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        Program PWSCF v.6.5 starts on  5Oct2023 at 11:24:31

        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

        Atomic positions and unit cell read from directory:
        ./tmp-hetero/
A.save/


        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        625     253      85               37579     9597     1785



        bravais-lattice index     =            4
        lattice parameter (alat)  =       4.7500  a.u.
        unit-cell volume          =      278.4407 (a.u.)^3
        number of atoms/cell      =            2
        number of atomic types    =            2
        number of electrons       =         8.00
        number of Kohn-Sham states=            8
        kinetic-energy cutoff     =      40.0000  Ry
        charge density cutoff     =     400.0000  Ry
        Exchange-correlation= PBE
                           (   1   4   3   4   0   0   0)

        celldm(1)=   4.750000  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)
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```
                     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 B  read from file:
     ./pseudo/B.pbe-n-rrkjus_psl.0.1.UPF
     MD5 check sum: 82e190d381d3269bb317afd43cf1db29
     Pseudo is Ultrasoft + core correction, Zval =  3.0
     Generated using "atomic" code by A. Dal Corso (Quantum ESPRESSO distribution)
     Using radial grid of 1059 points,  4 beta functions with:
                l(1) =   0
                l(2) =   0
                l(3) =   1
                l(4) =   1
     Q(r) pseudized with 0 coefficients


     PseudoPot. # 2 for N  read from file:
     ./pseudo/N.pbe-n-rrkjus_psl.0.1.UPF
     MD5 check sum: c8986a496cba5b831c7822586319e126
     Pseudo is Ultrasoft + core correction, Zval =  5.0
     Generated using "atomic" code by A. Dal Corso (Quantum ESPRESSO distribution)
     Using radial grid of 1085 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
        B              3.00    10.81000     B ( 1.00)
        N              5.00    14.01000     N ( 1.00)

     Starting magnetic structure
     atomic species   magnetization
        B              0.500
        N             -0.500

     12 Sym. Ops. (no inversion) found


                                   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 [0,1,0]

  cryst.   s( 2) = (     -1           0           0      )
                   (      1           1           0      )
                   (      0           0          -1      )
```

```
cart.    s( 2) = ( -1.0000000  0.0000000  0.0000000 )
                 (  0.0000000  1.0000000  0.0000000 )
                 (  0.0000000  0.0000000 -1.0000000 )


     isym =  3     120 deg rotation - cryst. axis [0,0,1]

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

cart.    s( 3) = ( -0.5000000 -0.8660254  0.0000000 )
                 (  0.8660254 -0.5000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )


     isym =  4     120 deg rotation - cryst. axis [0,0,-1]

cryst.   s( 4) = (    -1         -1          0      )
                 (     1          0          0      )
                 (     0          0          1      )

cart.    s( 4) = ( -0.5000000  0.8660254  0.0000000 )
                 ( -0.8660254 -0.5000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )


     isym =  5     180 deg rotation - cryst. axis [1,-1,0]

cryst.   s( 5) = (     0         -1          0      )
                 (    -1          0          0      )
                 (     0          0         -1      )

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


     isym =  6     180 deg rotation - cryst. axis [2,1,0]

cryst.   s( 6) = (     1          1          0      )
                 (     0         -1          0      )
                 (     0          0         -1      )

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


     isym =  7     inv. 180 deg rotation - cart. axis [0,0,1]

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

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


     isym =  8     inv. 180 deg rotation - cart. axis [1,0,0]
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cryst.    s( 8) = (      -1              0              0       )
                   (       1              1              0       )
                   (       0              0              1       )

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


      isym =  9     inv.  60 deg rotation - cryst. axis [0,0,1]

cryst.    s( 9) = (      -1             -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     inv.  60 deg rotation - cryst. axis [0,0,-1]

cryst.    s(10) = (       0              1              0       )
                   (      -1             -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     inv. 180 deg rotation - cryst. axis [0,1,0]

cryst.    s(11) = (       1              1              0       )
                   (       0             -1              0       )
                   (       0              0              1       )

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


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

cryst.    s(12) = (       0             -1              0       )
                   (      -1              0              0       )
                   (       0              0              1       )

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


      point group D_3h (-62m)
      there are  6 classes
      the character table:

       E     2C3   3C2   s_h   2S3   3s_v
A'_1   1.00  1.00  1.00  1.00  1.00  1.00
A'_2   1.00  1.00 -1.00  1.00  1.00 -1.00
E'     2.00 -1.00  0.00  2.00 -1.00  0.00
A''1   1.00  1.00  1.00 -1.00 -1.00 -1.00
```

```
A''2   1.00  1.00 -1.00 -1.00 -1.00  1.00
E''    2.00 -1.00  0.00 -2.00  1.00  0.00

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

      E        1
         identity
      2C3      3     4
         120 deg rotation - cryst. axis [0,0,1]
      3C2      2     6     5
         180 deg rotation - cart. axis [0,1,0]
      s_h      7
         inv. 180 deg rotation - cart. axis [0,0,1]
      2S3      9    10
         inv.  60 deg rotation - cryst. axis [0,0,1]
      3s_v     8    11    12
         inv. 180 deg rotation - cart. axis [1,0,0]

   Cartesian axes

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

   Crystallographic axes

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

   number of k points=   400  Marzari-Vanderbilt smearing, width (Ry)=  0.0010
                        cart. coord. in units 2pi/alat
        k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0025000
        k(    2) = (   0.0034247   0.0019772   0.0000000), wk =   0.0025000
        k(    3) = (   0.0068493   0.0039545   0.0000000), wk =   0.0025000
        k(    4) = (   0.0102740   0.0059317   0.0000000), wk =   0.0025000
        k(    5) = (   0.0136986   0.0079089   0.0000000), wk =   0.0025000
        k(    6) = (   0.0171233   0.0098861   0.0000000), wk =   0.0025000
        k(    7) = (   0.0205479   0.0118634   0.0000000), wk =   0.0025000
        k(    8) = (   0.0239726   0.0138406   0.0000000), wk =   0.0025000
        k(    9) = (   0.0273973   0.0158178   0.0000000), wk =   0.0025000
        k(   10) = (   0.0308219   0.0177950   0.0000000), wk =   0.0025000
        k(   11) = (   0.0342466   0.0197723   0.0000000), wk =   0.0025000
        k(   12) = (   0.0376712   0.0217495   0.0000000), wk =   0.0025000
        k(   13) = (   0.0410959   0.0237267   0.0000000), wk =   0.0025000
        k(   14) = (   0.0445205   0.0257040   0.0000000), wk =   0.0025000
        k(   15) = (   0.0479452   0.0276812   0.0000000), wk =   0.0025000
        k(   16) = (   0.0513699   0.0296584   0.0000000), wk =   0.0025000
        k(   17) = (   0.0547945   0.0316356   0.0000000), wk =   0.0025000
        k(   18) = (   0.0582192   0.0336129   0.0000000), wk =   0.0025000
        k(   19) = (   0.0616438   0.0355901   0.0000000), wk =   0.0025000
        k(   20) = (   0.0650685   0.0375673   0.0000000), wk =   0.0025000
        k(   21) = (   0.0684932   0.0395445   0.0000000), wk =   0.0025000
        k(   22) = (   0.0719178   0.0415218   0.0000000), wk =   0.0025000
        k(   23) = (   0.0753425   0.0434990   0.0000000), wk =   0.0025000
        k(   24) = (   0.0787671   0.0454762   0.0000000), wk =   0.0025000
        k(   25) = (   0.0821918   0.0474534   0.0000000), wk =   0.0025000
        k(   26) = (   0.0856164   0.0494307   0.0000000), wk =   0.0025000
        k(   27) = (   0.0890411   0.0514079   0.0000000), wk =   0.0025000
        k(   28) = (   0.0924658   0.0533851   0.0000000), wk =   0.0025000
        k(   29) = (   0.0958904   0.0553624   0.0000000), wk =   0.0025000
        k(   30) = (   0.0993151   0.0573396   0.0000000), wk =   0.0025000
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k(    31) = (    0.1027397    0.0593168    0.0000000), wk =    0.0025000
k(    32) = (    0.1061644    0.0612940    0.0000000), wk =    0.0025000
k(    33) = (    0.1095890    0.0632713    0.0000000), wk =    0.0025000
k(    34) = (    0.1130137    0.0652485    0.0000000), wk =    0.0025000
k(    35) = (    0.1164384    0.0672257    0.0000000), wk =    0.0025000
k(    36) = (    0.1198630    0.0692029    0.0000000), wk =    0.0025000
k(    37) = (    0.1232877    0.0711802    0.0000000), wk =    0.0025000
k(    38) = (    0.1267123    0.0731574    0.0000000), wk =    0.0025000
k(    39) = (    0.1301370    0.0751346    0.0000000), wk =    0.0025000
k(    40) = (    0.1335616    0.0771119    0.0000000), wk =    0.0025000
k(    41) = (    0.1369863    0.0790891    0.0000000), wk =    0.0025000
k(    42) = (    0.1404110    0.0810663    0.0000000), wk =    0.0025000
k(    43) = (    0.1438356    0.0830435    0.0000000), wk =    0.0025000
k(    44) = (    0.1472603    0.0850208    0.0000000), wk =    0.0025000
k(    45) = (    0.1506849    0.0869980    0.0000000), wk =    0.0025000
k(    46) = (    0.1541096    0.0889752    0.0000000), wk =    0.0025000
k(    47) = (    0.1575342    0.0909524    0.0000000), wk =    0.0025000
k(    48) = (    0.1609589    0.0929297    0.0000000), wk =    0.0025000
k(    49) = (    0.1643836    0.0949069    0.0000000), wk =    0.0025000
k(    50) = (    0.1678082    0.0968841    0.0000000), wk =    0.0025000
k(    51) = (    0.1712329    0.0988613    0.0000000), wk =    0.0025000
k(    52) = (    0.1746575    0.1008386    0.0000000), wk =    0.0025000
k(    53) = (    0.1780822    0.1028158    0.0000000), wk =    0.0025000
k(    54) = (    0.1815068    0.1047930    0.0000000), wk =    0.0025000
k(    55) = (    0.1849315    0.1067703    0.0000000), wk =    0.0025000
k(    56) = (    0.1883562    0.1087475    0.0000000), wk =    0.0025000
k(    57) = (    0.1917808    0.1107247    0.0000000), wk =    0.0025000
k(    58) = (    0.1952055    0.1127019    0.0000000), wk =    0.0025000
k(    59) = (    0.1986301    0.1146792    0.0000000), wk =    0.0025000
k(    60) = (    0.2020548    0.1166564    0.0000000), wk =    0.0025000
k(    61) = (    0.2054795    0.1186336    0.0000000), wk =    0.0025000
k(    62) = (    0.2089041    0.1206108    0.0000000), wk =    0.0025000
k(    63) = (    0.2123288    0.1225881    0.0000000), wk =    0.0025000
k(    64) = (    0.2157534    0.1245653    0.0000000), wk =    0.0025000
k(    65) = (    0.2191781    0.1265425    0.0000000), wk =    0.0025000
k(    66) = (    0.2226027    0.1285198    0.0000000), wk =    0.0025000
k(    67) = (    0.2260274    0.1304970    0.0000000), wk =    0.0025000
k(    68) = (    0.2294521    0.1324742    0.0000000), wk =    0.0025000
k(    69) = (    0.2328767    0.1344514    0.0000000), wk =    0.0025000
k(    70) = (    0.2363014    0.1364287    0.0000000), wk =    0.0025000
k(    71) = (    0.2397260    0.1384059    0.0000000), wk =    0.0025000
k(    72) = (    0.2431507    0.1403831    0.0000000), wk =    0.0025000
k(    73) = (    0.2465753    0.1423603    0.0000000), wk =    0.0025000
k(    74) = (    0.2500000    0.1443376    0.0000000), wk =    0.0025000
k(    75) = (    0.2534247    0.1463148    0.0000000), wk =    0.0025000
k(    76) = (    0.2568493    0.1482920    0.0000000), wk =    0.0025000
k(    77) = (    0.2602740    0.1502692    0.0000000), wk =    0.0025000
k(    78) = (    0.2636986    0.1522465    0.0000000), wk =    0.0025000
k(    79) = (    0.2671233    0.1542237    0.0000000), wk =    0.0025000
k(    80) = (    0.2705479    0.1562009    0.0000000), wk =    0.0025000
k(    81) = (    0.2739726    0.1581782    0.0000000), wk =    0.0025000
k(    82) = (    0.2773973    0.1601554    0.0000000), wk =    0.0025000
k(    83) = (    0.2808219    0.1621326    0.0000000), wk =    0.0025000
k(    84) = (    0.2842466    0.1641098    0.0000000), wk =    0.0025000
k(    85) = (    0.2876712    0.1660871    0.0000000), wk =    0.0025000
k(    86) = (    0.2910959    0.1680643    0.0000000), wk =    0.0025000
k(    87) = (    0.2945205    0.1700415    0.0000000), wk =    0.0025000
k(    88) = (    0.2979452    0.1720187    0.0000000), wk =    0.0025000
k(    89) = (    0.3013699    0.1739960    0.0000000), wk =    0.0025000
k(    90) = (    0.3047945    0.1759732    0.0000000), wk =    0.0025000
k(    91) = (    0.3082192    0.1779504    0.0000000), wk =    0.0025000
k(    92) = (    0.3116438    0.1799277    0.0000000), wk =    0.0025000
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k(   93) = (     0.3150685   0.1819049   0.0000000), wk =      0.0025000
k(   94) = (     0.3184932   0.1838821   0.0000000), wk =      0.0025000
k(   95) = (     0.3219178   0.1858593   0.0000000), wk =      0.0025000
k(   96) = (     0.3253425   0.1878366   0.0000000), wk =      0.0025000
k(   97) = (     0.3287671   0.1898138   0.0000000), wk =      0.0025000
k(   98) = (     0.3321918   0.1917910   0.0000000), wk =      0.0025000
k(   99) = (     0.3356164   0.1937682   0.0000000), wk =      0.0025000
k(  100) = (     0.3390411   0.1957455   0.0000000), wk =      0.0025000
k(  101) = (     0.3424658   0.1977227   0.0000000), wk =      0.0025000
k(  102) = (     0.3458904   0.1996999   0.0000000), wk =      0.0025000
k(  103) = (     0.3493151   0.2016771   0.0000000), wk =      0.0025000
k(  104) = (     0.3527397   0.2036544   0.0000000), wk =      0.0025000
k(  105) = (     0.3561644   0.2056316   0.0000000), wk =      0.0025000
k(  106) = (     0.3595890   0.2076088   0.0000000), wk =      0.0025000
k(  107) = (     0.3630137   0.2095861   0.0000000), wk =      0.0025000
k(  108) = (     0.3664384   0.2115633   0.0000000), wk =      0.0025000
k(  109) = (     0.3698630   0.2135405   0.0000000), wk =      0.0025000
k(  110) = (     0.3732877   0.2155177   0.0000000), wk =      0.0025000
k(  111) = (     0.3767123   0.2174950   0.0000000), wk =      0.0025000
k(  112) = (     0.3801370   0.2194722   0.0000000), wk =      0.0025000
k(  113) = (     0.3835616   0.2214494   0.0000000), wk =      0.0025000
k(  114) = (     0.3869863   0.2234266   0.0000000), wk =      0.0025000
k(  115) = (     0.3904110   0.2254039   0.0000000), wk =      0.0025000
k(  116) = (     0.3938356   0.2273811   0.0000000), wk =      0.0025000
k(  117) = (     0.3972603   0.2293583   0.0000000), wk =      0.0025000
k(  118) = (     0.4006849   0.2313356   0.0000000), wk =      0.0025000
k(  119) = (     0.4041096   0.2333128   0.0000000), wk =      0.0025000
k(  120) = (     0.4075342   0.2352900   0.0000000), wk =      0.0025000
k(  121) = (     0.4109589   0.2372672   0.0000000), wk =      0.0025000
k(  122) = (     0.4143836   0.2392445   0.0000000), wk =      0.0025000
k(  123) = (     0.4178082   0.2412217   0.0000000), wk =      0.0025000
k(  124) = (     0.4212329   0.2431989   0.0000000), wk =      0.0025000
k(  125) = (     0.4246575   0.2451761   0.0000000), wk =      0.0025000
k(  126) = (     0.4280822   0.2471534   0.0000000), wk =      0.0025000
k(  127) = (     0.4315068   0.2491306   0.0000000), wk =      0.0025000
k(  128) = (     0.4349315   0.2511078   0.0000000), wk =      0.0025000
k(  129) = (     0.4383562   0.2530850   0.0000000), wk =      0.0025000
k(  130) = (     0.4417808   0.2550623   0.0000000), wk =      0.0025000
k(  131) = (     0.4452055   0.2570395   0.0000000), wk =      0.0025000
k(  132) = (     0.4486301   0.2590167   0.0000000), wk =      0.0025000
k(  133) = (     0.4520548   0.2609940   0.0000000), wk =      0.0025000
k(  134) = (     0.4554795   0.2629712   0.0000000), wk =      0.0025000
k(  135) = (     0.4589041   0.2649484   0.0000000), wk =      0.0025000
k(  136) = (     0.4623288   0.2669256   0.0000000), wk =      0.0025000
k(  137) = (     0.4657534   0.2689029   0.0000000), wk =      0.0025000
k(  138) = (     0.4691781   0.2708801   0.0000000), wk =      0.0025000
k(  139) = (     0.4726027   0.2728573   0.0000000), wk =      0.0025000
k(  140) = (     0.4760274   0.2748345   0.0000000), wk =      0.0025000
k(  141) = (     0.4794521   0.2768118   0.0000000), wk =      0.0025000
k(  142) = (     0.4828767   0.2787890   0.0000000), wk =      0.0025000
k(  143) = (     0.4863014   0.2807662   0.0000000), wk =      0.0025000
k(  144) = (     0.4897260   0.2827435   0.0000000), wk =      0.0025000
k(  145) = (     0.4931507   0.2847207   0.0000000), wk =      0.0025000
k(  146) = (     0.4965753   0.2866979   0.0000000), wk =      0.0025000
k(  147) = (     0.5000000   0.2886751   0.0000000), wk =      0.0025000
k(  148) = (     0.4980158   0.2921117   0.0000000), wk =      0.0025000
k(  149) = (     0.4960317   0.2955482   0.0000000), wk =      0.0025000
k(  150) = (     0.4940475   0.2989848   0.0000000), wk =      0.0025000
k(  151) = (     0.4920633   0.3024213   0.0000000), wk =      0.0025000
k(  152) = (     0.4900792   0.3058578   0.0000000), wk =      0.0025000
k(  153) = (     0.4880950   0.3092944   0.0000000), wk =      0.0025000
k(  154) = (     0.4861108   0.3127309   0.0000000), wk =      0.0025000
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k(  155) = (     0.4841267    0.3161675    0.0000000), wk =     0.0025000
k(  156) = (     0.4821425    0.3196040    0.0000000), wk =     0.0025000
k(  157) = (     0.4801583    0.3230405    0.0000000), wk =     0.0025000
k(  158) = (     0.4781742    0.3264771    0.0000000), wk =     0.0025000
k(  159) = (     0.4761900    0.3299136    0.0000000), wk =     0.0025000
k(  160) = (     0.4742058    0.3333502    0.0000000), wk =     0.0025000
k(  161) = (     0.4722217    0.3367867    0.0000000), wk =     0.0025000
k(  162) = (     0.4702375    0.3402232    0.0000000), wk =     0.0025000
k(  163) = (     0.4682533    0.3436598    0.0000000), wk =     0.0025000
k(  164) = (     0.4662692    0.3470963    0.0000000), wk =     0.0025000
k(  165) = (     0.4642850    0.3505329    0.0000000), wk =     0.0025000
k(  166) = (     0.4623008    0.3539694    0.0000000), wk =     0.0025000
k(  167) = (     0.4603167    0.3574059    0.0000000), wk =     0.0025000
k(  168) = (     0.4583325    0.3608425    0.0000000), wk =     0.0025000
k(  169) = (     0.4563483    0.3642790    0.0000000), wk =     0.0025000
k(  170) = (     0.4543642    0.3677156    0.0000000), wk =     0.0025000
k(  171) = (     0.4523800    0.3711521    0.0000000), wk =     0.0025000
k(  172) = (     0.4503958    0.3745886    0.0000000), wk =     0.0025000
k(  173) = (     0.4484117    0.3780252    0.0000000), wk =     0.0025000
k(  174) = (     0.4464275    0.3814617    0.0000000), wk =     0.0025000
k(  175) = (     0.4444433    0.3848983    0.0000000), wk =     0.0025000
k(  176) = (     0.4424592    0.3883348    0.0000000), wk =     0.0025000
k(  177) = (     0.4404750    0.3917713    0.0000000), wk =     0.0025000
k(  178) = (     0.4384908    0.3952079    0.0000000), wk =     0.0025000
k(  179) = (     0.4365067    0.3986444    0.0000000), wk =     0.0025000
k(  180) = (     0.4345225    0.4020810    0.0000000), wk =     0.0025000
k(  181) = (     0.4325383    0.4055175    0.0000000), wk =     0.0025000
k(  182) = (     0.4305542    0.4089540    0.0000000), wk =     0.0025000
k(  183) = (     0.4285700    0.4123906    0.0000000), wk =     0.0025000
k(  184) = (     0.4265858    0.4158271    0.0000000), wk =     0.0025000
k(  185) = (     0.4246017    0.4192637    0.0000000), wk =     0.0025000
k(  186) = (     0.4226175    0.4227002    0.0000000), wk =     0.0025000
k(  187) = (     0.4206333    0.4261367    0.0000000), wk =     0.0025000
k(  188) = (     0.4186492    0.4295733    0.0000000), wk =     0.0025000
k(  189) = (     0.4166650    0.4330098    0.0000000), wk =     0.0025000
k(  190) = (     0.4146808    0.4364464    0.0000000), wk =     0.0025000
k(  191) = (     0.4126967    0.4398829    0.0000000), wk =     0.0025000
k(  192) = (     0.4107125    0.4433194    0.0000000), wk =     0.0025000
k(  193) = (     0.4087283    0.4467560    0.0000000), wk =     0.0025000
k(  194) = (     0.4067442    0.4501925    0.0000000), wk =     0.0025000
k(  195) = (     0.4047600    0.4536291    0.0000000), wk =     0.0025000
k(  196) = (     0.4027758    0.4570656    0.0000000), wk =     0.0025000
k(  197) = (     0.4007917    0.4605021    0.0000000), wk =     0.0025000
k(  198) = (     0.3988075    0.4639387    0.0000000), wk =     0.0025000
k(  199) = (     0.3968233    0.4673752    0.0000000), wk =     0.0025000
k(  200) = (     0.3948392    0.4708118    0.0000000), wk =     0.0025000
k(  201) = (     0.3928550    0.4742483    0.0000000), wk =     0.0025000
k(  202) = (     0.3908708    0.4776848    0.0000000), wk =     0.0025000
k(  203) = (     0.3888867    0.4811214    0.0000000), wk =     0.0025000
k(  204) = (     0.3869025    0.4845579    0.0000000), wk =     0.0025000
k(  205) = (     0.3849183    0.4879945    0.0000000), wk =     0.0025000
k(  206) = (     0.3829342    0.4914310    0.0000000), wk =     0.0025000
k(  207) = (     0.3809500    0.4948675    0.0000000), wk =     0.0025000
k(  208) = (     0.3789658    0.4983041    0.0000000), wk =     0.0025000
k(  209) = (     0.3769817    0.5017406    0.0000000), wk =     0.0025000
k(  210) = (     0.3749975    0.5051772    0.0000000), wk =     0.0025000
k(  211) = (     0.3730133    0.5086137    0.0000000), wk =     0.0025000
k(  212) = (     0.3710292    0.5120502    0.0000000), wk =     0.0025000
k(  213) = (     0.3690450    0.5154868    0.0000000), wk =     0.0025000
k(  214) = (     0.3670608    0.5189233    0.0000000), wk =     0.0025000
k(  215) = (     0.3650767    0.5223599    0.0000000), wk =     0.0025000
k(  216) = (     0.3630925    0.5257964    0.0000000), wk =     0.0025000
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k(  217) = (      0.3611083    0.5292329    0.0000000), wk =      0.0025000
k(  218) = (      0.3591242    0.5326695    0.0000000), wk =      0.0025000
k(  219) = (      0.3571400    0.5361060    0.0000000), wk =      0.0025000
k(  220) = (      0.3551558    0.5395426    0.0000000), wk =      0.0025000
k(  221) = (      0.3531717    0.5429791    0.0000000), wk =      0.0025000
k(  222) = (      0.3511875    0.5464156    0.0000000), wk =      0.0025000
k(  223) = (      0.3492033    0.5498522    0.0000000), wk =      0.0025000
k(  224) = (      0.3472192    0.5532887    0.0000000), wk =      0.0025000
k(  225) = (      0.3452350    0.5567253    0.0000000), wk =      0.0025000
k(  226) = (      0.3432508    0.5601618    0.0000000), wk =      0.0025000
k(  227) = (      0.3412667    0.5635983    0.0000000), wk =      0.0025000
k(  228) = (      0.3392825    0.5670349    0.0000000), wk =      0.0025000
k(  229) = (      0.3372983    0.5704714    0.0000000), wk =      0.0025000
k(  230) = (      0.3353142    0.5739080    0.0000000), wk =      0.0025000
k(  231) = (      0.3333300    0.5773445    0.0000000), wk =      0.0025000
k(  232) = (      0.3313576    0.5739283    0.0000000), wk =      0.0025000
k(  233) = (      0.3293853    0.5705120    0.0000000), wk =      0.0025000
k(  234) = (      0.3274129    0.5670958    0.0000000), wk =      0.0025000
k(  235) = (      0.3254405    0.5636795    0.0000000), wk =      0.0025000
k(  236) = (      0.3234682    0.5602633    0.0000000), wk =      0.0025000
k(  237) = (      0.3214958    0.5568471    0.0000000), wk =      0.0025000
k(  238) = (      0.3195234    0.5534308    0.0000000), wk =      0.0025000
k(  239) = (      0.3175511    0.5500146    0.0000000), wk =      0.0025000
k(  240) = (      0.3155787    0.5465983    0.0000000), wk =      0.0025000
k(  241) = (      0.3136063    0.5431821    0.0000000), wk =      0.0025000
k(  242) = (      0.3116340    0.5397659    0.0000000), wk =      0.0025000
k(  243) = (      0.3096616    0.5363496    0.0000000), wk =      0.0025000
k(  244) = (      0.3076892    0.5329334    0.0000000), wk =      0.0025000
k(  245) = (      0.3057169    0.5295171    0.0000000), wk =      0.0025000
k(  246) = (      0.3037445    0.5261009    0.0000000), wk =      0.0025000
k(  247) = (      0.3017721    0.5226847    0.0000000), wk =      0.0025000
k(  248) = (      0.2997998    0.5192684    0.0000000), wk =      0.0025000
k(  249) = (      0.2978274    0.5158522    0.0000000), wk =      0.0025000
k(  250) = (      0.2958550    0.5124359    0.0000000), wk =      0.0025000
k(  251) = (      0.2938827    0.5090197    0.0000000), wk =      0.0025000
k(  252) = (      0.2919103    0.5056035    0.0000000), wk =      0.0025000
k(  253) = (      0.2899379    0.5021872    0.0000000), wk =      0.0025000
k(  254) = (      0.2879656    0.4987710    0.0000000), wk =      0.0025000
k(  255) = (      0.2859932    0.4953547    0.0000000), wk =      0.0025000
k(  256) = (      0.2840208    0.4919385    0.0000000), wk =      0.0025000
k(  257) = (      0.2820485    0.4885223    0.0000000), wk =      0.0025000
k(  258) = (      0.2800761    0.4851060    0.0000000), wk =      0.0025000
k(  259) = (      0.2781037    0.4816898    0.0000000), wk =      0.0025000
k(  260) = (      0.2761314    0.4782735    0.0000000), wk =      0.0025000
k(  261) = (      0.2741590    0.4748573    0.0000000), wk =      0.0025000
k(  262) = (      0.2721866    0.4714411    0.0000000), wk =      0.0025000
k(  263) = (      0.2702143    0.4680248    0.0000000), wk =      0.0025000
k(  264) = (      0.2682419    0.4646086    0.0000000), wk =      0.0025000
k(  265) = (      0.2662695    0.4611923    0.0000000), wk =      0.0025000
k(  266) = (      0.2642972    0.4577761    0.0000000), wk =      0.0025000
k(  267) = (      0.2623248    0.4543599    0.0000000), wk =      0.0025000
k(  268) = (      0.2603524    0.4509436    0.0000000), wk =      0.0025000
k(  269) = (      0.2583801    0.4475274    0.0000000), wk =      0.0025000
k(  270) = (      0.2564077    0.4441112    0.0000000), wk =      0.0025000
k(  271) = (      0.2544353    0.4406949    0.0000000), wk =      0.0025000
k(  272) = (      0.2524630    0.4372787    0.0000000), wk =      0.0025000
k(  273) = (      0.2504906    0.4338624    0.0000000), wk =      0.0025000
k(  274) = (      0.2485182    0.4304462    0.0000000), wk =      0.0025000
k(  275) = (      0.2465459    0.4270300    0.0000000), wk =      0.0025000
k(  276) = (      0.2445735    0.4236137    0.0000000), wk =      0.0025000
k(  277) = (      0.2426011    0.4201975    0.0000000), wk =      0.0025000
k(  278) = (      0.2406288    0.4167812    0.0000000), wk =      0.0025000
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k(  279) = (     0.2386564    0.4133650    0.0000000), wk =     0.0025000
k(  280) = (     0.2366840    0.4099488    0.0000000), wk =     0.0025000
k(  281) = (     0.2347117    0.4065325    0.0000000), wk =     0.0025000
k(  282) = (     0.2327393    0.4031163    0.0000000), wk =     0.0025000
k(  283) = (     0.2307669    0.3997000    0.0000000), wk =     0.0025000
k(  284) = (     0.2287946    0.3962838    0.0000000), wk =     0.0025000
k(  285) = (     0.2268222    0.3928676    0.0000000), wk =     0.0025000
k(  286) = (     0.2248498    0.3894513    0.0000000), wk =     0.0025000
k(  287) = (     0.2228775    0.3860351    0.0000000), wk =     0.0025000
k(  288) = (     0.2209051    0.3826188    0.0000000), wk =     0.0025000
k(  289) = (     0.2189327    0.3792026    0.0000000), wk =     0.0025000
k(  290) = (     0.2169604    0.3757864    0.0000000), wk =     0.0025000
k(  291) = (     0.2149880    0.3723701    0.0000000), wk =     0.0025000
k(  292) = (     0.2130156    0.3689539    0.0000000), wk =     0.0025000
k(  293) = (     0.2110433    0.3655376    0.0000000), wk =     0.0025000
k(  294) = (     0.2090709    0.3621214    0.0000000), wk =     0.0025000
k(  295) = (     0.2070985    0.3587052    0.0000000), wk =     0.0025000
k(  296) = (     0.2051262    0.3552889    0.0000000), wk =     0.0025000
k(  297) = (     0.2031538    0.3518727    0.0000000), wk =     0.0025000
k(  298) = (     0.2011814    0.3484564    0.0000000), wk =     0.0025000
k(  299) = (     0.1992091    0.3450402    0.0000000), wk =     0.0025000
k(  300) = (     0.1972367    0.3416240    0.0000000), wk =     0.0025000
k(  301) = (     0.1952643    0.3382077    0.0000000), wk =     0.0025000
k(  302) = (     0.1932920    0.3347915    0.0000000), wk =     0.0025000
k(  303) = (     0.1913196    0.3313752    0.0000000), wk =     0.0025000
k(  304) = (     0.1893472    0.3279590    0.0000000), wk =     0.0025000
k(  305) = (     0.1873749    0.3245428    0.0000000), wk =     0.0025000
k(  306) = (     0.1854025    0.3211265    0.0000000), wk =     0.0025000
k(  307) = (     0.1834301    0.3177103    0.0000000), wk =     0.0025000
k(  308) = (     0.1814578    0.3142940    0.0000000), wk =     0.0025000
k(  309) = (     0.1794854    0.3108778    0.0000000), wk =     0.0025000
k(  310) = (     0.1775130    0.3074616    0.0000000), wk =     0.0025000
k(  311) = (     0.1755407    0.3040453    0.0000000), wk =     0.0025000
k(  312) = (     0.1735683    0.3006291    0.0000000), wk =     0.0025000
k(  313) = (     0.1715959    0.2972128    0.0000000), wk =     0.0025000
k(  314) = (     0.1696236    0.2937966    0.0000000), wk =     0.0025000
k(  315) = (     0.1676512    0.2903804    0.0000000), wk =     0.0025000
k(  316) = (     0.1656788    0.2869641    0.0000000), wk =     0.0025000
k(  317) = (     0.1637064    0.2835479    0.0000000), wk =     0.0025000
k(  318) = (     0.1617341    0.2801316    0.0000000), wk =     0.0025000
k(  319) = (     0.1597617    0.2767154    0.0000000), wk =     0.0025000
k(  320) = (     0.1577893    0.2732992    0.0000000), wk =     0.0025000
k(  321) = (     0.1558170    0.2698829    0.0000000), wk =     0.0025000
k(  322) = (     0.1538446    0.2664667    0.0000000), wk =     0.0025000
k(  323) = (     0.1518722    0.2630505    0.0000000), wk =     0.0025000
k(  324) = (     0.1498999    0.2596342    0.0000000), wk =     0.0025000
k(  325) = (     0.1479275    0.2562180    0.0000000), wk =     0.0025000
k(  326) = (     0.1459551    0.2528017    0.0000000), wk =     0.0025000
k(  327) = (     0.1439828    0.2493855    0.0000000), wk =     0.0025000
k(  328) = (     0.1420104    0.2459693    0.0000000), wk =     0.0025000
k(  329) = (     0.1400380    0.2425530    0.0000000), wk =     0.0025000
k(  330) = (     0.1380657    0.2391368    0.0000000), wk =     0.0025000
k(  331) = (     0.1360933    0.2357205    0.0000000), wk =     0.0025000
k(  332) = (     0.1341209    0.2323043    0.0000000), wk =     0.0025000
k(  333) = (     0.1321486    0.2288881    0.0000000), wk =     0.0025000
k(  334) = (     0.1301762    0.2254718    0.0000000), wk =     0.0025000
k(  335) = (     0.1282038    0.2220556    0.0000000), wk =     0.0025000
k(  336) = (     0.1262315    0.2186393    0.0000000), wk =     0.0025000
k(  337) = (     0.1242591    0.2152231    0.0000000), wk =     0.0025000
k(  338) = (     0.1222867    0.2118069    0.0000000), wk =     0.0025000
k(  339) = (     0.1203144    0.2083906    0.0000000), wk =     0.0025000
k(  340) = (     0.1183420    0.2049744    0.0000000), wk =     0.0025000
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k(  341) = (    0.1163696    0.2015581    0.0000000), wk =    0.0025000
k(  342) = (    0.1143973    0.1981419    0.0000000), wk =    0.0025000
k(  343) = (    0.1124249    0.1947257    0.0000000), wk =    0.0025000
k(  344) = (    0.1104525    0.1913094    0.0000000), wk =    0.0025000
k(  345) = (    0.1084802    0.1878932    0.0000000), wk =    0.0025000
k(  346) = (    0.1065078    0.1844769    0.0000000), wk =    0.0025000
k(  347) = (    0.1045354    0.1810607    0.0000000), wk =    0.0025000
k(  348) = (    0.1025631    0.1776445    0.0000000), wk =    0.0025000
k(  349) = (    0.1005907    0.1742282    0.0000000), wk =    0.0025000
k(  350) = (    0.0986183    0.1708120    0.0000000), wk =    0.0025000
k(  351) = (    0.0966460    0.1673957    0.0000000), wk =    0.0025000
k(  352) = (    0.0946736    0.1639795    0.0000000), wk =    0.0025000
k(  353) = (    0.0927012    0.1605633    0.0000000), wk =    0.0025000
k(  354) = (    0.0907289    0.1571470    0.0000000), wk =    0.0025000
k(  355) = (    0.0887565    0.1537308    0.0000000), wk =    0.0025000
k(  356) = (    0.0867841    0.1503145    0.0000000), wk =    0.0025000
k(  357) = (    0.0848118    0.1468983    0.0000000), wk =    0.0025000
k(  358) = (    0.0828394    0.1434821    0.0000000), wk =    0.0025000
k(  359) = (    0.0808670    0.1400658    0.0000000), wk =    0.0025000
k(  360) = (    0.0788947    0.1366496    0.0000000), wk =    0.0025000
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k(  362) = (    0.0749499    0.1298171    0.0000000), wk =    0.0025000
k(  363) = (    0.0729776    0.1264009    0.0000000), wk =    0.0025000
k(  364) = (    0.0710052    0.1229846    0.0000000), wk =    0.0025000
k(  365) = (    0.0690328    0.1195684    0.0000000), wk =    0.0025000
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k(  367) = (    0.0650881    0.1127359    0.0000000), wk =    0.0025000
k(  368) = (    0.0631157    0.1093197    0.0000000), wk =    0.0025000
k(  369) = (    0.0611434    0.1059034    0.0000000), wk =    0.0025000
k(  370) = (    0.0591710    0.1024872    0.0000000), wk =    0.0025000
k(  371) = (    0.0571986    0.0990709    0.0000000), wk =    0.0025000
k(  372) = (    0.0552263    0.0956547    0.0000000), wk =    0.0025000
k(  373) = (    0.0532539    0.0922385    0.0000000), wk =    0.0025000
k(  374) = (    0.0512815    0.0888222    0.0000000), wk =    0.0025000
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k(  377) = (    0.0453644    0.0785735    0.0000000), wk =    0.0025000
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k(  379) = (    0.0414197    0.0717410    0.0000000), wk =    0.0025000
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k(  382) = (    0.0355026    0.0614923    0.0000000), wk =    0.0025000
k(  383) = (    0.0335302    0.0580761    0.0000000), wk =    0.0025000
k(  384) = (    0.0315579    0.0546598    0.0000000), wk =    0.0025000
k(  385) = (    0.0295855    0.0512436    0.0000000), wk =    0.0025000
k(  386) = (    0.0276131    0.0478274    0.0000000), wk =    0.0025000
k(  387) = (    0.0256408    0.0444111    0.0000000), wk =    0.0025000
k(  388) = (    0.0236684    0.0409949    0.0000000), wk =    0.0025000
k(  389) = (    0.0216960    0.0375786    0.0000000), wk =    0.0025000
k(  390) = (    0.0197237    0.0341624    0.0000000), wk =    0.0025000
k(  391) = (    0.0177513    0.0307462    0.0000000), wk =    0.0025000
k(  392) = (    0.0157789    0.0273299    0.0000000), wk =    0.0025000
k(  393) = (    0.0138066    0.0239137    0.0000000), wk =    0.0025000
k(  394) = (    0.0118342    0.0204974    0.0000000), wk =    0.0025000
k(  395) = (    0.0098618    0.0170812    0.0000000), wk =    0.0025000
k(  396) = (    0.0078895    0.0136650    0.0000000), wk =    0.0025000
k(  397) = (    0.0059171    0.0102487    0.0000000), wk =    0.0025000
k(  398) = (    0.0039447    0.0068325    0.0000000), wk =    0.0025000
k(  399) = (    0.0019724    0.0034162    0.0000000), wk =    0.0025000
k(  400) = (    0.0000000    0.0000000    0.0000000), wk =    0.0025000

