



ICN2^R

Institut Català
de Nanociència
i Nanotecnologia



Vibrational Modes

Roberta Farris

Wednesday 4th October 2023

First steps with SIESTA: from zero to hero



Vibrational Modes of Benzene Molecule

🏠 » [Tutorials](#) » Vibration modes and phonons

Vibration modes and phonons

In this set of exercises we will use the method of finite-differences implemented in Siesta to compute force constants in real space. We will explore the cases of a crystal and a molecule. In the former case we will focus on the need of a supercell to represent the real-space force constants, while in the second we will understand how to visualize the vibrational modes.

- [Phonon dispersion of bulk Si](#)
- [Modes of vibration of the benzene molecule](#)

Vibrational Modes of Benzene Molecule

Step 1: Relax the structure.

The input file has been prepared for you in the file benzene.relax.fdf

```
%block Zmatrix
molecule
2 0 0 0  xm1 ym1  zm1  0 0 0
2 1 0 0  CC  90.0 60.0  0 0 0
2 2 1 0  CC  CCC  90.0  0 0 0
2 3 2 1  CC  CCC  0.0  0 0 0
2 4 3 2  CC  CCC  0.0  0 0 0
2 5 4 3  CC  CCC  0.0  0 0 0
1 1 2 3  CH  CCH 180.0  0 0 0
1 2 1 7  CH  CCH  0.0  0 0 0
1 3 2 8  CH  CCH  0.0  0 0 0
1 4 3 9  CH  CCH  0.0  0 0 0
1 5 4 10 CH  CCH  0.0  0 0 0
1 6 5 11 CH  CCH  0.0  0 0 0
constants
  ym1 5.00
  zm1 0.00
  CCC 120.0
  CCH 120.0
variables
  CC 1.390
  CH 1.090
constraints
  xm1 CC -1.0 3.903229
%endblock Zmatrix
```

Vibrational Modes of Benzene Molecule

Step 1: Relax the structure.

The input file has been prepared for you in the file benzene.relax.fdf

```
%block Zmatrix
molecule
2 0 0 0  xm1 ym1  zm1  0 0 0
2 1 0 0  CC  90.0 60.0  0 0 0
2 2 1 0  CC  CCC  90.0  0 0 0
2 3 2 1  CC  CCC  0.0  0 0 0
2 4 3 2  CC  CCC  0.0  0 0 0
2 5 4 3  CC  CCC  0.0  0 0 0
1 1 2 3  CH  CCH 180.0  0 0 0
1 2 1 7  CH  CCH  0.0  0 0 0
1 3 2 8  CH  CCH  0.0  0 0 0
1 4 3 9  CH  CCH  0.0  0 0 0
1 5 4 10 CH  CCH  0.0  0 0 0
1 6 5 11 CH  CCH  0.0  0 0 0
constants
  ym1 5.00
  zm1 0.00
  CCC 120.0
  CCH 120.0
variables
  CC 1.390
  CH 1.090
constraints
  xm1 CC -1.0 3.903229
%endblock Zmatrix
```

```
siesta benzene.relax.fdf > benzene.relax.out
```

Vibrational Modes of Benzene Molecule

Step 2: Compute the IFCs

There is already a prepared input file with the relaxed structure.
In principle, you should copy the relaxed coordinates and unit cell from the benzene.XV obtained in the previous step.

benzene.ifc.fdf

```
LatticeConstant      1.0 Bohr
%block LatticeVectors
20.932528150         0.000000000         0.000000000
0.000000000         19.551203193         0.000000000
0.000000000         0.000000000         10.714661844
%endblock LatticeVectors

AtomicCoordinatesFormat NotScaledCartesianBohr
%block AtomicCoordinatesAndAtomicSpecies
4.738724869         9.448634389         0.000000000         2         12.0107
6.057380810         11.732613477        -0.000000000         2         12.0107
8.694692693         11.732613477        -0.000000000         2         12.0107
10.013348634         9.448634389         -0.000000000         2         12.0107
8.694692693         7.164655301         -0.000000000         2         12.0107
6.057380810         7.164655301         -0.000000000         2         12.0107
2.647979028         9.448634389         -0.000000000         1         1.00794
5.012007889         13.543252488        -0.000000000         1         1.00794
9.740065613         13.543252488        -0.000000000         1         1.00794
12.104094475         9.448634389         -0.000000000         1         1.00794
9.740065613         5.354016289         -0.000000000         1         1.00794
5.012007889         5.354016289         -0.000000000         1         1.00794
%endblock AtomicCoordinatesAndAtomicSpecies
```

Vibrational Modes of Benzene Molecule

Step 2: Compute the IFCs

There is already a prepared input file with the relaxed structure.
In principle, you should copy the relaxed coordinates and unit cell from the benzene.XV obtained in the previous step.

