000000   0.5773503   1.5000000  )

 Crystallographic axes

   site n.     atom                  positions (cryst. coord.)
       1           C   tau(   1) = (  0.0000000  0.0000000  0.5000000  )
       2           C   tau(   2) = (  0.3333333  0.6666667  0.5000000  )

   number of k points=    37  Marzari-Vanderbilt smearing, width (Ry)=  0.0010
                     cart. coord. in units 2pi/alat
      k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0030864
      k(    2) = (   0.0000000   0.0641500   0.0000000), wk =   0.0185185
      k(    3) = (   0.0000000   0.1283001   0.0000000), wk =   0.0185185
      k(    4) = (   0.0000000   0.1924501   0.0000000), wk =   0.0185185
      k(    5) = (   0.0000000   0.2566001   0.0000000), wk =   0.0185185
      k(    6) = (   0.0000000   0.3207501   0.0000000), wk =   0.0185185
      k(    7) = (   0.0000000   0.3849002   0.0000000), wk =   0.0185185
      k(    8) = (   0.0000000   0.4490502   0.0000000), wk =   0.0185185
      k(    9) = (   0.0000000   0.5132002   0.0000000), wk =   0.0185185
      k(   10) = (   0.0000000  -0.5773503   0.0000000), wk =   0.0092593
      k(   11) = (   0.0555556   0.0962250   0.0000000), wk =   0.0185185
      k(   12) = (   0.0555556   0.1603751   0.0000000), wk =   0.0370370
      k(   13) = (   0.0555556   0.2245251   0.0000000), wk =   0.0370370
      k(   14) = (   0.0555556   0.2886751   0.0000000), wk =   0.0370370
      k(   15) = (   0.0555556   0.3528252   0.0000000), wk =   0.0370370
      k(   16) = (   0.0555556   0.4169752   0.0000000), wk =   0.0370370
      k(   17) = (   0.0555556   0.4811252   0.0000000), wk =   0.0370370
      k(   18) = (   0.0555556   0.5452753   0.0000000), wk =   0.0370370
      k(   19) = (   0.1111111   0.1924501   0.0000000), wk =   0.0185185
      k(   20) = (   0.1111111   0.2566001   0.0000000), wk =   0.0370370
```

```
     k(   21) = (   0.1111111   0.3207501   0.0000000), wk =   0.0370370
     k(   22) = (   0.1111111   0.3849002   0.0000000), wk =   0.0370370
     k(   23) = (   0.1111111   0.4490502   0.0000000), wk =   0.0370370
     k(   24) = (   0.1111111   0.5132002   0.0000000), wk =   0.0370370
     k(   25) = (   0.1111111   0.5773503   0.0000000), wk =   0.0185185
     k(   26) = (   0.1666667   0.2886751   0.0000000), wk =   0.0185185
     k(   27) = (   0.1666667   0.3528252   0.0000000), wk =   0.0370370
     k(   28) = (   0.1666667   0.4169752   0.0000000), wk =   0.0370370
     k(   29) = (   0.1666667   0.4811252   0.0000000), wk =   0.0370370
     k(   30) = (   0.1666667   0.5452753   0.0000000), wk =   0.0370370
     k(   31) = (   0.2222222   0.3849002   0.0000000), wk =   0.0185185
     k(   32) = (   0.2222222   0.4490502   0.0000000), wk =   0.0370370
     k(   33) = (   0.2222222   0.5132002   0.0000000), wk =   0.0370370
     k(   34) = (   0.2222222   0.5773503   0.0000000), wk =   0.0185185
     k(   35) = (   0.2777778   0.4811252   0.0000000), wk =   0.0185185
     k(   36) = (   0.2777778   0.5452753   0.0000000), wk =   0.0370370
     k(   37) = (   0.3333333   0.5773503   0.0000000), wk =   0.0061728