                  cryst. coord.
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k(    1) = (    0.0000000    0.0000000    0.0000000), wk =    0.0025000
k(    2) = (    0.0034247    0.0000000    0.0000000), wk =    0.0025000
k(    3) = (    0.0068493    0.0000000    0.0000000), wk =    0.0025000
k(    4) = (    0.0102740    0.0000000    0.0000000), wk =    0.0025000
k(    5) = (    0.0136986    0.0000000    0.0000000), wk =    0.0025000
k(    6) = (    0.0171233    0.0000000    0.0000000), wk =    0.0025000
k(    7) = (    0.0205479    0.0000000    0.0000000), wk =    0.0025000
k(    8) = (    0.0239726    0.0000000    0.0000000), wk =    0.0025000
k(    9) = (    0.0273973    0.0000000    0.0000000), wk =    0.0025000
k(   10) = (    0.0308219    0.0000000    0.0000000), wk =    0.0025000
k(   11) = (    0.0342466    0.0000000    0.0000000), wk =    0.0025000
k(   12) = (    0.0376712    0.0000000    0.0000000), wk =    0.0025000
k(   13) = (    0.0410959    0.0000000    0.0000000), wk =    0.0025000
k(   14) = (    0.0445205    0.0000000    0.0000000), wk =    0.0025000
k(   15) = (    0.0479452    0.0000000    0.0000000), wk =    0.0025000
k(   16) = (    0.0513699    0.0000000    0.0000000), wk =    0.0025000
k(   17) = (    0.0547945    0.0000000    0.0000000), wk =    0.0025000
k(   18) = (    0.0582192    0.0000000    0.0000000), wk =    0.0025000
k(   19) = (    0.0616438    0.0000000    0.0000000), wk =    0.0025000
k(   20) = (    0.0650685    0.0000000    0.0000000), wk =    0.0025000
k(   21) = (    0.0684932    0.0000000    0.0000000), wk =    0.0025000
k(   22) = (    0.0719178    0.0000000    0.0000000), wk =    0.0025000
k(   23) = (    0.0753425    0.0000000    0.0000000), wk =    0.0025000
k(   24) = (    0.0787671    0.0000000    0.0000000), wk =    0.0025000
k(   25) = (    0.0821918    0.0000000    0.0000000), wk =    0.0025000
k(   26) = (    0.0856164    0.0000000    0.0000000), wk =    0.0025000
k(   27) = (    0.0890411    0.0000000    0.0000000), wk =    0.0025000
k(   28) = (    0.0924658    0.0000000    0.0000000), wk =    0.0025000
k(   29) = (    0.0958904    0.0000000    0.0000000), wk =    0.0025000
k(   30) = (    0.0993151    0.0000000    0.0000000), wk =    0.0025000
k(   31) = (    0.1027397    0.0000000    0.0000000), wk =    0.0025000
k(   32) = (    0.1061644    0.0000000    0.0000000), wk =    0.0025000
k(   33) = (    0.1095890   -0.0000000    0.0000000), wk =    0.0025000
k(   34) = (    0.1130137    0.0000000    0.0000000), wk =    0.0025000
k(   35) = (    0.1164384    0.0000000    0.0000000), wk =    0.0025000
k(   36) = (    0.1198630    0.0000000    0.0000000), wk =    0.0025000
k(   37) = (    0.1232877    0.0000000    0.0000000), wk =    0.0025000
k(   38) = (    0.1267123    0.0000000    0.0000000), wk =    0.0025000
k(   39) = (    0.1301370    0.0000000    0.0000000), wk =    0.0025000
k(   40) = (    0.1335616    0.0000000    0.0000000), wk =    0.0025000
k(   41) = (    0.1369863    0.0000000    0.0000000), wk =    0.0025000
k(   42) = (    0.1404110    0.0000000    0.0000000), wk =    0.0025000
k(   43) = (    0.1438356    0.0000000    0.0000000), wk =    0.0025000
k(   44) = (    0.1472603    0.0000000    0.0000000), wk =    0.0025000
k(   45) = (    0.1506849    0.0000000    0.0000000), wk =    0.0025000
k(   46) = (    0.1541096    0.0000000    0.0000000), wk =    0.0025000
k(   47) = (    0.1575342    0.0000000    0.0000000), wk =    0.0025000
k(   48) = (    0.1609589    0.0000000    0.0000000), wk =    0.0025000
k(   49) = (    0.1643836    0.0000000    0.0000000), wk =    0.0025000
k(   50) = (    0.1678082    0.0000000    0.0000000), wk =    0.0025000
k(   51) = (    0.1712329    0.0000000    0.0000000), wk =    0.0025000
k(   52) = (    0.1746575    0.0000000    0.0000000), wk =    0.0025000
k(   53) = (    0.1780822    0.0000000    0.0000000), wk =    0.0025000
k(   54) = (    0.1815068    0.0000000    0.0000000), wk =    0.0025000
k(   55) = (    0.1849315    0.0000000    0.0000000), wk =    0.0025000
k(   56) = (    0.1883562    0.0000000    0.0000000), wk =    0.0025000
k(   57) = (    0.1917808    0.0000000    0.0000000), wk =    0.0025000
k(   58) = (    0.1952055    0.0000000    0.0000000), wk =    0.0025000
k(   59) = (    0.1986301    0.0000000    0.0000000), wk =    0.0025000
k(   60) = (    0.2020548    0.0000000    0.0000000), wk =    0.0025000
k(   61) = (    0.2054795    0.0000000    0.0000000), wk =    0.0025000
k(   62) = (    0.2089041    0.0000000    0.0000000), wk =    0.0025000
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k(   63) = (    0.2123288    0.0000000    0.0000000), wk =    0.0025000
k(   64) = (    0.2157534    0.0000000    0.0000000), wk =    0.0025000
k(   65) = (    0.2191781   -0.0000000    0.0000000), wk =    0.0025000
k(   66) = (    0.2226027    0.0000000    0.0000000), wk =    0.0025000
k(   67) = (    0.2260274    0.0000000    0.0000000), wk =    0.0025000
k(   68) = (    0.2294521    0.0000000    0.0000000), wk =    0.0025000
k(   69) = (    0.2328767    0.0000000    0.0000000), wk =    0.0025000
k(   70) = (    0.2363014    0.0000000    0.0000000), wk =    0.0025000
k(   71) = (    0.2397260    0.0000000    0.0000000), wk =    0.0025000
k(   72) = (    0.2431507    0.0000000    0.0000000), wk =    0.0025000
k(   73) = (    0.2465753    0.0000000    0.0000000), wk =    0.0025000
k(   74) = (    0.2500000    0.0000000    0.0000000), wk =    0.0025000
k(   75) = (    0.2534247    0.0000000    0.0000000), wk =    0.0025000
k(   76) = (    0.2568493    0.0000000    0.0000000), wk =    0.0025000
k(   77) = (    0.2602740    0.0000000    0.0000000), wk =    0.0025000
k(   78) = (    0.2636986    0.0000000    0.0000000), wk =    0.0025000
k(   79) = (    0.2671233    0.0000000    0.0000000), wk =    0.0025000
k(   80) = (    0.2705479    0.0000000    0.0000000), wk =    0.0025000
k(   81) = (    0.2739726    0.0000000    0.0000000), wk =    0.0025000
k(   82) = (    0.2773973    0.0000000    0.0000000), wk =    0.0025000
k(   83) = (    0.2808219    0.0000000    0.0000000), wk =    0.0025000
k(   84) = (    0.2842466    0.0000000    0.0000000), wk =    0.0025000
k(   85) = (    0.2876712    0.0000000    0.0000000), wk =    0.0025000
k(   86) = (    0.2910959    0.0000000    0.0000000), wk =    0.0025000
k(   87) = (    0.2945205    0.0000000    0.0000000), wk =    0.0025000
k(   88) = (    0.2979452    0.0000000    0.0000000), wk =    0.0025000
k(   89) = (    0.3013699    0.0000000    0.0000000), wk =    0.0025000
k(   90) = (    0.3047945    0.0000000    0.0000000), wk =    0.0025000
k(   91) = (    0.3082192    0.0000000    0.0000000), wk =    0.0025000
k(   92) = (    0.3116438    0.0000000    0.0000000), wk =    0.0025000
k(   93) = (    0.3150685    0.0000000    0.0000000), wk =    0.0025000
k(   94) = (    0.3184932    0.0000000    0.0000000), wk =    0.0025000
k(   95) = (    0.3219178    0.0000000    0.0000000), wk =    0.0025000
k(   96) = (    0.3253425    0.0000000    0.0000000), wk =    0.0025000
k(   97) = (    0.3287671    0.0000000    0.0000000), wk =    0.0025000
k(   98) = (    0.3321918    0.0000000    0.0000000), wk =    0.0025000
k(   99) = (    0.3356164    0.0000000    0.0000000), wk =    0.0025000
k(  100) = (    0.3390411    0.0000000    0.0000000), wk =    0.0025000
k(  101) = (    0.3424658    0.0000000    0.0000000), wk =    0.0025000
k(  102) = (    0.3458904    0.0000000    0.0000000), wk =    0.0025000
k(  103) = (    0.3493151    0.0000000    0.0000000), wk =    0.0025000
k(  104) = (    0.3527397    0.0000000    0.0000000), wk =    0.0025000
k(  105) = (    0.3561644    0.0000000    0.0000000), wk =    0.0025000
k(  106) = (    0.3595890    0.0000000    0.0000000), wk =    0.0025000
k(  107) = (    0.3630137    0.0000000    0.0000000), wk =    0.0025000
k(  108) = (    0.3664384    0.0000000    0.0000000), wk =    0.0025000
k(  109) = (    0.3698630    0.0000000    0.0000000), wk =    0.0025000
k(  110) = (    0.3732877    0.0000000    0.0000000), wk =    0.0025000
k(  111) = (    0.3767123    0.0000000    0.0000000), wk =    0.0025000
k(  112) = (    0.3801370    0.0000000    0.0000000), wk =    0.0025000
k(  113) = (    0.3835616    0.0000000    0.0000000), wk =    0.0025000
k(  114) = (    0.3869863    0.0000000    0.0000000), wk =    0.0025000
k(  115) = (    0.3904110    0.0000000    0.0000000), wk =    0.0025000
k(  116) = (    0.3938356    0.0000000    0.0000000), wk =    0.0025000
k(  117) = (    0.3972603    0.0000000    0.0000000), wk =    0.0025000
k(  118) = (    0.4006849    0.0000000    0.0000000), wk =    0.0025000
k(  119) = (    0.4041096    0.0000000    0.0000000), wk =    0.0025000
k(  120) = (    0.4075342    0.0000000    0.0000000), wk =    0.0025000
k(  121) = (    0.4109589    0.0000000    0.0000000), wk =    0.0025000
k(  122) = (    0.4143836    0.0000000    0.0000000), wk =    0.0025000
k(  123) = (    0.4178082    0.0000000    0.0000000), wk =    0.0025000
k(  124) = (    0.4212329    0.0000000    0.0000000), wk =    0.0025000
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k(  126) = (      0.4280822    0.0000000    0.0000000), wk =      0.0025000
k(  127) = (      0.4315068    0.0000000    0.0000000), wk =      0.0025000
k(  128) = (      0.4349315    0.0000000    0.0000000), wk =      0.0025000
k(  129) = (      0.4383562   -0.0000000    0.0000000), wk =      0.0025000
k(  130) = (      0.4417808    0.0000000    0.0000000), wk =      0.0025000
k(  131) = (      0.4452055    0.0000000    0.0000000), wk =      0.0025000
k(  132) = (      0.4486301   -0.0000000    0.0000000), wk =      0.0025000
k(  133) = (      0.4520548    0.0000000    0.0000000), wk =      0.0025000
k(  134) = (      0.4554795   -0.0000000    0.0000000), wk =      0.0025000
k(  135) = (      0.4589041    0.0000000    0.0000000), wk =      0.0025000
k(  136) = (      0.4623288    0.0000000    0.0000000), wk =      0.0025000
k(  137) = (      0.4657534   -0.0000000    0.0000000), wk =      0.0025000
k(  138) = (      0.4691781    0.0000000    0.0000000), wk =      0.0025000
k(  139) = (      0.4726027   -0.0000000    0.0000000), wk =      0.0025000
k(  140) = (      0.4760274    0.0000000    0.0000000), wk =      0.0025000
k(  141) = (      0.4794521    0.0000000    0.0000000), wk =      0.0025000
k(  142) = (      0.4828767    0.0000000    0.0000000), wk =      0.0025000
k(  143) = (      0.4863014    0.0000000    0.0000000), wk =      0.0025000
k(  144) = (      0.4897260   -0.0000000    0.0000000), wk =      0.0025000
k(  145) = (      0.4931507    0.0000000    0.0000000), wk =      0.0025000
k(  146) = (      0.4965753    0.0000000    0.0000000), wk =      0.0025000
k(  147) = (      0.5000000    0.0000000    0.0000000), wk =      0.0025000
k(  148) = (      0.4980158    0.0039682    0.0000000), wk =      0.0025000
k(  149) = (      0.4960317    0.0079364    0.0000000), wk =      0.0025000
k(  150) = (      0.4940475    0.0119046    0.0000000), wk =      0.0025000
k(  151) = (      0.4920633    0.0158729    0.0000000), wk =      0.0025000
k(  152) = (      0.4900792    0.0198411    0.0000000), wk =      0.0025000
k(  153) = (      0.4880950    0.0238093    0.0000000), wk =      0.0025000
k(  154) = (      0.4861108    0.0277775    0.0000000), wk =      0.0025000
k(  155) = (      0.4841267    0.0317457    0.0000000), wk =      0.0025000
k(  156) = (      0.4821425    0.0357139    0.0000000), wk =      0.0025000
k(  157) = (      0.4801583    0.0396821    0.0000000), wk =      0.0025000
k(  158) = (      0.4781742    0.0436504    0.0000000), wk =      0.0025000
k(  159) = (      0.4761900    0.0476186    0.0000000), wk =      0.0025000
k(  160) = (      0.4742058    0.0515868    0.0000000), wk =      0.0025000
k(  161) = (      0.4722217    0.0555550    0.0000000), wk =      0.0025000
k(  162) = (      0.4702375    0.0595232    0.0000000), wk =      0.0025000
k(  163) = (      0.4682533    0.0634914    0.0000000), wk =      0.0025000
k(  164) = (      0.4662692    0.0674596    0.0000000), wk =      0.0025000
k(  165) = (      0.4642850    0.0714279    0.0000000), wk =      0.0025000
k(  166) = (      0.4623008    0.0753961    0.0000000), wk =      0.0025000
k(  167) = (      0.4603167    0.0793643    0.0000000), wk =      0.0025000
k(  168) = (      0.4583325    0.0833325    0.0000000), wk =      0.0025000
k(  169) = (      0.4563483    0.0873007    0.0000000), wk =      0.0025000
k(  170) = (      0.4543642    0.0912689    0.0000000), wk =      0.0025000
k(  171) = (      0.4523800    0.0952371    0.0000000), wk =      0.0025000
k(  172) = (      0.4503958    0.0992054    0.0000000), wk =      0.0025000
k(  173) = (      0.4484117    0.1031736    0.0000000), wk =      0.0025000
k(  174) = (      0.4464275    0.1071418    0.0000000), wk =      0.0025000
k(  175) = (      0.4444433    0.1111100    0.0000000), wk =      0.0025000
k(  176) = (      0.4424592    0.1150782    0.0000000), wk =      0.0025000
k(  177) = (      0.4404750    0.1190464    0.0000000), wk =      0.0025000
k(  178) = (      0.4384908    0.1230146    0.0000000), wk =      0.0025000
k(  179) = (      0.4365067    0.1269829    0.0000000), wk =      0.0025000
k(  180) = (      0.4345225    0.1309511    0.0000000), wk =      0.0025000
k(  181) = (      0.4325383    0.1349193    0.0000000), wk =      0.0025000
k(  182) = (      0.4305542    0.1388875    0.0000000), wk =      0.0025000
k(  183) = (      0.4285700    0.1428557    0.0000000), wk =      0.0025000
k(  184) = (      0.4265858    0.1468239    0.0000000), wk =      0.0025000
k(  185) = (      0.4246017    0.1507921    0.0000000), wk =      0.0025000
k(  186) = (      0.4226175    0.1547604    0.0000000), wk =      0.0025000
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k(   187) = (     0.4206333    0.1587286    0.0000000), wk =     0.0025000
k(   188) = (     0.4186492    0.1626968    0.0000000), wk =     0.0025000
k(   189) = (     0.4166650    0.1666650    0.0000000), wk =     0.0025000
k(   190) = (     0.4146808    0.1706332    0.0000000), wk =     0.0025000
k(   191) = (     0.4126967    0.1746014    0.0000000), wk =     0.0025000
k(   192) = (     0.4107125    0.1785696    0.0000000), wk =     0.0025000
k(   193) = (     0.4087283    0.1825379    0.0000000), wk =     0.0025000
k(   194) = (     0.4067442    0.1865061    0.0000000), wk =     0.0025000
k(   195) = (     0.4047600    0.1904743    0.0000000), wk =     0.0025000
k(   196) = (     0.4027758    0.1944425    0.0000000), wk =     0.0025000
k(   197) = (     0.4007917    0.1984107    0.0000000), wk =     0.0025000
k(   198) = (     0.3988075    0.2023789    0.0000000), wk =     0.0025000
k(   199) = (     0.3968233    0.2063471    0.0000000), wk =     0.0025000
k(   200) = (     0.3948392    0.2103154    0.0000000), wk =     0.0025000
k(   201) = (     0.3928550    0.2142836    0.0000000), wk =     0.0025000
k(   202) = (     0.3908708    0.2182518    0.0000000), wk =     0.0025000
k(   203) = (     0.3888867    0.2222200    0.0000000), wk =     0.0025000
k(   204) = (     0.3869025    0.2261882    0.0000000), wk =     0.0025000
k(   205) = (     0.3849183    0.2301564    0.0000000), wk =     0.0025000
k(   206) = (     0.3829342    0.2341246    0.0000000), wk =     0.0025000
k(   207) = (     0.3809500    0.2380929    0.0000000), wk =     0.0025000
k(   208) = (     0.3789658    0.2420611    0.0000000), wk =     0.0025000
k(   209) = (     0.3769817    0.2460293    0.0000000), wk =     0.0025000
k(   210) = (     0.3749975    0.2499975    0.0000000), wk =     0.0025000
k(   211) = (     0.3730133    0.2539657    0.0000000), wk =     0.0025000
k(   212) = (     0.3710292    0.2579339    0.0000000), wk =     0.0025000
k(   213) = (     0.3690450    0.2619021    0.0000000), wk =     0.0025000
k(   214) = (     0.3670608    0.2658704    0.0000000), wk =     0.0025000
k(   215) = (     0.3650767    0.2698386    0.0000000), wk =     0.0025000
k(   216) = (     0.3630925    0.2738068    0.0000000), wk =     0.0025000
k(   217) = (     0.3611083    0.2777750    0.0000000), wk =     0.0025000
k(   218) = (     0.3591242    0.2817432    0.0000000), wk =     0.0025000
k(   219) = (     0.3571400    0.2857114    0.0000000), wk =     0.0025000
k(   220) = (     0.3551558    0.2896796    0.0000000), wk =     0.0025000
k(   221) = (     0.3531717    0.2936479    0.0000000), wk =     0.0025000
k(   222) = (     0.3511875    0.2976161    0.0000000), wk =     0.0025000
k(   223) = (     0.3492033    0.3015843    0.0000000), wk =     0.0025000
k(   224) = (     0.3472192    0.3055525    0.0000000), wk =     0.0025000
k(   225) = (     0.3452350    0.3095207    0.0000000), wk =     0.0025000
k(   226) = (     0.3432508    0.3134889    0.0000000), wk =     0.0025000
k(   227) = (     0.3412667    0.3174571    0.0000000), wk =     0.0025000
k(   228) = (     0.3392825    0.3214254    0.0000000), wk =     0.0025000
k(   229) = (     0.3372983    0.3253936    0.0000000), wk =     0.0025000
k(   230) = (     0.3353142    0.3293618    0.0000000), wk =     0.0025000
k(   231) = (     0.3333300    0.3333300    0.0000000), wk =     0.0025000
k(   232) = (     0.3313576    0.3313576    0.0000000), wk =     0.0025000
k(   233) = (     0.3293853    0.3293853    0.0000000), wk =     0.0025000
k(   234) = (     0.3274129    0.3274129    0.0000000), wk =     0.0025000
k(   235) = (     0.3254405    0.3254405    0.0000000), wk =     0.0025000
k(   236) = (     0.3234682    0.3234682    0.0000000), wk =     0.0025000
k(   237) = (     0.3214958    0.3214958    0.0000000), wk =     0.0025000
k(   238) = (     0.3195234    0.3195234    0.0000000), wk =     0.0025000
k(   239) = (     0.3175511    0.3175511    0.0000000), wk =     0.0025000
k(   240) = (     0.3155787    0.3155787    0.0000000), wk =     0.0025000
k(   241) = (     0.3136063    0.3136063    0.0000000), wk =     0.0025000
k(   242) = (     0.3116340    0.3116340    0.0000000), wk =     0.0025000
k(   243) = (     0.3096616    0.3096616    0.0000000), wk =     0.0025000
k(   244) = (     0.3076892    0.3076892    0.0000000), wk =     0.0025000
k(   245) = (     0.3057169    0.3057169    0.0000000), wk =     0.0025000
k(   246) = (     0.3037445    0.3037445    0.0000000), wk =     0.0025000
k(   247) = (     0.3017721    0.3017721    0.0000000), wk =     0.0025000
k(   248) = (     0.2997998    0.2997998    0.0000000), wk =     0.0025000
```

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k(  249) = (     0.2978274    0.2978274    0.0000000), wk =    0.0025000
k(  250) = (     0.2958550    0.2958550    0.0000000), wk =    0.0025000
k(  251) = (     0.2938827    0.2938827    0.0000000), wk =    0.0025000
k(  252) = (     0.2919103    0.2919103    0.0000000), wk =    0.0025000
k(  253) = (     0.2899379    0.2899379    0.0000000), wk =    0.0025000
k(  254) = (     0.2879656    0.2879656    0.0000000), wk =    0.0025000
k(  255) = (     0.2859932    0.2859932    0.0000000), wk =    0.0025000
k(  256) = (     0.2840208    0.2840208    0.0000000), wk =    0.0025000
k(  257) = (     0.2820485    0.2820485    0.0000000), wk =    0.0025000
k(  258) = (     0.2800761    0.2800761    0.0000000), wk =    0.0025000
k(  259) = (     0.2781037    0.2781037    0.0000000), wk =    0.0025000
k(  260) = (     0.2761314    0.2761314    0.0000000), wk =    0.0025000
k(  261) = (     0.2741590    0.2741590    0.0000000), wk =    0.0025000
k(  262) = (     0.2721866    0.2721866    0.0000000), wk =    0.0025000
k(  263) = (     0.2702143    0.2702143    0.0000000), wk =    0.0025000
k(  264) = (     0.2682419    0.2682419    0.0000000), wk =    0.0025000
k(  265) = (     0.2662695    0.2662695    0.0000000), wk =    0.0025000
k(  266) = (     0.2642972    0.2642972    0.0000000), wk =    0.0025000
k(  267) = (     0.2623248    0.2623248    0.0000000), wk =    0.0025000
k(  268) = (     0.2603524    0.2603524    0.0000000), wk =    0.0025000
k(  269) = (     0.2583801    0.2583801    0.0000000), wk =    0.0025000
k(  270) = (     0.2564077    0.2564077    0.0000000), wk =    0.0025000
k(  271) = (     0.2544353    0.2544353    0.0000000), wk =    0.0025000
k(  272) = (     0.2524630    0.2524630    0.0000000), wk =    0.0025000
k(  273) = (     0.2504906    0.2504906    0.0000000), wk =    0.0025000
k(  274) = (     0.2485182    0.2485182    0.0000000), wk =    0.0025000
k(  275) = (     0.2465459    0.2465459    0.0000000), wk =    0.0025000
k(  276) = (     0.2445735    0.2445735    0.0000000), wk =    0.0025000
k(  277) = (     0.2426011    0.2426011    0.0000000), wk =    0.0025000
k(  278) = (     0.2406288    0.2406288    0.0000000), wk =    0.0025000
k(  279) = (     0.2386564    0.2386564    0.0000000), wk =    0.0025000
k(  280) = (     0.2366840    0.2366840    0.0000000), wk =    0.0025000
k(  281) = (     0.2347117    0.2347117    0.0000000), wk =    0.0025000
k(  282) = (     0.2327393    0.2327393    0.0000000), wk =    0.0025000
k(  283) = (     0.2307669    0.2307669    0.0000000), wk =    0.0025000
k(  284) = (     0.2287946    0.2287946    0.0000000), wk =    0.0025000
k(  285) = (     0.2268222    0.2268222    0.0000000), wk =    0.0025000
k(  286) = (     0.2248498    0.2248498    0.0000000), wk =    0.0025000
k(  287) = (     0.2228775    0.2228775    0.0000000), wk =    0.0025000
k(  288) = (     0.2209051    0.2209051    0.0000000), wk =    0.0025000
k(  289) = (     0.2189327    0.2189327    0.0000000), wk =    0.0025000
k(  290) = (     0.2169604    0.2169604    0.0000000), wk =    0.0025000
k(  291) = (     0.2149880    0.2149880    0.0000000), wk =    0.0025000
k(  292) = (     0.2130156    0.2130156    0.0000000), wk =    0.0025000
k(  293) = (     0.2110433    0.2110433    0.0000000), wk =    0.0025000
k(  294) = (     0.2090709    0.2090709    0.0000000), wk =    0.0025000
k(  295) = (     0.2070985    0.2070985    0.0000000), wk =    0.0025000
k(  296) = (     0.2051262    0.2051262    0.0000000), wk =    0.0025000
k(  297) = (     0.2031538    0.2031538    0.0000000), wk =    0.0025000
k(  298) = (     0.2011814    0.2011814    0.0000000), wk =    0.0025000
k(  299) = (     0.1992091    0.1992091    0.0000000), wk =    0.0025000
k(  300) = (     0.1972367    0.1972367    0.0000000), wk =    0.0025000
k(  301) = (     0.1952643    0.1952643    0.0000000), wk =    0.0025000
k(  302) = (     0.1932920    0.1932920    0.0000000), wk =    0.0025000
k(  303) = (     0.1913196    0.1913196    0.0000000), wk =    0.0025000
k(  304) = (     0.1893472    0.1893472    0.0000000), wk =    0.0025000
k(  305) = (     0.1873749    0.1873749    0.0000000), wk =    0.0025000
k(  306) = (     0.1854025    0.1854025    0.0000000), wk =    0.0025000
k(  307) = (     0.1834301    0.1834301    0.0000000), wk =    0.0025000
k(  308) = (     0.1814578    0.1814578    0.0000000), wk =    0.0025000
k(  309) = (     0.1794854    0.1794854    0.0000000), wk =    0.0025000
k(  310) = (     0.1775130    0.1775130    0.0000000), wk =    0.0025000
```

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k(  311) = (     0.1755407    0.1755407    0.0000000), wk =     0.0025000
k(  312) = (     0.1735683    0.1735683    0.0000000), wk =     0.0025000
k(  313) = (     0.1715959    0.1715959    0.0000000), wk =     0.0025000
k(  314) = (     0.1696236    0.1696236    0.0000000), wk =     0.0025000
k(  315) = (     0.1676512    0.1676512    0.0000000), wk =     0.0025000
k(  316) = (     0.1656788    0.1656788    0.0000000), wk =     0.0025000
k(  317) = (     0.1637064    0.1637064    0.0000000), wk =     0.0025000
k(  318) = (     0.1617341    0.1617341    0.0000000), wk =     0.0025000
k(  319) = (     0.1597617    0.1597617    0.0000000), wk =     0.0025000
k(  320) = (     0.1577893    0.1577893    0.0000000), wk =     0.0025000
k(  321) = (     0.1558170    0.1558170    0.0000000), wk =     0.0025000
k(  322) = (     0.1538446    0.1538446    0.0000000), wk =     0.0025000
k(  323) = (     0.1518722    0.1518722    0.0000000), wk =     0.0025000
k(  324) = (     0.1498999    0.1498999    0.0000000), wk =     0.0025000
k(  325) = (     0.1479275    0.1479275    0.0000000), wk =     0.0025000
k(  326) = (     0.1459551    0.1459551    0.0000000), wk =     0.0025000
k(  327) = (     0.1439828    0.1439828    0.0000000), wk =     0.0025000
k(  328) = (     0.1420104    0.1420104    0.0000000), wk =     0.0025000
k(  329) = (     0.1400380    0.1400380    0.0000000), wk =     0.0025000
k(  330) = (     0.1380657    0.1380657    0.0000000), wk =     0.0025000
k(  331) = (     0.1360933    0.1360933    0.0000000), wk =     0.0025000
k(  332) = (     0.1341209    0.1341209    0.0000000), wk =     0.0025000
k(  333) = (     0.1321486    0.1321486    0.0000000), wk =     0.0025000
k(  334) = (     0.1301762    0.1301762    0.0000000), wk =     0.0025000
k(  335) = (     0.1282038    0.1282038    0.0000000), wk =     0.0025000
k(  336) = (     0.1262315    0.1262315    0.0000000), wk =     0.0025000
k(  337) = (     0.1242591    0.1242591    0.0000000), wk =     0.0025000
k(  338) = (     0.1222867    0.1222867    0.0000000), wk =     0.0025000
k(  339) = (     0.1203144    0.1203144    0.0000000), wk =     0.0025000
k(  340) = (     0.1183420    0.1183420    0.0000000), wk =     0.0025000
k(  341) = (     0.1163696    0.1163696    0.0000000), wk =     0.0025000
k(  342) = (     0.1143973    0.1143973    0.0000000), wk =     0.0025000
k(  343) = (     0.1124249    0.1124249    0.0000000), wk =     0.0025000
k(  344) = (     0.1104525    0.1104525    0.0000000), wk =     0.0025000
k(  345) = (     0.1084802    0.1084802    0.0000000), wk =     0.0025000
k(  346) = (     0.1065078    0.1065078    0.0000000), wk =     0.0025000
k(  347) = (     0.1045354    0.1045354    0.0000000), wk =     0.0025000
k(  348) = (     0.1025631    0.1025631    0.0000000), wk =     0.0025000
k(  349) = (     0.1005907    0.1005907    0.0000000), wk =     0.0025000
k(  350) = (     0.0986183    0.0986183    0.0000000), wk =     0.0025000
k(  351) = (     0.0966460    0.0966460    0.0000000), wk =     0.0025000
k(  352) = (     0.0946736    0.0946736    0.0000000), wk =     0.0025000
k(  353) = (     0.0927012    0.0927012    0.0000000), wk =     0.0025000
k(  354) = (     0.0907289    0.0907289    0.0000000), wk =     0.0025000
k(  355) = (     0.0887565    0.0887565    0.0000000), wk =     0.0025000
k(  356) = (     0.0867841    0.0867841    0.0000000), wk =     0.0025000
k(  357) = (     0.0848118    0.0848118    0.0000000), wk =     0.0025000
k(  358) = (     0.0828394    0.0828394    0.0000000), wk =     0.0025000
k(  359) = (     0.0808670    0.0808670    0.0000000), wk =     0.0025000
k(  360) = (     0.0788947    0.0788947    0.0000000), wk =     0.0025000
k(  361) = (     0.0769223    0.0769223    0.0000000), wk =     0.0025000
k(  362) = (     0.0749499    0.0749499    0.0000000), wk =     0.0025000
k(  363) = (     0.0729776    0.0729776    0.0000000), wk =     0.0025000
k(  364) = (     0.0710052    0.0710052    0.0000000), wk =     0.0025000
k(  365) = (     0.0690328    0.0690328    0.0000000), wk =     0.0025000
k(  366) = (     0.0670605    0.0670605    0.0000000), wk =     0.0025000
k(  367) = (     0.0650881    0.0650881    0.0000000), wk =     0.0025000
k(  368) = (     0.0631157    0.0631157    0.0000000), wk =     0.0025000
k(  369) = (     0.0611434    0.0611434    0.0000000), wk =     0.0025000
k(  370) = (     0.0591710    0.0591710    0.0000000), wk =     0.0025000
k(  371) = (     0.0571986    0.0571986    0.0000000), wk =     0.0025000
k(  372) = (     0.0552263    0.0552263    0.0000000), wk =     0.0025000
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k( 373) = (   0.0532539   0.0532539   0.0000000), wk =   0.0025000
k( 374) = (   0.0512815   0.0512815   0.0000000), wk =   0.0025000
k( 375) = (   0.0493092   0.0493092   0.0000000), wk =   0.0025000
k( 376) = (   0.0473368   0.0473368   0.0000000), wk =   0.0025000
k( 377) = (   0.0453644   0.0453644   0.0000000), wk =   0.0025000
k( 378) = (   0.0433921   0.0433921   0.0000000), wk =   0.0025000
k( 379) = (   0.0414197   0.0414197   0.0000000), wk =   0.0025000
k( 380) = (   0.0394473   0.0394473   0.0000000), wk =   0.0025000
k( 381) = (   0.0374750   0.0374750   0.0000000), wk =   0.0025000
k( 382) = (   0.0355026   0.0355026   0.0000000), wk =   0.0025000
k( 383) = (   0.0335302   0.0335302   0.0000000), wk =   0.0025000
k( 384) = (   0.0315579   0.0315579   0.0000000), wk =   0.0025000
k( 385) = (   0.0295855   0.0295855   0.0000000), wk =   0.0025000
k( 386) = (   0.0276131   0.0276131   0.0000000), wk =   0.0025000
k( 387) = (   0.0256408   0.0256408   0.0000000), wk =   0.0025000
k( 388) = (   0.0236684   0.0236684   0.0000000), wk =   0.0025000
k( 389) = (   0.0216960   0.0216960   0.0000000), wk =   0.0025000
k( 390) = (   0.0197237   0.0197237   0.0000000), wk =   0.0025000
k( 391) = (   0.0177513   0.0177513   0.0000000), wk =   0.0025000
k( 392) = (   0.0157789   0.0157789   0.0000000), wk =   0.0025000
k( 393) = (   0.0138066   0.0138066   0.0000000), wk =   0.0025000
k( 394) = (   0.0118342   0.0118342   0.0000000), wk =   0.0025000
k( 395) = (   0.0098618   0.0098618   0.0000000), wk =   0.0025000
k( 396) = (   0.0078895   0.0078895   0.0000000), wk =   0.0025000
k( 397) = (   0.0059171   0.0059171   0.0000000), wk =   0.0025000
k( 398) = (   0.0039447   0.0039447   0.0000000), wk =   0.0025000
k( 399) = (   0.0019724   0.0019724   0.0000000), wk =   0.0025000
k( 400) = (   0.0000000   0.0000000   0.0000000), wk =   0.0025000

Dense  grid:    37579 G-vectors     FFT dimensions: (  32,  32,  96)

