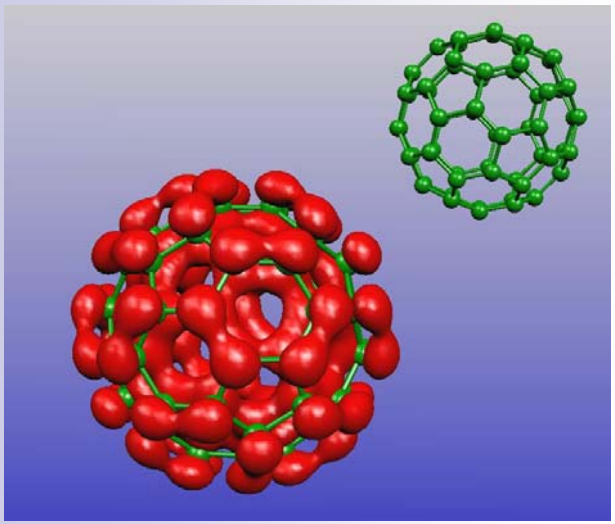
Example 2



Molecular C_{60}

Instructions (I)

- Have a look at the input file (C60.fdf)
  - PAO.Basis
  - Input coordinates
  - Lattice vectors (remember this is a molecular system)
  - Save.DRHO, save.LDOS, …
  - CG relaxation: modify the input to 0 CG steps
- Run & converge
- Use grid2cube (or grid2xfs) to generate contours

Instructions (II)

- Input file (grid2cube.dat)

```
C60
ldos
10.0    10.0    10.0
1
unformatted
```

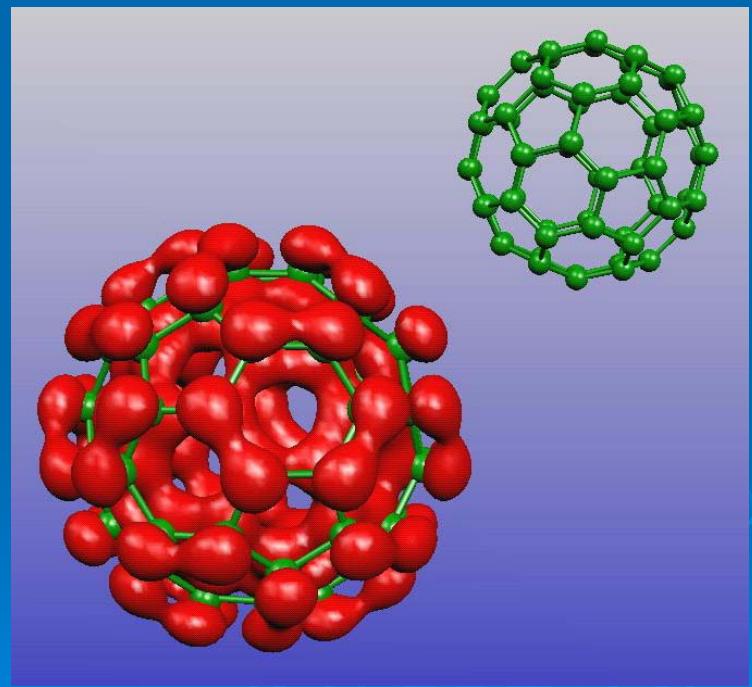
- Run the utility

```
grid2cube < grid2cube.dat
```

- Check you now have a C60.ldos.cube file

Instructions (III)

- Execute xcrysden
- File → Open Structure → open XSF
  - Choose .xsf file
- Tools → Data Grid → OK
- Check “Display isosurface”
  - Set isovalue = 0.009
  - Tab “Plane #1”
    - “color basis” → Rainbow
    - “display color plane”,
    - “transparent color plane”,
    - “display thermometer”,
    - “display isolines”.
  - Tab “Isolines” → Isoline Color → Property Color



Instructions (IV)

Measure interatomic distances & angles

- click “Distance” → pick 2 atoms → click “done”
- Click “Angle” → pick 3 atoms → click “done”

There are two C-C distances (pentagons & hectagons)

Instructions (V)

Use constraints in the CG relaxation:

1. Modify constr.f subroutine in siesta/Src
2. Add a new block in the fdf:

```
%block GeometryConstraints
        routine constr
%endblock GeometryConstraints
```

File Edit View Terminal Go Help

```
c $Id: constr.f,v 1.6 2003/06/23 09:46:16 ordejon Exp $

      subroutine constr( cell, na, isa, amass, xa, stress, fa, ntcon )
c *********************************************************************
c User-written routine to implement specific geometric constraints,
c by orthogonalizing the forces and stress to undesired changes.
c Arguments:
c real*8  cell(3,3)    : input lattice vectors (Bohr)
c integer na           : input number of atoms
c integer isa(na)      : input species indexes
c real*8  amass(na)    : input atomic masses
c real*8  xa(3,na)     : input atomic cartesian coordinates (Bohr)
c real*8  stress( 3,3) : input/output stress tensor (Ry/Bohr**3)
c real*8  fa(3,na)     : input/output atomic forces (Ry/Bohr)
c integer ntcon        : total number of positions constr. imposed
c *********************************************************************
      implicit         none
      integer          na, isa(na), ntcon,ia
      double precision amass(na), cell(3,3), fa(3,na),
     .                 stress(3,3), xa(3,na)

c Write here your problem-specific code.

      do ia = 1,na
        fa(1,ia) = 0.d0
        fa(2,ia) = 0.d0
      enddo

      end
```

constr.f

Instructions (VI)

- Increase number of CG steps in input file
- Run siesta to obtain the relaxed atomic positions with the constraint geometry (icosahedral symmetry). The constr.f file is included in the directory.
- Obtain the new interatomic distances & angles