                    cryst. coord.
     k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0030864
     k(    2) = (   0.0000000   0.0555556   0.0000000), wk =   0.0185185
     k(    3) = (   0.0000000   0.1111111   0.0000000), wk =   0.0185185
     k(    4) = (   0.0000000   0.1666667   0.0000000), wk =   0.0185185
     k(    5) = (   0.0000000   0.2222222   0.0000000), wk =   0.0185185
     k(    6) = (   0.0000000   0.2777778   0.0000000), wk =   0.0185185
     k(    7) = (   0.0000000   0.3333333   0.0000000), wk =   0.0185185
     k(    8) = (   0.0000000   0.3888889   0.0000000), wk =   0.0185185
     k(    9) = (   0.0000000   0.4444444   0.0000000), wk =   0.0185185
     k(   10) = (   0.0000000  -0.5000000   0.0000000), wk =   0.0092593
     k(   11) = (   0.0555556   0.0555556   0.0000000), wk =   0.0185185
     k(   12) = (   0.0555556   0.1111111   0.0000000), wk =   0.0370370
     k(   13) = (   0.0555556   0.1666667   0.0000000), wk =   0.0370370
     k(   14) = (   0.0555556   0.2222222   0.0000000), wk =   0.0370370
     k(   15) = (   0.0555556   0.2777778   0.0000000), wk =   0.0370370
     k(   16) = (   0.0555556   0.3333333   0.0000000), wk =   0.0370370
     k(   17) = (   0.0555556   0.3888889   0.0000000), wk =   0.0370370
     k(   18) = (   0.0555556   0.4444444   0.0000000), wk =   0.0370370
     k(   19) = (   0.1111111   0.1111111   0.0000000), wk =   0.0185185
     k(   20) = (   0.1111111   0.1666667   0.0000000), wk =   0.0370370
     k(   21) = (   0.1111111   0.2222222   0.0000000), wk =   0.0370370
     k(   22) = (   0.1111111   0.2777778   0.0000000), wk =   0.0370370
     k(   23) = (   0.1111111   0.3333333   0.0000000), wk =   0.0370370
     k(   24) = (   0.1111111   0.3888889   0.0000000), wk =   0.0370370
     k(   25) = (   0.1111111   0.4444444   0.0000000), wk =   0.0185185
     k(   26) = (   0.1666667   0.1666667   0.0000000), wk =   0.0185185
     k(   27) = (   0.1666667   0.2222222   0.0000000), wk =   0.0370370
     k(   28) = (   0.1666667   0.2777778   0.0000000), wk =   0.0370370
     k(   29) = (   0.1666667   0.3333333   0.0000000), wk =   0.0370370
     k(   30) = (   0.1666667   0.3888889   0.0000000), wk =   0.0370370
     k(   31) = (   0.2222222   0.2222222   0.0000000), wk =   0.0185185
     k(   32) = (   0.2222222   0.2777778   0.0000000), wk =   0.0370370
     k(   33) = (   0.2222222   0.3333333   0.0000000), wk =   0.0370370
     k(   34) = (   0.2222222   0.3888889   0.0000000), wk =   0.0185185
     k(   35) = (   0.2777778   0.2777778   0.0000000), wk =   0.0185185
     k(   36) = (   0.2777778   0.3333333   0.0000000), wk =   0.0370370
     k(   37) = (   0.3333333   0.3333333   0.0000000), wk =   0.0061728

   Dense  grid:    42167 G-vectors     FFT dimensions: (  36,  36,  96)

   Smooth grid:    10667 G-vectors     FFT dimensions: (  24,  24,  60)

   Dynamical RAM for                wfc:       0.16 MB
```

```
     Dynamical RAM for     wfc (w. buffer):      12.19 MB

     Dynamical RAM for           str. fact:       0.64 MB

     Dynamical RAM for           local pot:       0.00 MB

     Dynamical RAM for          nlocal pot:       0.33 MB

     Dynamical RAM for                qrad:       0.36 MB

     Dynamical RAM for          rho,v,vnew:       9.56 MB

     Dynamical RAM for               rhoin:       3.19 MB

     Dynamical RAM for             rho*nmix:      20.59 MB

     Dynamical RAM for           G-vectors:       2.49 MB

     Dynamical RAM for          h,s,v(r/c):       0.05 MB

     Dynamical RAM for          <psi|beta>:       0.00 MB

     Dynamical RAM for                 psi:       0.65 MB

     Dynamical RAM for                hpsi:       0.65 MB

     Dynamical RAM for                spsi:       0.65 MB

     Dynamical RAM for      wfcinit/wfcrot:       0.33 MB

     Dynamical RAM for           addusdens:      29.60 MB

     Dynamical RAM for          addusforce:      30.89 MB

     Dynamical RAM for         addusstress:      33.14 MB

     Estimated static dynamical RAM per process >      56.33 MB

     Estimated max dynamical RAM per process >      89.47 MB
     Generating pointlists ...
     new r_m :   0.2382 (alat units)  1.1074 (a.u.) for type    1