Smooth grid:     9597 G-vectors     FFT dimensions: (  20,  20,  60)

Dynamical RAM for                   wfc:        0.15 MB

Dynamical RAM for      wfc (w. buffer):        0.15 MB

Dynamical RAM for             str. fact:        1.15 MB

Dynamical RAM for             local pot:        0.00 MB

Dynamical RAM for            nlocal pot:        0.29 MB

Dynamical RAM for                  qrad:        0.69 MB

Dynamical RAM for            rho,v,vnew:        7.94 MB

Dynamical RAM for             G-vectors:        2.22 MB

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

Dynamical RAM for            <psi|beta>:        0.00 MB

Dynamical RAM for                   psi:        0.58 MB

Dynamical RAM for                  hpsi:        0.58 MB

Dynamical RAM for                  spsi:        0.58 MB

Dynamical RAM for        wfcinit/wfcrot:        0.29 MB

Dynamical RAM for             addusdens:       25.80 MB
```

```
Estimated static dynamical RAM per process >      18.66 MB

Estimated max dynamical RAM per process >      44.46 MB
Generating pointlists ...
new r_m :   0.2382 (alat units)  1.1312 (a.u.) for type    1
new r_m :   0.2382 (alat units)  1.1312 (a.u.) for type    2

Check: negative core charge=   -0.000009

The potential is recalculated from file :
./tmp-hetero/A.save/charge-density

Starting wfcs are    8 randomized atomic wfcs

Band Structure Calculation
Davidson diagonalization with overlap

Computing kpt #:     1  of   800
total cpu time spent up to now is       3.7 secs

Computing kpt #:     2  of   800
total cpu time spent up to now is       3.7 secs

Computing kpt #:     3  of   800
total cpu time spent up to now is       3.8 secs

Computing kpt #:     4  of   800
total cpu time spent up to now is       3.9 secs

Computing kpt #:     5  of   800
total cpu time spent up to now is       4.0 secs

Computing kpt #:     6  of   800
total cpu time spent up to now is       4.1 secs

Computing kpt #:     7  of   800
total cpu time spent up to now is       4.1 secs

Computing kpt #:     8  of   800
total cpu time spent up to now is       4.2 secs

Computing kpt #:     9  of   800
total cpu time spent up to now is       4.3 secs

Computing kpt #:    10  of   800
total cpu time spent up to now is       4.4 secs

Computing kpt #:    11  of   800
total cpu time spent up to now is       4.5 secs

Computing kpt #:    12  of   800
total cpu time spent up to now is       4.6 secs

Computing kpt #:    13  of   800
total cpu time spent up to now is       4.7 secs

Computing kpt #:    14  of   800
total cpu time spent up to now is       4.8 secs

Computing kpt #:    15  of   800
total cpu time spent up to now is       4.9 secs
```

```
Computing kpt #:    16  of    800
total cpu time spent up to now is       4.9 secs

Computing kpt #:    17  of    800
total cpu time spent up to now is       5.0 secs

Computing kpt #:    18  of    800
total cpu time spent up to now is       5.1 secs

Computing kpt #:    19  of    800
total cpu time spent up to now is       5.2 secs

Computing kpt #:    20  of    800
total cpu time spent up to now is       5.2 secs

Computing kpt #:    21  of    800
total cpu time spent up to now is       5.3 secs

Computing kpt #:    22  of    800
total cpu time spent up to now is       5.4 secs

Computing kpt #:    23  of    800
total cpu time spent up to now is       5.5 secs

Computing kpt #:    24  of    800
total cpu time spent up to now is       5.6 secs

Computing kpt #:    25  of    800
total cpu time spent up to now is       5.7 secs

Computing kpt #:    26  of    800
total cpu time spent up to now is       5.7 secs

Computing kpt #:    27  of    800
total cpu time spent up to now is       5.8 secs

Computing kpt #:    28  of    800
total cpu time spent up to now is       5.9 secs

Computing kpt #:    29  of    800
total cpu time spent up to now is       6.0 secs

Computing kpt #:    30  of    800
total cpu time spent up to now is       6.1 secs

Computing kpt #:    31  of    800
total cpu time spent up to now is       6.1 secs

Computing kpt #:    32  of    800
total cpu time spent up to now is       6.2 secs

Computing kpt #:    33  of    800
total cpu time spent up to now is       6.3 secs

Computing kpt #:    34  of    800
total cpu time spent up to now is       6.4 secs

Computing kpt #:    35  of    800
total cpu time spent up to now is       6.5 secs

Computing kpt #:    36  of    800
```

```
        total cpu time spent up to now is        6.5 secs

Computing kpt #:     37  of    800
        total cpu time spent up to now is        6.6 secs

Computing kpt #:     38  of    800
        total cpu time spent up to now is        6.7 secs

Computing kpt #:     39  of    800
        total cpu time spent up to now is        6.8 secs

Computing kpt #:     40  of    800
        total cpu time spent up to now is        6.9 secs

Computing kpt #:     41  of    800
        total cpu time spent up to now is        7.0 secs

Computing kpt #:     42  of    800
        total cpu time spent up to now is        7.1 secs

Computing kpt #:     43  of    800
        total cpu time spent up to now is        7.2 secs

Computing kpt #:     44  of    800
        total cpu time spent up to now is        7.3 secs

Computing kpt #:     45  of    800
        total cpu time spent up to now is        7.4 secs

Computing kpt #:     46  of    800
        total cpu time spent up to now is        7.5 secs

Computing kpt #:     47  of    800
        total cpu time spent up to now is        7.6 secs

Computing kpt #:     48  of    800
        total cpu time spent up to now is        7.7 secs

Computing kpt #:     49  of    800
        total cpu time spent up to now is        7.8 secs

Computing kpt #:     50  of    800
        total cpu time spent up to now is        7.9 secs

Computing kpt #:     51  of    800
        total cpu time spent up to now is        8.0 secs

Computing kpt #:     52  of    800
        total cpu time spent up to now is        8.1 secs

Computing kpt #:     53  of    800
        total cpu time spent up to now is        8.2 secs

Computing kpt #:     54  of    800
        total cpu time spent up to now is        8.3 secs

Computing kpt #:     55  of    800
        total cpu time spent up to now is        8.4 secs

Computing kpt #:     56  of    800
        total cpu time spent up to now is        8.5 secs
```

```
Computing kpt #:    57  of    800
total cpu time spent up to now is        8.7 secs

Computing kpt #:    58  of    800
total cpu time spent up to now is        8.8 secs

Computing kpt #:    59  of    800
total cpu time spent up to now is        8.9 secs

Computing kpt #:    60  of    800
total cpu time spent up to now is        9.0 secs

Computing kpt #:    61  of    800
total cpu time spent up to now is        9.1 secs

Computing kpt #:    62  of    800
total cpu time spent up to now is        9.2 secs

Computing kpt #:    63  of    800
total cpu time spent up to now is        9.3 secs

Computing kpt #:    64  of    800
total cpu time spent up to now is        9.4 secs

Computing kpt #:    65  of    800
total cpu time spent up to now is        9.5 secs

Computing kpt #:    66  of    800
total cpu time spent up to now is        9.6 secs

Computing kpt #:    67  of    800
total cpu time spent up to now is        9.7 secs

Computing kpt #:    68  of    800
total cpu time spent up to now is        9.8 secs

Computing kpt #:    69  of    800
total cpu time spent up to now is        9.8 secs

Computing kpt #:    70  of    800
total cpu time spent up to now is       10.0 secs

Computing kpt #:    71  of    800
total cpu time spent up to now is       10.1 secs

Computing kpt #:    72  of    800
total cpu time spent up to now is       10.2 secs

Computing kpt #:    73  of    800
total cpu time spent up to now is       10.3 secs

Computing kpt #:    74  of    800
total cpu time spent up to now is       10.4 secs

Computing kpt #:    75  of    800
total cpu time spent up to now is       10.5 secs

Computing kpt #:    76  of    800
total cpu time spent up to now is       10.6 secs

