```
CalculationMode = gs_start

units = 'eVA'
```

and under which operating system (in this case, my desktop, called `g32`

Let us know take a look at the Output box 2, to see how the code pursues its calculation. The first step is to obtain a reasonably good starting density and KS orbitals to feed in the self consistent (SCF) procedure. For this purpose, `octopus` performs an initial calculation restricted to the basis set

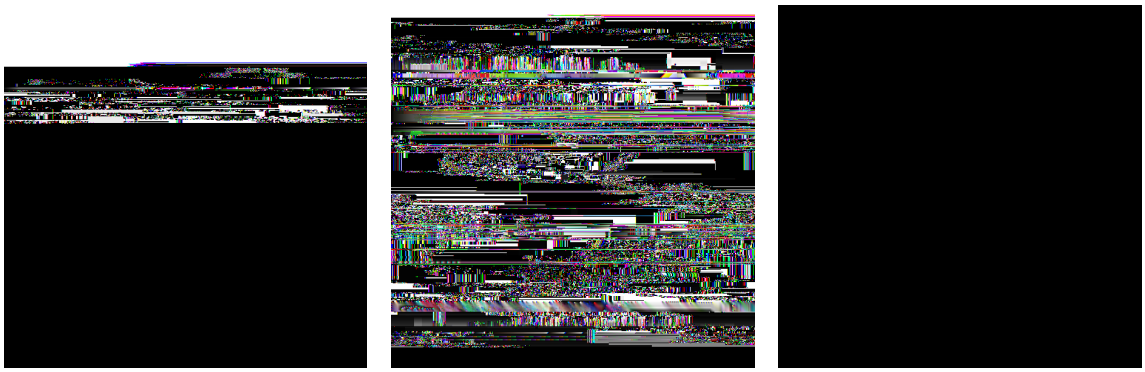

Figure 1: Second, third, and fourth KS orbitals of the Nitrogen atom, showing the expected *p* symmetry.

```
************
SCF CYCLE ITER #    7
 abs_dens =  2.57E-06 abs_ev =  1.98E-04
 rel_dens =  5.15E-07 rel_ev =  9.23E-05
Matrix vector products:    108
Converged eigenvectors:      0
Eigenvalues [eV]
 #st   Eigenvalue    Occupation      Error (  1)
   1
   r0Tm 60R9301())-0.77499(8)-0.4.9301]TJ 9.479399(8)-0.449301]TJ 9.487499(8)-0.449301]TJ 9.447499(8)-0.479341E
   ra0Tm 60R9301())-0.77499(8)-0.4.9301]TJ 9.479399(8)-0.449301]TJ 9.487499(8)-0.449301]TJ 9.447499(8)-0.479341E
   rE0Tm 60R9301())-0.77499(8)-0.4.9301]TJ 9.479399(8)-0.449301]TJ 9.487499(8)-0.449301]TJ 9.447499(8)-0.479341E
```

```
Sysgem name: sysgem

Mesh:
  Type = sphere
  Radius  [A] =   5.000
  Spacing [A] = ( 0.180, 0.1     180)    e7499(s)-0.47l7499     .40582   ume/pint [A^3] =  0.0
  # inner mesh =  89727
  Grid C7499(s)-0.4utf [eV       160.595

Exchange and crrelagin fu      als:
      Exchange    : :DA         -relag.
      Correlagin : :DA         1

SCF cnverged in    7        gins

Eigenvalues [eV]
 #st   Eigenvalue       upgin
   1   -18.378882        2.000000
   2    -7.248448        1.000000
   3    -7.248448        1.000000
   4    -7.24844         1.000000

Energy:
      In-in            0.00000000
      Eigenva      =    -58.50310712
      P7geng       =   -144.61568022
      Exchar       =    -51.46568858
      Corre     n =     -7.28085027
      Tgal         =   -261.86532618

Diple [A]                     [Debye]
      <x         6.19852E-17      2.97728E
      <          7.85171E-17      3.77134E
      <     =    1.15262E-16      5.53628

Angul      mengum L [adimensi7nal]
         =    79301(.)-0.477499(1)-0.4      +00
         =    79301(.)-0.477499(1)-0.       +00
         =    79301(.)-0.477499(1)-0        +00

        ^2 =    5.99516E+00

C     gence:
      abs_dens = 2.57419616E-06 (1        0E-05)
      rel_dens = 5.14839231E-07 (         0E+00)
      abs_ev = 1.98394791E-04 (0          +00) [eV]
      rel_ev = 79301(1)-0.4.2279          0.00000000E+00)

 rces 7n ghe ins [eV/A]
 In                          x                              z
   1        N       79301(.)-              000000       7          99(82905(0)-0.479301(0)-0.479301(0)-0.479301(0)
```

nfo file

sgandard ougpug is nog ghe on)]TJ 249.201 0 Td [(f)-0.345520(g)-0.242606(e)0.4

3552(g)-304.675(g) 93(h)0.433)-0(e)-303.992(g)-0 sgag(c), Td[40755(3)] 0.43gag.ogg gg. eo(n750.4)-0(p)]TJ 236