     Initial potential from superposition of free atoms

     starting charge    7.99989, renormalised to    8.00000
     Starting wfcs are    8 randomized atomic wfcs

     total cpu time spent up to now is        2.9 secs

     Self-consistent Calculation

     iteration #  1     ecut=    45.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.00E-02,  avg # of iterations =  4.6

     total cpu time spent up to now is        9.6 secs

     total energy              =     -22.71773151 Ry
     Harris-Foulkes estimate   =     -22.62352664 Ry
     estimated scf accuracy    <       0.28188478 Ry
```

```
     total magnetization       =     0.23 Bohr mag/cell
     absolute magnetization    =     0.26 Bohr mag/cell

     iteration #  2     ecut=    45.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  3.52E-03,  avg # of iterations =  2.4

     total cpu time spent up to now is       14.0 secs

     total energy              =     -22.78776602 Ry
     Harris-Foulkes estimate   =     -22.76061961 Ry
     estimated scf accuracy    <       0.01291763 Ry

     total magnetization       =     0.01 Bohr mag/cell
     absolute magnetization    =     0.05 Bohr mag/cell

     iteration #  3     ecut=    45.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.61E-04,  avg # of iterations =  3.0

     total cpu time spent up to now is       18.7 secs

     total energy              =     -22.79052770 Ry
     Harris-Foulkes estimate   =     -22.78833037 Ry
     estimated scf accuracy    <       0.00086503 Ry

     total magnetization       =     0.01 Bohr mag/cell
     absolute magnetization    =     0.03 Bohr mag/cell

     iteration #  4     ecut=    45.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.08E-05,  avg # of iterations =  3.2

     total cpu time spent up to now is       23.6 secs

     total energy              =     -22.79062700 Ry
     Harris-Foulkes estimate   =     -22.79061457 Ry
     estimated scf accuracy    <       0.00000500 Ry

     total magnetization       =     0.01 Bohr mag/cell
     absolute magnetization    =     0.01 Bohr mag/cell

     iteration #  5     ecut=    45.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  6.25E-08,  avg # of iterations =  2.5

     total cpu time spent up to now is       28.5 secs

     total energy              =     -22.79063186 Ry
     Harris-Foulkes estimate   =     -22.79063093 Ry
     estimated scf accuracy    <       0.00000028 Ry

     total magnetization       =     0.01 Bohr mag/cell
     absolute magnetization    =     0.01 Bohr mag/cell

     iteration #  6     ecut=    45.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  3.49E-09,  avg # of iterations =  2.2

     total cpu time spent up to now is       33.1 secs

     total energy              =     -22.79063218 Ry
```

```
     Harris-Foulkes estimate   =     -22.79063214 Ry
     estimated scf accuracy    <       0.00000001 Ry

     total magnetization       =     0.01 Bohr mag/cell
     absolute magnetization    =     0.01 Bohr mag/cell

     iteration #  7     ecut=    45.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
     ethr =  1.27E-10,  avg # of iterations =  2.8

     Magnetic moment per site:
     atom:    1    charge:    1.7094    magn:    0.0023    constr:    0.0000
     atom:    2    charge:    1.7094    magn:    0.0023    constr:    0.0000

     total cpu time spent up to now is       38.0 secs

     End of self-consistent calculation

 ------ SPIN UP ------------


          k = 0.0000 0.0000 0.0000 (  1301 PWs)   bands (ev):

   -18.6339  -6.7494  -2.1633  -2.1633   3.7766   7.1287   9.2229   9.2229

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.0000 0.0642 0.0000 (  1295 PWs)   bands (ev):

   -18.5608  -6.6619  -2.4594  -2.3200   3.8762   7.2240   9.2364   9.5386

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.0000 0.1283 0.0000 (  1309 PWs)   bands (ev):