Computing kpt #:    77  of    800
total cpu time spent up to now is       10.7 secs
```

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Computing kpt #:     78  of    800
total cpu time spent up to now is       10.8 secs

Computing kpt #:     79  of    800
total cpu time spent up to now is       10.9 secs

Computing kpt #:     80  of    800
total cpu time spent up to now is       11.0 secs

Computing kpt #:     81  of    800
total cpu time spent up to now is       11.1 secs

Computing kpt #:     82  of    800
total cpu time spent up to now is       11.1 secs

Computing kpt #:     83  of    800
total cpu time spent up to now is       11.2 secs

Computing kpt #:     84  of    800
total cpu time spent up to now is       11.3 secs

Computing kpt #:     85  of    800
total cpu time spent up to now is       11.4 secs

Computing kpt #:     86  of    800
total cpu time spent up to now is       11.5 secs

Computing kpt #:     87  of    800
total cpu time spent up to now is       11.6 secs

Computing kpt #:     88  of    800
total cpu time spent up to now is       11.7 secs

Computing kpt #:     89  of    800
total cpu time spent up to now is       11.8 secs

Computing kpt #:     90  of    800
total cpu time spent up to now is       11.9 secs

Computing kpt #:     91  of    800
total cpu time spent up to now is       12.0 secs

Computing kpt #:     92  of    800
total cpu time spent up to now is       12.1 secs

Computing kpt #:     93  of    800
total cpu time spent up to now is       12.2 secs

Computing kpt #:     94  of    800
total cpu time spent up to now is       12.3 secs

Computing kpt #:     95  of    800
total cpu time spent up to now is       12.4 secs

Computing kpt #:     96  of    800
total cpu time spent up to now is       12.5 secs

Computing kpt #:     97  of    800
total cpu time spent up to now is       12.6 secs

Computing kpt #:     98  of    800
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      total cpu time spent up to now is        12.7 secs

Computing kpt #:    99  of    800
      total cpu time spent up to now is        12.8 secs

Computing kpt #:   100  of    800
      total cpu time spent up to now is        12.9 secs

Computing kpt #:   101  of    800
      total cpu time spent up to now is        13.0 secs

Computing kpt #:   102  of    800
      total cpu time spent up to now is        13.1 secs

Computing kpt #:   103  of    800
      total cpu time spent up to now is        13.2 secs

Computing kpt #:   104  of    800
      total cpu time spent up to now is        13.2 secs

Computing kpt #:   105  of    800
      total cpu time spent up to now is        13.4 secs

Computing kpt #:   106  of    800
      total cpu time spent up to now is        13.4 secs

Computing kpt #:   107  of    800
      total cpu time spent up to now is        13.6 secs

Computing kpt #:   108  of    800
      total cpu time spent up to now is        13.6 secs

Computing kpt #:   109  of    800
      total cpu time spent up to now is        13.7 secs

Computing kpt #:   110  of    800
      total cpu time spent up to now is        13.9 secs

Computing kpt #:   111  of    800
      total cpu time spent up to now is        14.0 secs

Computing kpt #:   112  of    800
      total cpu time spent up to now is        14.1 secs

Computing kpt #:   113  of    800
      total cpu time spent up to now is        14.2 secs

Computing kpt #:   114  of    800
      total cpu time spent up to now is        14.3 secs

Computing kpt #:   115  of    800
      total cpu time spent up to now is        14.4 secs

Computing kpt #:   116  of    800
      total cpu time spent up to now is        14.5 secs

Computing kpt #:   117  of    800
      total cpu time spent up to now is        14.6 secs

Computing kpt #:   118  of    800
      total cpu time spent up to now is        14.7 secs
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Computing kpt #:   119  of   800
total cpu time spent up to now is       14.8 secs

Computing kpt #:   120  of   800
total cpu time spent up to now is       14.9 secs

Computing kpt #:   121  of   800
total cpu time spent up to now is       15.0 secs

Computing kpt #:   122  of   800
total cpu time spent up to now is       15.1 secs

Computing kpt #:   123  of   800
total cpu time spent up to now is       15.2 secs

Computing kpt #:   124  of   800
total cpu time spent up to now is       15.3 secs

Computing kpt #:   125  of   800
total cpu time spent up to now is       15.4 secs

Computing kpt #:   126  of   800
total cpu time spent up to now is       15.5 secs

Computing kpt #:   127  of   800
total cpu time spent up to now is       15.6 secs

Computing kpt #:   128  of   800
total cpu time spent up to now is       15.7 secs

Computing kpt #:   129  of   800
total cpu time spent up to now is       15.8 secs

Computing kpt #:   130  of   800
total cpu time spent up to now is       15.9 secs

Computing kpt #:   131  of   800
total cpu time spent up to now is       16.0 secs

Computing kpt #:   132  of   800
total cpu time spent up to now is       16.1 secs

Computing kpt #:   133  of   800
total cpu time spent up to now is       16.3 secs

Computing kpt #:   134  of   800
total cpu time spent up to now is       16.4 secs

Computing kpt #:   135  of   800
total cpu time spent up to now is       16.5 secs

Computing kpt #:   136  of   800
total cpu time spent up to now is       16.6 secs

Computing kpt #:   137  of   800
total cpu time spent up to now is       16.7 secs

Computing kpt #:   138  of   800
total cpu time spent up to now is       16.8 secs

Computing kpt #:   139  of   800
total cpu time spent up to now is       17.0 secs
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Computing kpt #:   140  of   800
total cpu time spent up to now is      17.1 secs

Computing kpt #:   141  of   800
total cpu time spent up to now is      17.2 secs

Computing kpt #:   142  of   800
total cpu time spent up to now is      17.3 secs

Computing kpt #:   143  of   800
total cpu time spent up to now is      17.4 secs

Computing kpt #:   144  of   800
total cpu time spent up to now is      17.5 secs

Computing kpt #:   145  of   800
total cpu time spent up to now is      17.6 secs

Computing kpt #:   146  of   800
total cpu time spent up to now is      17.7 secs

Computing kpt #:   147  of   800
total cpu time spent up to now is      17.8 secs

Computing kpt #:   148  of   800
total cpu time spent up to now is      17.9 secs

Computing kpt #:   149  of   800
total cpu time spent up to now is      18.0 secs

Computing kpt #:   150  of   800
total cpu time spent up to now is      18.1 secs

Computing kpt #:   151  of   800
total cpu time spent up to now is      18.2 secs

Computing kpt #:   152  of   800
total cpu time spent up to now is      18.3 secs

Computing kpt #:   153  of   800
total cpu time spent up to now is      18.4 secs

Computing kpt #:   154  of   800
total cpu time spent up to now is      18.5 secs

Computing kpt #:   155  of   800
total cpu time spent up to now is      18.6 secs

Computing kpt #:   156  of   800
total cpu time spent up to now is      18.7 secs

Computing kpt #:   157  of   800
total cpu time spent up to now is      18.8 secs

Computing kpt #:   158  of   800
total cpu time spent up to now is      18.9 secs

Computing kpt #:   159  of   800
total cpu time spent up to now is      19.0 secs

Computing kpt #:   160  of   800
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total cpu time spent up to now is        19.1 secs

Computing kpt #:    161  of    800
total cpu time spent up to now is        19.2 secs

Computing kpt #:    162  of    800
total cpu time spent up to now is        19.3 secs

Computing kpt #:    163  of    800
total cpu time spent up to now is        19.4 secs

Computing kpt #:    164  of    800
total cpu time spent up to now is        19.5 secs

Computing kpt #:    165  of    800
total cpu time spent up to now is        19.6 secs

Computing kpt #:    166  of    800
total cpu time spent up to now is        19.7 secs

Computing kpt #:    167  of    800
total cpu time spent up to now is        19.8 secs

Computing kpt #:    168  of    800
total cpu time spent up to now is        20.0 secs

Computing kpt #:    169  of    800
total cpu time spent up to now is        20.1 secs

Computing kpt #:    170  of    800
total cpu time spent up to now is        20.2 secs

Computing kpt #:    171  of    800
total cpu time spent up to now is        20.3 secs

Computing kpt #:    172  of    800
total cpu time spent up to now is        20.4 secs

Computing kpt #:    173  of    800
total cpu time spent up to now is        20.5 secs

Computing kpt #:    174  of    800
total cpu time spent up to now is        20.6 secs

Computing kpt #:    175  of    800
total cpu time spent up to now is        20.7 secs

Computing kpt #:    176  of    800
total cpu time spent up to now is        20.9 secs

Computing kpt #:    177  of    800
total cpu time spent up to now is        21.0 secs

Computing kpt #:    178  of    800
total cpu time spent up to now is        21.1 secs

Computing kpt #:    179  of    800
total cpu time spent up to now is        21.2 secs

Computing kpt #:    180  of    800
total cpu time spent up to now is        21.3 secs
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Computing kpt #:   181  of   800
total cpu time spent up to now is       21.4 secs

Computing kpt #:   182  of   800
total cpu time spent up to now is       21.5 secs

Computing kpt #:   183  of   800
total cpu time spent up to now is       21.6 secs

Computing kpt #:   184  of   800
total cpu time spent up to now is       21.8 secs

Computing kpt #:   185  of   800
total cpu time spent up to now is       21.9 secs

Computing kpt #:   186  of   800
total cpu time spent up to now is       22.0 secs

Computing kpt #:   187  of   800
total cpu time spent up to now is       22.1 secs

Computing kpt #:   188  of   800
total cpu time spent up to now is       22.2 secs

Computing kpt #:   189  of   800
total cpu time spent up to now is       22.4 secs

Computing kpt #:   190  of   800
total cpu time spent up to now is       22.5 secs

Computing kpt #:   191  of   800
total cpu time spent up to now is       22.6 secs

Computing kpt #:   192  of   800
total cpu time spent up to now is       22.7 secs

Computing kpt #:   193  of   800
total cpu time spent up to now is       22.9 secs

Computing kpt #:   194  of   800
total cpu time spent up to now is       23.0 secs

Computing kpt #:   195  of   800
total cpu time spent up to now is       23.1 secs

Computing kpt #:   196  of   800
total cpu time spent up to now is       23.2 secs

Computing kpt #:   197  of   800
total cpu time spent up to now is       23.3 secs

Computing kpt #:   198  of   800
total cpu time spent up to now is       23.4 secs

Computing kpt #:   199  of   800
total cpu time spent up to now is       23.5 secs

Computing kpt #:   200  of   800
total cpu time spent up to now is       23.6 secs

Computing kpt #:   201  of   800
total cpu time spent up to now is       23.7 secs
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Computing kpt #:   202  of   800
total cpu time spent up to now is       23.9 secs

Computing kpt #:   203  of   800
total cpu time spent up to now is       24.0 secs

Computing kpt #:   204  of   800
total cpu time spent up to now is       24.1 secs

Computing kpt #:   205  of   800
total cpu time spent up to now is       24.2 secs

Computing kpt #:   206  of   800
total cpu time spent up to now is       24.3 secs

Computing kpt #:   207  of   800
total cpu time spent up to now is       24.4 secs

Computing kpt #:   208  of   800
total cpu time spent up to now is       24.5 secs

Computing kpt #:   209  of   800
total cpu time spent up to now is       24.6 secs

Computing kpt #:   210  of   800
total cpu time spent up to now is       24.7 secs

Computing kpt #:   211  of   800
total cpu time spent up to now is       24.9 secs

Computing kpt #:   212  of   800
total cpu time spent up to now is       25.0 secs

Computing kpt #:   213  of   800
total cpu time spent up to now is       25.1 secs

Computing kpt #:   214  of   800
total cpu time spent up to now is       25.2 secs

Computing kpt #:   215  of   800
total cpu time spent up to now is       25.3 secs

Computing kpt #:   216  of   800
total cpu time spent up to now is       25.5 secs

Computing kpt #:   217  of   800
total cpu time spent up to now is       25.6 secs

Computing kpt #:   218  of   800
total cpu time spent up to now is       25.7 secs

Computing kpt #:   219  of   800
total cpu time spent up to now is       25.8 secs

Computing kpt #:   220  of   800
total cpu time spent up to now is       25.9 secs

Computing kpt #:   221  of   800
total cpu time spent up to now is       26.0 secs

Computing kpt #:   222  of   800
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     total cpu time spent up to now is        26.1 secs

Computing kpt #:   223  of   800
     total cpu time spent up to now is        26.2 secs

Computing kpt #:   224  of   800
     total cpu time spent up to now is        26.3 secs

Computing kpt #:   225  of   800
     total cpu time spent up to now is        26.4 secs

Computing kpt #:   226  of   800
     total cpu time spent up to now is        26.5 secs

Computing kpt #:   227  of   800
     total cpu time spent up to now is        26.7 secs

Computing kpt #:   228  of   800
     total cpu time spent up to now is        26.8 secs

Computing kpt #:   229  of   800
     total cpu time spent up to now is        26.9 secs

Computing kpt #:   230  of   800
     total cpu time spent up to now is        27.0 secs

Computing kpt #:   231  of   800
     total cpu time spent up to now is        27.1 secs

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     total cpu time spent up to now is        27.2 secs

Computing kpt #:   233  of   800
     total cpu time spent up to now is        27.4 secs

Computing kpt #:   234  of   800
     total cpu time spent up to now is        27.5 secs

Computing kpt #:   235  of   800
     total cpu time spent up to now is        27.6 secs

Computing kpt #:   236  of   800
     total cpu time spent up to now is        27.7 secs

Computing kpt #:   237  of   800
     total cpu time spent up to now is        27.8 secs

Computing kpt #:   238  of   800
     total cpu time spent up to now is        27.9 secs

Computing kpt #:   239  of   800
     total cpu time spent up to now is        28.0 secs

Computing kpt #:   240  of   800
     total cpu time spent up to now is        28.2 secs

Computing kpt #:   241  of   800
     total cpu time spent up to now is        28.3 secs

Computing kpt #:   242  of   800
     total cpu time spent up to now is        28.4 secs
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Computing kpt #:   243  of   800
total cpu time spent up to now is      28.5 secs

Computing kpt #:   244  of   800
total cpu time spent up to now is      28.6 secs

Computing kpt #:   245  of   800
total cpu time spent up to now is      28.7 secs

Computing kpt #:   246  of   800
total cpu time spent up to now is      28.8 secs

Computing kpt #:   247  of   800
total cpu time spent up to now is      28.9 secs

Computing kpt #:   248  of   800
total cpu time spent up to now is      29.1 secs

Computing kpt #:   249  of   800
total cpu time spent up to now is      29.2 secs

Computing kpt #:   250  of   800
total cpu time spent up to now is      29.3 secs

Computing kpt #:   251  of   800
total cpu time spent up to now is      29.4 secs

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total cpu time spent up to now is      29.5 secs

Computing kpt #:   253  of   800
total cpu time spent up to now is      29.6 secs

Computing kpt #:   254  of   800
total cpu time spent up to now is      29.7 secs

Computing kpt #:   255  of   800
total cpu time spent up to now is      29.9 secs

Computing kpt #:   256  of   800
total cpu time spent up to now is      30.0 secs

Computing kpt #:   257  of   800
total cpu time spent up to now is      30.1 secs

Computing kpt #:   258  of   800
total cpu time spent up to now is      30.2 secs

Computing kpt #:   259  of   800
total cpu time spent up to now is      30.4 secs

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total cpu time spent up to now is      30.5 secs

Computing kpt #:   261  of   800
total cpu time spent up to now is      30.6 secs

Computing kpt #:   262  of   800
total cpu time spent up to now is      30.7 secs

Computing kpt #:   263  of   800
total cpu time spent up to now is      30.8 secs
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Computing kpt #:   264  of   800
total cpu time spent up to now is       30.9 secs

Computing kpt #:   265  of   800
total cpu time spent up to now is       31.0 secs

Computing kpt #:   266  of   800
total cpu time spent up to now is       31.1 secs

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total cpu time spent up to now is       31.3 secs

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total cpu time spent up to now is       31.4 secs

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total cpu time spent up to now is       31.5 secs

Computing kpt #:   271  of   800
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Computing kpt #:   273  of   800
total cpu time spent up to now is       31.8 secs

Computing kpt #:   274  of   800
total cpu time spent up to now is       32.0 secs

Computing kpt #:   275  of   800
total cpu time spent up to now is       32.1 secs

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total cpu time spent up to now is       32.2 secs

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total cpu time spent up to now is       32.3 secs

Computing kpt #:   278  of   800
total cpu time spent up to now is       32.4 secs

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total cpu time spent up to now is       32.5 secs

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total cpu time spent up to now is       32.6 secs

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total cpu time spent up to now is       32.7 secs

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total cpu time spent up to now is       32.7 secs

Computing kpt #:   283  of   800
total cpu time spent up to now is       32.9 secs

Computing kpt #:   284  of   800
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        total cpu time spent up to now is        32.9 secs

Computing kpt #:    285  of    800
        total cpu time spent up to now is        33.0 secs

Computing kpt #:    286  of    800
        total cpu time spent up to now is        33.1 secs

Computing kpt #:    287  of    800
        total cpu time spent up to now is        33.2 secs

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        total cpu time spent up to now is        33.3 secs

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        total cpu time spent up to now is        33.4 secs

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        total cpu time spent up to now is        33.9 secs

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        total cpu time spent up to now is        34.1 secs

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        total cpu time spent up to now is        34.3 secs

Computing kpt #:    299  of    800
        total cpu time spent up to now is        34.4 secs

Computing kpt #:    300  of    800
        total cpu time spent up to now is        34.5 secs

Computing kpt #:    301  of    800
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Computing kpt #:    302  of    800
        total cpu time spent up to now is        34.6 secs

Computing kpt #:    303  of    800
        total cpu time spent up to now is        34.7 secs

Computing kpt #:    304  of    800
        total cpu time spent up to now is        34.8 secs
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Computing kpt #:   305  of   800
total cpu time spent up to now is      34.9 secs

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total cpu time spent up to now is      35.1 secs

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total cpu time spent up to now is      35.9 secs

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total cpu time spent up to now is      36.0 secs

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total cpu time spent up to now is      36.1 secs

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total cpu time spent up to now is      36.3 secs

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total cpu time spent up to now is      36.4 secs

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total cpu time spent up to now is      36.5 secs

Computing kpt #:   320  of   800
total cpu time spent up to now is      36.6 secs

Computing kpt #:   321  of   800
total cpu time spent up to now is      36.7 secs

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total cpu time spent up to now is      36.8 secs

Computing kpt #:   323  of   800
total cpu time spent up to now is      36.9 secs

Computing kpt #:   324  of   800
total cpu time spent up to now is      37.0 secs

Computing kpt #:   325  of   800
total cpu time spent up to now is      37.0 secs
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Computing kpt #:   326  of   800
total cpu time spent up to now is       37.1 secs

Computing kpt #:   327  of   800
total cpu time spent up to now is       37.2 secs

Computing kpt #:   328  of   800
total cpu time spent up to now is       37.3 secs

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total cpu time spent up to now is       37.4 secs

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total cpu time spent up to now is       37.5 secs

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Computing kpt #:   332  of   800
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Computing kpt #:   333  of   800
total cpu time spent up to now is       37.7 secs

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total cpu time spent up to now is       38.0 secs

Computing kpt #:   336  of   800
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Computing kpt #:   338  of   800
total cpu time spent up to now is       38.2 secs

Computing kpt #:   339  of   800
total cpu time spent up to now is       38.4 secs

Computing kpt #:   340  of   800
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Computing kpt #:   344  of   800
total cpu time spent up to now is       38.9 secs

Computing kpt #:   345  of   800
total cpu time spent up to now is       39.0 secs

Computing kpt #:   346  of   800
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      total cpu time spent up to now is        39.1 secs

Computing kpt #:   347  of   800
      total cpu time spent up to now is        39.2 secs

Computing kpt #:   348  of   800
      total cpu time spent up to now is        39.4 secs

Computing kpt #:   349  of   800
      total cpu time spent up to now is        39.5 secs

Computing kpt #:   350  of   800
      total cpu time spent up to now is        39.6 secs

Computing kpt #:   351  of   800
      total cpu time spent up to now is        39.7 secs

Computing kpt #:   352  of   800
      total cpu time spent up to now is        39.8 secs

Computing kpt #:   353  of   800
      total cpu time spent up to now is        39.9 secs

Computing kpt #:   354  of   800
      total cpu time spent up to now is        40.0 secs

Computing kpt #:   355  of   800
      total cpu time spent up to now is        40.0 secs

Computing kpt #:   356  of   800
      total cpu time spent up to now is        40.1 secs

Computing kpt #:   357  of   800
      total cpu time spent up to now is        40.3 secs

Computing kpt #:   358  of   800
      total cpu time spent up to now is        40.3 secs

Computing kpt #:   359  of   800
      total cpu time spent up to now is        40.4 secs

Computing kpt #:   360  of   800
      total cpu time spent up to now is        40.5 secs

Computing kpt #:   361  of   800
      total cpu time spent up to now is        40.6 secs

Computing kpt #:   362  of   800
      total cpu time spent up to now is        40.7 secs

Computing kpt #:   363  of   800
      total cpu time spent up to now is        40.8 secs

Computing kpt #:   364  of   800
      total cpu time spent up to now is        40.9 secs

Computing kpt #:   365  of   800
      total cpu time spent up to now is        41.0 secs

Computing kpt #:   366  of   800
      total cpu time spent up to now is        41.0 secs
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Computing kpt #:    367  of    800
total cpu time spent up to now is        41.1 secs

Computing kpt #:    368  of    800
total cpu time spent up to now is        41.2 secs

Computing kpt #:    369  of    800
total cpu time spent up to now is        41.3 secs

Computing kpt #:    370  of    800
total cpu time spent up to now is        41.4 secs

Computing kpt #:    371  of    800
total cpu time spent up to now is        41.5 secs

Computing kpt #:    372  of    800
total cpu time spent up to now is        41.6 secs

Computing kpt #:    373  of    800
total cpu time spent up to now is        41.7 secs

Computing kpt #:    374  of    800
total cpu time spent up to now is        41.8 secs

Computing kpt #:    375  of    800
total cpu time spent up to now is        41.9 secs

Computing kpt #:    376  of    800
total cpu time spent up to now is        42.0 secs

Computing kpt #:    377  of    800
total cpu time spent up to now is        42.1 secs

Computing kpt #:    378  of    800
total cpu time spent up to now is        42.2 secs

Computing kpt #:    379  of    800
total cpu time spent up to now is        42.3 secs

Computing kpt #:    380  of    800
total cpu time spent up to now is        42.4 secs

Computing kpt #:    381  of    800
total cpu time spent up to now is        42.5 secs

Computing kpt #:    382  of    800
total cpu time spent up to now is        42.6 secs

Computing kpt #:    383  of    800
total cpu time spent up to now is        42.7 secs

Computing kpt #:    384  of    800
total cpu time spent up to now is        42.8 secs

Computing kpt #:    385  of    800
total cpu time spent up to now is        43.0 secs

Computing kpt #:    386  of    800
total cpu time spent up to now is        43.1 secs

Computing kpt #:    387  of    800
total cpu time spent up to now is        43.1 secs
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Computing kpt #:   388  of   800
total cpu time spent up to now is       43.2 secs

Computing kpt #:   389  of   800
total cpu time spent up to now is       43.4 secs

Computing kpt #:   390  of   800
total cpu time spent up to now is       43.5 secs

Computing kpt #:   391  of   800
total cpu time spent up to now is       43.6 secs

Computing kpt #:   392  of   800
total cpu time spent up to now is       43.7 secs

Computing kpt #:   393  of   800
total cpu time spent up to now is       43.8 secs

Computing kpt #:   394  of   800
total cpu time spent up to now is       43.9 secs

Computing kpt #:   395  of   800
total cpu time spent up to now is       43.9 secs

Computing kpt #:   396  of   800
total cpu time spent up to now is       44.1 secs

Computing kpt #:   397  of   800
total cpu time spent up to now is       44.1 secs

Computing kpt #:   398  of   800
total cpu time spent up to now is       44.2 secs

Computing kpt #:   399  of   800
total cpu time spent up to now is       44.3 secs

Computing kpt #:   400  of   800
total cpu time spent up to now is       44.4 secs

Computing kpt #:   401  of   800
total cpu time spent up to now is       44.5 secs

Computing kpt #:   402  of   800
total cpu time spent up to now is       44.6 secs

Computing kpt #:   403  of   800
total cpu time spent up to now is       44.7 secs

Computing kpt #:   404  of   800
total cpu time spent up to now is       44.8 secs

Computing kpt #:   405  of   800
total cpu time spent up to now is       44.9 secs

Computing kpt #:   406  of   800
total cpu time spent up to now is       44.9 secs

Computing kpt #:   407  of   800
total cpu time spent up to now is       45.0 secs

Computing kpt #:   408  of   800
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total cpu time spent up to now is        45.1 secs

Computing kpt #:    409  of    800
total cpu time spent up to now is        45.2 secs

Computing kpt #:    410  of    800
total cpu time spent up to now is        45.3 secs

Computing kpt #:    411  of    800
total cpu time spent up to now is        45.4 secs

Computing kpt #:    412  of    800
total cpu time spent up to now is        45.4 secs

Computing kpt #:    413  of    800
total cpu time spent up to now is        45.5 secs

Computing kpt #:    414  of    800
total cpu time spent up to now is        45.6 secs

Computing kpt #:    415  of    800
total cpu time spent up to now is        45.7 secs

Computing kpt #:    416  of    800
total cpu time spent up to now is        45.8 secs

Computing kpt #:    417  of    800
total cpu time spent up to now is        45.9 secs

Computing kpt #:    418  of    800
total cpu time spent up to now is        46.0 secs

Computing kpt #:    419  of    800
total cpu time spent up to now is        46.1 secs

Computing kpt #:    420  of    800
total cpu time spent up to now is        46.1 secs

Computing kpt #:    421  of    800
total cpu time spent up to now is        46.2 secs

Computing kpt #:    422  of    800
total cpu time spent up to now is        46.3 secs

Computing kpt #:    423  of    800
total cpu time spent up to now is        46.4 secs

Computing kpt #:    424  of    800
total cpu time spent up to now is        46.5 secs

Computing kpt #:    425  of    800
total cpu time spent up to now is        46.6 secs

Computing kpt #:    426  of    800
total cpu time spent up to now is        46.7 secs

Computing kpt #:    427  of    800
total cpu time spent up to now is        46.8 secs

Computing kpt #:    428  of    800
total cpu time spent up to now is        46.9 secs
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Computing kpt #:    429  of    800
total cpu time spent up to now is       47.0 secs

Computing kpt #:    430  of    800
total cpu time spent up to now is       47.1 secs

Computing kpt #:    431  of    800
total cpu time spent up to now is       47.1 secs

Computing kpt #:    432  of    800
total cpu time spent up to now is       47.2 secs

Computing kpt #:    433  of    800
total cpu time spent up to now is       47.3 secs

Computing kpt #:    434  of    800
total cpu time spent up to now is       47.4 secs

Computing kpt #:    435  of    800
total cpu time spent up to now is       47.5 secs

Computing kpt #:    436  of    800
total cpu time spent up to now is       47.6 secs

Computing kpt #:    437  of    800
total cpu time spent up to now is       47.7 secs

Computing kpt #:    438  of    800
total cpu time spent up to now is       47.8 secs

Computing kpt #:    439  of    800
total cpu time spent up to now is       47.9 secs

Computing kpt #:    440  of    800
total cpu time spent up to now is       48.0 secs

Computing kpt #:    441  of    800
total cpu time spent up to now is       48.1 secs

Computing kpt #:    442  of    800
total cpu time spent up to now is       48.1 secs

Computing kpt #:    443  of    800
total cpu time spent up to now is       48.2 secs

Computing kpt #:    444  of    800
total cpu time spent up to now is       48.4 secs

Computing kpt #:    445  of    800
total cpu time spent up to now is       48.4 secs

Computing kpt #:    446  of    800
total cpu time spent up to now is       48.5 secs

Computing kpt #:    447  of    800
total cpu time spent up to now is       48.6 secs

Computing kpt #:    448  of    800
total cpu time spent up to now is       48.8 secs

Computing kpt #:    449  of    800
total cpu time spent up to now is       48.9 secs
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Computing kpt #:   450  of   800
total cpu time spent up to now is       49.0 secs

Computing kpt #:   451  of   800
total cpu time spent up to now is       49.1 secs

Computing kpt #:   452  of   800
total cpu time spent up to now is       49.2 secs

Computing kpt #:   453  of   800
total cpu time spent up to now is       49.3 secs

Computing kpt #:   454  of   800
total cpu time spent up to now is       49.4 secs

Computing kpt #:   455  of   800
total cpu time spent up to now is       49.6 secs

Computing kpt #:   456  of   800
total cpu time spent up to now is       49.7 secs

Computing kpt #:   457  of   800
total cpu time spent up to now is       49.8 secs

Computing kpt #:   458  of   800
total cpu time spent up to now is       49.9 secs

Computing kpt #:   459  of   800
total cpu time spent up to now is       50.0 secs

Computing kpt #:   460  of   800
total cpu time spent up to now is       50.1 secs

Computing kpt #:   461  of   800
total cpu time spent up to now is       50.3 secs

Computing kpt #:   462  of   800
total cpu time spent up to now is       50.4 secs

Computing kpt #:   463  of   800
total cpu time spent up to now is       50.5 secs

Computing kpt #:   464  of   800
total cpu time spent up to now is       50.6 secs

Computing kpt #:   465  of   800
total cpu time spent up to now is       50.7 secs

Computing kpt #:   466  of   800
total cpu time spent up to now is       50.7 secs

Computing kpt #:   467  of   800
total cpu time spent up to now is       50.9 secs

Computing kpt #:   468  of   800
total cpu time spent up to now is       51.0 secs

Computing kpt #:   469  of   800
total cpu time spent up to now is       51.1 secs

Computing kpt #:   470  of   800
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total cpu time spent up to now is        51.2 secs

Computing kpt #:    471  of    800
total cpu time spent up to now is        51.3 secs

Computing kpt #:    472  of    800
total cpu time spent up to now is        51.4 secs

Computing kpt #:    473  of    800
total cpu time spent up to now is        51.5 secs

Computing kpt #:    474  of    800
total cpu time spent up to now is        51.6 secs

Computing kpt #:    475  of    800
total cpu time spent up to now is        51.7 secs

Computing kpt #:    476  of    800
total cpu time spent up to now is        51.7 secs

Computing kpt #:    477  of    800
total cpu time spent up to now is        51.8 secs

Computing kpt #:    478  of    800
total cpu time spent up to now is        51.9 secs

Computing kpt #:    479  of    800
total cpu time spent up to now is        52.0 secs

Computing kpt #:    480  of    800
total cpu time spent up to now is        52.1 secs

Computing kpt #:    481  of    800
total cpu time spent up to now is        52.2 secs

Computing kpt #:    482  of    800
total cpu time spent up to now is        52.3 secs

Computing kpt #:    483  of    800
total cpu time spent up to now is        52.4 secs

Computing kpt #:    484  of    800
total cpu time spent up to now is        52.5 secs

Computing kpt #:    485  of    800
total cpu time spent up to now is        52.6 secs

Computing kpt #:    486  of    800
total cpu time spent up to now is        52.7 secs

Computing kpt #:    487  of    800
total cpu time spent up to now is        52.8 secs

Computing kpt #:    488  of    800
total cpu time spent up to now is        52.9 secs

Computing kpt #:    489  of    800
total cpu time spent up to now is        53.0 secs

Computing kpt #:    490  of    800
total cpu time spent up to now is        53.1 secs
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Computing kpt #:   491  of   800
total cpu time spent up to now is       53.2 secs

Computing kpt #:   492  of   800
total cpu time spent up to now is       53.3 secs

Computing kpt #:   493  of   800
total cpu time spent up to now is       53.4 secs

Computing kpt #:   494  of   800
total cpu time spent up to now is       53.5 secs

Computing kpt #:   495  of   800
total cpu time spent up to now is       53.6 secs

Computing kpt #:   496  of   800
total cpu time spent up to now is       53.7 secs

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total cpu time spent up to now is       53.8 secs

Computing kpt #:   498  of   800
total cpu time spent up to now is       53.9 secs

Computing kpt #:   499  of   800
total cpu time spent up to now is       54.0 secs

Computing kpt #:   500  of   800
total cpu time spent up to now is       54.1 secs

Computing kpt #:   501  of   800
total cpu time spent up to now is       54.2 secs

Computing kpt #:   502  of   800
total cpu time spent up to now is       54.3 secs

Computing kpt #:   503  of   800
total cpu time spent up to now is       54.4 secs

Computing kpt #:   504  of   800
total cpu time spent up to now is       54.5 secs

Computing kpt #:   505  of   800
total cpu time spent up to now is       54.6 secs

Computing kpt #:   506  of   800
total cpu time spent up to now is       54.7 secs

Computing kpt #:   507  of   800
total cpu time spent up to now is       54.8 secs

Computing kpt #:   508  of   800
total cpu time spent up to now is       54.9 secs

Computing kpt #:   509  of   800
total cpu time spent up to now is       55.0 secs

Computing kpt #:   510  of   800
total cpu time spent up to now is       55.1 secs

Computing kpt #:   511  of   800
total cpu time spent up to now is       55.2 secs
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Computing kpt #:    512  of    800
total cpu time spent up to now is        55.3 secs

Computing kpt #:    513  of    800
total cpu time spent up to now is        55.4 secs

Computing kpt #:    514  of    800
total cpu time spent up to now is        55.5 secs

Computing kpt #:    515  of    800
total cpu time spent up to now is        55.6 secs

Computing kpt #:    516  of    800
total cpu time spent up to now is        55.7 secs

Computing kpt #:    517  of    800
total cpu time spent up to now is        55.8 secs

Computing kpt #:    518  of    800
total cpu time spent up to now is        55.9 secs

Computing kpt #:    519  of    800
total cpu time spent up to now is        56.0 secs

Computing kpt #:    520  of    800
total cpu time spent up to now is        56.1 secs

Computing kpt #:    521  of    800
total cpu time spent up to now is        56.2 secs

Computing kpt #:    522  of    800
total cpu time spent up to now is        56.3 secs

Computing kpt #:    523  of    800
total cpu time spent up to now is        56.4 secs

Computing kpt #:    524  of    800
total cpu time spent up to now is        56.5 secs

Computing kpt #:    525  of    800
total cpu time spent up to now is        56.6 secs

Computing kpt #:    526  of    800
total cpu time spent up to now is        56.7 secs

Computing kpt #:    527  of    800
total cpu time spent up to now is        56.8 secs

Computing kpt #:    528  of    800
total cpu time spent up to now is        56.9 secs

Computing kpt #:    529  of    800
total cpu time spent up to now is        57.0 secs

Computing kpt #:    530  of    800
total cpu time spent up to now is        57.2 secs

Computing kpt #:    531  of    800
total cpu time spent up to now is        57.3 secs

Computing kpt #:    532  of    800
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total cpu time spent up to now is        57.4 secs

Computing kpt #:   533  of   800
total cpu time spent up to now is        57.5 secs

Computing kpt #:   534  of   800
total cpu time spent up to now is        57.7 secs

Computing kpt #:   535  of   800
total cpu time spent up to now is        57.8 secs

Computing kpt #:   536  of   800
total cpu time spent up to now is        57.9 secs

Computing kpt #:   537  of   800
total cpu time spent up to now is        58.0 secs

Computing kpt #:   538  of   800
total cpu time spent up to now is        58.1 secs

Computing kpt #:   539  of   800
total cpu time spent up to now is        58.2 secs

Computing kpt #:   540  of   800
total cpu time spent up to now is        58.3 secs

Computing kpt #:   541  of   800
total cpu time spent up to now is        58.4 secs

Computing kpt #:   542  of   800
total cpu time spent up to now is        58.5 secs

Computing kpt #:   543  of   800
total cpu time spent up to now is        58.6 secs

Computing kpt #:   544  of   800
total cpu time spent up to now is        58.7 secs

Computing kpt #:   545  of   800
total cpu time spent up to now is        58.8 secs

Computing kpt #:   546  of   800
total cpu time spent up to now is        58.9 secs

Computing kpt #:   547  of   800
total cpu time spent up to now is        59.0 secs

Computing kpt #:   548  of   800
total cpu time spent up to now is        59.1 secs

Computing kpt #:   549  of   800
total cpu time spent up to now is        59.2 secs

Computing kpt #:   550  of   800
total cpu time spent up to now is        59.3 secs

Computing kpt #:   551  of   800
total cpu time spent up to now is        59.5 secs

Computing kpt #:   552  of   800
total cpu time spent up to now is        59.6 secs
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Computing kpt #:   553  of   800
total cpu time spent up to now is       59.7 secs

Computing kpt #:   554  of   800
total cpu time spent up to now is       59.8 secs

Computing kpt #:   555  of   800
total cpu time spent up to now is       59.9 secs

Computing kpt #:   556  of   800
total cpu time spent up to now is       60.0 secs

Computing kpt #:   557  of   800
total cpu time spent up to now is       60.1 secs

Computing kpt #:   558  of   800
total cpu time spent up to now is       60.2 secs

Computing kpt #:   559  of   800
total cpu time spent up to now is       60.3 secs

Computing kpt #:   560  of   800
total cpu time spent up to now is       60.4 secs

Computing kpt #:   561  of   800
total cpu time spent up to now is       60.5 secs

Computing kpt #:   562  of   800
total cpu time spent up to now is       60.6 secs

Computing kpt #:   563  of   800
total cpu time spent up to now is       60.7 secs

Computing kpt #:   564  of   800
total cpu time spent up to now is       60.8 secs

Computing kpt #:   565  of   800
total cpu time spent up to now is       60.9 secs

Computing kpt #:   566  of   800
total cpu time spent up to now is       61.0 secs

Computing kpt #:   567  of   800
total cpu time spent up to now is       61.1 secs

Computing kpt #:   568  of   800
total cpu time spent up to now is       61.2 secs

Computing kpt #:   569  of   800
total cpu time spent up to now is       61.4 secs

Computing kpt #:   570  of   800
total cpu time spent up to now is       61.5 secs

Computing kpt #:   571  of   800
total cpu time spent up to now is       61.6 secs

Computing kpt #:   572  of   800
total cpu time spent up to now is       61.7 secs

Computing kpt #:   573  of   800
total cpu time spent up to now is       61.8 secs
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Computing kpt #:   574  of   800
total cpu time spent up to now is      61.9 secs

Computing kpt #:   575  of   800
total cpu time spent up to now is      62.0 secs

Computing kpt #:   576  of   800
total cpu time spent up to now is      62.1 secs

Computing kpt #:   577  of   800
total cpu time spent up to now is      62.3 secs

Computing kpt #:   578  of   800
total cpu time spent up to now is      62.4 secs

Computing kpt #:   579  of   800
total cpu time spent up to now is      62.5 secs

Computing kpt #:   580  of   800
total cpu time spent up to now is      62.6 secs

Computing kpt #:   581  of   800
total cpu time spent up to now is      62.7 secs

Computing kpt #:   582  of   800
total cpu time spent up to now is      62.8 secs

Computing kpt #:   583  of   800
total cpu time spent up to now is      62.9 secs

Computing kpt #:   584  of   800
total cpu time spent up to now is      63.0 secs

Computing kpt #:   585  of   800
total cpu time spent up to now is      63.2 secs

Computing kpt #:   586  of   800
total cpu time spent up to now is      63.3 secs

Computing kpt #:   587  of   800
total cpu time spent up to now is      63.4 secs

Computing kpt #:   588  of   800
total cpu time spent up to now is      63.5 secs

Computing kpt #:   589  of   800
total cpu time spent up to now is      63.7 secs

Computing kpt #:   590  of   800
total cpu time spent up to now is      63.8 secs

Computing kpt #:   591  of   800
total cpu time spent up to now is      63.9 secs

Computing kpt #:   592  of   800
total cpu time spent up to now is      64.1 secs

Computing kpt #:   593  of   800
total cpu time spent up to now is      64.2 secs

Computing kpt #:   594  of   800
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     total cpu time spent up to now is        64.3 secs

Computing kpt #:    595  of    800
     total cpu time spent up to now is        64.5 secs

Computing kpt #:    596  of    800
     total cpu time spent up to now is        64.6 secs

Computing kpt #:    597  of    800
     total cpu time spent up to now is        64.7 secs

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     total cpu time spent up to now is        64.8 secs

Computing kpt #:    599  of    800
     total cpu time spent up to now is        64.9 secs

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Computing kpt #:    601  of    800
     total cpu time spent up to now is        65.1 secs

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     total cpu time spent up to now is        65.4 secs

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     total cpu time spent up to now is        65.5 secs

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     total cpu time spent up to now is        65.7 secs

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     total cpu time spent up to now is        65.8 secs

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     total cpu time spent up to now is        65.9 secs

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     total cpu time spent up to now is        66.2 secs

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     total cpu time spent up to now is        66.4 secs

Computing kpt #:    613  of    800
     total cpu time spent up to now is        66.5 secs

Computing kpt #:    614  of    800
     total cpu time spent up to now is        66.6 secs
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Computing kpt #:   615  of   800
total cpu time spent up to now is       66.7 secs

Computing kpt #:   616  of   800
total cpu time spent up to now is       66.8 secs

Computing kpt #:   617  of   800
total cpu time spent up to now is       67.0 secs

Computing kpt #:   618  of   800
total cpu time spent up to now is       67.1 secs

Computing kpt #:   619  of   800
total cpu time spent up to now is       67.2 secs

Computing kpt #:   620  of   800
total cpu time spent up to now is       67.3 secs

Computing kpt #:   621  of   800
total cpu time spent up to now is       67.4 secs

Computing kpt #:   622  of   800
total cpu time spent up to now is       67.5 secs

Computing kpt #:   623  of   800
total cpu time spent up to now is       67.6 secs

Computing kpt #:   624  of   800
total cpu time spent up to now is       67.7 secs

Computing kpt #:   625  of   800
total cpu time spent up to now is       67.9 secs

Computing kpt #:   626  of   800
total cpu time spent up to now is       68.0 secs

Computing kpt #:   627  of   800
total cpu time spent up to now is       68.1 secs

Computing kpt #:   628  of   800
total cpu time spent up to now is       68.2 secs

Computing kpt #:   629  of   800
total cpu time spent up to now is       68.3 secs

Computing kpt #:   630  of   800
total cpu time spent up to now is       68.4 secs

Computing kpt #:   631  of   800
total cpu time spent up to now is       68.5 secs

Computing kpt #:   632  of   800
total cpu time spent up to now is       68.7 secs

Computing kpt #:   633  of   800
total cpu time spent up to now is       68.8 secs

Computing kpt #:   634  of   800
total cpu time spent up to now is       68.9 secs

Computing kpt #:   635  of   800
total cpu time spent up to now is       69.0 secs
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Computing kpt #:   636  of   800
total cpu time spent up to now is        69.1 secs

Computing kpt #:   637  of   800
total cpu time spent up to now is        69.2 secs

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total cpu time spent up to now is        69.3 secs

Computing kpt #:   639  of   800
total cpu time spent up to now is        69.4 secs

Computing kpt #:   640  of   800
total cpu time spent up to now is        69.5 secs

Computing kpt #:   641  of   800
total cpu time spent up to now is        69.7 secs

Computing kpt #:   642  of   800
total cpu time spent up to now is        69.8 secs

Computing kpt #:   643  of   800
total cpu time spent up to now is        69.9 secs

Computing kpt #:   644  of   800
total cpu time spent up to now is        70.0 secs

Computing kpt #:   645  of   800
total cpu time spent up to now is        70.1 secs

Computing kpt #:   646  of   800
total cpu time spent up to now is        70.2 secs

Computing kpt #:   647  of   800
total cpu time spent up to now is        70.4 secs

Computing kpt #:   648  of   800
total cpu time spent up to now is        70.5 secs

Computing kpt #:   649  of   800
total cpu time spent up to now is        70.6 secs

Computing kpt #:   650  of   800
total cpu time spent up to now is        70.7 secs

Computing kpt #:   651  of   800
total cpu time spent up to now is        70.8 secs

Computing kpt #:   652  of   800
total cpu time spent up to now is        70.9 secs

Computing kpt #:   653  of   800
total cpu time spent up to now is        71.0 secs

Computing kpt #:   654  of   800
total cpu time spent up to now is        71.1 secs

Computing kpt #:   655  of   800
total cpu time spent up to now is        71.2 secs

Computing kpt #:   656  of   800
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total cpu time spent up to now is        71.4 secs

Computing kpt #:    657  of    800
total cpu time spent up to now is        71.5 secs

Computing kpt #:    658  of    800
total cpu time spent up to now is        71.6 secs

Computing kpt #:    659  of    800
total cpu time spent up to now is        71.7 secs

Computing kpt #:    660  of    800
total cpu time spent up to now is        71.8 secs

Computing kpt #:    661  of    800
total cpu time spent up to now is        71.9 secs

Computing kpt #:    662  of    800
total cpu time spent up to now is        72.0 secs

Computing kpt #:    663  of    800
total cpu time spent up to now is        72.1 secs

Computing kpt #:    664  of    800
total cpu time spent up to now is        72.2 secs

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total cpu time spent up to now is        72.3 secs

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total cpu time spent up to now is        72.4 secs

Computing kpt #:    667  of    800
total cpu time spent up to now is        72.5 secs

Computing kpt #:    668  of    800
total cpu time spent up to now is        72.6 secs

Computing kpt #:    669  of    800
total cpu time spent up to now is        72.7 secs

Computing kpt #:    670  of    800
total cpu time spent up to now is        72.8 secs

Computing kpt #:    671  of    800
total cpu time spent up to now is        72.9 secs

Computing kpt #:    672  of    800
total cpu time spent up to now is        73.0 secs

Computing kpt #:    673  of    800
total cpu time spent up to now is        73.1 secs

Computing kpt #:    674  of    800
total cpu time spent up to now is        73.2 secs

Computing kpt #:    675  of    800
total cpu time spent up to now is        73.3 secs

Computing kpt #:    676  of    800
total cpu time spent up to now is        73.4 secs
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Computing kpt #:   677  of   800
total cpu time spent up to now is      73.5 secs

Computing kpt #:   678  of   800
total cpu time spent up to now is      73.6 secs

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total cpu time spent up to now is      73.7 secs

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total cpu time spent up to now is      73.8 secs

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total cpu time spent up to now is      73.9 secs

Computing kpt #:   682  of   800
total cpu time spent up to now is      74.0 secs

Computing kpt #:   683  of   800
total cpu time spent up to now is      74.1 secs

Computing kpt #:   684  of   800
total cpu time spent up to now is      74.2 secs

Computing kpt #:   685  of   800
total cpu time spent up to now is      74.3 secs

Computing kpt #:   686  of   800
total cpu time spent up to now is      74.4 secs

Computing kpt #:   687  of   800
total cpu time spent up to now is      74.5 secs

Computing kpt #:   688  of   800
total cpu time spent up to now is      74.6 secs

Computing kpt #:   689  of   800
total cpu time spent up to now is      74.7 secs

Computing kpt #:   690  of   800
total cpu time spent up to now is      74.8 secs

Computing kpt #:   691  of   800
total cpu time spent up to now is      74.9 secs

Computing kpt #:   692  of   800
total cpu time spent up to now is      75.0 secs

Computing kpt #:   693  of   800
total cpu time spent up to now is      75.1 secs

Computing kpt #:   694  of   800
total cpu time spent up to now is      75.2 secs

Computing kpt #:   695  of   800
total cpu time spent up to now is      75.3 secs

Computing kpt #:   696  of   800
total cpu time spent up to now is      75.4 secs

Computing kpt #:   697  of   800
total cpu time spent up to now is      75.5 secs
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Computing kpt #:    698  of    800
total cpu time spent up to now is        75.5 secs

Computing kpt #:    699  of    800
total cpu time spent up to now is        75.6 secs

Computing kpt #:    700  of    800
total cpu time spent up to now is        75.7 secs

Computing kpt #:    701  of    800
total cpu time spent up to now is        75.8 secs

Computing kpt #:    702  of    800
total cpu time spent up to now is        75.9 secs

Computing kpt #:    703  of    800
total cpu time spent up to now is        76.0 secs

Computing kpt #:    704  of    800
total cpu time spent up to now is        76.1 secs

Computing kpt #:    705  of    800
total cpu time spent up to now is        76.2 secs

Computing kpt #:    706  of    800
total cpu time spent up to now is        76.3 secs

Computing kpt #:    707  of    800
total cpu time spent up to now is        76.4 secs

Computing kpt #:    708  of    800
total cpu time spent up to now is        76.5 secs

Computing kpt #:    709  of    800
total cpu time spent up to now is        76.6 secs

Computing kpt #:    710  of    800
total cpu time spent up to now is        76.7 secs

Computing kpt #:    711  of    800
total cpu time spent up to now is        76.8 secs

Computing kpt #:    712  of    800
total cpu time spent up to now is        76.9 secs

Computing kpt #:    713  of    800
total cpu time spent up to now is        77.0 secs

Computing kpt #:    714  of    800
total cpu time spent up to now is        77.1 secs

Computing kpt #:    715  of    800
total cpu time spent up to now is        77.2 secs

Computing kpt #:    716  of    800
total cpu time spent up to now is        77.3 secs

Computing kpt #:    717  of    800
total cpu time spent up to now is        77.4 secs

Computing kpt #:    718  of    800
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total cpu time spent up to now is        77.5 secs

Computing kpt #:    719  of    800
total cpu time spent up to now is        77.6 secs

Computing kpt #:    720  of    800
total cpu time spent up to now is        77.7 secs

Computing kpt #:    721  of    800
total cpu time spent up to now is        77.8 secs

Computing kpt #:    722  of    800
total cpu time spent up to now is        77.9 secs

Computing kpt #:    723  of    800
total cpu time spent up to now is        78.0 secs

Computing kpt #:    724  of    800
total cpu time spent up to now is        78.1 secs

Computing kpt #:    725  of    800
total cpu time spent up to now is        78.2 secs

Computing kpt #:    726  of    800
total cpu time spent up to now is        78.3 secs

Computing kpt #:    727  of    800
total cpu time spent up to now is        78.4 secs

Computing kpt #:    728  of    800
total cpu time spent up to now is        78.5 secs

Computing kpt #:    729  of    800
total cpu time spent up to now is        78.6 secs

Computing kpt #:    730  of    800
total cpu time spent up to now is        78.7 secs

Computing kpt #:    731  of    800
total cpu time spent up to now is        78.9 secs

Computing kpt #:    732  of    800
total cpu time spent up to now is        79.0 secs

Computing kpt #:    733  of    800
total cpu time spent up to now is        79.0 secs

Computing kpt #:    734  of    800
total cpu time spent up to now is        79.1 secs

Computing kpt #:    735  of    800
total cpu time spent up to now is        79.2 secs

Computing kpt #:    736  of    800
total cpu time spent up to now is        79.3 secs

Computing kpt #:    737  of    800
total cpu time spent up to now is        79.4 secs

Computing kpt #:    738  of    800
total cpu time spent up to now is        79.5 secs
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Computing kpt #:    739  of    800
total cpu time spent up to now is        79.6 secs

Computing kpt #:    740  of    800
total cpu time spent up to now is        79.7 secs

Computing kpt #:    741  of    800
total cpu time spent up to now is        79.8 secs

Computing kpt #:    742  of    800
total cpu time spent up to now is        79.9 secs

Computing kpt #:    743  of    800
total cpu time spent up to now is        80.0 secs

Computing kpt #:    744  of    800
total cpu time spent up to now is        80.1 secs

Computing kpt #:    745  of    800
total cpu time spent up to now is        80.2 secs

Computing kpt #:    746  of    800
total cpu time spent up to now is        80.3 secs

Computing kpt #:    747  of    800
total cpu time spent up to now is        80.4 secs

Computing kpt #:    748  of    800
total cpu time spent up to now is        80.6 secs

Computing kpt #:    749  of    800
total cpu time spent up to now is        80.7 secs

Computing kpt #:    750  of    800
total cpu time spent up to now is        80.8 secs

Computing kpt #:    751  of    800
total cpu time spent up to now is        80.9 secs

Computing kpt #:    752  of    800
total cpu time spent up to now is        81.0 secs

Computing kpt #:    753  of    800
total cpu time spent up to now is        81.1 secs

Computing kpt #:    754  of    800
total cpu time spent up to now is        81.2 secs

Computing kpt #:    755  of    800
total cpu time spent up to now is        81.3 secs

Computing kpt #:    756  of    800
total cpu time spent up to now is        81.4 secs

Computing kpt #:    757  of    800
total cpu time spent up to now is        81.4 secs

Computing kpt #:    758  of    800
total cpu time spent up to now is        81.5 secs

Computing kpt #:    759  of    800
total cpu time spent up to now is        81.6 secs
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Computing kpt #:   760  of   800
total cpu time spent up to now is       81.7 secs

Computing kpt #:   761  of   800
total cpu time spent up to now is       81.8 secs

Computing kpt #:   762  of   800
total cpu time spent up to now is       81.9 secs

Computing kpt #:   763  of   800
total cpu time spent up to now is       82.0 secs

Computing kpt #:   764  of   800
total cpu time spent up to now is       82.1 secs

Computing kpt #:   765  of   800
total cpu time spent up to now is       82.1 secs

Computing kpt #:   766  of   800
total cpu time spent up to now is       82.2 secs

Computing kpt #:   767  of   800
total cpu time spent up to now is       82.3 secs

Computing kpt #:   768  of   800
total cpu time spent up to now is       82.4 secs

Computing kpt #:   769  of   800
total cpu time spent up to now is       82.5 secs

Computing kpt #:   770  of   800
total cpu time spent up to now is       82.6 secs

Computing kpt #:   771  of   800
total cpu time spent up to now is       82.7 secs

Computing kpt #:   772  of   800
total cpu time spent up to now is       82.7 secs

Computing kpt #:   773  of   800
total cpu time spent up to now is       82.8 secs

Computing kpt #:   774  of   800
total cpu time spent up to now is       82.9 secs

Computing kpt #:   775  of   800
total cpu time spent up to now is       83.0 secs

Computing kpt #:   776  of   800
total cpu time spent up to now is       83.1 secs

Computing kpt #:   777  of   800
total cpu time spent up to now is       83.2 secs

Computing kpt #:   778  of   800
total cpu time spent up to now is       83.2 secs

Computing kpt #:   779  of   800
total cpu time spent up to now is       83.3 secs

Computing kpt #:   780  of   800
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    total cpu time spent up to now is        83.4 secs

Computing kpt #:   781  of    800
    total cpu time spent up to now is        83.5 secs

Computing kpt #:   782  of    800
    total cpu time spent up to now is        83.6 secs

Computing kpt #:   783  of    800
    total cpu time spent up to now is        83.7 secs

Computing kpt #:   784  of    800
    total cpu time spent up to now is        83.8 secs

Computing kpt #:   785  of    800
    total cpu time spent up to now is        83.9 secs

Computing kpt #:   786  of    800
    total cpu time spent up to now is        84.0 secs

Computing kpt #:   787  of    800
    total cpu time spent up to now is        84.1 secs

Computing kpt #:   788  of    800
    total cpu time spent up to now is        84.2 secs

Computing kpt #:   789  of    800
    total cpu time spent up to now is        84.3 secs

Computing kpt #:   790  of    800
    total cpu time spent up to now is        84.4 secs

Computing kpt #:   791  of    800
    total cpu time spent up to now is        84.5 secs

Computing kpt #:   792  of    800
    total cpu time spent up to now is        84.6 secs

Computing kpt #:   793  of    800
    total cpu time spent up to now is        84.7 secs

Computing kpt #:   794  of    800
    total cpu time spent up to now is        84.8 secs

Computing kpt #:   795  of    800
    total cpu time spent up to now is        84.9 secs

Computing kpt #:   796  of    800
    total cpu time spent up to now is        85.0 secs

Computing kpt #:   797  of    800
    total cpu time spent up to now is        85.1 secs

Computing kpt #:   798  of    800
    total cpu time spent up to now is        85.1 secs

Computing kpt #:   799  of    800
    total cpu time spent up to now is        85.2 secs

Computing kpt #:   800  of    800
    total cpu time spent up to now is        85.3 secs
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    ethr =  1.25E-10,  avg # of iterations = 21.8

    total cpu time spent up to now is       85.3 secs

    End of band structure calculation
 ------ SPIN UP ------------


       k = 0.0000 0.0000 0.0000 (  1205 PWs)   bands (ev):

  -18.7874  -6.3756  -2.5513  -2.5513   3.0788   6.2375   7.8080  10.3196

       k = 0.0034 0.0020 0.0000 (  1205 PWs)   bands (ev):

  -18.7871  -6.3753  -2.5523  -2.5518   3.0792   6.2378   7.8084  10.3195

       k = 0.0068 0.0040 0.0000 (  1205 PWs)   bands (ev):

  -18.7865  -6.3744  -2.5553  -2.5531   3.0803   6.2387   7.8097  10.3191

       k = 0.0103 0.0059 0.0000 (  1201 PWs)   bands (ev):

  -18.7853  -6.3729  -2.5601  -2.5554   3.0823   6.2401   7.8118  10.3185

       k = 0.0137 0.0079 0.0000 (  1193 PWs)   bands (ev):

  -18.7838  -6.3708  -2.5669  -2.5585   3.0850   6.2421   7.8148  10.3180

       k = 0.0171 0.0099 0.0000 (  1189 PWs)   bands (ev):

  -18.7817  -6.3680  -2.5757  -2.5626   3.0885   6.2447   7.8185  10.3169

       k = 0.0205 0.0119 0.0000 (  1189 PWs)   bands (ev):

  -18.7793  -6.3647  -2.5865  -2.5676   3.0928   6.2478   7.8231  10.3155

       k = 0.0240 0.0138 0.0000 (  1187 PWs)   bands (ev):

  -18.7763  -6.3607  -2.5994  -2.5734   3.0979   6.2515   7.8286  10.3137

       k = 0.0274 0.0158 0.0000 (  1187 PWs)   bands (ev):

  -18.7730  -6.3562  -2.6140  -2.5802   3.1037   6.2558   7.8348  10.3118

       k = 0.0308 0.0178 0.0000 (  1183 PWs)   bands (ev):

  -18.7692  -6.3511  -2.6306  -2.5878   3.1104   6.2606   7.8419  10.3098

       k = 0.0342 0.0198 0.0000 (  1189 PWs)   bands (ev):

  -18.7649  -6.3454  -2.6491  -2.5963   3.1177   6.2660   7.8498  10.3072

       k = 0.0377 0.0217 0.0000 (  1189 PWs)   bands (ev):

  -18.7602  -6.3391  -2.6695  -2.6057   3.1259   6.2719   7.8584  10.3048

       k = 0.0411 0.0237 0.0000 (  1189 PWs)   bands (ev):

  -18.7551  -6.3321  -2.6917  -2.6159   3.1348   6.2784   7.8678  10.3021

       k = 0.0445 0.0257 0.0000 (  1189 PWs)   bands (ev):
```

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-18.7495   -6.3246   -2.7157   -2.6270    3.1445    6.2854    7.8780   10.2992
        k = 0.0479 0.0277 0.0000 (   1193 PWs)    bands (ev):
-18.7434   -6.3165   -2.7415   -2.6390    3.1549    6.2930    7.8890   10.2960
        k = 0.0514 0.0297 0.0000 (   1191 PWs)    bands (ev):
-18.7369   -6.3078   -2.7691   -2.6517    3.1661    6.3011    7.9007   10.2932
        k = 0.0548 0.0316 0.0000 (   1191 PWs)    bands (ev):
-18.7300   -6.2985   -2.7984   -2.6652    3.1781    6.3098    7.9132   10.2898
        k = 0.0582 0.0336 0.0000 (   1191 PWs)    bands (ev):
-18.7226   -6.2886   -2.8295   -2.6795    3.1908    6.3190    7.9263   10.2863
        k = 0.0616 0.0356 0.0000 (   1187 PWs)    bands (ev):
-18.7148   -6.2780   -2.8622   -2.6944    3.2043    6.3287    7.9402   10.2827
        k = 0.0651 0.0376 0.0000 (   1191 PWs)    bands (ev):
-18.7065   -6.2670   -2.8966   -2.7102    3.2185    6.3390    7.9547   10.2789
        k = 0.0685 0.0395 0.0000 (   1191 PWs)    bands (ev):
-18.6978   -6.2553   -2.9327   -2.7267    3.2334    6.3498    7.9700   10.2751
        k = 0.0719 0.0415 0.0000 (   1191 PWs)    bands (ev):
-18.6887   -6.2430   -2.9703   -2.7440    3.2491    6.3611    7.9858   10.2712
        k = 0.0753 0.0435 0.0000 (   1191 PWs)    bands (ev):
-18.6791   -6.2301   -3.0095   -2.7619    3.2655    6.3729    8.0023   10.2672
        k = 0.0788 0.0455 0.0000 (   1191 PWs)    bands (ev):
-18.6691   -6.2166   -3.0503   -2.7805    3.2827    6.3851    8.0195   10.2631
        k = 0.0822 0.0475 0.0000 (   1191 PWs)    bands (ev):
-18.6586   -6.2025   -3.0925   -2.7998    3.3006    6.3979    8.0372   10.2590
        k = 0.0856 0.0494 0.0000 (   1191 PWs)    bands (ev):
-18.6477   -6.1879   -3.1362   -2.8197    3.3192    6.4112    8.0555   10.2549
        k = 0.0890 0.0514 0.0000 (   1191 PWs)    bands (ev):
-18.6364   -6.1726   -3.1813   -2.8402    3.3385    6.4249    8.0744   10.2508
        k = 0.0925 0.0534 0.0000 (   1191 PWs)    bands (ev):
-18.6246   -6.1568   -3.2278   -2.8613    3.3586    6.4391    8.0938   10.2468
        k = 0.0959 0.0554 0.0000 (   1191 PWs)    bands (ev):
-18.6124   -6.1404   -3.2756   -2.8830    3.3794    6.4538    8.1137   10.2427
```

```
       k = 0.0993 0.0573 0.0000 (  1189 PWs)    bands (ev):

 -18.5997  -6.1234  -3.3248  -2.9052    3.4009    6.4689    8.1342   10.2389
       k = 0.1027 0.0593 0.0000 (  1187 PWs)    bands (ev):

 -18.5867  -6.1058  -3.3752  -2.9280    3.4231    6.4844    8.1551   10.2354
       k = 0.1062 0.0613 0.0000 (  1187 PWs)    bands (ev):

 -18.5732  -6.0876  -3.4269  -2.9513    3.4461    6.5003    8.1764   10.2316
       k = 0.1096 0.0633 0.0000 (  1187 PWs)    bands (ev):

 -18.5592  -6.0689  -3.4798  -2.9752    3.4697    6.5167    8.1982   10.2280
       k = 0.1130 0.0652 0.0000 (  1187 PWs)    bands (ev):

 -18.5449  -6.0496  -3.5339  -2.9995    3.4941    6.5334    8.2204   10.2245
       k = 0.1164 0.0672 0.0000 (  1187 PWs)    bands (ev):

 -18.5301  -6.0296  -3.5891  -3.0243    3.5192    6.5505    8.2429   10.2212
       k = 0.1199 0.0692 0.0000 (  1189 PWs)    bands (ev):

 -18.5149  -6.0092  -3.6455  -3.0495    3.5449    6.5679    8.2658   10.2179
       k = 0.1233 0.0712 0.0000 (  1189 PWs)    bands (ev):

 -18.4992  -5.9881  -3.7029  -3.0751    3.5714    6.5857    8.2890   10.2151
       k = 0.1267 0.0732 0.0000 (  1189 PWs)    bands (ev):

 -18.4832  -5.9665  -3.7613  -3.1012    3.5986    6.6037    8.3125   10.2125
       k = 0.1301 0.0751 0.0000 (  1189 PWs)    bands (ev):

 -18.4667  -5.9443  -3.8207  -3.1276    3.6264    6.6221    8.3362   10.2102
       k = 0.1336 0.0771 0.0000 (  1187 PWs)    bands (ev):

 -18.4498  -5.9215  -3.8810  -3.1543    3.6550    6.6407    8.3602   10.2087
       k = 0.1370 0.0791 0.0000 (  1187 PWs)    bands (ev):

 -18.4325  -5.8982  -3.9423  -3.1814    3.6843    6.6595    8.3843   10.2071
       k = 0.1404 0.0811 0.0000 (  1187 PWs)    bands (ev):

 -18.4148  -5.8743  -4.0045  -3.2089    3.7142    6.6786    8.4086   10.2059
       k = 0.1438 0.0830 0.0000 (  1186 PWs)    bands (ev):

 -18.3967  -5.8498  -4.0675  -3.2366    3.7449    6.6978    8.4331   10.2054
       k = 0.1473 0.0850 0.0000 (  1186 PWs)    bands (ev):

 -18.3781  -5.8248  -4.1313  -3.2646    3.7762    6.7171    8.4576   10.2051
       k = 0.1507 0.0870 0.0000 (  1186 PWs)    bands (ev):
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-18.3592   -5.7992   -4.1959   -3.2928    3.8083    6.7366    8.4821   10.2054
        k = 0.1541 0.0890 0.0000 (   1186 PWs)    bands (ev):
-18.3398   -5.7731   -4.2613   -3.3213    3.8410    6.7561    8.5066   10.2063
        k = 0.1575 0.0910 0.0000 (   1186 PWs)    bands (ev):
-18.3201   -5.7464   -4.3274   -3.3500    3.8744    6.7756    8.5311   10.2078
        k = 0.1610 0.0929 0.0000 (   1182 PWs)    bands (ev):
-18.2999   -5.7192   -4.3942   -3.3790    3.9085    6.7951    8.5555   10.2100
        k = 0.1644 0.0949 0.0000 (   1182 PWs)    bands (ev):
-18.2793   -5.6914   -4.4616   -3.4081    3.9433    6.8145    8.5798   10.2129
        k = 0.1678 0.0969 0.0000 (   1182 PWs)    bands (ev):
-18.2584   -5.6631   -4.5297   -3.4373    3.9788    6.8338    8.6039   10.2165
        k = 0.1712 0.0989 0.0000 (   1182 PWs)    bands (ev):
-18.2370   -5.6342   -4.5984   -3.4668    4.0149    6.8529    8.6277   10.2209
        k = 0.1747 0.1008 0.0000 (   1182 PWs)    bands (ev):
-18.2153   -5.6048   -4.6677   -3.4963    4.0518    6.8716    8.6513   10.2264
        k = 0.1781 0.1028 0.0000 (   1182 PWs)    bands (ev):
-18.1932   -5.5748   -4.7375   -3.5260    4.0893    6.8901    8.6745   10.2326
        k = 0.1815 0.1048 0.0000 (   1182 PWs)    bands (ev):
-18.1707   -5.5444   -4.8078   -3.5557    4.1275    6.9081    8.6973   10.2398
        k = 0.1849 0.1068 0.0000 (   1182 PWs)    bands (ev):
-18.1478   -5.5134   -4.8786   -3.5856    4.1663    6.9256    8.7197   10.2481
        k = 0.1884 0.1087 0.0000 (   1182 PWs)    bands (ev):
-18.1245   -5.4819   -4.9498   -3.6155    4.2059    6.9426    8.7415   10.2242
        k = 0.1918 0.1107 0.0000 (   1182 PWs)    bands (ev):
-18.1009   -5.4498   -5.0214   -3.6454    4.2461    6.9588    8.7629   10.1796
        k = 0.1952 0.1127 0.0000 (   1178 PWs)    bands (ev):
-18.0769   -5.4173   -5.0934   -3.6753    4.2870    6.9742    8.7837   10.1356
        k = 0.1986 0.1147 0.0000 (   1178 PWs)    bands (ev):
-18.0525   -5.3842   -5.1658   -3.7054    4.3286    6.9888    8.8038   10.0924
        k = 0.2021 0.1167 0.0000 (   1178 PWs)    bands (ev):
-18.0277   -5.3506   -5.2386   -3.7354    4.3708    7.0023    8.8232   10.0500
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      k = 0.2055 0.1186 0.0000 (   1178 PWs)   bands (ev):