benzene.ifc.fdf

```
LatticeConstant      1.0 Bohr
%block LatticeVectors
20.932528150         0.000000000         0.000000000
0.000000000         19.551203193         0.000000000
0.000000000         0.000000000         10.714661844
%endblock LatticeVectors

AtomicCoordinatesFormat NotScaledCartesianBohr
%block AtomicCoordinatesAndAtomicSpecies
4.738724863         11.448634389         -0.000000000         2         12.0107
6.057380810         11.732613477         -0.000000000         2         12.0107
8.694692693         11.732613477         -0.000000000         2         12.0107
10.013348634         9.448634389         -0.000000000         2         12.0107
8.694692693         7.164655301         -0.000000000         2         12.0107
6.057380810         7.164655301         -0.000000000         2         12.0107
2.647979028         9.448634389         -0.000000000         1         1.00794
5.012007889         13.543252488         -0.000000000         1         1.00794
9.740065613         13.543252488         -0.000000000         1         1.00794
12.104094475         9.448634389         -0.000000000         1         1.00794
9.740065613         5.354016289         -0.000000000         1         1.00794
5.012007889         5.354016289         -0.000000000         1         1.00794
%endblock AtomicCoordinatesAndAtomicSpecies
```

siesta < benzene.ifc.fdf > benzene.ifc.out

Vibrational Modes of Benzene Molecule

Step 3: Compute the dynamical matrix at Gamma

In the case of a molecule, only the Gamma point is relevant. It is specified in the same way as to compute the electronic band structure, in the same file benzene.ifc.fdf

```
Eigenvectors .true. # Compute both phonon eigenvalues and eigenvectors
BandLinesScale pi/a
%block BandLines
1 0.0 0.0 0.0 \Gamma # Only the Gamma point (enough for a molecule)
%endblock BandLines
```

```
vibra < benzene.ifc.fdf > vibra.out
```

Vibrational Modes of Benzene Molecule

Step 4: Visualize the normal modes:

Needed files:

- benzene.XV
- benzene.vectors

You need to specify:

- units of lattice vectors(Angstroms or Bohr)
- the zero of the coordinates
- the unit cell lattice vectors
- modes to visualize (the first and the last)
- the amplitude
- the steps of the animation

It is already done in vib2xsf.dat for you. Run: **vib2xsf < vib2xsf.dat**

*By Andrei Postnikov

Vibrational Modes of Benzene Molecule

Step 5: XCrysden

Output files:

- Benzene.Mode_*.XSF: contains a static structures (as in .XV), with arrors added to each atom to indicate displacement pattern.
- Benzene.Mode_*.AXSF: contains the animation of a phonon, for a defined amplitude and number of steps.

Vibrational Modes of Benzene Molecule

Step 5: XCrySDen

Output files:

- [Benzene.Mode_*.XSF](#): contains a static structures (as in .XV), with errors added to each atom to indicate displacement pattern.
- [Benzene.Mode_*.AXSF](#): contains the animation of a phonon, for a defined amplitude and number of steps.



XCrySDen ...
X-window CRYstalline Structures and DENsities

[Home](#) | [About](#) | [Description](#) | [Documentation](#) | [Download](#) | [News](#) | [Links](#)

XCrySDen

XCrySDen is a **crystalline and molecular structure visualisation program** aiming at display of isosurfaces and contours, which can be superimposed on crystalline structures and interactively rotated and manipulated. It runs on GNU/Linux.

XCrySDen has been also ported to Mac OS (requires X11) and Windows (requires either [CYGWIN](#) or [WSL](#)).

The name of the program stands for *Crystalline Structures and Densities* and *X* because it runs under the X-Window environment.

[Read more...](#) | [See screenshots ...](#)

Latest version: [1.6.2](#)

Vibrational Modes of Benzene Molecule

Step 5: XCrySDen

Output files:

- Benzene.Mode_*.XSF: contains a static structures (as in .XV), with errors added to each atom to indicate displacement pattern.
- Benzene.Mode_*.AXSF: contains the animation of a phonon, for a defined amplitude and number of steps.

...And have fun!



XCrySDen ...
X-window CRYstalline Structures and DENsities

[Home](#) | [About](#) | [Description](#) | [Documentation](#) | [Download](#) | [News](#) | [Links](#)

XCrySDen

XCrySDen is a **crystalline and molecular structure visualisation program** aiming at display of isosurfaces and contours, which can be superimposed on crystalline structures and interactively rotated and manipulated. It runs on GNU/Linux.

XCrySDen has been also ported to Mac OS (requires X11) and Windows (requires either [CYGWIN](#) or [WSL](#)).

The name of the program stands for *Crystalline Structures and Densities* and *X* because it runs under the X-Window environment.

[Read more...](#) | [See screenshots...](#)

Latest version: [1.6.2](#)

Vibrational Modes of Benzene Molecule

Results: examples of two modes....