   -18.3420  -6.4004  -3.2739  -2.7365   4.1748   7.5090   9.2645   9.8846

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.0000 0.1925 0.0000 (  1323 PWs)   bands (ev):

   -17.9785  -5.9681  -4.4445  -3.2970   4.6726   7.9782   9.2232  10.2916

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.0000 0.2566 0.0000 (  1321 PWs)   bands (ev):

   -17.4722  -5.8161  -5.3713  -3.8928   5.3687   8.5396   9.0319   9.0805

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.0000 0.3208 0.0000 (  1319 PWs)   bands (ev):

   -16.8262  -7.2747  -4.6218  -4.4477   6.2620   7.3758   8.8820   9.5282

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000
```

```
       k = 0.0000 0.3849 0.0000 (  1330 PWs)   bands (ev):

-16.0454  -8.7430  -4.9139  -3.7428   5.8304   7.3480   8.6848  10.5336

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.4491 0.0000 (  1328 PWs)   bands (ev):

-15.1393 -10.1665  -5.2628  -2.7861   4.3488   8.4428   8.7080  11.7009

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.5132 0.0000 (  1326 PWs)   bands (ev):

-14.1371 -11.4885  -5.4779  -1.8953   3.1250   8.3934  10.1212  12.9801

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000-0.5774 0.0000 (  1332 PWs)   bands (ev):

-13.3722 -12.3616  -5.5505  -1.4690   2.5849   8.3590  11.6929  11.8412

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.0962 0.0000 (  1301 PWs)   bands (ev):

-18.4149  -6.4874  -2.9879  -2.6337   4.0753   7.4142   9.3254   9.7941

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.1604 0.0000 (  1322 PWs)   bands (ev):

-18.1238  -6.1404  -3.9278  -3.1758   4.4736   7.7924   9.4447  10.1854

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.2245 0.0000 (  1324 PWs)   bands (ev):

-17.6889  -5.6255  -5.1571  -3.7969   5.0708   8.3452   9.4317   9.5201

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.2887 0.0000 (  1328 PWs)   bands (ev):

-17.1127  -6.5461  -4.9513  -4.3991   5.8659   8.0483   9.1512   9.2905

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.3528 0.0000 (  1321 PWs)   bands (ev):

-16.3992  -7.9944  -4.9249  -4.1340   6.5500   6.8569   9.0994  10.0573

  occupation numbers
```

```
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.4170 0.0000 (  1329 PWs)   bands (ev):

-15.5551  -9.4324  -5.3408  -3.2070   5.0392   8.0360   8.9244  11.1376

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.4811 0.0000 (  1330 PWs)   bands (ev):

-14.5957 -10.8058  -5.6270  -2.2535   3.6661   8.7546   9.4457  12.3434

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.5453 0.0000 (  1330 PWs)   bands (ev):

-13.5997 -12.0139  -5.7726  -1.5204   2.7143   8.6935  10.9908  12.7146

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.1925 0.0000 (  1331 PWs)   bands (ev):

-17.7612  -5.7106  -4.8243  -3.8818   4.9716   8.2611   9.7187   9.8545

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.2566 0.0000 (  1329 PWs)   bands (ev):

-17.2565  -5.9581  -5.1173  -4.6235   5.6680   8.4692   8.9237  10.0965

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.3208 0.0000 (  1327 PWs)   bands (ev):

-16.6128  -7.2694  -5.2648  -4.3720   6.5616   7.0897   9.7394  10.0510

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.3849 0.0000 (  1332 PWs)   bands (ev):

-15.8355  -8.6537  -5.7747  -3.4967   5.6411   7.6496   9.8964  10.7138

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.4491 0.0000 (  1336 PWs)   bands (ev):

-14.9345 -10.0282  -6.1447  -2.5407   4.2327   8.9233   9.7491  11.7977

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.5132 0.0000 (  1339 PWs)   bands (ev):

-13.9402 -11.3207  -6.3691  -1.6409   3.0438   9.6182  10.4125  12.8705
```

```
  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.5774 0.0000 (  1341 PWs)   bands (ev):