-18.0027  -5.3166  -5.3117  -3.7654    4.4137   7.0146   8.8419  10.0088
      k = 0.2089 0.1206 0.0000 (   1178 PWs)   bands (ev):

-17.9772  -5.3850  -5.2820  -3.7953    4.4573   7.0256   8.8599   9.9687
      k = 0.2123 0.1226 0.0000 (   1178 PWs)   bands (ev):

-17.9514  -5.4586  -5.2469  -3.8253    4.5015   7.0352   8.8770   9.9301
      k = 0.2158 0.1246 0.0000 (   1178 PWs)   bands (ev):

-17.9252  -5.5325  -5.2114  -3.8552    4.5464   7.0432   8.8934   9.8929
      k = 0.2192 0.1265 0.0000 (   1178 PWs)   bands (ev):

-17.8988  -5.6065  -5.1753  -3.8850    4.5920   7.0495   8.9089   9.8575
      k = 0.2226 0.1285 0.0000 (   1174 PWs)   bands (ev):

-17.8719  -5.6808  -5.1388  -3.9147    4.6382   7.0539   8.9236   9.8240
      k = 0.2260 0.1305 0.0000 (   1172 PWs)   bands (ev):

-17.8447  -5.7552  -5.1018  -3.9443    4.6851   7.0563   8.9374   9.7926
      k = 0.2295 0.1325 0.0000 (   1172 PWs)   bands (ev):

-17.8173  -5.8297  -5.0643  -3.9739    4.7327   7.0564   8.9504   9.7633
      k = 0.2329 0.1345 0.0000 (   1172 PWs)   bands (ev):

-17.7894  -5.9044  -5.0264  -4.0033    4.7809   7.0543   8.9625   9.7365
      k = 0.2363 0.1364 0.0000 (   1172 PWs)   bands (ev):

-17.7613  -5.9792  -4.9880  -4.0326    4.8297   7.0496   8.9738   9.7122
      k = 0.2397 0.1384 0.0000 (   1176 PWs)   bands (ev):

-17.7329  -6.0542  -4.9492  -4.0617    4.8792   7.0423   8.9841   9.6906
      k = 0.2432 0.1404 0.0000 (   1176 PWs)   bands (ev):

-17.7042  -6.1291  -4.9099  -4.0907    4.9294   7.0323   8.9937   9.6719
      k = 0.2466 0.1424 0.0000 (   1176 PWs)   bands (ev):

-17.6751  -6.2040  -4.8702  -4.1195    4.9802   7.0196   9.0026   9.6562
      k = 0.2500 0.1443 0.0000 (   1168 PWs)   bands (ev):

-17.6458  -6.2789  -4.8300  -4.1481    5.0316   7.0039   9.0108   9.6437
      k = 0.2534 0.1463 0.0000 (   1186 PWs)   bands (ev):

-17.6162  -6.3540  -4.7895  -4.1768    5.0837   6.9850   9.0179   9.6337
      k = 0.2568 0.1483 0.0000 (   1186 PWs)   bands (ev):
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  -17.5863   -6.4288   -4.7486   -4.2051    5.1363    6.9634    9.0245    9.6274
        k = 0.2603 0.1503 0.0000 (   1186 PWs)    bands (ev):
  -17.5561   -6.5036   -4.7072   -4.2332    5.1897    6.9388    9.0306    9.6243
        k = 0.2637 0.1522 0.0000 (   1186 PWs)    bands (ev):
  -17.5257   -6.5783   -4.6654   -4.2611    5.2436    6.9113    9.0360    9.6245
        k = 0.2671 0.1542 0.0000 (   1186 PWs)    bands (ev):
  -17.4950   -6.6529   -4.6233   -4.2887    5.2982    6.8808    9.0409    9.6278
        k = 0.2705 0.1562 0.0000 (   1182 PWs)    bands (ev):
  -17.4641   -6.7273   -4.5807   -4.3161    5.3534    6.8475    9.0452    9.6344
        k = 0.2740 0.1582 0.0000 (   1182 PWs)    bands (ev):
  -17.4329   -6.8016   -4.5378   -4.3432    5.4092    6.8114    9.0491    9.6441
        k = 0.2774 0.1602 0.0000 (   1184 PWs)    bands (ev):
  -17.4015   -6.8757   -4.4945   -4.3702    5.4656    6.7727    9.0524    9.6568
        k = 0.2808 0.1621 0.0000 (   1188 PWs)    bands (ev):
  -17.3699   -6.9497   -4.4509   -4.3969    5.5226    6.7313    9.0553    9.6724
        k = 0.2842 0.1641 0.0000 (   1188 PWs)    bands (ev):
  -17.3380   -7.0235   -4.4233   -4.4070    5.5801    6.6876    9.0578    9.6909
        k = 0.2877 0.1661 0.0000 (   1188 PWs)    bands (ev):
  -17.3060   -7.0969   -4.4494   -4.3627    5.6383    6.6415    9.0601    9.7122
        k = 0.2911 0.1681 0.0000 (   1192 PWs)    bands (ev):
  -17.2737   -7.1701   -4.4754   -4.3181    5.6970    6.5933    9.0620    9.7361
        k = 0.2945 0.1700 0.0000 (   1192 PWs)    bands (ev):
  -17.2413   -7.2430   -4.5009   -4.2732    5.7563    6.5430    9.0637    9.7625
        k = 0.2979 0.1720 0.0000 (   1192 PWs)    bands (ev):
  -17.2087   -7.3156   -4.5262   -4.2280    5.8162    6.4909    9.0651    9.7913
        k = 0.3014 0.1740 0.0000 (   1192 PWs)    bands (ev):
  -17.1760   -7.3879   -4.5511   -4.1826    5.8766    6.4370    9.0664    9.8224
        k = 0.3048 0.1760 0.0000 (   1192 PWs)    bands (ev):
  -17.1431   -7.4598   -4.5757   -4.1368    5.9375    6.3815    9.0676    9.8557
        k = 0.3082 0.1780 0.0000 (   1192 PWs)    bands (ev):
  -17.1101   -7.5314   -4.6000   -4.0909    5.9990    6.3245    9.0687    9.8911
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     k = 0.3116 0.1799 0.0000 (   1192 PWs)   bands (ev):

 -17.0769  -7.6025  -4.6240  -4.0446   6.0610   6.2661   9.0696   9.9284
     k = 0.3151 0.1819 0.0000 (   1192 PWs)   bands (ev):

 -17.0437  -7.6732  -4.6477  -3.9982   6.1234   6.2065   9.0706   9.9676
     k = 0.3185 0.1839 0.0000 (   1192 PWs)   bands (ev):

 -17.0103  -7.7435  -4.6710  -3.9516   6.1458   6.1863   9.0715  10.0086
     k = 0.3219 0.1859 0.0000 (   1192 PWs)   bands (ev):

 -16.9769  -7.8133  -4.6940  -3.9048   6.0842   6.2497   9.0725  10.0513
     k = 0.3253 0.1878 0.0000 (   1192 PWs)   bands (ev):

 -16.9434  -7.8826  -4.7166  -3.8578   6.0216   6.3135   9.0736  10.0956
     k = 0.3288 0.1898 0.0000 (   1196 PWs)   bands (ev):

 -16.9098  -7.9514  -4.7390  -3.8107   5.9583   6.3778   9.0747  10.1413
     k = 0.3322 0.1918 0.0000 (   1196 PWs)   bands (ev):

 -16.8763  -8.0197  -4.7609  -3.7635   5.8943   6.4424   9.0760  10.1886
     k = 0.3356 0.1938 0.0000 (   1196 PWs)   bands (ev):

 -16.8427  -8.0874  -4.7824  -3.7161   5.8298   6.5074   9.0775  10.2372
     k = 0.3390 0.1957 0.0000 (   1192 PWs)   bands (ev):

 -16.8090  -8.1545  -4.8036  -3.6687   5.7648   6.5727   9.0793  10.2871
     k = 0.3425 0.1977 0.0000 (   1192 PWs)   bands (ev):

 -16.7755  -8.2210  -4.8244  -3.6212   5.6994   6.6383   9.0814  10.3382
     k = 0.3459 0.1997 0.0000 (   1194 PWs)   bands (ev):

 -16.7420  -8.2869  -4.8448  -3.5737   5.6337   6.7041   9.0837  10.3905
     k = 0.3493 0.2017 0.0000 (   1194 PWs)   bands (ev):

 -16.7085  -8.3520  -4.8648  -3.5261   5.5677   6.7702   9.0865  10.4440
     k = 0.3527 0.2037 0.0000 (   1194 PWs)   bands (ev):

 -16.6751  -8.4165  -4.8845  -3.4786   5.5017   6.8364   9.0897  10.4985
     k = 0.3562 0.2056 0.0000 (   1194 PWs)   bands (ev):

 -16.6418  -8.4802  -4.9037  -3.4312   5.4356   6.9027   9.0934  10.5540
     k = 0.3596 0.2076 0.0000 (   1194 PWs)   bands (ev):

 -16.6087  -8.5432  -4.9226  -3.3838   5.3696   6.9691   9.0977  10.6105
     k = 0.3630 0.2096 0.0000 (   1194 PWs)   bands (ev):
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-16.5756  -8.6054  -4.9410  -3.3365   5.3036   7.0355   9.1027  10.6678
         k = 0.3664 0.2116 0.0000 (   1194 PWs)   bands (ev):
-16.5428  -8.6667  -4.9591  -3.2894   5.2379   7.1018   9.1083  10.7261
         k = 0.3699 0.2135 0.0000 (   1194 PWs)   bands (ev):
-16.5102  -8.7272  -4.9767  -3.2424   5.1724   7.1679   9.1148  10.7852
         k = 0.3733 0.2155 0.0000 (   1194 PWs)   bands (ev):
-16.4778  -8.7868  -4.9939  -3.1956   5.1072   7.2338   9.1222  10.8451
         k = 0.3767 0.2175 0.0000 (   1194 PWs)   bands (ev):
-16.4456  -8.8456  -5.0107  -3.1491   5.0425   7.2992   9.1306  10.9057
         k = 0.3801 0.2195 0.0000 (   1194 PWs)   bands (ev):
-16.4137  -8.9033  -5.0271  -3.1029   4.9782   7.3642   9.1402  10.9671
         k = 0.3836 0.2214 0.0000 (   1186 PWs)   bands (ev):
-16.3821  -8.9601  -5.0430  -3.0570   4.9145   7.4286   9.1511  11.0291
         k = 0.3870 0.2234 0.0000 (   1188 PWs)   bands (ev):
-16.3509  -9.0159  -5.0585  -3.0114   4.8512   7.4922   9.1633  11.0916
         k = 0.3904 0.2254 0.0000 (   1188 PWs)   bands (ev):
-16.3200  -9.0706  -5.0736  -2.9663   4.7888   7.5548   9.1772  11.1548
         k = 0.3938 0.2274 0.0000 (   1188 PWs)   bands (ev):
-16.2896  -9.1242  -5.0882  -2.9216   4.7271   7.6164   9.1928  11.2185
         k = 0.3973 0.2294 0.0000 (   1196 PWs)   bands (ev):
-16.2596  -9.1767  -5.1025  -2.8774   4.6662   7.6766   9.2103  11.2827
         k = 0.4007 0.2313 0.0000 (   1196 PWs)   bands (ev):
-16.2300  -9.2281  -5.1163  -2.8338   4.6062   7.7354   9.2300  11.3474
         k = 0.4041 0.2333 0.0000 (   1200 PWs)   bands (ev):
-16.2010  -9.2783  -5.1296  -2.7908   4.5469   7.7924   9.2520  11.4124
         k = 0.4075 0.2353 0.0000 (   1200 PWs)   bands (ev):
-16.1724  -9.3272  -5.1425  -2.7485   4.4890   7.8476   9.2766  11.4777
         k = 0.4110 0.2373 0.0000 (   1192 PWs)   bands (ev):
-16.1444  -9.3747  -5.1549  -2.7067   4.4324   7.9007   9.3040  11.5434
         k = 0.4144 0.2392 0.0000 (   1192 PWs)   bands (ev):
-16.1171  -9.4210  -5.1669  -2.6659   4.3769   7.9514   9.3343  11.6093
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        k = 0.4178 0.2412 0.0000 (   1192 PWs)   bands (ev):

 -16.0904  -9.4660  -5.1784  -2.6258    4.3226    7.9996    9.3678   11.6754

        k = 0.4212 0.2432 0.0000 (   1196 PWs)   bands (ev):

 -16.0644  -9.5095  -5.1895  -2.5867    4.2696    8.0451    9.4045   11.7416

        k = 0.4247 0.2452 0.0000 (   1196 PWs)   bands (ev):

 -16.0391  -9.5516  -5.2001  -2.5485    4.2182    8.0879    9.4447   11.8078

        k = 0.4281 0.2472 0.0000 (   1196 PWs)   bands (ev):

 -16.0146  -9.5922  -5.2103  -2.5113    4.1683    8.1278    9.4883   11.8739

        k = 0.4315 0.2491 0.0000 (   1196 PWs)   bands (ev):

 -15.9909  -9.6313  -5.2200  -2.4753    4.1199    8.1648    9.5354   11.9399

        k = 0.4349 0.2511 0.0000 (   1196 PWs)   bands (ev):

 -15.9680  -9.6688  -5.2292  -2.4403    4.0733    8.1988    9.5861   12.0056

        k = 0.4384 0.2531 0.0000 (   1194 PWs)   bands (ev):

 -15.9459  -9.7047  -5.2380  -2.4066    4.0284    8.2300    9.6402   12.0710

        k = 0.4418 0.2551 0.0000 (   1194 PWs)   bands (ev):

 -15.9248  -9.7389  -5.2463  -2.3742    3.9854    8.2584    9.6975   12.1359

        k = 0.4452 0.2570 0.0000 (   1194 PWs)   bands (ev):

 -15.9047  -9.7714  -5.2542  -2.3432    3.9443    8.2841    9.7581   12.2001

        k = 0.4486 0.2590 0.0000 (   1194 PWs)   bands (ev):

 -15.8856  -9.8022  -5.2615  -2.3136    3.9051    8.3073    9.8216   12.2635

        k = 0.4521 0.2610 0.0000 (   1196 PWs)   bands (ev):

 -15.8675  -9.8312  -5.2685  -2.2855    3.8681    8.3280    9.8880   12.3259

        k = 0.4555 0.2630 0.0000 (   1192 PWs)   bands (ev):

 -15.8504  -9.8584  -5.2749  -2.2590    3.8332    8.3466    9.9570   12.3517

        k = 0.4589 0.2649 0.0000 (   1192 PWs)   bands (ev):

 -15.8345  -9.8838  -5.2808  -2.2341    3.8006    8.3631   10.0284   12.2544

        k = 0.4623 0.2669 0.0000 (   1196 PWs)   bands (ev):

 -15.8197  -9.9073  -5.2863  -2.2110    3.7702    8.3777   10.1020   12.1570

        k = 0.4658 0.2689 0.0000 (   1188 PWs)   bands (ev):

 -15.8060  -9.9288  -5.2912  -2.1896    3.7424    8.3906   10.1776   12.0598

        k = 0.4692 0.2709 0.0000 (   1188 PWs)   bands (ev):
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 -15.7936  -9.9484  -5.2957  -2.1700   3.7169   8.4018  10.2547  11.9631
        k = 0.4726 0.2729 0.0000 (  1188 PWs)   bands (ev):
 -15.7824  -9.9661  -5.2998  -2.1524   3.6939   8.4115  10.3333  11.8671
        k = 0.4760 0.2748 0.0000 (  1184 PWs)   bands (ev):
 -15.7724  -9.9817  -5.3034  -2.1366   3.6735   8.4198  10.4129  11.7723
        k = 0.4795 0.2768 0.0000 (  1184 PWs)   bands (ev):
 -15.7637  -9.9953  -5.3065  -2.1229   3.6557   8.4268  10.4930  11.6791
        k = 0.4829 0.2788 0.0000 (  1184 PWs)   bands (ev):
 -15.7564 -10.0068  -5.3091  -2.1112   3.6405   8.4326  10.5728  11.5882
        k = 0.4863 0.2808 0.0000 (  1184 PWs)   bands (ev):
 -15.7503 -10.0163  -5.3113  -2.1016   3.6280   8.4373  10.6513  11.5007
        k = 0.4897 0.2827 0.0000 (  1188 PWs)   bands (ev):
 -15.7456 -10.0236  -5.3130  -2.0941   3.6183   8.4408  10.7262  11.4188
        k = 0.4932 0.2847 0.0000 (  1192 PWs)   bands (ev):
 -15.7422 -10.0289  -5.3142  -2.0887   3.6113   8.4433  10.7933  11.3467
        k = 0.4966 0.2867 0.0000 (  1192 PWs)   bands (ev):
 -15.7402 -10.0321  -5.3149  -2.0855   3.6071   8.4448  10.8437  11.2933
        k = 0.5000 0.2887 0.0000 (  1192 PWs)   bands (ev):
 -15.7395 -10.0332  -5.3152  -2.0844   3.6057   8.4453  10.8635  11.2725
        k = 0.4980 0.2921 0.0000 (  1192 PWs)   bands (ev):
 -15.7393 -10.0330  -5.3161  -2.0842   3.6057   8.4466  10.8638  11.2730
        k = 0.4960 0.2955 0.0000 (  1192 PWs)   bands (ev):
 -15.7389 -10.0324  -5.3189  -2.0835   3.6059   8.4504  10.8648  11.2744
        k = 0.4940 0.2990 0.0000 (  1192 PWs)   bands (ev):
 -15.7381 -10.0315  -5.3235  -2.0824   3.6062   8.4568  10.8665  11.2767
        k = 0.4921 0.3024 0.0000 (  1188 PWs)   bands (ev):
 -15.7371 -10.0302  -5.3300  -2.0808   3.6066   8.4658  10.8688  11.2799
        k = 0.4901 0.3059 0.0000 (  1192 PWs)   bands (ev):
 -15.7357 -10.0286  -5.3385  -2.0788   3.6070   8.4772  10.8718  11.2840
        k = 0.4881 0.3093 0.0000 (  1192 PWs)   bands (ev):
 -15.7341 -10.0266  -5.3487  -2.0764   3.6076   8.4912  10.8754  11.2890
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       k = 0.4861 0.3127 0.0000 (  1192 PWs)   bands (ev):

 -15.7321 -10.0242  -5.3607  -2.0735   3.6082   8.5077  10.8797  11.2950
       k = 0.4841 0.3162 0.0000 (  1192 PWs)   bands (ev):

 -15.7299 -10.0215  -5.3744  -2.0702   3.6090   8.5267  10.8846  11.3019
       k = 0.4821 0.3196 0.0000 (  1196 PWs)   bands (ev):

 -15.7274 -10.0183  -5.3900  -2.0665   3.6097   8.5481  10.8903  11.3097
       k = 0.4802 0.3230 0.0000 (  1196 PWs)   bands (ev):

 -15.7246 -10.0149  -5.4074  -2.0623   3.6107   8.5719  10.8965  11.3185
       k = 0.4782 0.3265 0.0000 (  1190 PWs)   bands (ev):

 -15.7214 -10.0110  -5.4264  -2.0577   3.6118   8.5980  10.9035  11.3283
       k = 0.4762 0.3299 0.0000 (  1190 PWs)   bands (ev):

 -15.7180 -10.0068  -5.4471  -2.0527   3.6129   8.6265  10.9111  11.3389
       k = 0.4742 0.3334 0.0000 (  1190 PWs)   bands (ev):

 -15.7143 -10.0022  -5.4695  -2.0472   3.6141   8.6573  10.9194  11.3506
       k = 0.4722 0.3368 0.0000 (  1190 PWs)   bands (ev):

 -15.7103  -9.9973  -5.4935  -2.0413   3.6154   8.6903  10.9283  11.3632
       k = 0.4702 0.3402 0.0000 (  1190 PWs)   bands (ev):

 -15.7061  -9.9920  -5.5191  -2.0350   3.6167   8.7256  10.9379  11.3768
       k = 0.4683 0.3437 0.0000 (  1190 PWs)   bands (ev):

 -15.7015  -9.9863  -5.5462  -2.0283   3.6181   8.7629  10.9481  11.3913
       k = 0.4663 0.3471 0.0000 (  1198 PWs)   bands (ev):

 -15.6968  -9.9803  -5.5750  -2.0212   3.6193   8.8023  10.9591  11.4068
       k = 0.4643 0.3505 0.0000 (  1196 PWs)   bands (ev):

 -15.6917  -9.9740  -5.6051  -2.0136   3.6209   8.8437  10.9707  11.4234
       k = 0.4623 0.3540 0.0000 (  1200 PWs)   bands (ev):

 -15.6863  -9.9672  -5.6367  -2.0056   3.6224   8.8871  10.9829  11.4410
       k = 0.4603 0.3574 0.0000 (  1200 PWs)   bands (ev):

 -15.6807  -9.9601  -5.6697  -1.9973   3.6239   8.9324  10.9958  11.4596
       k = 0.4583 0.3608 0.0000 (  1204 PWs)   bands (ev):

 -15.6748  -9.9527  -5.7041  -1.9885   3.6254   8.9794  11.0094  11.4793
       k = 0.4563 0.3643 0.0000 (  1204 PWs)   bands (ev):
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-15.6687   -9.9448   -5.7398   -1.9794    3.6269    9.0283   11.0237   11.5000
       k = 0.4544 0.3677 0.0000 (   1204 PWs)    bands (ev):
-15.6623   -9.9366   -5.7767   -1.9698    3.6285    9.0787   11.0386   11.5218
       k = 0.4524 0.3712 0.0000 (   1204 PWs)    bands (ev):
-15.6556   -9.9281   -5.8148   -1.9599    3.6301    9.1308   11.0542   11.5447
       k = 0.4504 0.3746 0.0000 (   1204 PWs)    bands (ev):
-15.6487   -9.9192   -5.8541   -1.9496    3.6317    9.1844   11.0705   11.5687
       k = 0.4484 0.3780 0.0000 (   1204 PWs)    bands (ev):
-15.6416   -9.9100   -5.8945   -1.9389    3.6332    9.2394   11.0875   11.5939
       k = 0.4464 0.3815 0.0000 (   1204 PWs)    bands (ev):
-15.6342   -9.9004   -5.9360   -1.9279    3.6347    9.2958   11.1051   11.6202
       k = 0.4444 0.3849 0.0000 (   1204 PWs)    bands (ev):
-15.6266   -9.8904   -5.9785   -1.9165    3.6362    9.3533   11.1234   11.6477
       k = 0.4425 0.3883 0.0000 (   1204 PWs)    bands (ev):
-15.6188   -9.8801   -6.0220   -1.9047    3.6376    9.4121   11.1424   11.6764
       k = 0.4405 0.3918 0.0000 (   1204 PWs)    bands (ev):
-15.6107   -9.8694   -6.0664   -1.8926    3.6389    9.4719   11.1621   11.7063
       k = 0.4385 0.3952 0.0000 (   1204 PWs)    bands (ev):
-15.6025   -9.8584   -6.1117   -1.8802    3.6402    9.5326   11.1825   11.7375
       k = 0.4365 0.3986 0.0000 (   1204 PWs)    bands (ev):
-15.5940   -9.8470   -6.1578   -1.8675    3.6414    9.5942   11.2036   11.7699
       k = 0.4345 0.4021 0.0000 (   1204 PWs)    bands (ev):
-15.5854   -9.8353   -6.2047   -1.8544    3.6425    9.6566   11.2253   11.8037
       k = 0.4325 0.4055 0.0000 (   1196 PWs)    bands (ev):
-15.5765   -9.8233   -6.2522   -1.8410    3.6435    9.7199   11.2478   11.8389
       k = 0.4306 0.4090 0.0000 (   1196 PWs)    bands (ev):
-15.5675   -9.8109   -6.3005   -1.8273    3.6443    9.7834   11.2710   11.8753
       k = 0.4286 0.4124 0.0000 (   1192 PWs)    bands (ev):
-15.5583   -9.7981   -6.3494   -1.8134    3.6450    9.8475   11.2949   11.9132
       k = 0.4266 0.4158 0.0000 (   1192 PWs)    bands (ev):
-15.5490   -9.7850   -6.3989   -1.7992    3.6456    9.9118   11.3195   11.9524
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      k = 0.4246 0.4193 0.0000 (  1192 PWs)   bands (ev):

 -15.5394  -9.7716  -6.4489  -1.7847   3.6460   9.9763  11.3448  11.9930

      k = 0.4226 0.4227 0.0000 (  1196 PWs)   bands (ev):

 -15.5298  -9.7579  -6.4995  -1.7699   3.6462  10.0409  11.3708  12.0351

      k = 0.4206 0.4261 0.0000 (  1204 PWs)   bands (ev):

 -15.5200  -9.7438  -6.5505  -1.7549   3.6461  10.1055  11.3976  12.0786

      k = 0.4186 0.4296 0.0000 (  1204 PWs)   bands (ev):

 -15.5101  -9.7294  -6.6018  -1.7397   3.6459  10.1700  11.4251  12.1236

      k = 0.4167 0.4330 0.0000 (  1204 PWs)   bands (ev):

 -15.5000  -9.7147  -6.6535  -1.7243   3.6456  10.2342  11.4534  12.1701

      k = 0.4147 0.4364 0.0000 (  1204 PWs)   bands (ev):

 -15.4898  -9.6996  -6.7055  -1.7086   3.6450  10.2982  11.4824  12.2107

      k = 0.4127 0.4399 0.0000 (  1204 PWs)   bands (ev):

 -15.4796  -9.6843  -6.7576  -1.6928   3.6442  10.3616  11.5122  12.1756

      k = 0.4107 0.4433 0.0000 (  1204 PWs)   bands (ev):

 -15.4692  -9.6686  -6.8100  -1.6768   3.6432  10.4246  11.5427  12.1400

      k = 0.4087 0.4468 0.0000 (  1200 PWs)   bands (ev):

 -15.4588  -9.6526  -6.8626  -1.6607   3.6420  10.4869  11.5740  12.1041

      k = 0.4067 0.4502 0.0000 (  1200 PWs)   bands (ev):

 -15.4483  -9.6363  -6.9152  -1.6444   3.6405  10.5485  11.6061  12.0680

      k = 0.4048 0.4536 0.0000 (  1198 PWs)   bands (ev):

 -15.4378  -9.6197  -6.9679  -1.6280   3.6387  10.6093  11.6389  12.0316

      k = 0.4028 0.4571 0.0000 (  1198 PWs)   bands (ev):

 -15.4272  -9.6028  -7.0205  -1.6115   3.6367  10.6692  11.6725  11.9952

      k = 0.4008 0.4605 0.0000 (  1198 PWs)   bands (ev):

 -15.4166  -9.5856  -7.0731  -1.5950   3.6344  10.7282  11.7069  11.9588

      k = 0.3988 0.4639 0.0000 (  1198 PWs)   bands (ev):

 -15.4060  -9.5682  -7.1256  -1.5784   3.6319  10.7862  11.7421  11.9225

      k = 0.3968 0.4674 0.0000 (  1206 PWs)   bands (ev):

 -15.3954  -9.5505  -7.1781  -1.5617   3.6289  10.8431  11.7781  11.8863

      k = 0.3948 0.4708 0.0000 (  1206 PWs)   bands (ev):
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-15.3848   -9.5325   -7.2303   -1.5450    3.6258   10.8989   11.8149   11.8504
         k = 0.3929 0.4742 0.0000 (   1206 PWs)    bands (ev):
-15.3743   -9.5143   -7.2822   -1.5283    3.6225   10.9536   11.8149   11.8524
         k = 0.3909 0.4777 0.0000 (   1206 PWs)    bands (ev):
-15.3638   -9.4958   -7.3338   -1.5117    3.6189   11.0072   11.7799   11.8907
         k = 0.3889 0.4811 0.0000 (   1207 PWs)    bands (ev):
-15.3534   -9.4771   -7.3850   -1.4951    3.6150   11.0596   11.7454   11.9298
         k = 0.3869 0.4846 0.0000 (   1207 PWs)    bands (ev):
-15.3430   -9.4582   -7.4359   -1.4787    3.6108   11.1108   11.7115   11.9697
         k = 0.3849 0.4880 0.0000 (   1195 PWs)    bands (ev):
-15.3327   -9.4390   -7.4862   -1.4622    3.6067   11.1608   11.6782   12.0103
         k = 0.3829 0.4914 0.0000 (   1197 PWs)    bands (ev):
-15.3226   -9.4198   -7.5361   -1.4460    3.6021   11.2096   11.6458   12.0516
         k = 0.3810 0.4949 0.0000 (   1191 PWs)    bands (ev):
-15.3126   -9.4003   -7.5853   -1.4299    3.5975   11.2572   11.6141   12.0937
         k = 0.3790 0.4983 0.0000 (   1191 PWs)    bands (ev):
-15.3028   -9.3807   -7.6339   -1.4140    3.5925   11.3036   11.5834   12.1364
         k = 0.3770 0.5017 0.0000 (   1191 PWs)    bands (ev):
-15.2931   -9.3610   -7.6818   -1.3984    3.5872   11.3488   11.5535   12.1798
         k = 0.3750 0.5052 0.0000 (   1195 PWs)    bands (ev):
-15.2836   -9.3412   -7.7290   -1.3830    3.5818   11.3928   11.5247   12.2239
         k = 0.3730 0.5086 0.0000 (   1191 PWs)    bands (ev):
-15.2744   -9.3214   -7.7752   -1.3680    3.5762   11.4357   11.4970   12.2686
         k = 0.3710 0.5121 0.0000 (   1191 PWs)    bands (ev):
-15.2654   -9.3016   -7.8205   -1.3533    3.5705   11.4704   11.4773   12.3139
         k = 0.3690 0.5155 0.0000 (   1191 PWs)    bands (ev):
-15.2566   -9.2818   -7.8649   -1.3389    3.5647   11.4450   11.5177   12.3597
         k = 0.3671 0.5189 0.0000 (   1193 PWs)    bands (ev):
-15.2481   -9.2621   -7.9081   -1.3250    3.5589   11.4207   11.5568   12.4061
         k = 0.3651 0.5224 0.0000 (   1193 PWs)    bands (ev):
-15.2399   -9.2425   -7.9501   -1.3115    3.5530   11.3978   11.5948   12.4529
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       k = 0.3631 0.5258 0.0000 (   1193 PWs)   bands (ev):

 -15.2321  -9.2232  -7.9909  -1.2985    3.5470   11.3761   11.6315   12.5001

       k = 0.3611 0.5292 0.0000 (   1197 PWs)   bands (ev):

 -15.2245  -9.2042  -8.0302  -1.2860    3.5412   11.3557   11.6668   12.5477

       k = 0.3591 0.5327 0.0000 (   1193 PWs)   bands (ev):

 -15.2174  -9.1855  -8.0679  -1.2741    3.5353   11.3367   11.7009   12.5957

       k = 0.3571 0.5361 0.0000 (   1193 PWs)   bands (ev):

 -15.2106  -9.1673  -8.1040  -1.2628    3.5296   11.3191   11.7336   12.6438

       k = 0.3552 0.5395 0.0000 (   1193 PWs)   bands (ev):

 -15.2042  -9.1497  -8.1382  -1.2522    3.5241   11.3029   11.7647   12.6921

       k = 0.3532 0.5430 0.0000 (   1193 PWs)   bands (ev):

 -15.1983  -9.1329  -8.1704  -1.2423    3.5188   11.2881   11.7943   12.7403

       k = 0.3512 0.5464 0.0000 (   1191 PWs)   bands (ev):

 -15.1928  -9.1169  -8.2005  -1.2331    3.5137   11.2747   11.8223   12.7884

       k = 0.3492 0.5499 0.0000 (   1191 PWs)   bands (ev):

 -15.1878  -9.1021  -8.2281  -1.2246    3.5089   11.2627   11.8484   12.8360

       k = 0.3472 0.5533 0.0000 (   1187 PWs)   bands (ev):

 -15.1833  -9.0884  -8.2531  -1.2171    3.5046   11.2522   11.8725   12.8830

       k = 0.3452 0.5567 0.0000 (   1187 PWs)   bands (ev):

 -15.1793  -9.0761  -8.2753  -1.2103    3.5006   11.2431   11.8944   12.9288

       k = 0.3433 0.5602 0.0000 (   1187 PWs)   bands (ev):

 -15.1759  -9.0655  -8.2944  -1.2045    3.4970   11.2355   11.9140   12.9727

       k = 0.3413 0.5636 0.0000 (   1187 PWs)   bands (ev):

 -15.1730  -9.0566  -8.3104  -1.1997    3.4940   11.2292   11.9308   13.0138

       k = 0.3393 0.5670 0.0000 (   1187 PWs)   bands (ev):

 -15.1708  -9.0496  -8.3229  -1.1959    3.4915   11.2244   11.9446   13.0504

       k = 0.3373 0.5705 0.0000 (   1197 PWs)   bands (ev):

 -15.1692  -9.0447  -8.3319  -1.1931    3.4896   11.2210   11.9550   13.0802

       k = 0.3353 0.5739 0.0000 (   1197 PWs)   bands (ev):

 -15.1682  -9.0417  -8.3372  -1.1914    3.4885   11.2189   11.9616   13.1001

       k = 0.3333 0.5773 0.0000 (   1197 PWs)   bands (ev):
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-15.1679   -9.0408   -8.3390   -1.1908    3.4881   11.2183   11.9640   13.1072
        k = 0.3314 0.5739 0.0000 (   1197 PWs)    bands (ev):
-15.1682   -9.0417   -8.3373   -1.1914    3.4885   11.2189   11.9615   13.1004
        k = 0.3294 0.5705 0.0000 (   1197 PWs)    bands (ev):
-15.1692   -9.0443   -8.3322   -1.1932    3.4897   11.2209   11.9537   13.0819
        k = 0.3274 0.5671 0.0000 (   1193 PWs)    bands (ev):
-15.1710   -9.0483   -8.3240   -1.1962    3.4919   11.2241   11.9401   13.0557
        k = 0.3254 0.5637 0.0000 (   1193 PWs)    bands (ev):
-15.1734   -9.0537   -8.3129   -1.2004    3.4950   11.2285   11.9201   13.0255
        k = 0.3235 0.5603 0.0000 (   1185 PWs)    bands (ev):
-15.1766   -9.0599   -8.2991   -1.2059    3.4992   11.2341   11.8933   12.9944
        k = 0.3215 0.5568 0.0000 (   1185 PWs)    bands (ev):
-15.1806   -9.0669   -8.2829   -1.2127    3.5043   11.2408   11.8596   12.9644
        k = 0.3195 0.5534 0.0000 (   1187 PWs)    bands (ev):
-15.1853   -9.0743   -8.2645   -1.2208    3.5105   11.2485   11.8190   12.9366
        k = 0.3176 0.5500 0.0000 (   1183 PWs)    bands (ev):
-15.1909   -9.0819   -8.2441   -1.2303    3.5179   11.2573   11.7716   12.9119
        k = 0.3156 0.5466 0.0000 (   1183 PWs)    bands (ev):
-15.1972   -9.0895   -8.2220   -1.2411    3.5264   11.2671   11.7177   12.8902
        k = 0.3136 0.5432 0.0000 (   1187 PWs)    bands (ev):
-15.2044   -9.0968   -8.1983   -1.2533    3.5361   11.2777   11.6580   12.8717
        k = 0.3116 0.5398 0.0000 (   1187 PWs)    bands (ev):
-15.2124   -9.1037   -8.1732   -1.2668    3.5470   11.2892   11.5929   12.8559
        k = 0.3097 0.5363 0.0000 (   1187 PWs)    bands (ev):
-15.2212   -9.1101   -8.1469   -1.2818    3.5591   11.3014   11.5232   12.8426
        k = 0.3077 0.5329 0.0000 (   1193 PWs)    bands (ev):
-15.2309   -9.1158   -8.1194   -1.2982    3.5724   11.3142   11.4494   12.8312
        k = 0.3057 0.5295 0.0000 (   1193 PWs)    bands (ev):
-15.2414   -9.1207   -8.0909   -1.3159    3.5871   11.3277   11.3722   12.8215
        k = 0.3037 0.5261 0.0000 (   1193 PWs)    bands (ev):
-15.2527   -9.1246   -8.0614   -1.3350    3.6032   11.2921   11.3416   12.8128
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      k = 0.3018 0.5227 0.0000 (  1193 PWs)   bands (ev):