-13.1850 -12.1775  -6.4444  -1.2019   2.5055   9.5878  11.9558  12.1192

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.2887 0.0000 (  1335 PWs)   bands (ev):

-16.6842  -6.8741  -5.5452  -4.4518   6.4630   7.2988   9.6221  10.8900

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.3528 0.0000 (  1336 PWs)   bands (ev):

-15.9765  -7.9841  -6.3087  -3.6441   6.0097   7.4535  10.4767  11.1917

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.4170 0.0000 (  1336 PWs)   bands (ev):

-15.1411  -9.2388  -6.8405  -2.7240   4.6836   8.6358  11.1125  11.4125

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.4811 0.0000 (  1342 PWs)   bands (ev):

-14.1948 -10.5153  -7.1765  -1.7644   3.4285   9.9997  10.9930  12.2757

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.5453 0.0000 (  1338 PWs)   bands (ev):

-13.2181 -11.6696  -7.3407  -0.9982   2.5063  10.8983  11.5529  12.7842

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.2222 0.3849 0.0000 (  1333 PWs)   bands (ev):

-15.2104  -8.7801  -7.2791  -2.7868   4.8601   8.5380  11.2684  12.3400

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.2222 0.4491 0.0000 (  1347 PWs)   bands (ev):

-14.3266  -9.7803  -7.9370  -1.8389   3.6900   9.8078  11.9120  12.5420

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.2222 0.5132 0.0000 (  1347 PWs)   bands (ev):

-13.3575 -10.8960  -8.2761  -0.9070   2.6171  11.2431  12.1755  12.4425
```

```
     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2222 0.5774 0.0000 (  1347 PWs)   bands (ev):

   -12.6244 -11.6903  -8.3801  -0.4059   2.0674  12.2051  12.3650  12.7017

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2778 0.4811 0.0000 (  1355 PWs)   bands (ev):

   -13.4128 -10.4053  -8.8197  -0.8844   2.6802  11.1478  11.9395  13.8219

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2778 0.5453 0.0000 (  1349 PWs)   bands (ev):

   -12.4750 -11.2212  -9.2508  -0.0052   1.7785  11.7822  12.5915  13.6479

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.3333 0.5774 0.0000 (  1365 PWs)   bands (ev):

   -11.6946 -11.6946  -9.7020   0.9006   0.9006  11.6038  13.6441  13.6441

     occupation numbers
     1.0000   1.0000   1.0000   0.9663   0.9663   0.0000   0.0000   0.0000

 ------ SPIN DOWN ----------


          k = 0.0000 0.0000 0.0000 (  1301 PWs)   bands (ev):

   -18.6260  -6.7295  -2.1601  -2.1601   3.7795   7.1345   9.2255   9.2255

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.0000 0.0642 0.0000 (  1295 PWs)   bands (ev):

   -18.5530  -6.6420  -2.4560  -2.3168   3.8791   7.2298   9.2394   9.5413

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.0000 0.1283 0.0000 (  1309 PWs)   bands (ev):

   -18.3342  -6.3803  -3.2700  -2.7333   4.1778   7.5149   9.2682   9.8880

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.0000 0.1925 0.0000 (  1323 PWs)   bands (ev):

   -17.9707  -5.9478  -4.4401  -3.2939   4.6755   7.9841   9.2283  10.3231

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000
```

```
       k = 0.0000 0.2566 0.0000 (  1321 PWs)   bands (ev):

-17.4645  -5.8112  -5.3507  -3.8897   5.3718   8.5500   9.0573   9.0871

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.3208 0.0000 (  1319 PWs)   bands (ev):

-16.8185  -7.2693  -4.6009  -4.4446   6.2650   7.4030   8.8899   9.5351

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.3849 0.0000 (  1330 PWs)   bands (ev):

-16.0378  -8.7373  -4.9109  -3.7213   5.8562   7.3512   8.6935  10.5404

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.4491 0.0000 (  1328 PWs)   bands (ev):

-15.1317 -10.1605  -5.2598  -2.7640   4.3730   8.4514   8.7121  11.7079

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000 0.5132 0.0000 (  1326 PWs)   bands (ev):

-14.1293 -11.4826  -5.4749  -1.8722   3.1479   8.4034  10.1245  12.9878

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0000-0.5774 0.0000 (  1332 PWs)   bands (ev):

-13.3636 -12.3565  -5.5475  -1.4454   2.6070   8.3691  11.6973  11.8438

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.0962 0.0000 (  1301 PWs)   bands (ev):

-18.4071  -6.4674  -2.9841  -2.6305   4.0782   7.4201   9.3287   9.7975

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.1604 0.0000 (  1322 PWs)   bands (ev):

-18.1160  -6.1202  -3.9236  -3.1726   4.4766   7.7983   9.4487  10.1888

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.2245 0.0000 (  1324 PWs)   bands (ev):

-17.6811  -5.6051  -5.1523  -3.7937   5.0738   8.3513   9.4372   9.5505

  occupation numbers
```

```
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.2887 0.0000 (  1328 PWs)   bands (ev):

-17.1050  -6.5408  -4.9306  -4.3960   5.8689   8.0759   9.1585   9.2975

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.3528 0.0000 (  1321 PWs)   bands (ev):

-16.3916  -7.9888  -4.9218  -4.1128   6.5767   6.8600   9.1076  10.0640

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.4170 0.0000 (  1329 PWs)   bands (ev):

-15.5475  -9.4265  -5.3377  -3.1852   5.0643   8.0394   8.9333  11.1445

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.4811 0.0000 (  1330 PWs)   bands (ev):

-14.5881 -10.7998  -5.6239  -2.2309   3.6898   8.7643   9.4488  12.3508

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.0556 0.5453 0.0000 (  1330 PWs)   bands (ev):

-13.5916 -12.0082  -5.7694  -1.4969   2.7368   8.7034  10.9943  12.7183

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.1925 0.0000 (  1331 PWs)   bands (ev):

-17.7535  -5.6902  -4.8196  -3.8786   4.9746   8.2671   9.7496   9.8585

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.2566 0.0000 (  1329 PWs)   bands (ev):

-17.2487  -5.9529  -5.0966  -4.6203   5.6711   8.4978   8.9307  10.1015

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.3208 0.0000 (  1327 PWs)   bands (ev):

-16.6051  -7.2638  -5.2615  -4.3509   6.5647   7.1175   9.7458  10.0579

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.3849 0.0000 (  1332 PWs)   bands (ev):

-15.8279  -8.6479  -5.7714  -3.4751   5.6675   7.6528   9.9046  10.7205
```

```
  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.4491 0.0000 (  1336 PWs)   bands (ev):

-14.9270 -10.0222  -6.1413  -2.5184   4.2576   8.9268   9.7578  11.8049

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.5132 0.0000 (  1339 PWs)   bands (ev):

-13.9325 -11.3147  -6.3657  -1.6178   3.0673   9.6277  10.4158  12.8785

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1111 0.5774 0.0000 (  1341 PWs)   bands (ev):

-13.1764 -12.1723  -6.4409  -1.1782   2.5283   9.5974  11.9604  12.1217

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.2887 0.0000 (  1335 PWs)   bands (ev):

-16.6765  -6.8684  -5.5421  -4.4308   6.4661   7.3273   9.6283  10.8946

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.3528 0.0000 (  1336 PWs)   bands (ev):

-15.9689  -7.9780  -6.3054  -3.6227   6.0371   7.4567  10.4831  11.1980

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.4170 0.0000 (  1336 PWs)   bands (ev):

-15.1336  -9.2326  -6.8370  -2.7020   4.7097   8.6391  11.1204  11.4193

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.4811 0.0000 (  1342 PWs)   bands (ev):

-14.1873 -10.5090  -7.1729  -1.7416   3.4533  10.0032  11.0016  12.2830

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.1667 0.5453 0.0000 (  1338 PWs)   bands (ev):

-13.2101 -11.6638  -7.3370  -0.9745   2.5300  10.9076  11.5565  12.7919

  occupation numbers
  1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

       k = 0.2222 0.3849 0.0000 (  1333 PWs)   bands (ev):

-15.2029  -8.7735  -7.2760  -2.7649   4.8867   8.5413  11.2750  12.3451
```

```
     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2222 0.4491 0.0000 (  1347 PWs)   bands (ev):