-15.2649  -9.1276  -8.0311  -1.3555   3.6206  11.2095  11.3560  12.8050

      k = 0.2998 0.5193 0.0000 (  1193 PWs)   bands (ev):

-15.2779  -9.1295  -7.9999  -1.3773   3.6393  11.1248  11.3706  12.7977

      k = 0.2978 0.5159 0.0000 (  1193 PWs)   bands (ev):

-15.2918  -9.1303  -7.9680  -1.4005   3.6594  11.0385  11.3853  12.7906

      k = 0.2959 0.5124 0.0000 (  1189 PWs)   bands (ev):

-15.3065  -9.1299  -7.9354  -1.4249   3.6808  10.9508  11.4002  12.7834

      k = 0.2939 0.5090 0.0000 (  1199 PWs)   bands (ev):

-15.3221  -9.1284  -7.9022  -1.4508   3.7035  10.8619  11.4149  12.7759

      k = 0.2919 0.5056 0.0000 (  1199 PWs)   bands (ev):

-15.3384  -9.1256  -7.8684  -1.4778   3.7276  10.7721  11.4294  12.7681

      k = 0.2899 0.5022 0.0000 (  1199 PWs)   bands (ev):

-15.3556  -9.1215  -7.8340  -1.5062   3.7531  10.6816  11.4435  12.7598

      k = 0.2880 0.4988 0.0000 (  1199 PWs)   bands (ev):

-15.3737  -9.1161  -7.7991  -1.5357   3.7799  10.5905  11.4571  12.7508

      k = 0.2860 0.4954 0.0000 (  1197 PWs)   bands (ev):

-15.3925  -9.1093  -7.7636  -1.5665   3.8080  10.4991  11.4701  12.7410

      k = 0.2840 0.4919 0.0000 (  1205 PWs)   bands (ev):

-15.4121  -9.1013  -7.7277  -1.5984   3.8373  10.4073  11.4822  12.7303

      k = 0.2820 0.4885 0.0000 (  1205 PWs)   bands (ev):

-15.4325  -9.0920  -7.6913  -1.6315   3.8680  10.3153  11.4933  12.7188

      k = 0.2801 0.4851 0.0000 (  1205 PWs)   bands (ev):

-15.4537  -9.0813  -7.6544  -1.6656   3.9000  10.2232  11.5032  12.7063

      k = 0.2781 0.4817 0.0000 (  1205 PWs)   bands (ev):

-15.4756  -9.0692  -7.6171  -1.7008   3.9332  10.1311  11.5117  12.6928

      k = 0.2761 0.4783 0.0000 (  1197 PWs)   bands (ev):

-15.4982  -9.0558  -7.5794  -1.7370   3.9677  10.0391  11.5187  12.6782

      k = 0.2742 0.4749 0.0000 (  1197 PWs)   bands (ev):

-15.5216  -9.0411  -7.5413  -1.7742   4.0034   9.9472  11.5240  12.6626

      k = 0.2722 0.4714 0.0000 (  1197 PWs)   bands (ev):
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  -15.5456   -9.0250   -7.5028   -1.8124    4.0402    9.8554   11.5274   12.6458
        k = 0.2702 0.4680 0.0000 (   1195 PWs)    bands (ev):
  -15.5703   -9.0077   -7.4639   -1.8514    4.0781    9.7638   11.5288   12.6279
        k = 0.2682 0.4646 0.0000 (   1195 PWs)    bands (ev):
  -15.5957   -8.9890   -7.4247   -1.8913    4.1172    9.6725   11.5279   12.6088
        k = 0.2663 0.4612 0.0000 (   1195 PWs)    bands (ev):
  -15.6217   -8.9690   -7.3850   -1.9321    4.1573    9.5814   11.5247   12.5885
        k = 0.2643 0.4578 0.0000 (   1199 PWs)    bands (ev):
  -15.6484   -8.9477   -7.3451   -1.9736    4.1986    9.4907   11.5191   12.5669
        k = 0.2623 0.4544 0.0000 (   1199 PWs)    bands (ev):
  -15.6756   -8.9252   -7.3049   -2.0158    4.2409    9.4003   11.5109   12.5442
        k = 0.2604 0.4509 0.0000 (   1195 PWs)    bands (ev):
  -15.7034   -8.9014   -7.2642   -2.0588    4.2843    9.3104   11.5002   12.5202
        k = 0.2584 0.4475 0.0000 (   1195 PWs)    bands (ev):
  -15.7317   -8.8764   -7.2233   -2.1025    4.3285    9.2208   11.4867   12.4949
        k = 0.2564 0.4441 0.0000 (   1195 PWs)    bands (ev):
  -15.7606   -8.8501   -7.1821   -2.1467    4.3737    9.1316   11.4706   12.4683
        k = 0.2544 0.4407 0.0000 (   1195 PWs)    bands (ev):
  -15.7900   -8.8227   -7.1407   -2.1916    4.4198    9.0429   11.4519   12.4404
        k = 0.2525 0.4373 0.0000 (   1195 PWs)    bands (ev):
  -15.8198   -8.7941   -7.0989   -2.2370    4.4668    8.9547   11.4305   12.4111
        k = 0.2505 0.4339 0.0000 (   1195 PWs)    bands (ev):
  -15.8502   -8.7643   -7.0568   -2.2830    4.5146    8.8669   11.4065   12.3805
        k = 0.2485 0.4304 0.0000 (   1195 PWs)    bands (ev):
  -15.8809   -8.7334   -7.0145   -2.3294    4.5633    8.7797   11.3801   12.3484
        k = 0.2465 0.4270 0.0000 (   1195 PWs)    bands (ev):
  -15.9121   -8.7013   -6.9718   -2.3763    4.6127    8.6929   11.3513   12.3149
        k = 0.2446 0.4236 0.0000 (   1195 PWs)    bands (ev):
  -15.9436   -8.6681   -6.9290   -2.4236    4.6629    8.6067   11.3203   12.2798
        k = 0.2426 0.4202 0.0000 (   1195 PWs)    bands (ev):
  -15.9756   -8.6339   -6.8858   -2.4712    4.7137    8.5210   11.2871   12.2433
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    k = 0.2406 0.4168 0.0000 (   1197 PWs)   bands (ev):

-16.0079   -8.5986   -6.8425   -2.5193     4.7653     8.4359   11.2519   12.2051

    k = 0.2387 0.4134 0.0000 (   1197 PWs)   bands (ev):

-16.0405   -8.5623   -6.7989   -2.5676     4.8175     8.3513   11.2149   12.1654

    k = 0.2367 0.4099 0.0000 (   1197 PWs)   bands (ev):

-16.0734   -8.5249   -6.7550   -2.6163     4.8703     8.2673   11.1762   12.1240

    k = 0.2347 0.4065 0.0000 (   1197 PWs)   bands (ev):

-16.1066   -8.4866   -6.7109   -2.6652     4.9236     8.1839   11.1360   12.0811

    k = 0.2327 0.4031 0.0000 (   1189 PWs)   bands (ev):

-16.1400   -8.4471   -6.6665   -2.7143     4.9776     8.1010   11.0945   12.0365

    k = 0.2308 0.3997 0.0000 (   1189 PWs)   bands (ev):

-16.1737   -8.4069   -6.6220   -2.7636     5.0320     8.0188   11.0517   11.9904

    k = 0.2288 0.3963 0.0000 (   1185 PWs)   bands (ev):

-16.2075   -8.3656   -6.5773   -2.8131     5.0870     7.9371   11.0079   11.9428

    k = 0.2268 0.3929 0.0000 (   1185 PWs)   bands (ev):

-16.2416   -8.3235   -6.5323   -2.8628     5.1423     7.8560   10.9630   11.8938

    k = 0.2248 0.3895 0.0000 (   1185 PWs)   bands (ev):

-16.2759   -8.2804   -6.4872   -2.9125     5.1980     7.7756   10.9174   11.8434

    k = 0.2229 0.3860 0.0000 (   1185 PWs)   bands (ev):

-16.3103   -8.2365   -6.4419   -2.9624     5.2540     7.6958   10.8712   11.7919

    k = 0.2209 0.3826 0.0000 (   1179 PWs)   bands (ev):

-16.3449   -8.1917   -6.3963   -3.0124     5.3107     7.6165   10.8245   11.7393

    k = 0.2189 0.3792 0.0000 (   1179 PWs)   bands (ev):

-16.3796   -8.1461   -6.3507   -3.0624     5.3673     7.5379   10.7773   11.6858

    k = 0.2170 0.3758 0.0000 (   1179 PWs)   bands (ev):

-16.4144   -8.0997   -6.3049   -3.1124     5.4241     7.4600   10.7298   11.6315

    k = 0.2150 0.3724 0.0000 (   1179 PWs)   bands (ev):

-16.4493   -8.0525   -6.2589   -3.1624     5.4811     7.3826   10.6821   11.5765

    k = 0.2130 0.3690 0.0000 (   1183 PWs)   bands (ev):

-16.4842   -8.0045   -6.2128   -3.2125     5.5382     7.3060   10.6344   11.5209

    k = 0.2110 0.3655 0.0000 (   1183 PWs)   bands (ev):
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   -16.5192   -7.9557   -6.1665   -3.2625    5.5953    7.2299   10.5867   11.4649
          k = 0.2091 0.3621 0.0000 (   1183 PWs)    bands (ev):
   -16.5543   -7.9062   -6.1201   -3.3124    5.6526    7.1545   10.5392   11.4085
          k = 0.2071 0.3587 0.0000 (   1183 PWs)    bands (ev):
   -16.5893   -7.8560   -6.0736   -3.3623    5.7098    7.0797   10.4918   11.3519
          k = 0.2051 0.3553 0.0000 (   1183 PWs)    bands (ev):
   -16.6244   -7.8051   -6.0269   -3.4121    5.7669    7.0056   10.4449   11.2951
          k = 0.2032 0.3519 0.0000 (   1183 PWs)    bands (ev):
   -16.6595   -7.7535   -5.9801   -3.4618    5.8239    6.9322   10.3983   11.2382
          k = 0.2012 0.3485 0.0000 (   1183 PWs)    bands (ev):
   -16.6945   -7.7013   -5.9333   -3.5113    5.8807    6.8594   10.3523   11.1812
          k = 0.1992 0.3450 0.0000 (   1183 PWs)    bands (ev):
   -16.7295   -7.6484   -5.8863   -3.5607    5.9372    6.7872   10.3069   11.1243
          k = 0.1972 0.3416 0.0000 (   1183 PWs)    bands (ev):
   -16.7645   -7.5948   -5.8392   -3.6100    5.9935    6.7158   10.2621   11.0674
          k = 0.1953 0.3382 0.0000 (   1183 PWs)    bands (ev):
   -16.7994   -7.5407   -5.7921   -3.6591    6.0493    6.6450   10.2182   11.0107
          k = 0.1933 0.3348 0.0000 (   1183 PWs)    bands (ev):
   -16.8342   -7.4859   -5.7448   -3.7080    6.1047    6.5748   10.1752   10.9541
          k = 0.1913 0.3314 0.0000 (   1183 PWs)    bands (ev):
   -16.8689   -7.4306   -5.6975   -3.7566    6.1595    6.5053   10.1331   10.8976
          k = 0.1893 0.3280 0.0000 (   1187 PWs)    bands (ev):
   -16.9035   -7.3747   -5.6502   -3.8052    6.2137    6.4365   10.0921   10.8414
          k = 0.1874 0.3245 0.0000 (   1187 PWs)    bands (ev):
   -16.9380   -7.3183   -5.6028   -3.8534    6.2673    6.3684   10.0523   10.7855
          k = 0.1854 0.3211 0.0000 (   1187 PWs)    bands (ev):
   -16.9724   -7.2613   -5.5554   -3.9014    6.3009    6.3200   10.0137   10.7298
          k = 0.1834 0.3177 0.0000 (   1187 PWs)    bands (ev):
   -17.0067   -7.2038   -5.5079   -3.9492    6.2341    6.3719    9.9765   10.6744
          k = 0.1815 0.3143 0.0000 (   1187 PWs)    bands (ev):
   -17.0408   -7.1458   -5.4605   -3.9967    6.1680    6.4227    9.9408   10.6194
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      k = 0.1795 0.3109 0.0000 (   1183 PWs)   bands (ev):

 -17.0747  -7.0873  -5.4129  -4.0439   6.1026   6.4725   9.9067  10.5647
      k = 0.1775 0.3075 0.0000 (   1183 PWs)   bands (ev):

 -17.1085  -7.0284  -5.3654  -4.0908   6.0379   6.5211   9.8742  10.5103
      k = 0.1755 0.3040 0.0000 (   1183 PWs)   bands (ev):

 -17.1421  -6.9691  -5.3179  -4.1374   5.9738   6.5684   9.8435  10.4563
      k = 0.1736 0.3006 0.0000 (   1187 PWs)   bands (ev):

 -17.1755  -6.9093  -5.2704  -4.1838   5.9104   6.6142   9.8147  10.4027
      k = 0.1716 0.2972 0.0000 (   1187 PWs)   bands (ev):

 -17.2087  -6.8491  -5.2230  -4.2298   5.8477   6.6586   9.7880  10.3495
      k = 0.1696 0.2938 0.0000 (   1185 PWs)   bands (ev):

 -17.2418  -6.7885  -5.1756  -4.2754   5.7857   6.7014   9.7635  10.2967
      k = 0.1677 0.2904 0.0000 (   1185 PWs)   bands (ev):

 -17.2746  -6.7275  -5.1282  -4.3207   5.7243   6.7423   9.7411  10.2443
      k = 0.1657 0.2870 0.0000 (   1185 PWs)   bands (ev):

 -17.3072  -6.6661  -5.0809  -4.3657   5.6637   6.7813   9.7211  10.1924
      k = 0.1637 0.2835 0.0000 (   1189 PWs)   bands (ev):

 -17.3395  -6.6044  -5.0337  -4.4103   5.6037   6.8183   9.7036  10.1408
      k = 0.1617 0.2801 0.0000 (   1193 PWs)   bands (ev):

 -17.3717  -6.5424  -4.9866  -4.4546   5.5444   6.8532   9.6886  10.0898
      k = 0.1598 0.2767 0.0000 (   1189 PWs)   bands (ev):

 -17.4035  -6.4799  -4.9394  -4.4985   5.4859   6.8859   9.6764  10.0392
      k = 0.1578 0.2733 0.0000 (   1189 PWs)   bands (ev):

 -17.4352  -6.4173  -4.8925  -4.5420   5.4280   6.9162   9.6668   9.9890
      k = 0.1558 0.2699 0.0000 (   1189 PWs)   bands (ev):

 -17.4665  -6.3544  -4.8456  -4.5851   5.3708   6.9441   9.6601   9.9393
      k = 0.1538 0.2665 0.0000 (   1189 PWs)   bands (ev):

 -17.4977  -6.2912  -4.7989  -4.6278   5.3143   6.9695   9.6563   9.8902
      k = 0.1519 0.2631 0.0000 (   1189 PWs)   bands (ev):

 -17.5285  -6.2277  -4.7523  -4.6701   5.2584   6.9924   9.6554   9.8414
      k = 0.1499 0.2596 0.0000 (   1185 PWs)   bands (ev):
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-17.5590   -6.1640   -4.7119   -4.7058    5.2033    7.0127    9.6575    9.7932
         k = 0.1479 0.2562 0.0000 (   1185 PWs)    bands (ev):
-17.5893   -6.1001   -4.7534   -4.6595    5.1489    7.0304    9.6626    9.7455
         k = 0.1460 0.2528 0.0000 (   1189 PWs)    bands (ev):
-17.6193   -6.0360   -4.7945   -4.6134    5.0951    7.0455    9.6705    9.6983
         k = 0.1440 0.2494 0.0000 (   1189 PWs)    bands (ev):
-17.6490   -5.9717   -4.8351   -4.5675    5.0421    7.0580    9.6516    9.6813
         k = 0.1420 0.2460 0.0000 (   1189 PWs)    bands (ev):
-17.6784   -5.9073   -4.8753   -4.5217    4.9897    7.0680    9.6054    9.6951
         k = 0.1400 0.2426 0.0000 (   1189 PWs)    bands (ev):
-17.7075   -5.8427   -4.9150   -4.4762    4.9381    7.0755    9.5597    9.7116
         k = 0.1381 0.2391 0.0000 (   1183 PWs)    bands (ev):
-17.7363   -5.7780   -4.9542   -4.4308    4.8871    7.0806    9.5145    9.7309
         k = 0.1361 0.2357 0.0000 (   1183 PWs)    bands (ev):
-17.7647   -5.7132   -4.9931   -4.3857    4.8368    7.0833    9.4699    9.7527
         k = 0.1341 0.2323 0.0000 (   1183 PWs)    bands (ev):
-17.7929   -5.6483   -5.0314   -4.3409    4.7872    7.0839    9.4257    9.7770
         k = 0.1321 0.2289 0.0000 (   1179 PWs)    bands (ev):
-17.8207   -5.5833   -5.0693   -4.2962    4.7384    7.0823    9.3821    9.8035
         k = 0.1302 0.2255 0.0000 (   1179 PWs)    bands (ev):
-17.8481   -5.5183   -5.1067   -4.2519    4.6902    7.0788    9.3391    9.8323
         k = 0.1282 0.2221 0.0000 (   1179 PWs)    bands (ev):
-17.8753   -5.4532   -5.1436   -4.2078    4.6427    7.0734    9.2965    9.8631
         k = 0.1262 0.2186 0.0000 (   1177 PWs)    bands (ev):
-17.9021   -5.3881   -5.1801   -4.1640    4.5959    7.0663    9.2545    9.8957
         k = 0.1243 0.2152 0.0000 (   1177 PWs)    bands (ev):
-17.9285   -5.3231   -5.2161   -4.1206    4.5498    7.0576    9.2131    9.9301
         k = 0.1223 0.2118 0.0000 (   1181 PWs)    bands (ev):
-17.9547   -5.2581   -5.2516   -4.0775    4.5044    7.0474    9.1721    9.9661
         k = 0.1203 0.2084 0.0000 (   1181 PWs)    bands (ev):
-17.9804   -5.2865   -5.1932   -4.0348    4.4597    7.0359    9.1318   10.0035
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      k = 0.1183 0.2050 0.0000 (   1181 PWs)   bands (ev):

 -18.0058   -5.3210   -5.1283   -3.9923    4.4157    7.0232    9.0919   10.0422

      k = 0.1164 0.2016 0.0000 (   1181 PWs)   bands (ev):

 -18.0309   -5.3550   -5.0636   -3.9503    4.3724    7.0094    9.0527   10.0821

      k = 0.1144 0.1981 0.0000 (   1181 PWs)   bands (ev):

 -18.0555   -5.3885   -4.9990   -3.9086    4.3298    6.9946    9.0139   10.1229

      k = 0.1124 0.1947 0.0000 (   1181 PWs)   bands (ev):

 -18.0798   -5.4214   -4.9345   -3.8673    4.2879    6.9789    8.9758   10.1646

      k = 0.1105 0.1913 0.0000 (   1181 PWs)   bands (ev):

 -18.1038   -5.4539   -4.8702   -3.8263    4.2467    6.9625    8.9381   10.2071

      k = 0.1085 0.1879 0.0000 (   1181 PWs)   bands (ev):

 -18.1274   -5.4858   -4.8060   -3.7858    4.2062    6.9454    8.9011   10.2503

      k = 0.1065 0.1845 0.0000 (   1181 PWs)   bands (ev):

 -18.1505   -5.5172   -4.7422   -3.7458    4.1664    6.9278    8.8646   10.2939

      k = 0.1045 0.1811 0.0000 (   1181 PWs)   bands (ev):

 -18.1734   -5.5481   -4.6785   -3.7061    4.1273    6.9096    8.8286   10.3380

      k = 0.1026 0.1776 0.0000 (   1181 PWs)   bands (ev):

 -18.1958   -5.5784   -4.6152   -3.6670    4.0889    6.8910    8.7932   10.3823

      k = 0.1006 0.1742 0.0000 (   1177 PWs)   bands (ev):

 -18.2178   -5.6083   -4.5520   -3.6282    4.0512    6.8721    8.7584   10.3906

      k = 0.0986 0.1708 0.0000 (   1177 PWs)   bands (ev):

 -18.2395   -5.6375   -4.4893   -3.5900    4.0142    6.8530    8.7242   10.3793

      k = 0.0966 0.1674 0.0000 (   1177 PWs)   bands (ev):

 -18.2608   -5.6663   -4.4269   -3.5523    3.9779    6.8336    8.6905   10.3685

      k = 0.0947 0.1640 0.0000 (   1177 PWs)   bands (ev):

 -18.2816   -5.6945   -4.3649   -3.5151    3.9423    6.8140    8.6573   10.3585

      k = 0.0927 0.1606 0.0000 (   1183 PWs)   bands (ev):

 -18.3021   -5.7222   -4.3034   -3.4784    3.9074    6.7944    8.6248   10.3487

      k = 0.0907 0.1571 0.0000 (   1183 PWs)   bands (ev):

 -18.3222   -5.7493   -4.2423   -3.4422    3.8732    6.7747    8.5928   10.3398

      k = 0.0888 0.1537 0.0000 (   1183 PWs)   bands (ev):
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  -18.3419  -5.7759  -4.1817  -3.4066    3.8397    6.7551    8.5613   10.3316
         k = 0.0868 0.1503 0.0000 (   1183 PWs)    bands (ev):
  -18.3611  -5.8019  -4.1216  -3.3715    3.8069    6.7354    8.5305   10.3240
         k = 0.0848 0.1469 0.0000 (   1189 PWs)    bands (ev):
  -18.3800  -5.8274  -4.0621  -3.3371    3.7748    6.7159    8.5002   10.3163
         k = 0.0828 0.1435 0.0000 (   1189 PWs)    bands (ev):
  -18.3985  -5.8523  -4.0031  -3.3032    3.7434    6.6965    8.4705   10.3098
         k = 0.0809 0.1401 0.0000 (   1189 PWs)    bands (ev):
  -18.4165  -5.8766  -3.9447  -3.2699    3.7127    6.6772    8.4414   10.3040
         k = 0.0789 0.1366 0.0000 (   1185 PWs)    bands (ev):
  -18.4342  -5.9004  -3.8868  -3.2371    3.6827    6.6582    8.4129   10.2990
         k = 0.0769 0.1332 0.0000 (   1185 PWs)    bands (ev):
  -18.4514  -5.9236  -3.8297  -3.2051    3.6534    6.6393    8.3849   10.2943
         k = 0.0749 0.1298 0.0000 (   1185 PWs)    bands (ev):
  -18.4682  -5.9463  -3.7734  -3.1736    3.6248    6.6207    8.3575   10.2900
         k = 0.0730 0.1264 0.0000 (   1185 PWs)    bands (ev):
  -18.4846  -5.9684  -3.7178  -3.1429    3.5970    6.6024    8.3308   10.2863
         k = 0.0710 0.1230 0.0000 (   1185 PWs)    bands (ev):
  -18.5006  -5.9899  -3.6630  -3.1128    3.5698    6.5843    8.3046   10.2832
         k = 0.0690 0.1196 0.0000 (   1185 PWs)    bands (ev):
  -18.5162  -6.0109  -3.6090  -3.0833    3.5434    6.5666    8.2790   10.2805
         k = 0.0671 0.1162 0.0000 (   1181 PWs)    bands (ev):
  -18.5313  -6.0312  -3.5559  -3.0546    3.5176    6.5492    8.2540   10.2782
         k = 0.0651 0.1127 0.0000 (   1185 PWs)    bands (ev):
  -18.5460  -6.0511  -3.5038  -3.0266    3.4926    6.5322    8.2296   10.2759
         k = 0.0631 0.1093 0.0000 (   1185 PWs)    bands (ev):
  -18.5603  -6.0703  -3.4526  -2.9992    3.4683    6.5155    8.2058   10.2746
         k = 0.0611 0.1059 0.0000 (   1185 PWs)    bands (ev):
  -18.5742  -6.0890  -3.4024  -2.9726    3.4447    6.4992    8.1827   10.2736
         k = 0.0592 0.1025 0.0000 (   1185 PWs)    bands (ev):
  -18.5876  -6.1070  -3.3531  -2.9467    3.4218    6.4833    8.1601   10.2731
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        k = 0.0572 0.0991 0.0000 (   1185 PWs)    bands (ev):

  -18.6006   -6.1245   -3.3050   -2.9216    3.3996    6.4679    8.1382   10.2729
        k = 0.0552 0.0957 0.0000 (   1185 PWs)    bands (ev):

  -18.6132   -6.1415   -3.2580   -2.8972    3.3782    6.4528    8.1169   10.2732
        k = 0.0533 0.0922 0.0000 (   1185 PWs)    bands (ev):

  -18.6254   -6.1578   -3.2121   -2.8735    3.3575    6.4382    8.0962   10.2737
        k = 0.0513 0.0888 0.0000 (   1185 PWs)    bands (ev):

  -18.6371   -6.1736   -3.1674   -2.8506    3.3374    6.4241    8.0762   10.2745
        k = 0.0493 0.0854 0.0000 (   1185 PWs)    bands (ev):

  -18.6484   -6.1887   -3.1239   -2.8286    3.3182    6.4104    8.0568   10.2756
        k = 0.0473 0.0820 0.0000 (   1185 PWs)    bands (ev):

  -18.6592   -6.2033   -3.0818   -2.8073    3.2996    6.3972    8.0381   10.2770
        k = 0.0454 0.0786 0.0000 (   1185 PWs)    bands (ev):

  -18.6696   -6.2173   -3.0409   -2.7867    3.2818    6.3845    8.0200   10.2786
        k = 0.0434 0.0752 0.0000 (   1185 PWs)    bands (ev):

  -18.6796   -6.2307   -3.0014   -2.7671    3.2647    6.3722    8.0026   10.2805
        k = 0.0414 0.0717 0.0000 (   1185 PWs)    bands (ev):

  -18.6891   -6.2436   -2.9633   -2.7482    3.2483    6.3605    7.9859   10.2824
        k = 0.0394 0.0683 0.0000 (   1185 PWs)    bands (ev):

  -18.6982   -6.2558   -2.9267   -2.7301    3.2327    6.3492    7.9699   10.2846
        k = 0.0375 0.0649 0.0000 (   1185 PWs)    bands (ev):

  -18.7069   -6.2674   -2.8916   -2.7129    3.2178    6.3385    7.9546   10.2869
        k = 0.0355 0.0615 0.0000 (   1185 PWs)    bands (ev):

  -18.7151   -6.2785   -2.8579   -2.6965    3.2037    6.3283    7.9399   10.2892
        k = 0.0335 0.0581 0.0000 (   1185 PWs)    bands (ev):

  -18.7229   -6.2889   -2.8259   -2.6810    3.1903    6.3186    7.9260   10.2917
        k = 0.0316 0.0547 0.0000 (   1185 PWs)    bands (ev):

  -18.7303   -6.2988   -2.7955   -2.6663    3.1776    6.3095    7.9129   10.2937
        k = 0.0296 0.0512 0.0000 (   1185 PWs)    bands (ev):

  -18.7372   -6.3081   -2.7667   -2.6525    3.1657    6.3008    7.9004   10.2961
        k = 0.0276 0.0478 0.0000 (   1185 PWs)    bands (ev):
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  -18.7436  -6.3167  -2.7396  -2.6395   3.1546   6.2927   7.8887  10.2986
        k = 0.0256 0.0444 0.0000 (   1185 PWs)   bands (ev):
  -18.7496  -6.3248  -2.7141  -2.6274   3.1442   6.2852   7.8778  10.3010
        k = 0.0237 0.0410 0.0000 (   1185 PWs)   bands (ev):
  -18.7552  -6.3323  -2.6904  -2.6162   3.1345   6.2782   7.8676  10.3034
        k = 0.0217 0.0376 0.0000 (   1185 PWs)   bands (ev):
  -18.7603  -6.3392  -2.6685  -2.6058   3.1257   6.2717   7.8582  10.3057
        k = 0.0197 0.0342 0.0000 (   1193 PWs)   bands (ev):
  -18.7650  -6.3456  -2.6484  -2.5965   3.1176   6.2658   7.8496  10.3079
        k = 0.0178 0.0307 0.0000 (   1193 PWs)   bands (ev):
  -18.7693  -6.3513  -2.6301  -2.5879   3.1102   6.2605   7.8417  10.3099
        k = 0.0158 0.0273 0.0000 (   1193 PWs)   bands (ev):
  -18.7731  -6.3563  -2.6137  -2.5803   3.1036   6.2557   7.8347  10.3118
        k = 0.0138 0.0239 0.0000 (   1187 PWs)   bands (ev):
  -18.7764  -6.3608  -2.5990  -2.5734   3.0978   6.2514   7.8285  10.3142
        k = 0.0118 0.0205 0.0000 (   1187 PWs)   bands (ev):
  -18.7793  -6.3647  -2.5863  -2.5675   3.0928   6.2478   7.8231  10.3157
        k = 0.0099 0.0171 0.0000 (   1193 PWs)   bands (ev):
  -18.7818  -6.3681  -2.5756  -2.5626   3.0885   6.2446   7.8185  10.3168
        k = 0.0079 0.0137 0.0000 (   1193 PWs)   bands (ev):
  -18.7838  -6.3708  -2.5668  -2.5585   3.0850   6.2421   7.8147  10.3179
        k = 0.0059 0.0102 0.0000 (   1201 PWs)   bands (ev):
  -18.7854  -6.3729  -2.5601  -2.5554   3.0823   6.2401   7.8118  10.3186
        k = 0.0039 0.0068 0.0000 (   1205 PWs)   bands (ev):
  -18.7865  -6.3744  -2.5552  -2.5531   3.0803   6.2387   7.8097  10.3191
        k = 0.0020 0.0034 0.0000 (   1205 PWs)   bands (ev):
  -18.7871  -6.3753  -2.5523  -2.5518   3.0792   6.2378   7.8084  10.3195
        k = 0.0000 0.0000 0.0000 (   1205 PWs)   bands (ev):
  -18.7874  -6.3756  -2.5513  -2.5513   3.0788   6.2375   7.8080  10.3196
  ------ SPIN DOWN ----------
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       k = 0.0000 0.0000 0.0000 (   1205 PWs)   bands (ev):

 -18.7874  -6.3756  -2.5513  -2.5513   3.0788   6.2375   7.8080  10.3196

       k = 0.0034 0.0020 0.0000 (   1205 PWs)   bands (ev):

 -18.7871  -6.3753  -2.5523  -2.5518   3.0792   6.2378   7.8085  10.3195

       k = 0.0068 0.0040 0.0000 (   1205 PWs)   bands (ev):

 -18.7865  -6.3744  -2.5552  -2.5531   3.0804   6.2387   7.8097  10.3191

       k = 0.0103 0.0059 0.0000 (   1201 PWs)   bands (ev):

 -18.7854  -6.3729  -2.5601  -2.5554   3.0823   6.2401   7.8118  10.3185

       k = 0.0137 0.0079 0.0000 (   1193 PWs)   bands (ev):

 -18.7838  -6.3708  -2.5669  -2.5585   3.0850   6.2421   7.8148  10.3180

       k = 0.0171 0.0099 0.0000 (   1189 PWs)   bands (ev):

 -18.7818  -6.3680  -2.5757  -2.5626   3.0886   6.2447   7.8186  10.3169

       k = 0.0205 0.0119 0.0000 (   1189 PWs)   bands (ev):

 -18.7793  -6.3647  -2.5865  -2.5676   3.0928   6.2478   7.8232  10.3155

       k = 0.0240 0.0138 0.0000 (   1187 PWs)   bands (ev):

 -18.7763  -6.3607  -2.5994  -2.5734   3.0979   6.2515   7.8286  10.3136

       k = 0.0274 0.0158 0.0000 (   1187 PWs)   bands (ev):

 -18.7730  -6.3562  -2.6140  -2.5802   3.1038   6.2558   7.8349  10.3118

       k = 0.0308 0.0178 0.0000 (   1183 PWs)   bands (ev):

 -18.7692  -6.3511  -2.6306  -2.5878   3.1104   6.2606   7.8419  10.3098

       k = 0.0342 0.0198 0.0000 (   1189 PWs)   bands (ev):

 -18.7649  -6.3454  -2.6491  -2.5963   3.1178   6.2660   7.8498  10.3072

       k = 0.0377 0.0217 0.0000 (   1189 PWs)   bands (ev):

 -18.7602  -6.3391  -2.6695  -2.6057   3.1259   6.2719   7.8584  10.3047

       k = 0.0411 0.0237 0.0000 (   1189 PWs)   bands (ev):

 -18.7551  -6.3322  -2.6917  -2.6159   3.1348   6.2784   7.8679  10.3021

       k = 0.0445 0.0257 0.0000 (   1189 PWs)   bands (ev):

 -18.7495  -6.3246  -2.7157  -2.6269   3.1445   6.2854   7.8781  10.2992

       k = 0.0479 0.0277 0.0000 (   1193 PWs)   bands (ev):

 -18.7434  -6.3165  -2.7415  -2.6390   3.1550   6.2930   7.8890  10.2960

       k = 0.0514 0.0297 0.0000 (   1191 PWs)   bands (ev):
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 -18.7369  -6.3078  -2.7690  -2.6517   3.1662   6.3011   7.9007  10.2932

      k = 0.0548 0.0316 0.0000 (  1191 PWs)   bands (ev):

 -18.7300  -6.2985  -2.7984  -2.6652   3.1781   6.3098   7.9132  10.2898

      k = 0.0582 0.0336 0.0000 (  1191 PWs)   bands (ev):

 -18.7226  -6.2886  -2.8295  -2.6794   3.1908   6.3190   7.9263  10.2863

      k = 0.0616 0.0356 0.0000 (  1187 PWs)   bands (ev):

 -18.7148  -6.2780  -2.8622  -2.6944   3.2043   6.3287   7.9402  10.2827

      k = 0.0651 0.0376 0.0000 (  1191 PWs)   bands (ev):

 -18.7065  -6.2670  -2.8966  -2.7102   3.2185   6.3390   7.9548  10.2789

      k = 0.0685 0.0395 0.0000 (  1191 PWs)   bands (ev):

 -18.6978  -6.2553  -2.9327  -2.7267   3.2334   6.3498   7.9700  10.2751

      k = 0.0719 0.0415 0.0000 (  1191 PWs)   bands (ev):

 -18.6887  -6.2430  -2.9703  -2.7440   3.2491   6.3611   7.9858  10.2712

      k = 0.0753 0.0435 0.0000 (  1191 PWs)   bands (ev):

 -18.6791  -6.2301  -3.0095  -2.7619   3.2655   6.3729   8.0024  10.2672

      k = 0.0788 0.0455 0.0000 (  1191 PWs)   bands (ev):

 -18.6691  -6.2166  -3.0503  -2.7805   3.2827   6.3851   8.0195  10.2631

      k = 0.0822 0.0475 0.0000 (  1191 PWs)   bands (ev):

 -18.6586  -6.2025  -3.0925  -2.7998   3.3006   6.3979   8.0372  10.2590

      k = 0.0856 0.0494 0.0000 (  1191 PWs)   bands (ev):

 -18.6477  -6.1879  -3.1362  -2.8197   3.3192   6.4112   8.0555  10.2549

      k = 0.0890 0.0514 0.0000 (  1191 PWs)   bands (ev):

 -18.6364  -6.1726  -3.1813  -2.8402   3.3386   6.4249   8.0744  10.2508

      k = 0.0925 0.0534 0.0000 (  1191 PWs)   bands (ev):

 -18.6246  -6.1568  -3.2278  -2.8613   3.3586   6.4391   8.0938  10.2468

      k = 0.0959 0.0554 0.0000 (  1191 PWs)   bands (ev):

 -18.6124  -6.1404  -3.2756  -2.8830   3.3794   6.4538   8.1137  10.2427

      k = 0.0993 0.0573 0.0000 (  1189 PWs)   bands (ev):

 -18.5997  -6.1234  -3.3248  -2.9052   3.4009   6.4689   8.1342  10.2389

      k = 0.1027 0.0593 0.0000 (  1187 PWs)   bands (ev):

 -18.5867  -6.1058  -3.3752  -2.9280   3.4232   6.4844   8.1551  10.2354
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      k = 0.1062 0.0613 0.0000 (   1187 PWs)    bands (ev):

 -18.5732  -6.0876  -3.4269  -2.9513    3.4461    6.5003    8.1764   10.2316

      k = 0.1096 0.0633 0.0000 (   1187 PWs)    bands (ev):

 -18.5592  -6.0689  -3.4798  -2.9752    3.4697    6.5167    8.1982   10.2280

      k = 0.1130 0.0652 0.0000 (   1187 PWs)    bands (ev):

 -18.5449  -6.0496  -3.5339  -2.9995    3.4941    6.5334    8.2204   10.2245

      k = 0.1164 0.0672 0.0000 (   1187 PWs)    bands (ev):

 -18.5301  -6.0296  -3.5891  -3.0243    3.5192    6.5505    8.2429   10.2212

      k = 0.1199 0.0692 0.0000 (   1189 PWs)    bands (ev):

 -18.5149  -6.0092  -3.6455  -3.0495    3.5449    6.5679    8.2658   10.2179

      k = 0.1233 0.0712 0.0000 (   1189 PWs)    bands (ev):

 -18.4993  -5.9881  -3.7029  -3.0751    3.5714    6.5857    8.2890   10.2151

      k = 0.1267 0.0732 0.0000 (   1189 PWs)    bands (ev):

 -18.4832  -5.9665  -3.7613  -3.1012    3.5986    6.6037    8.3125   10.2125

      k = 0.1301 0.0751 0.0000 (   1189 PWs)    bands (ev):

 -18.4667  -5.9443  -3.8207  -3.1276    3.6265    6.6221    8.3362   10.2102

      k = 0.1336 0.0771 0.0000 (   1187 PWs)    bands (ev):

 -18.4498  -5.9215  -3.8810  -3.1543    3.6550    6.6407    8.3602   10.2086

      k = 0.1370 0.0791 0.0000 (   1187 PWs)    bands (ev):

 -18.4325  -5.8982  -3.9423  -3.1814    3.6843    6.6595    8.3843   10.2071

      k = 0.1404 0.0811 0.0000 (   1187 PWs)    bands (ev):

 -18.4148  -5.8743  -4.0045  -3.2089    3.7143    6.6786    8.4087   10.2059

      k = 0.1438 0.0830 0.0000 (   1186 PWs)    bands (ev):

 -18.3967  -5.8498  -4.0675  -3.2366    3.7449    6.6978    8.4331   10.2054

      k = 0.1473 0.0850 0.0000 (   1186 PWs)    bands (ev):

 -18.3781  -5.8248  -4.1313  -3.2646    3.7763    6.7171    8.4576   10.2051

      k = 0.1507 0.0870 0.0000 (   1186 PWs)    bands (ev):

 -18.3592  -5.7992  -4.1959  -3.2928    3.8083    6.7366    8.4821   10.2054

      k = 0.1541 0.0890 0.0000 (   1186 PWs)    bands (ev):

 -18.3398  -5.7731  -4.2613  -3.3213    3.8410    6.7561    8.5067   10.2063

      k = 0.1575 0.0910 0.0000 (   1186 PWs)    bands (ev):
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   -18.3201   -5.7464   -4.3274   -3.3500    3.8744    6.7756    8.5311   10.2078
        k = 0.1610 0.0929 0.0000 (   1182 PWs)   bands (ev):
   -18.2999   -5.7192   -4.3942   -3.3790    3.9085    6.7951    8.5556   10.2100
        k = 0.1644 0.0949 0.0000 (   1182 PWs)   bands (ev):
   -18.2793   -5.6914   -4.4616   -3.4081    3.9433    6.8145    8.5798   10.2129
        k = 0.1678 0.0969 0.0000 (   1182 PWs)   bands (ev):
   -18.2584   -5.6631   -4.5297   -3.4373    3.9788    6.8338    8.6039   10.2165
        k = 0.1712 0.0989 0.0000 (   1182 PWs)   bands (ev):
   -18.2370   -5.6342   -4.5984   -3.4668    4.0149    6.8529    8.6277   10.2209
        k = 0.1747 0.1008 0.0000 (   1182 PWs)   bands (ev):
   -18.2153   -5.6048   -4.6677   -3.4963    4.0518    6.8716    8.6513   10.2264
        k = 0.1781 0.1028 0.0000 (   1182 PWs)   bands (ev):
   -18.1932   -5.5748   -4.7375   -3.5260    4.0893    6.8901    8.6745   10.2326
        k = 0.1815 0.1048 0.0000 (   1182 PWs)   bands (ev):
   -18.1707   -5.5444   -4.8078   -3.5557    4.1275    6.9081    8.6973   10.2398
        k = 0.1849 0.1068 0.0000 (   1182 PWs)   bands (ev):
   -18.1478   -5.5134   -4.8786   -3.5856    4.1663    6.9256    8.7197   10.2481
        k = 0.1884 0.1087 0.0000 (   1182 PWs)   bands (ev):
   -18.1245   -5.4819   -4.9498   -3.6155    4.2059    6.9426    8.7416   10.2242
        k = 0.1918 0.1107 0.0000 (   1182 PWs)   bands (ev):
   -18.1009   -5.4498   -5.0214   -3.6454    4.2461    6.9588    8.7629   10.1796
        k = 0.1952 0.1127 0.0000 (   1178 PWs)   bands (ev):
   -18.0769   -5.4173   -5.0934   -3.6753    4.2870    6.9742    8.7837   10.1356
        k = 0.1986 0.1147 0.0000 (   1178 PWs)   bands (ev):
   -18.0525   -5.3842   -5.1658   -3.7053    4.3286    6.9888    8.8038   10.0924
        k = 0.2021 0.1167 0.0000 (   1178 PWs)   bands (ev):
   -18.0278   -5.3507   -5.2386   -3.7354    4.3708    7.0023    8.8232   10.0501
        k = 0.2055 0.1186 0.0000 (   1178 PWs)   bands (ev):
   -18.0027   -5.3166   -5.3116   -3.7654    4.4137    7.0146    8.8419   10.0088
        k = 0.2089 0.1206 0.0000 (   1178 PWs)   bands (ev):
   -17.9772   -5.3850   -5.2820   -3.7953    4.4573    7.0256    8.8599    9.9688
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      k = 0.2123 0.1226 0.0000 (   1178 PWs)   bands (ev):

 -17.9514  -5.4586  -5.2469  -3.8253    4.5015    7.0352    8.8770    9.9301

      k = 0.2158 0.1246 0.0000 (   1178 PWs)   bands (ev):

 -17.9253  -5.5325  -5.2114  -3.8552    4.5465    7.0432    8.8934    9.8930

      k = 0.2192 0.1265 0.0000 (   1178 PWs)   bands (ev):

 -17.8988  -5.6065  -5.1754  -3.8850    4.5920    7.0495    8.9089    9.8575

      k = 0.2226 0.1285 0.0000 (   1174 PWs)   bands (ev):

 -17.8719  -5.6808  -5.1388  -3.9147    4.6383    7.0539    8.9236    9.8240

      k = 0.2260 0.1305 0.0000 (   1172 PWs)   bands (ev):

 -17.8448  -5.7552  -5.1018  -3.9443    4.6851    7.0563    8.9374    9.7926

      k = 0.2295 0.1325 0.0000 (   1172 PWs)   bands (ev):

 -17.8173  -5.8297  -5.0643  -3.9739    4.7327    7.0564    8.9504    9.7634

      k = 0.2329 0.1345 0.0000 (   1172 PWs)   bands (ev):

 -17.7895  -5.9044  -5.0264  -4.0033    4.7809    7.0543    8.9625    9.7365

      k = 0.2363 0.1364 0.0000 (   1172 PWs)   bands (ev):

 -17.7613  -5.9792  -4.9880  -4.0326    4.8297    7.0496    8.9738    9.7123

      k = 0.2397 0.1384 0.0000 (   1176 PWs)   bands (ev):

 -17.7329  -6.0542  -4.9492  -4.0617    4.8792    7.0423    8.9841    9.6906

      k = 0.2432 0.1404 0.0000 (   1176 PWs)   bands (ev):

 -17.7042  -6.1291  -4.9100  -4.0907    4.9294    7.0323    8.9937    9.6719

      k = 0.2466 0.1424 0.0000 (   1176 PWs)   bands (ev):

 -17.6751  -6.2040  -4.8703  -4.1195    4.9802    7.0196    9.0026    9.6562

      k = 0.2500 0.1443 0.0000 (   1168 PWs)   bands (ev):

 -17.6458  -6.2789  -4.8300  -4.1481    5.0316    7.0039    9.0108    9.6437

      k = 0.2534 0.1463 0.0000 (   1186 PWs)   bands (ev):

 -17.6162  -6.3540  -4.7895  -4.1768    5.0837    6.9850    9.0179    9.6337

      k = 0.2568 0.1483 0.0000 (   1186 PWs)   bands (ev):

 -17.5863  -6.4288  -4.7486  -4.2051    5.1364    6.9634    9.0246    9.6274

      k = 0.2603 0.1503 0.0000 (   1186 PWs)   bands (ev):

 -17.5561  -6.5036  -4.7072  -4.2332    5.1897    6.9388    9.0306    9.6243

      k = 0.2637 0.1522 0.0000 (   1186 PWs)   bands (ev):
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   -17.5257   -6.5783   -4.6654   -4.2611    5.2436    6.9113    9.0360    9.6245

          k = 0.2671 0.1542 0.0000 (   1186 PWs)    bands (ev):

   -17.4950   -6.6528   -4.6233   -4.2887    5.2982    6.8808    9.0409    9.6279

          k = 0.2705 0.1562 0.0000 (   1182 PWs)    bands (ev):

   -17.4641   -6.7273   -4.5807   -4.3161    5.3534    6.8475    9.0452    9.6344

          k = 0.2740 0.1582 0.0000 (   1182 PWs)    bands (ev):

   -17.4329   -6.8016   -4.5378   -4.3432    5.4092    6.8114    9.0491    9.6441

          k = 0.2774 0.1602 0.0000 (   1184 PWs)    bands (ev):

   -17.4015   -6.8757   -4.4946   -4.3702    5.4656    6.7727    9.0524    9.6568

          k = 0.2808 0.1621 0.0000 (   1188 PWs)    bands (ev):

   -17.3699   -6.9496   -4.4509   -4.3969    5.5226    6.7314    9.0553    9.6724

          k = 0.2842 0.1641 0.0000 (   1188 PWs)    bands (ev):

   -17.3380   -7.0235   -4.4233   -4.4070    5.5802    6.6876    9.0578    9.6909

          k = 0.2877 0.1661 0.0000 (   1188 PWs)    bands (ev):

   -17.3060   -7.0969   -4.4494   -4.3627    5.6383    6.6415    9.0601    9.7122

          k = 0.2911 0.1681 0.0000 (   1192 PWs)    bands (ev):

   -17.2738   -7.1701   -4.4754   -4.3181    5.6971    6.5933    9.0620    9.7361

          k = 0.2945 0.1700 0.0000 (   1192 PWs)    bands (ev):

   -17.2413   -7.2430   -4.5009   -4.2732    5.7564    6.5430    9.0637    9.7625

          k = 0.2979 0.1720 0.0000 (   1192 PWs)    bands (ev):

   -17.2088   -7.3156   -4.5261   -4.2280    5.8162    6.4909    9.0652    9.7913

          k = 0.3014 0.1740 0.0000 (   1192 PWs)    bands (ev):

   -17.1760   -7.3879   -4.5511   -4.1826    5.8766    6.4370    9.0665    9.8224

          k = 0.3048 0.1760 0.0000 (   1192 PWs)    bands (ev):

   -17.1431   -7.4598   -4.5757   -4.1368    5.9376    6.3815    9.0676    9.8557

          k = 0.3082 0.1780 0.0000 (   1192 PWs)    bands (ev):

   -17.1101   -7.5314   -4.6000   -4.0909    5.9990    6.3245    9.0687    9.8911

          k = 0.3116 0.1799 0.0000 (   1192 PWs)    bands (ev):

   -17.0769   -7.6025   -4.6240   -4.0447    6.0610    6.2661    9.0696    9.9285

          k = 0.3151 0.1819 0.0000 (   1192 PWs)    bands (ev):

   -17.0437   -7.6732   -4.6477   -3.9982    6.1234    6.2065    9.0706    9.9677
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      k = 0.3185 0.1839 0.0000 (   1192 PWs)    bands (ev):

-17.0103   -7.7435   -4.6710   -3.9516    6.1459    6.1863    9.0715   10.0087

      k = 0.3219 0.1859 0.0000 (   1192 PWs)    bands (ev):

-16.9769   -7.8133   -4.6940   -3.9048    6.0842    6.2497    9.0725   10.0513

      k = 0.3253 0.1878 0.0000 (   1192 PWs)    bands (ev):

-16.9434   -7.8826   -4.7166   -3.8578    6.0216    6.3135    9.0736   10.0956

      k = 0.3288 0.1898 0.0000 (   1196 PWs)    bands (ev):

-16.9099   -7.9514   -4.7390   -3.8107    5.9583    6.3778    9.0747   10.1414

      k = 0.3322 0.1918 0.0000 (   1196 PWs)    bands (ev):

-16.8763   -8.0197   -4.7609   -3.7635    5.8943    6.4424    9.0760   10.1886

      k = 0.3356 0.1938 0.0000 (   1196 PWs)    bands (ev):

-16.8427   -8.0874   -4.7824   -3.7161    5.8298    6.5074    9.0775   10.2372

      k = 0.3390 0.1957 0.0000 (   1192 PWs)    bands (ev):

-16.8091   -8.1545   -4.8036   -3.6687    5.7648    6.5727    9.0794   10.2871

      k = 0.3425 0.1977 0.0000 (   1192 PWs)    bands (ev):

-16.7755   -8.2210   -4.8244   -3.6212    5.6994    6.6383    9.0814   10.3383

      k = 0.3459 0.1997 0.0000 (   1194 PWs)    bands (ev):

-16.7420   -8.2869   -4.8448   -3.5737    5.6337    6.7041    9.0837   10.3906

      k = 0.3493 0.2017 0.0000 (   1194 PWs)    bands (ev):

-16.7085   -8.3520   -4.8648   -3.5262    5.5678    6.7702    9.0865   10.4440

      k = 0.3527 0.2037 0.0000 (   1194 PWs)    bands (ev):

-16.6751   -8.4165   -4.8845   -3.4786    5.5017    6.8364    9.0897   10.4985

      k = 0.3562 0.2056 0.0000 (   1194 PWs)    bands (ev):

-16.6418   -8.4802   -4.9037   -3.4312    5.4357    6.9028    9.0934   10.5540

      k = 0.3596 0.2076 0.0000 (   1194 PWs)    bands (ev):

-16.6087   -8.5432   -4.9226   -3.3838    5.3696    6.9692    9.0977   10.6105

      k = 0.3630 0.2096 0.0000 (   1194 PWs)    bands (ev):

-16.5757   -8.6053   -4.9410   -3.3365    5.3037    7.0355    9.1027   10.6679

      k = 0.3664 0.2116 0.0000 (   1194 PWs)    bands (ev):

-16.5428   -8.6667   -4.9591   -3.2894    5.2379    7.1018    9.1083   10.7261

      k = 0.3699 0.2135 0.0000 (   1194 PWs)    bands (ev):
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  -16.5102   -8.7272   -4.9767   -3.2424    5.1724    7.1679    9.1148   10.7852
        k = 0.3733 0.2155 0.0000 (   1194 PWs)    bands (ev):
  -16.4778   -8.7868   -4.9939   -3.1957    5.1073    7.2338    9.1222   10.8451
        k = 0.3767 0.2175 0.0000 (   1194 PWs)    bands (ev):
  -16.4456   -8.8455   -5.0107   -3.1492    5.0425    7.2993    9.1306   10.9057
        k = 0.3801 0.2195 0.0000 (   1194 PWs)    bands (ev):
  -16.4137   -8.9033   -5.0271   -3.1029    4.9782    7.3642    9.1402   10.9671
        k = 0.3836 0.2214 0.0000 (   1186 PWs)    bands (ev):
  -16.3821   -8.9601   -5.0430   -3.0570    4.9145    7.4286    9.1511   11.0291
        k = 0.3870 0.2234 0.0000 (   1188 PWs)    bands (ev):
  -16.3509   -9.0159   -5.0585   -3.0115    4.8513    7.4922    9.1633   11.0917
        k = 0.3904 0.2254 0.0000 (   1188 PWs)    bands (ev):
  -16.3201   -9.0706   -5.0736   -2.9663    4.7888    7.5548    9.1772   11.1548
        k = 0.3938 0.2274 0.0000 (   1188 PWs)    bands (ev):
  -16.2896   -9.1242   -5.0882   -2.9216    4.7272    7.6164    9.1928   11.2186
        k = 0.3973 0.2294 0.0000 (   1196 PWs)    bands (ev):
  -16.2596   -9.1767   -5.1025   -2.8775    4.6662    7.6766    9.2103   11.2827
        k = 0.4007 0.2313 0.0000 (   1196 PWs)    bands (ev):
  -16.2300   -9.2281   -5.1163   -2.8338    4.6063    7.7354    9.2300   11.3474
        k = 0.4041 0.2333 0.0000 (   1200 PWs)    bands (ev):
  -16.2010   -9.2783   -5.1296   -2.7909    4.5470    7.7925    9.2520   11.4124
        k = 0.4075 0.2353 0.0000 (   1200 PWs)    bands (ev):
  -16.1724   -9.3271   -5.1425   -2.7485    4.4891    7.8476    9.2766   11.4777
        k = 0.4110 0.2373 0.0000 (   1192 PWs)    bands (ev):
  -16.1445   -9.3747   -5.1549   -2.7068    4.4324    7.9007    9.3040   11.5435
        k = 0.4144 0.2392 0.0000 (   1192 PWs)    bands (ev):
  -16.1171   -9.4210   -5.1669   -2.6659    4.3769    7.9514    9.3343   11.6094
        k = 0.4178 0.2412 0.0000 (   1192 PWs)    bands (ev):
  -16.0904   -9.4660   -5.1784   -2.6259    4.3226    7.9996    9.3678   11.6754
        k = 0.4212 0.2432 0.0000 (   1196 PWs)    bands (ev):
  -16.0644   -9.5095   -5.1895   -2.5867    4.2697    8.0452    9.4045   11.7416
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     k = 0.4247 0.2452 0.0000 (   1196 PWs)    bands (ev):

 -16.0391  -9.5516  -5.2001  -2.5485    4.2182    8.0879   9.4447  11.8078

     k = 0.4281 0.2472 0.0000 (   1196 PWs)    bands (ev):

 -16.0146  -9.5922  -5.2103  -2.5114    4.1683    8.1278   9.4883  11.8739

     k = 0.4315 0.2491 0.0000 (   1196 PWs)    bands (ev):

 -15.9909  -9.6313  -5.2200  -2.4753    4.1200    8.1648   9.5354  11.9399

     k = 0.4349 0.2511 0.0000 (   1196 PWs)    bands (ev):

 -15.9680  -9.6688  -5.2292  -2.4404    4.0733    8.1988   9.5861  12.0056

     k = 0.4384 0.2531 0.0000 (   1194 PWs)    bands (ev):

 -15.9459  -9.7046  -5.2380  -2.4067    4.0285    8.2300   9.6402  12.0710

     k = 0.4418 0.2551 0.0000 (   1194 PWs)    bands (ev):

 -15.9248  -9.7389  -5.2463  -2.3743    3.9854    8.2584   9.6975  12.1359

     k = 0.4452 0.2570 0.0000 (   1194 PWs)    bands (ev):

 -15.9047  -9.7714  -5.2542  -2.3432    3.9443    8.2841   9.7581  12.2001

     k = 0.4486 0.2590 0.0000 (   1194 PWs)    bands (ev):

 -15.8856  -9.8022  -5.2615  -2.3136    3.9052    8.3073   9.8216  12.2635

     k = 0.4521 0.2610 0.0000 (   1196 PWs)    bands (ev):

 -15.8675  -9.8312  -5.2684  -2.2856    3.8681    8.3281   9.8880  12.3259

     k = 0.4555 0.2630 0.0000 (   1192 PWs)    bands (ev):

 -15.8504  -9.8584  -5.2749  -2.2590    3.8332    8.3466   9.9570  12.3517

     k = 0.4589 0.2649 0.0000 (   1192 PWs)    bands (ev):

 -15.8345  -9.8838  -5.2808  -2.2342    3.8006    8.3631  10.0284  12.2544

     k = 0.4623 0.2669 0.0000 (   1196 PWs)    bands (ev):

 -15.8197  -9.9073  -5.2863  -2.2110    3.7703    8.3777  10.1020  12.1570

     k = 0.4658 0.2689 0.0000 (   1188 PWs)    bands (ev):

 -15.8060  -9.9288  -5.2912  -2.1896    3.7425    8.3906  10.1776  12.0598

     k = 0.4692 0.2709 0.0000 (   1188 PWs)    bands (ev):

 -15.7936  -9.9484  -5.2957  -2.1701    3.7170    8.4018  10.2548  11.9631

     k = 0.4726 0.2729 0.0000 (   1188 PWs)    bands (ev):

 -15.7824  -9.9661  -5.2998  -2.1524    3.6939    8.4115  10.3333  11.8671

     k = 0.4760 0.2748 0.0000 (   1184 PWs)    bands (ev):
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   -15.7724   -9.9817   -5.3034   -2.1367    3.6735    8.4198   10.4129   11.7723

          k = 0.4795 0.2768 0.0000 (   1184 PWs)    bands (ev):

   -15.7637   -9.9953   -5.3065   -2.1229    3.6557    8.4269   10.4930   11.6791

          k = 0.4829 0.2788 0.0000 (   1184 PWs)    bands (ev):

   -15.7564  -10.0068   -5.3091   -2.1112    3.6405    8.4326   10.5728   11.5882

          k = 0.4863 0.2808 0.0000 (   1184 PWs)    bands (ev):

   -15.7503  -10.0163   -5.3113   -2.1016    3.6281    8.4373   10.6513   11.5007

          k = 0.4897 0.2827 0.0000 (   1188 PWs)    bands (ev):

   -15.7456  -10.0236   -5.3130   -2.0941    3.6183    8.4408   10.7262   11.4188

          k = 0.4932 0.2847 0.0000 (   1192 PWs)    bands (ev):

   -15.7422  -10.0289   -5.3142   -2.0887    3.6113    8.4433   10.7933   11.3467

          k = 0.4966 0.2867 0.0000 (   1192 PWs)    bands (ev):

   -15.7402  -10.0321   -5.3149   -2.0855    3.6071    8.4448   10.8438   11.2933

          k = 0.5000 0.2887 0.0000 (   1192 PWs)    bands (ev):

   -15.7395  -10.0332   -5.3152   -2.0844    3.6057    8.4453   10.8635   11.2725

          k = 0.4980 0.2921 0.0000 (   1192 PWs)    bands (ev):

   -15.7394  -10.0330   -5.3161   -2.0842    3.6058    8.4466   10.8638   11.2730

          k = 0.4960 0.2955 0.0000 (   1192 PWs)    bands (ev):

   -15.7389  -10.0324   -5.3189   -2.0835    3.6059    8.4505   10.8648   11.2744

          k = 0.4940 0.2990 0.0000 (   1192 PWs)    bands (ev):

   -15.7382  -10.0315   -5.3235   -2.0824    3.6062    8.4569   10.8665   11.2767

          k = 0.4921 0.3024 0.0000 (   1188 PWs)    bands (ev):

   -15.7371  -10.0302   -5.3300   -2.0809    3.6066    8.4658   10.8688   11.2799

          k = 0.4901 0.3059 0.0000 (   1192 PWs)    bands (ev):

   -15.7358  -10.0286   -5.3385   -2.0789    3.6070    8.4772   10.8718   11.2840

          k = 0.4881 0.3093 0.0000 (   1192 PWs)    bands (ev):

   -15.7341  -10.0266   -5.3487   -2.0764    3.6076    8.4912   10.8754   11.2890

          k = 0.4861 0.3127 0.0000 (   1192 PWs)    bands (ev):

   -15.7322  -10.0242   -5.3607   -2.0736    3.6083    8.5077   10.8797   11.2950

          k = 0.4841 0.3162 0.0000 (   1192 PWs)    bands (ev):

   -15.7299  -10.0214   -5.3744   -2.0703    3.6091    8.5267   10.8847   11.3019
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      k = 0.4821 0.3196 0.0000 (   1196 PWs)   bands (ev):

 -15.7274 -10.0183   -5.3900   -2.0665    3.6097    8.5481   10.8903   11.3098

      k = 0.4802 0.3230 0.0000 (   1196 PWs)   bands (ev):

 -15.7246 -10.0149   -5.4073   -2.0624    3.6107    8.5719   10.8966   11.3185

      k = 0.4782 0.3265 0.0000 (   1190 PWs)   bands (ev):

 -15.7214 -10.0110   -5.4264   -2.0577    3.6119    8.5981   10.9035   11.3283

      k = 0.4762 0.3299 0.0000 (   1190 PWs)   bands (ev):

 -15.7180 -10.0068   -5.4471   -2.0527    3.6130    8.6266   10.9111   11.3389

      k = 0.4742 0.3334 0.0000 (   1190 PWs)   bands (ev):

 -15.7143 -10.0022   -5.4695   -2.0472    3.6142    8.6573   10.9194   11.3506

      k = 0.4722 0.3368 0.0000 (   1190 PWs)   bands (ev):

 -15.7103   -9.9973   -5.4935   -2.0413    3.6155    8.6904   10.9283   11.3632

      k = 0.4702 0.3402 0.0000 (   1190 PWs)   bands (ev):

 -15.7061   -9.9920   -5.5191   -2.0350    3.6168    8.7256   10.9379   11.3768

      k = 0.4683 0.3437 0.0000 (   1190 PWs)   bands (ev):

 -15.7015   -9.9863   -5.5462   -2.0283    3.6182    8.7629   10.9482   11.3913

      k = 0.4663 0.3471 0.0000 (   1198 PWs)   bands (ev):

 -15.6968   -9.9803   -5.5750   -2.0212    3.6194    8.8023   10.9591   11.4068

      k = 0.4643 0.3505 0.0000 (   1196 PWs)   bands (ev):

 -15.6917   -9.9740   -5.6051   -2.0136    3.6209    8.8437   10.9707   11.4234

      k = 0.4623 0.3540 0.0000 (   1200 PWs)   bands (ev):

 -15.6863   -9.9672   -5.6367   -2.0057    3.6224    8.8871   10.9829   11.4410

      k = 0.4603 0.3574 0.0000 (   1200 PWs)   bands (ev):

 -15.6807   -9.9601   -5.6697   -1.9973    3.6240    8.9324   10.9958   11.4596

      k = 0.4583 0.3608 0.0000 (   1204 PWs)   bands (ev):

 -15.6748   -9.9526   -5.7041   -1.9886    3.6254    8.9794   11.0094   11.4793

      k = 0.4563 0.3643 0.0000 (   1204 PWs)   bands (ev):

 -15.6687   -9.9448   -5.7398   -1.9794    3.6270    9.0283   11.0237   11.5000

      k = 0.4544 0.3677 0.0000 (   1204 PWs)   bands (ev):

 -15.6623   -9.9366   -5.7767   -1.9699    3.6286    9.0788   11.0386   11.5218

      k = 0.4524 0.3712 0.0000 (   1204 PWs)   bands (ev):
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 -15.6556   -9.9281   -5.8148   -1.9599    3.6302    9.1308   11.0542   11.5447

          k = 0.4504 0.3746 0.0000 (   1204 PWs)    bands (ev):

 -15.6487   -9.9192   -5.8541   -1.9496    3.6317    9.1844   11.0705   11.5687

          k = 0.4484 0.3780 0.0000 (   1204 PWs)    bands (ev):

 -15.6416   -9.9100   -5.8945   -1.9390    3.6333    9.2394   11.0875   11.5939

          k = 0.4464 0.3815 0.0000 (   1204 PWs)    bands (ev):

 -15.6342   -9.9003   -5.9360   -1.9279    3.6348    9.2958   11.1051   11.6202

          k = 0.4444 0.3849 0.0000 (   1204 PWs)    bands (ev):

 -15.6266   -9.8904   -5.9785   -1.9165    3.6363    9.3534   11.1234   11.6477

          k = 0.4425 0.3883 0.0000 (   1204 PWs)    bands (ev):

 -15.6188   -9.8801   -6.0220   -1.9048    3.6377    9.4121   11.1424   11.6764

          k = 0.4405 0.3918 0.0000 (   1204 PWs)    bands (ev):

 -15.6108   -9.8694   -6.0664   -1.8927    3.6390    9.4719   11.1621   11.7063

          k = 0.4385 0.3952 0.0000 (   1204 PWs)    bands (ev):

 -15.6025   -9.8584   -6.1117   -1.8803    3.6403    9.5326   11.1825   11.7375

          k = 0.4365 0.3986 0.0000 (   1204 PWs)    bands (ev):

 -15.5941   -9.8470   -6.1578   -1.8675    3.6414    9.5943   11.2036   11.7699

          k = 0.4345 0.4021 0.0000 (   1204 PWs)    bands (ev):

 -15.5854   -9.8353   -6.2047   -1.8544    3.6425    9.6566   11.2253   11.8037

          k = 0.4325 0.4055 0.0000 (   1196 PWs)    bands (ev):

 -15.5766   -9.8233   -6.2522   -1.8411    3.6435    9.7199   11.2478   11.8389

          k = 0.4306 0.4090 0.0000 (   1196 PWs)    bands (ev):

 -15.5675   -9.8109   -6.3005   -1.8274    3.6444    9.7835   11.2710   11.8753

          k = 0.4286 0.4124 0.0000 (   1192 PWs)    bands (ev):

 -15.5583   -9.7981   -6.3494   -1.8134    3.6451    9.8475   11.2949   11.9132

          k = 0.4266 0.4158 0.0000 (   1192 PWs)    bands (ev):

 -15.5490   -9.7850   -6.3989   -1.7992    3.6456    9.9118   11.3195   11.9524

          k = 0.4246 0.4193 0.0000 (   1192 PWs)    bands (ev):

 -15.5395   -9.7716   -6.4489   -1.7847    3.6460    9.9763   11.3448   11.9930

          k = 0.4226 0.4227 0.0000 (   1196 PWs)    bands (ev):

 -15.5298   -9.7579   -6.4995   -1.7700    3.6462   10.0409   11.3709   12.0351
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        k = 0.4206 0.4261 0.0000 (  1204 PWs)   bands (ev):

 -15.5200   -9.7438   -6.5505   -1.7550    3.6461   10.1055   11.3976   12.0786

        k = 0.4186 0.4296 0.0000 (  1204 PWs)   bands (ev):

 -15.5101   -9.7294   -6.6018   -1.7398    3.6460   10.1700   11.4251   12.1236

        k = 0.4167 0.4330 0.0000 (  1204 PWs)   bands (ev):

 -15.5000   -9.7147   -6.6535   -1.7243    3.6456   10.2343   11.4534   12.1701

        k = 0.4147 0.4364 0.0000 (  1204 PWs)   bands (ev):

 -15.4899   -9.6996   -6.7054   -1.7087    3.6451   10.2982   11.4824   12.2107

        k = 0.4127 0.4399 0.0000 (  1204 PWs)   bands (ev):

 -15.4796   -9.6843   -6.7576   -1.6929    3.6443   10.3617   11.5122   12.1756

        k = 0.4107 0.4433 0.0000 (  1204 PWs)   bands (ev):

 -15.4693   -9.6686   -6.8100   -1.6769    3.6433   10.4246   11.5427   12.1400

        k = 0.4087 0.4468 0.0000 (  1200 PWs)   bands (ev):

 -15.4588   -9.6526   -6.8625   -1.6607    3.6420   10.4870   11.5740   12.1041

        k = 0.4067 0.4502 0.0000 (  1200 PWs)   bands (ev):

 -15.4483   -9.6363   -6.9152   -1.6445    3.6405   10.5486   11.6061   12.0680

        k = 0.4048 0.4536 0.0000 (  1198 PWs)   bands (ev):

 -15.4378   -9.6197   -6.9678   -1.6281    3.6388   10.6094   11.6389   12.0316

        k = 0.4028 0.4571 0.0000 (  1198 PWs)   bands (ev):

 -15.4272   -9.6028   -7.0205   -1.6116    3.6367   10.6693   11.6725   11.9952

        k = 0.4008 0.4605 0.0000 (  1198 PWs)   bands (ev):

 -15.4166   -9.5856   -7.0731   -1.5950    3.6345   10.7283   11.7069   11.9588

        k = 0.3988 0.4639 0.0000 (  1198 PWs)   bands (ev):

 -15.4060   -9.5682   -7.1256   -1.5784    3.6319   10.7862   11.7421   11.9225

        k = 0.3968 0.4674 0.0000 (  1206 PWs)   bands (ev):

 -15.3954   -9.5505   -7.1781   -1.5617    3.6290   10.8431   11.7781   11.8863

        k = 0.3948 0.4708 0.0000 (  1206 PWs)   bands (ev):

 -15.3849   -9.5325   -7.2303   -1.5451    3.6259   10.8990   11.8149   11.8504

        k = 0.3929 0.4742 0.0000 (  1206 PWs)   bands (ev):

 -15.3743   -9.5143   -7.2822   -1.5284    3.6226   10.9537   11.8149   11.8524

        k = 0.3909 0.4777 0.0000 (  1206 PWs)   bands (ev):
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  -15.3638   -9.4958   -7.3338   -1.5118    3.6189   11.0072   11.7799   11.8907

         k = 0.3889 0.4811 0.0000 (   1207 PWs)    bands (ev):

  -15.3534   -9.4771   -7.3850   -1.4952    3.6150   11.0596   11.7454   11.9298

         k = 0.3869 0.4846 0.0000 (   1207 PWs)    bands (ev):

  -15.3431   -9.4582   -7.4359   -1.4787    3.6109   11.1108   11.7115   11.9697

         k = 0.3849 0.4880 0.0000 (   1195 PWs)    bands (ev):

  -15.3328   -9.4390   -7.4862   -1.4623    3.6068   11.1608   11.6783   12.0103

         k = 0.3829 0.4914 0.0000 (   1197 PWs)    bands (ev):

  -15.3227   -9.4198   -7.5361   -1.4461    3.6021   11.2096   11.6458   12.0516

         k = 0.3810 0.4949 0.0000 (   1191 PWs)    bands (ev):

  -15.3126   -9.4003   -7.5853   -1.4299    3.5976   11.2572   11.6141   12.0937

         k = 0.3790 0.4983 0.0000 (   1191 PWs)    bands (ev):

  -15.3028   -9.3807   -7.6339   -1.4141    3.5925   11.3036   11.5834   12.1364

         k = 0.3770 0.5017 0.0000 (   1191 PWs)    bands (ev):

  -15.2931   -9.3610   -7.6818   -1.3985    3.5873   11.3488   11.5535   12.1798

         k = 0.3750 0.5052 0.0000 (   1195 PWs)    bands (ev):

  -15.2837   -9.3412   -7.7290   -1.3831    3.5819   11.3928   11.5247   12.2239

         k = 0.3730 0.5086 0.0000 (   1191 PWs)    bands (ev):

  -15.2744   -9.3214   -7.7752   -1.3680    3.5763   11.4357   11.4970   12.2686

         k = 0.3710 0.5121 0.0000 (   1191 PWs)    bands (ev):

  -15.2654   -9.3016   -7.8205   -1.3533    3.5706   11.4704   11.4773   12.3139

         k = 0.3690 0.5155 0.0000 (   1191 PWs)    bands (ev):

  -15.2566   -9.2818   -7.8648   -1.3390    3.5648   11.4450   11.5177   12.3597

         k = 0.3671 0.5189 0.0000 (   1193 PWs)    bands (ev):

  -15.2482   -9.2621   -7.9081   -1.3250    3.5589   11.4207   11.5569   12.4061

         k = 0.3651 0.5224 0.0000 (   1193 PWs)    bands (ev):

  -15.2400   -9.2425   -7.9501   -1.3115    3.5530   11.3978   11.5948   12.4529

         k = 0.3631 0.5258 0.0000 (   1193 PWs)    bands (ev):

  -15.2321   -9.2232   -7.9909   -1.2985    3.5471   11.3761   11.6315   12.5002

         k = 0.3611 0.5292 0.0000 (   1197 PWs)    bands (ev):

  -15.2246   -9.2042   -8.0302   -1.2861    3.5412   11.3557   11.6669   12.5477
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       k = 0.3591 0.5327 0.0000 (   1193 PWs)   bands (ev):

 -15.2174   -9.1855   -8.0679   -1.2742    3.5354   11.3367   11.7010   12.5957

       k = 0.3571 0.5361 0.0000 (   1193 PWs)   bands (ev):

 -15.2106   -9.1673   -8.1040   -1.2629    3.5297   11.3191   11.7336   12.6438

       k = 0.3552 0.5395 0.0000 (   1193 PWs)   bands (ev):

 -15.2042   -9.1497   -8.1382   -1.2522    3.5242   11.3029   11.7648   12.6921

       k = 0.3532 0.5430 0.0000 (   1193 PWs)   bands (ev):

 -15.1983   -9.1329   -8.1704   -1.2423    3.5188   11.2881   11.7944   12.7403

       k = 0.3512 0.5464 0.0000 (   1191 PWs)   bands (ev):

 -15.1928   -9.1169   -8.2004   -1.2331    3.5138   11.2747   11.8223   12.7884

       k = 0.3492 0.5499 0.0000 (   1191 PWs)   bands (ev):

 -15.1878   -9.1021   -8.2281   -1.2247    3.5090   11.2627   11.8484   12.8360

       k = 0.3472 0.5533 0.0000 (   1187 PWs)   bands (ev):