   -14.3191  -9.7736  -7.9336  -1.8162   3.7157   9.8112  11.9188  12.5497

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2222 0.5132 0.0000 (  1347 PWs)   bands (ev):

   -13.3499 -10.8895  -8.2725  -0.8835   2.6419  11.2469  12.1821  12.4510

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2222 0.5774 0.0000 (  1347 PWs)   bands (ev):

   -12.6162 -11.6845  -8.3765  -0.3819   2.0916  12.2116  12.3743  12.7068

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2778 0.4811 0.0000 (  1355 PWs)   bands (ev):

   -13.4052 -10.3980  -8.8167  -0.8611   2.7055  11.1515  11.9457  13.8471

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.2778 0.5453 0.0000 (  1349 PWs)   bands (ev):

   -12.4672 -11.2141  -9.2478   0.0188   1.8032  11.7879  12.5960  13.6570

     occupation numbers
     1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

          k = 0.3333 0.5774 0.0000 (  1365 PWs)   bands (ev):

   -11.6867 -11.6867  -9.6997   0.9251   0.9251  11.6090  13.6514  13.6514

     occupation numbers
     1.0000   1.0000   1.0000   0.0337   0.0337   0.0000   0.0000   0.0000

     the Fermi energy is     0.9120 ev

!    total energy              =     -22.79063219 Ry
     Harris-Foulkes estimate   =     -22.79063219 Ry
     estimated scf accuracy    <          6.2E-10 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =     -56.46141515 Ry
     hartree contribution      =      30.37605896 Ry
     xc contribution           =      -7.02479511 Ry
     ewald contribution        =      10.31951897 Ry
     smearing contrib. (-TS)   =       0.00000013 Ry

     total magnetization       =     0.01 Bohr mag/cell
     absolute magnetization    =     0.01 Bohr mag/cell
```

```
     convergence has been achieved in   7 iterations

     Forces acting on atoms (cartesian axes, Ry/au):

     atom    1 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =     0.00000000    0.00000000    0.00000000
     The non-local contrib.  to forces
     atom    1 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =     0.00000000   -0.00000000    0.00000000
     The ionic contribution  to forces
     atom    1 type  1   force =    -0.00000006    0.00000000   -0.00000000
     atom    2 type  1   force =     0.00000006   -0.00000000    0.00000000
     The local contribution  to forces
     atom    1 type  1   force =     0.00000000   -0.00000000    0.00000000
     atom    2 type  1   force =     0.00000005   -0.00000000    0.00000000
     The core correction contribution to forces
     atom    1 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =     0.00000000    0.00000000    0.00000000
     The Hubbard contrib.    to forces
     atom    1 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =     0.00000000    0.00000000    0.00000000
     The SCF correction term to forces
     atom    1 type  1   force =    -0.00000000    0.00000000   -0.00000000
     atom    2 type  1   force =     0.00000000   -0.00000000   -0.00000000

     Total force =     0.000000     Total SCF correction =     0.000000


     Computing stress (Cartesian axis) and pressure

          total   stress  (Ry/bohr**3)                   (kbar)     P=        1.84
    0.00001942   0.00000000   0.00000000           2.86        0.00        0.00
    0.00000000   0.00001942   0.00000000           0.00        2.86        0.00
    0.00000000   0.00000000  -0.00000130           0.00        0.00       -0.19

     kinetic stress (kbar)   4817.03     -0.00      0.00
                               -0.00   4817.03      0.00
                                0.00      0.00   5573.53

     local   stress (kbar) -36991.27      0.00     -0.00
                                0.00 -36991.27     -0.00
                               -0.00     -0.00  40189.32

     nonloc. stress (kbar)   -211.97      0.00      0.00
                                0.00   -211.97      0.00
                                0.00      0.00   -209.36

     hartree stress (kbar)  16640.39     -0.00      0.00
                               -0.00  16640.39     -0.00
                                0.00     -0.00 -16174.79

     exc-cor stress (kbar)  -1215.31     -0.00      0.00
                               -0.00  -1215.31      0.00
                                0.00      0.00  -1262.26

     corecor stress (kbar)      0.00      0.00      0.00
                                0.00      0.00      0.00
                                0.00      0.00      0.00

     ewald   stress (kbar)  16963.98     -0.00      0.00
                               -0.00  16963.98      0.00
```

```
                            0.00      0.00 -28116.62

     hubbard stress (kbar)      0.00      0.00      0.00
                                0.00      0.00      0.00
                                0.00      0.00      0.00

     london  stress (kbar)      0.00      0.00      0.00
                                0.00      0.00      0.00
                                0.00      0.00      0.00

     DFT-D3  stress (kbar)      0.00      0.00      0.00
                                0.00      0.00      0.00
                                0.00      0.00      0.00

     XDM     stress (kbar)      0.00      0.00      0.00
                                0.00      0.00      0.00
                                0.00      0.00      0.00

     dft-nl  stress (kbar)      0.00      0.00      0.00
                                0.00      0.00      0.00
                                0.00      0.00      0.00

     TS-vdW  stress (kbar)      0.00      0.00      0.00
                                0.00      0.00      0.00
                                0.00      0.00      0.00


     Writing output data file ./tmp-hetero/A.save/

     init_run     :      2.90s CPU      2.83s WALL (       1 calls)
     electrons    :     41.43s CPU     35.15s WALL (       1 calls)
     forces       :      0.42s CPU      0.38s WALL (       1 calls)
     stress       :      1.65s CPU      1.45s WALL (       1 calls)

     Called by init_run:
     wfcinit      :      1.69s CPU      1.42s WALL (       1 calls)
     wfcinit:atom :      0.04s CPU      0.03s WALL (      74 calls)
     wfcinit:wfcr :      1.46s CPU      1.23s WALL (      74 calls)
     potinit      :      0.71s CPU      0.77s WALL (       1 calls)
     hinit0       :      0.37s CPU      0.42s WALL (       1 calls)

     Called by electrons:
     c_bands      :     30.38s CPU     25.06s WALL (       7 calls)
     sum_band     :      6.40s CPU      5.17s WALL (       7 calls)
     v_of_rho     :      4.59s CPU      4.87s WALL (       8 calls)
     v_h          :      0.05s CPU      0.06s WALL (       8 calls)
     v_xc         :      4.55s CPU      4.81s WALL (       8 calls)
     newd         :      0.36s CPU      0.42s WALL (       8 calls)
     mix_rho      :      0.23s CPU      0.18s WALL (       7 calls)

     Called by c_bands:
     init_us_2    :      0.86s CPU      0.69s WALL (    1258 calls)
     cegterg      :     29.60s CPU     24.43s WALL (     518 calls)

     Called by sum_band:
     sum_band:bec :      0.01s CPU      0.01s WALL (     518 calls)
     addusdens    :      0.52s CPU      0.39s WALL (       7 calls)

     Called by *egterg:
     h_psi        :     27.61s CPU     23.00s WALL (    2123 calls)
     s_psi        :      0.39s CPU      0.28s WALL (    2123 calls)
```

```
     g_psi        :      0.11s CPU      0.08s WALL (    1531 calls)
     cdiaghg      :      1.06s CPU      0.88s WALL (    2049 calls)
     cegterg:over :      0.76s CPU      0.57s WALL (    1531 calls)
     cegterg:upda :      0.57s CPU      0.44s WALL (    1531 calls)
     cegterg:last :      0.15s CPU      0.12s WALL (     520 calls)

     Called by h_psi:
     h_psi:calbec :      0.48s CPU      0.40s WALL (    2123 calls)
     vloc_psi     :     26.63s CPU     22.23s WALL (    2123 calls)
     add_vuspsi   :      0.42s CPU      0.31s WALL (    2123 calls)

     General routines
     calbec       :      0.74s CPU      0.61s WALL (    3011 calls)
     fft          :      1.24s CPU      1.26s WALL (     207 calls)
     ffts         :      0.07s CPU      0.06s WALL (      30 calls)
     fftw         :     29.11s CPU     24.40s WALL (   27340 calls)
     interpolate  :      0.13s CPU      0.14s WALL (      16 calls)

     Parallel routines

     PWSCF        :     46.55s CPU     40.09s WALL


   This run was terminated on:  19:27:32  25Oct2023

=------------------------------------------------------------------------------=
   JOB DONE.
=------------------------------------------------------------------------------=
```