 -15.1833   -9.0884   -8.2531   -1.2171    3.5046   11.2522   11.8725   12.8830

       k = 0.3452 0.5567 0.0000 (   1187 PWs)   bands (ev):

 -15.1793   -9.0761   -8.2753   -1.2104    3.5006   11.2431   11.8945   12.9288

       k = 0.3433 0.5602 0.0000 (   1187 PWs)   bands (ev):

 -15.1759   -9.0655   -8.2944   -1.2046    3.4971   11.2355   11.9140   12.9727

       k = 0.3413 0.5636 0.0000 (   1187 PWs)   bands (ev):

 -15.1731   -9.0566   -8.3103   -1.1998    3.4941   11.2292   11.9308   13.0138

       k = 0.3393 0.5670 0.0000 (   1187 PWs)   bands (ev):

 -15.1708   -9.0496   -8.3228   -1.1959    3.4916   11.2244   11.9447   13.0504

       k = 0.3373 0.5705 0.0000 (   1197 PWs)   bands (ev):

 -15.1692   -9.0447   -8.3318   -1.1932    3.4897   11.2210   11.9551   13.0802

       k = 0.3353 0.5739 0.0000 (   1197 PWs)   bands (ev):

 -15.1682   -9.0417   -8.3372   -1.1915    3.4885   11.2190   11.9617   13.1001

       k = 0.3333 0.5773 0.0000 (   1197 PWs)   bands (ev):

 -15.1679   -9.0408   -8.3390   -1.1909    3.4882   11.2183   11.9640   13.1072

       k = 0.3314 0.5739 0.0000 (   1197 PWs)   bands (ev):

 -15.1682   -9.0417   -8.3373   -1.1915    3.4886   11.2189   11.9615   13.1004

       k = 0.3294 0.5705 0.0000 (   1197 PWs)   bands (ev):
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    -15.1693   -9.0443   -8.3322   -1.1932    3.4898   11.2209   11.9537   13.0819

        k = 0.3274 0.5671 0.0000 (   1193 PWs)    bands (ev):

    -15.1710   -9.0484   -8.3240   -1.1962    3.4920   11.2241   11.9401   13.0557

        k = 0.3254 0.5637 0.0000 (   1193 PWs)    bands (ev):

    -15.1735   -9.0537   -8.3129   -1.2004    3.4950   11.2285   11.9201   13.0255

        k = 0.3235 0.5603 0.0000 (   1185 PWs)    bands (ev):

    -15.1766   -9.0599   -8.2991   -1.2059    3.4992   11.2341   11.8934   12.9944

        k = 0.3215 0.5568 0.0000 (   1185 PWs)    bands (ev):

    -15.1806   -9.0669   -8.2828   -1.2127    3.5044   11.2408   11.8597   12.9644

        k = 0.3195 0.5534 0.0000 (   1187 PWs)    bands (ev):

    -15.1854   -9.0743   -8.2644   -1.2209    3.5106   11.2485   11.8190   12.9367

        k = 0.3176 0.5500 0.0000 (   1183 PWs)    bands (ev):

    -15.1909   -9.0819   -8.2441   -1.2303    3.5180   11.2573   11.7716   12.9119

        k = 0.3156 0.5466 0.0000 (   1183 PWs)    bands (ev):

    -15.1972   -9.0895   -8.2220   -1.2411    3.5264   11.2671   11.7177   12.8902

        k = 0.3136 0.5432 0.0000 (   1187 PWs)    bands (ev):

    -15.2044   -9.0968   -8.1983   -1.2533    3.5361   11.2777   11.6580   12.8717

        k = 0.3116 0.5398 0.0000 (   1187 PWs)    bands (ev):

    -15.2124   -9.1037   -8.1732   -1.2669    3.5470   11.2892   11.5929   12.8559

        k = 0.3097 0.5363 0.0000 (   1187 PWs)    bands (ev):

    -15.2212   -9.1101   -8.1469   -1.2818    3.5592   11.3014   11.5232   12.8426

        k = 0.3077 0.5329 0.0000 (   1193 PWs)    bands (ev):

    -15.2309   -9.1158   -8.1194   -1.2982    3.5724   11.3143   11.4494   12.8313

        k = 0.3057 0.5295 0.0000 (   1193 PWs)    bands (ev):

    -15.2414   -9.1207   -8.0909   -1.3159    3.5872   11.3277   11.3722   12.8215

        k = 0.3037 0.5261 0.0000 (   1193 PWs)    bands (ev):

    -15.2527   -9.1246   -8.0614   -1.3350    3.6032   11.2921   11.3416   12.8129

        k = 0.3018 0.5227 0.0000 (   1193 PWs)    bands (ev):

    -15.2649   -9.1276   -8.0310   -1.3555    3.6206   11.2095   11.3560   12.8051

        k = 0.2998 0.5193 0.0000 (   1193 PWs)    bands (ev):

    -15.2779   -9.1295   -7.9999   -1.3773    3.6394   11.1248   11.3706   12.7977
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       k = 0.2978 0.5159 0.0000 (  1193 PWs)   bands (ev):

 -15.2918  -9.1303  -7.9680  -1.4005   3.6595  11.0385  11.3853  12.7906

       k = 0.2959 0.5124 0.0000 (  1189 PWs)   bands (ev):

 -15.3065  -9.1299  -7.9354  -1.4250   3.6809  10.9508  11.4002  12.7834

       k = 0.2939 0.5090 0.0000 (  1199 PWs)   bands (ev):

 -15.3221  -9.1284  -7.9022  -1.4508   3.7036  10.8619  11.4149  12.7760

       k = 0.2919 0.5056 0.0000 (  1199 PWs)   bands (ev):

 -15.3385  -9.1256  -7.8684  -1.4779   3.7277  10.7721  11.4294  12.7682

       k = 0.2899 0.5022 0.0000 (  1199 PWs)   bands (ev):

 -15.3557  -9.1215  -7.8340  -1.5062   3.7532  10.6816  11.4435  12.7598

       k = 0.2880 0.4988 0.0000 (  1199 PWs)   bands (ev):

 -15.3737  -9.1161  -7.7991  -1.5358   3.7800  10.5906  11.4571  12.7508

       k = 0.2860 0.4954 0.0000 (  1197 PWs)   bands (ev):

 -15.3925  -9.1093  -7.7636  -1.5665   3.8081  10.4991  11.4701  12.7411

       k = 0.2840 0.4919 0.0000 (  1205 PWs)   bands (ev):

 -15.4122  -9.1013  -7.7277  -1.5985   3.8374  10.4073  11.4822  12.7303

       k = 0.2820 0.4885 0.0000 (  1205 PWs)   bands (ev):

 -15.4325  -9.0920  -7.6913  -1.6315   3.8681  10.3153  11.4933  12.7188

       k = 0.2801 0.4851 0.0000 (  1205 PWs)   bands (ev):

 -15.4537  -9.0813  -7.6544  -1.6657   3.9001  10.2232  11.5032  12.7063

       k = 0.2781 0.4817 0.0000 (  1205 PWs)   bands (ev):

 -15.4756  -9.0692  -7.6171  -1.7009   3.9333  10.1311  11.5117  12.6928

       k = 0.2761 0.4783 0.0000 (  1197 PWs)   bands (ev):

 -15.4982  -9.0558  -7.5794  -1.7371   3.9678  10.0391  11.5187  12.6783

       k = 0.2742 0.4749 0.0000 (  1197 PWs)   bands (ev):

 -15.5216  -9.0411  -7.5413  -1.7743   4.0034   9.9472  11.5240  12.6626

       k = 0.2722 0.4714 0.0000 (  1197 PWs)   bands (ev):

 -15.5456  -9.0250  -7.5028  -1.8124   4.0402   9.8554  11.5274  12.6458

       k = 0.2702 0.4680 0.0000 (  1195 PWs)   bands (ev):

 -15.5703  -9.0077  -7.4639  -1.8514   4.0782   9.7638  11.5288  12.6279

       k = 0.2682 0.4646 0.0000 (  1195 PWs)   bands (ev):
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   -15.5957   -8.9890   -7.4247   -1.8913    4.1173    9.6725   11.5279   12.6088

        k = 0.2663 0.4612 0.0000 (   1195 PWs)    bands (ev):

   -15.6217   -8.9690   -7.3850   -1.9321    4.1574    9.5814   11.5247   12.5885

        k = 0.2643 0.4578 0.0000 (   1199 PWs)    bands (ev):

   -15.6484   -8.9477   -7.3451   -1.9736    4.1986    9.4907   11.5191   12.5670

        k = 0.2623 0.4544 0.0000 (   1199 PWs)    bands (ev):

   -15.6756   -8.9252   -7.3049   -2.0159    4.2409    9.4004   11.5109   12.5442

        k = 0.2604 0.4509 0.0000 (   1195 PWs)    bands (ev):

   -15.7034   -8.9014   -7.2642   -2.0589    4.2843    9.3104   11.5002   12.5202

        k = 0.2584 0.4475 0.0000 (   1195 PWs)    bands (ev):

   -15.7317   -8.8764   -7.2233   -2.1025    4.3286    9.2208   11.4868   12.4949

        k = 0.2564 0.4441 0.0000 (   1195 PWs)    bands (ev):

   -15.7606   -8.8501   -7.1821   -2.1468    4.3738    9.1317   11.4707   12.4684

        k = 0.2544 0.4407 0.0000 (   1195 PWs)    bands (ev):

   -15.7900   -8.8227   -7.1406   -2.1916    4.4199    9.0430   11.4519   12.4404

        k = 0.2525 0.4373 0.0000 (   1195 PWs)    bands (ev):

   -15.8198   -8.7941   -7.0989   -2.2370    4.4669    8.9547   11.4305   12.4112

        k = 0.2505 0.4339 0.0000 (   1195 PWs)    bands (ev):

   -15.8502   -8.7643   -7.0568   -2.2830    4.5147    8.8670   11.4066   12.3805

        k = 0.2485 0.4304 0.0000 (   1195 PWs)    bands (ev):

   -15.8809   -8.7333   -7.0145   -2.3294    4.5633    8.7797   11.3801   12.3485

        k = 0.2465 0.4270 0.0000 (   1195 PWs)    bands (ev):

   -15.9121   -8.7013   -6.9718   -2.3763    4.6127    8.6930   11.3513   12.3149

        k = 0.2446 0.4236 0.0000 (   1195 PWs)    bands (ev):

   -15.9437   -8.6681   -6.9290   -2.4236    4.6629    8.6067   11.3203   12.2799

        k = 0.2426 0.4202 0.0000 (   1195 PWs)    bands (ev):

   -15.9756   -8.6339   -6.8858   -2.4713    4.7138    8.5211   11.2871   12.2433

        k = 0.2406 0.4168 0.0000 (   1197 PWs)    bands (ev):

   -16.0079   -8.5986   -6.8425   -2.5193    4.7653    8.4359   11.2519   12.2052

        k = 0.2387 0.4134 0.0000 (   1197 PWs)    bands (ev):

   -16.0405   -8.5623   -6.7989   -2.5677    4.8175    8.3513   11.2149   12.1654
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        k = 0.2367 0.4099 0.0000 (   1197 PWs)    bands (ev):

  -16.0734   -8.5249   -6.7550   -2.6163    4.8703    8.2673   11.1762   12.1241

        k = 0.2347 0.4065 0.0000 (   1197 PWs)    bands (ev):

  -16.1066   -8.4866   -6.7109   -2.6652    4.9237    8.1839   11.1360   12.0811

        k = 0.2327 0.4031 0.0000 (   1189 PWs)    bands (ev):

  -16.1400   -8.4471   -6.6665   -2.7143    4.9776    8.1010   11.0945   12.0366

        k = 0.2308 0.3997 0.0000 (   1189 PWs)    bands (ev):

  -16.1737   -8.4068   -6.6220   -2.7636    5.0320    8.0188   11.0517   11.9904

        k = 0.2288 0.3963 0.0000 (   1185 PWs)    bands (ev):

  -16.2075   -8.3656   -6.5773   -2.8131    5.0871    7.9371   11.0079   11.9428

        k = 0.2268 0.3929 0.0000 (   1185 PWs)    bands (ev):

  -16.2416   -8.3235   -6.5323   -2.8628    5.1424    7.8561   10.9631   11.8938

        k = 0.2248 0.3895 0.0000 (   1185 PWs)    bands (ev):

  -16.2759   -8.2804   -6.4872   -2.9126    5.1980    7.7756   10.9175   11.8435

        k = 0.2229 0.3860 0.0000 (   1185 PWs)    bands (ev):

  -16.3103   -8.2365   -6.4419   -2.9624    5.2540    7.6958   10.8712   11.7919

        k = 0.2209 0.3826 0.0000 (   1179 PWs)    bands (ev):

  -16.3449   -8.1917   -6.3963   -3.0124    5.3107    7.6165   10.8245   11.7394

        k = 0.2189 0.3792 0.0000 (   1179 PWs)    bands (ev):

  -16.3796   -8.1461   -6.3507   -3.0624    5.3673    7.5380   10.7773   11.6859

        k = 0.2170 0.3758 0.0000 (   1179 PWs)    bands (ev):

  -16.4144   -8.0997   -6.3049   -3.1124    5.4241    7.4600   10.7298   11.6315

        k = 0.2150 0.3724 0.0000 (   1179 PWs)    bands (ev):

  -16.4493   -8.0525   -6.2589   -3.1625    5.4811    7.3827   10.6821   11.5765

        k = 0.2130 0.3690 0.0000 (   1183 PWs)    bands (ev):

  -16.4842   -8.0045   -6.2128   -3.2125    5.5382    7.3060   10.6344   11.5209

        k = 0.2110 0.3655 0.0000 (   1183 PWs)    bands (ev):

  -16.5192   -7.9557   -6.1665   -3.2625    5.5954    7.2299   10.5867   11.4649

        k = 0.2091 0.3621 0.0000 (   1183 PWs)    bands (ev):

  -16.5543   -7.9062   -6.1201   -3.3124    5.6526    7.1545   10.5392   11.4085

        k = 0.2071 0.3587 0.0000 (   1183 PWs)    bands (ev):
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   -16.5894   -7.8560   -6.0736   -3.3623    5.7098    7.0798   10.4919   11.3519

         k = 0.2051 0.3553 0.0000 (   1183 PWs)    bands (ev):

   -16.6244   -7.8051   -6.0269   -3.4121    5.7669    7.0056   10.4449   11.2951

         k = 0.2032 0.3519 0.0000 (   1183 PWs)    bands (ev):

   -16.6595   -7.7535   -5.9801   -3.4618    5.8239    6.9322   10.3983   11.2382

         k = 0.2012 0.3485 0.0000 (   1183 PWs)    bands (ev):

   -16.6945   -7.7013   -5.9332   -3.5113    5.8807    6.8594   10.3523   11.1812

         k = 0.1992 0.3450 0.0000 (   1183 PWs)    bands (ev):

   -16.7295   -7.6484   -5.8863   -3.5607    5.9373    6.7873   10.3069   11.1243

         k = 0.1972 0.3416 0.0000 (   1183 PWs)    bands (ev):

   -16.7645   -7.5948   -5.8392   -3.6100    5.9935    6.7158   10.2622   11.0674

         k = 0.1953 0.3382 0.0000 (   1183 PWs)    bands (ev):

   -16.7994   -7.5407   -5.7921   -3.6591    6.0493    6.6450   10.2182   11.0107

         k = 0.1933 0.3348 0.0000 (   1183 PWs)    bands (ev):

   -16.8342   -7.4859   -5.7448   -3.7080    6.1047    6.5748   10.1752   10.9541

         k = 0.1913 0.3314 0.0000 (   1183 PWs)    bands (ev):

   -16.8689   -7.4306   -5.6975   -3.7567    6.1596    6.5053   10.1331   10.8977

         k = 0.1893 0.3280 0.0000 (   1187 PWs)    bands (ev):

   -16.9035   -7.3747   -5.6502   -3.8052    6.2138    6.4365   10.0921   10.8415

         k = 0.1874 0.3245 0.0000 (   1187 PWs)    bands (ev):

   -16.9381   -7.3183   -5.6028   -3.8534    6.2673    6.3684   10.0523   10.7855

         k = 0.1854 0.3211 0.0000 (   1187 PWs)    bands (ev):

   -16.9724   -7.2613   -5.5554   -3.9014    6.3009    6.3200   10.0137   10.7298

         k = 0.1834 0.3177 0.0000 (   1187 PWs)    bands (ev):

   -17.0067   -7.2038   -5.5079   -3.9492    6.2342    6.3719    9.9765   10.6745

         k = 0.1815 0.3143 0.0000 (   1187 PWs)    bands (ev):

   -17.0408   -7.1458   -5.4604   -3.9967    6.1681    6.4227    9.9408   10.6194

         k = 0.1795 0.3109 0.0000 (   1183 PWs)    bands (ev):

   -17.0747   -7.0873   -5.4129   -4.0439    6.1026    6.4725    9.9067   10.5647

         k = 0.1775 0.3075 0.0000 (   1183 PWs)    bands (ev):

   -17.1085   -7.0284   -5.3654   -4.0908    6.0379    6.5211    9.8742   10.5103
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```
        k = 0.1755 0.3040 0.0000 (   1183 PWs)   bands (ev):

-17.1421  -6.9691  -5.3179  -4.1374   5.9738   6.5684   9.8436  10.4563

        k = 0.1736 0.3006 0.0000 (   1187 PWs)   bands (ev):

-17.1755  -6.9093  -5.2704  -4.1838   5.9104   6.6142   9.8147  10.4027

        k = 0.1716 0.2972 0.0000 (   1187 PWs)   bands (ev):

-17.2088  -6.8491  -5.2230  -4.2298   5.8477   6.6586   9.7880  10.3495

        k = 0.1696 0.2938 0.0000 (   1185 PWs)   bands (ev):

-17.2418  -6.7884  -5.1756  -4.2754   5.7857   6.7014   9.7635  10.2967

        k = 0.1677 0.2904 0.0000 (   1185 PWs)   bands (ev):

-17.2746  -6.7275  -5.1282  -4.3208   5.7243   6.7423   9.7411  10.2443

        k = 0.1657 0.2870 0.0000 (   1185 PWs)   bands (ev):

-17.3072  -6.6661  -5.0809  -4.3657   5.6637   6.7813   9.7211  10.1924

        k = 0.1637 0.2835 0.0000 (   1189 PWs)   bands (ev):

-17.3395  -6.6044  -5.0337  -4.4103   5.6037   6.8183   9.7036  10.1409

        k = 0.1617 0.2801 0.0000 (   1193 PWs)   bands (ev):

-17.3717  -6.5424  -4.9866  -4.4546   5.5445   6.8532   9.6886  10.0898

        k = 0.1598 0.2767 0.0000 (   1189 PWs)   bands (ev):

-17.4036  -6.4799  -4.9394  -4.4985   5.4859   6.8859   9.6764  10.0392

        k = 0.1578 0.2733 0.0000 (   1189 PWs)   bands (ev):

-17.4352  -6.4173  -4.8925  -4.5420   5.4280   6.9162   9.6669   9.9890

        k = 0.1558 0.2699 0.0000 (   1189 PWs)   bands (ev):

-17.4666  -6.3544  -4.8456  -4.5851   5.3708   6.9441   9.6602   9.9394

        k = 0.1538 0.2665 0.0000 (   1189 PWs)   bands (ev):

-17.4977  -6.2912  -4.7989  -4.6278   5.3143   6.9695   9.6564   9.8902

        k = 0.1519 0.2631 0.0000 (   1189 PWs)   bands (ev):

-17.5285  -6.2277  -4.7523  -4.6701   5.2584   6.9924   9.6555   9.8415

        k = 0.1499 0.2596 0.0000 (   1185 PWs)   bands (ev):

-17.5591  -6.1640  -4.7119  -4.7058   5.2033   7.0127   9.6576   9.7933

        k = 0.1479 0.2562 0.0000 (   1185 PWs)   bands (ev):

-17.5893  -6.1001  -4.7534  -4.6595   5.1489   7.0304   9.6626   9.7455

        k = 0.1460 0.2528 0.0000 (   1189 PWs)   bands (ev):
```

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-17.6193  -6.0360  -4.7945  -4.6134    5.0951    7.0455    9.6705    9.6983

          k = 0.1440 0.2494 0.0000 (   1189 PWs)    bands (ev):

-17.6490  -5.9717  -4.8351  -4.5675    5.0421    7.0580    9.6516    9.6814

          k = 0.1420 0.2460 0.0000 (   1189 PWs)    bands (ev):

-17.6784  -5.9073  -4.8753  -4.5217    4.9897    7.0680    9.6054    9.6951

          k = 0.1400 0.2426 0.0000 (   1189 PWs)    bands (ev):

-17.7075  -5.8427  -4.9150  -4.4762    4.9381    7.0754    9.5597    9.7116

          k = 0.1381 0.2391 0.0000 (   1183 PWs)    bands (ev):

-17.7363  -5.7780  -4.9543  -4.4308    4.8871    7.0806    9.5145    9.7310

          k = 0.1361 0.2357 0.0000 (   1183 PWs)    bands (ev):

-17.7647  -5.7132  -4.9931  -4.3857    4.8368    7.0833    9.4699    9.7528

          k = 0.1341 0.2323 0.0000 (   1183 PWs)    bands (ev):

-17.7929  -5.6483  -5.0314  -4.3409    4.7873    7.0839    9.4257    9.7770

          k = 0.1321 0.2289 0.0000 (   1179 PWs)    bands (ev):

-17.8207  -5.5833  -5.0693  -4.2962    4.7384    7.0823    9.3822    9.8036

          k = 0.1302 0.2255 0.0000 (   1179 PWs)    bands (ev):

-17.8482  -5.5183  -5.1067  -4.2519    4.6902    7.0788    9.3391    9.8323

          k = 0.1282 0.2221 0.0000 (   1179 PWs)    bands (ev):

-17.8753  -5.4532  -5.1437  -4.2078    4.6427    7.0734    9.2965    9.8631

          k = 0.1262 0.2186 0.0000 (   1177 PWs)    bands (ev):

-17.9021  -5.3881  -5.1801  -4.1640    4.5959    7.0663    9.2546    9.8958

          k = 0.1243 0.2152 0.0000 (   1177 PWs)    bands (ev):

-17.9285  -5.3231  -5.2161  -4.1206    4.5498    7.0576    9.2131    9.9302

          k = 0.1223 0.2118 0.0000 (   1181 PWs)    bands (ev):

-17.9547  -5.2581  -5.2516  -4.0775    4.5044    7.0474    9.1722    9.9661

          k = 0.1203 0.2084 0.0000 (   1181 PWs)    bands (ev):

-17.9804  -5.2865  -5.1932  -4.0348    4.4597    7.0359    9.1318   10.0035

          k = 0.1183 0.2050 0.0000 (   1181 PWs)    bands (ev):

-18.0058  -5.3210  -5.1283  -3.9923    4.4157    7.0232    9.0920   10.0422

          k = 0.1164 0.2016 0.0000 (   1181 PWs)    bands (ev):

-18.0309  -5.3550  -5.0636  -3.9503    4.3724    7.0094    9.0527   10.0821
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      k = 0.1144 0.1981 0.0000 (   1181 PWs)   bands (ev):

 -18.0555   -5.3885   -4.9990   -3.9086    4.3298    6.9946    9.0140   10.1229

      k = 0.1124 0.1947 0.0000 (   1181 PWs)   bands (ev):

 -18.0799   -5.4214   -4.9345   -3.8672    4.2879    6.9789    8.9758   10.1647

      k = 0.1105 0.1913 0.0000 (   1181 PWs)   bands (ev):

 -18.1038   -5.4539   -4.8702   -3.8263    4.2467    6.9625    8.9382   10.2072

      k = 0.1085 0.1879 0.0000 (   1181 PWs)   bands (ev):

 -18.1274   -5.4858   -4.8060   -3.7858    4.2062    6.9454    8.9011   10.2503

      k = 0.1065 0.1845 0.0000 (   1181 PWs)   bands (ev):

 -18.1506   -5.5172   -4.7422   -3.7458    4.1664    6.9278    8.8646   10.2939

      k = 0.1045 0.1811 0.0000 (   1181 PWs)   bands (ev):

 -18.1734   -5.5481   -4.6785   -3.7061    4.1273    6.9096    8.8286   10.3380

      k = 0.1026 0.1776 0.0000 (   1181 PWs)   bands (ev):

 -18.1958   -5.5785   -4.6151   -3.6670    4.0889    6.8910    8.7933   10.3823

      k = 0.1006 0.1742 0.0000 (   1177 PWs)   bands (ev):

 -18.2178   -5.6083   -4.5520   -3.6282    4.0512    6.8721    8.7584   10.3906

      k = 0.0986 0.1708 0.0000 (   1177 PWs)   bands (ev):

 -18.2395   -5.6376   -4.4893   -3.5900    4.0142    6.8530    8.7242   10.3793

      k = 0.0966 0.1674 0.0000 (   1177 PWs)   bands (ev):

 -18.2608   -5.6663   -4.4269   -3.5523    3.9779    6.8336    8.6905   10.3685

      k = 0.0947 0.1640 0.0000 (   1177 PWs)   bands (ev):

 -18.2816   -5.6945   -4.3649   -3.5151    3.9423    6.8140    8.6573   10.3585

      k = 0.0927 0.1606 0.0000 (   1183 PWs)   bands (ev):

 -18.3021   -5.7222   -4.3034   -3.4784    3.9074    6.7944    8.6248   10.3487

      k = 0.0907 0.1571 0.0000 (   1183 PWs)   bands (ev):

 -18.3222   -5.7493   -4.2423   -3.4422    3.8732    6.7747    8.5928   10.3398

      k = 0.0888 0.1537 0.0000 (   1183 PWs)   bands (ev):

 -18.3419   -5.7759   -4.1817   -3.4066    3.8397    6.7551    8.5614   10.3316

      k = 0.0868 0.1503 0.0000 (   1183 PWs)   bands (ev):

 -18.3612   -5.8019   -4.1216   -3.3715    3.8069    6.7354    8.5305   10.3240

      k = 0.0848 0.1469 0.0000 (   1189 PWs)   bands (ev):
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    -18.3800   -5.8274   -4.0621   -3.3371    3.7748    6.7159    8.5002   10.3163

        k = 0.0828 0.1435 0.0000 (   1189 PWs)    bands (ev):

    -18.3985   -5.8523   -4.0031   -3.3032    3.7434    6.6965    8.4705   10.3098

        k = 0.0809 0.1401 0.0000 (   1189 PWs)    bands (ev):

    -18.4166   -5.8766   -3.9447   -3.2699    3.7127    6.6772    8.4414   10.3040

        k = 0.0789 0.1366 0.0000 (   1185 PWs)    bands (ev):

    -18.4342   -5.9004   -3.8868   -3.2371    3.6827    6.6581    8.4129   10.2990

        k = 0.0769 0.1332 0.0000 (   1185 PWs)    bands (ev):

    -18.4514   -5.9236   -3.8297   -3.2051    3.6534    6.6393    8.3849   10.2943

        k = 0.0749 0.1298 0.0000 (   1185 PWs)    bands (ev):

    -18.4682   -5.9463   -3.7734   -3.1736    3.6249    6.6207    8.3576   10.2900

        k = 0.0730 0.1264 0.0000 (   1185 PWs)    bands (ev):

    -18.4846   -5.9684   -3.7178   -3.1429    3.5970    6.6023    8.3308   10.2863

        k = 0.0710 0.1230 0.0000 (   1185 PWs)    bands (ev):

    -18.5006   -5.9899   -3.6630   -3.1128    3.5698    6.5843    8.3046   10.2831

        k = 0.0690 0.1196 0.0000 (   1185 PWs)    bands (ev):

    -18.5162   -6.0109   -3.6090   -3.0833    3.5434    6.5666    8.2790   10.2804

        k = 0.0671 0.1162 0.0000 (   1181 PWs)    bands (ev):

    -18.5313   -6.0312   -3.5559   -3.0546    3.5176    6.5492    8.2540   10.2782

        k = 0.0651 0.1127 0.0000 (   1185 PWs)    bands (ev):

    -18.5460   -6.0511   -3.5038   -3.0266    3.4926    6.5321    8.2296   10.2759

        k = 0.0631 0.1093 0.0000 (   1185 PWs)    bands (ev):

    -18.5603   -6.0703   -3.4526   -2.9992    3.4683    6.5155    8.2059   10.2745

        k = 0.0611 0.1059 0.0000 (   1185 PWs)    bands (ev):

    -18.5742   -6.0890   -3.4023   -2.9726    3.4447    6.4992    8.1827   10.2736

        k = 0.0592 0.1025 0.0000 (   1185 PWs)    bands (ev):

    -18.5876   -6.1070   -3.3531   -2.9467    3.4218    6.4833    8.1601   10.2731

        k = 0.0572 0.0991 0.0000 (   1185 PWs)    bands (ev):

    -18.6006   -6.1246   -3.3050   -2.9215    3.3996    6.4679    8.1382   10.2729

        k = 0.0552 0.0957 0.0000 (   1185 PWs)    bands (ev):

    -18.6132   -6.1415   -3.2579   -2.8971    3.3782    6.4528    8.1169   10.2731
```

```
     k = 0.0533 0.0922 0.0000 (   1185 PWs)   bands (ev):

 -18.6254  -6.1578  -3.2121  -2.8735    3.3575    6.4382    8.0962   10.2737

     k = 0.0513 0.0888 0.0000 (   1185 PWs)   bands (ev):

 -18.6371  -6.1736  -3.1674  -2.8506    3.3375    6.4241    8.0762   10.2745

     k = 0.0493 0.0854 0.0000 (   1185 PWs)   bands (ev):

 -18.6484  -6.1887  -3.1239  -2.8285    3.3182    6.4104    8.0568   10.2756

     k = 0.0473 0.0820 0.0000 (   1185 PWs)   bands (ev):

 -18.6592  -6.2033  -3.0818  -2.8072    3.2996    6.3972    8.0381   10.2770

     k = 0.0454 0.0786 0.0000 (   1185 PWs)   bands (ev):

 -18.6696  -6.2173  -3.0409  -2.7867    3.2818    6.3845    8.0200   10.2786

     k = 0.0434 0.0752 0.0000 (   1185 PWs)   bands (ev):

 -18.6796  -6.2307  -3.0014  -2.7670    3.2647    6.3722    8.0026   10.2804

     k = 0.0414 0.0717 0.0000 (   1185 PWs)   bands (ev):

 -18.6891  -6.2436  -2.9633  -2.7482    3.2483    6.3605    7.9859   10.2824

     k = 0.0394 0.0683 0.0000 (   1185 PWs)   bands (ev):

 -18.6982  -6.2558  -2.9267  -2.7301    3.2327    6.3492    7.9699   10.2846

     k = 0.0375 0.0649 0.0000 (   1185 PWs)   bands (ev):

 -18.7069  -6.2674  -2.8916  -2.7129    3.2178    6.3385    7.9546   10.2869

     k = 0.0355 0.0615 0.0000 (   1185 PWs)   bands (ev):

 -18.7151  -6.2785  -2.8579  -2.6965    3.2037    6.3283    7.9400   10.2892

     k = 0.0335 0.0581 0.0000 (   1185 PWs)   bands (ev):

 -18.7229  -6.2890  -2.8259  -2.6810    3.1903    6.3186    7.9261   10.2917

     k = 0.0316 0.0547 0.0000 (   1185 PWs)   bands (ev):

 -18.7303  -6.2988  -2.7955  -2.6663    3.1776    6.3095    7.9129   10.2936

     k = 0.0296 0.0512 0.0000 (   1185 PWs)   bands (ev):

 -18.7372  -6.3081  -2.7667  -2.6525    3.1657    6.3008    7.9004   10.2961

     k = 0.0276 0.0478 0.0000 (   1185 PWs)   bands (ev):

 -18.7436  -6.3167  -2.7395  -2.6395    3.1546    6.2927    7.8887   10.2986

     k = 0.0256 0.0444 0.0000 (   1185 PWs)   bands (ev):

 -18.7496  -6.3248  -2.7141  -2.6274    3.1442    6.2852    7.8778   10.3010

     k = 0.0237 0.0410 0.0000 (   1185 PWs)   bands (ev):
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 -18.7552  -6.3323  -2.6904  -2.6162    3.1346    6.2782    7.8676   10.3034

      k = 0.0217 0.0376 0.0000 (   1185 PWs)    bands (ev):

 -18.7603  -6.3392  -2.6685  -2.6058    3.1257    6.2717    7.8582   10.3057

      k = 0.0197 0.0342 0.0000 (   1193 PWs)    bands (ev):

 -18.7650  -6.3456  -2.6484  -2.5965    3.1176    6.2658    7.8496   10.3079

      k = 0.0178 0.0307 0.0000 (   1193 PWs)    bands (ev):

 -18.7693  -6.3513  -2.6301  -2.5879    3.1102    6.2605    7.8417   10.3099

      k = 0.0158 0.0273 0.0000 (   1193 PWs)    bands (ev):

 -18.7731  -6.3564  -2.6137  -2.5803    3.1036    6.2557    7.8347   10.3118

      k = 0.0138 0.0239 0.0000 (   1187 PWs)    bands (ev):

 -18.7764  -6.3608  -2.5990  -2.5734    3.0978    6.2514    7.8285   10.3142

      k = 0.0118 0.0205 0.0000 (   1187 PWs)    bands (ev):

 -18.7793  -6.3647  -2.5863  -2.5675    3.0928    6.2478    7.8231   10.3157

      k = 0.0099 0.0171 0.0000 (   1193 PWs)    bands (ev):

 -18.7818  -6.3681  -2.5756  -2.5626    3.0885    6.2446    7.8185   10.3168

      k = 0.0079 0.0137 0.0000 (   1193 PWs)    bands (ev):

 -18.7838  -6.3708  -2.5668  -2.5585    3.0850    6.2421    7.8147   10.3179

      k = 0.0059 0.0102 0.0000 (   1201 PWs)    bands (ev):

 -18.7854  -6.3729  -2.5601  -2.5554    3.0823    6.2401    7.8118   10.3186

      k = 0.0039 0.0068 0.0000 (   1205 PWs)    bands (ev):

 -18.7865  -6.3744  -2.5552  -2.5531    3.0804    6.2387    7.8097   10.3191

      k = 0.0020 0.0034 0.0000 (   1205 PWs)    bands (ev):

 -18.7872  -6.3753  -2.5523  -2.5518    3.0792    6.2378    7.8085   10.3195

      k = 0.0000 0.0000 0.0000 (   1205 PWs)    bands (ev):

 -18.7874  -6.3756  -2.5513  -2.5513    3.0788    6.2375    7.8080   10.3196

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

   init_run     :      1.98s CPU      2.04s WALL (       1 calls)
   electrons    :    101.95s CPU     81.77s WALL (       1 calls)

   Called by init_run:
   wfcinit      :      0.00s CPU      0.00s WALL (       1 calls)
   wfcinit:atom :      0.39s CPU      0.33s WALL (     800 calls)
   wfcinit:wfcr :      4.72s CPU      3.84s WALL (     800 calls)
   potinit      :      0.53s CPU      0.57s WALL (       1 calls)
   hinit0       :      1.16s CPU      1.16s WALL (       1 calls)
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      Called by electrons:
      c_bands      :     101.93s CPU      81.75s WALL (        1 calls)
      v_of_rho     :       0.49s CPU       0.49s WALL (        1 calls)
      v_h          :       0.01s CPU       0.01s WALL (        1 calls)
      v_xc         :       0.48s CPU       0.49s WALL (        1 calls)
      newd         :       0.07s CPU       0.09s WALL (        1 calls)

      Called by c_bands:
      init_us_2    :       0.52s CPU       0.44s WALL (      800 calls)
      cegterg      :      94.30s CPU      75.35s WALL (     1297 calls)

      Called by sum_band:

      Called by *egterg:
      h_psi        :      62.87s CPU      50.59s WALL (    19543 calls)
      s_psi        :       2.92s CPU       2.33s WALL (    19543 calls)
      g_psi        :       1.17s CPU       0.86s WALL (    17446 calls)
      cdiaghg      :      11.23s CPU       9.54s WALL (    18246 calls)
      cegterg:over :       8.36s CPU       6.64s WALL (    17446 calls)
      cegterg:upda :       6.42s CPU       4.99s WALL (    17446 calls)
      cegterg:last :       3.86s CPU       2.66s WALL (     3979 calls)

      Called by h_psi:
      h_psi:calbec :       3.33s CPU       2.82s WALL (    19543 calls)
      vloc_psi     :      55.97s CPU      44.91s WALL (    19543 calls)
      add_vuspsi   :       3.03s CPU       2.49s WALL (    19543 calls)

      General routines
      calbec       :       3.24s CPU       2.75s WALL (    19543 calls)
      fft          :       0.17s CPU       0.17s WALL (       23 calls)
      ffts         :       0.00s CPU       0.00s WALL (        2 calls)
      fftw         :      44.55s CPU      35.90s WALL (   192906 calls)
      interpolate  :       0.02s CPU       0.02s WALL (        2 calls)
      davcio       :       0.22s CPU       0.21s WALL (     1600 calls)

      Parallel routines

      PWSCF        :     1m45.88s CPU    1m26.88s WALL


   This run was terminated on:  11:25:57   5Oct2023

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