

# CONVIV Interface And Layout

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# From a Computer Point of View

- CONVIV is written in FORTRAN.
- FORTRAN is (so far) not (really) well designed to parse input files.
- Accordingly, CONVIV can be somewhat delicate to start with.

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# From a Chemist Point of View

- CONVIV allows to investigate the spectroscopy of a molecule through the VMFCI method.
- We need to provide CONVIV with the information about the molecule.
- We need to describe the VMFCI steps we want to take.
- And even if we are not specialist in Quantum Chemistry.
- So, we want a (smart) "black box".

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Sorry, I'm a C++ programmer...

# Configuration Files Format for CONVIVIAL

- We chose the JSON format (JavaScript Object Notation, see <http://www.json.org>)
- A very simple syntax to read and write arrays or associative arrays of strings, floating point numbers, booleans,...
- It's a text format that can be modified with a simple text editor.

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# Interface Builder

- We chose the **Fast Light ToolKit** (<http://www.fltk.org>)
  - A very permissive license.
  - No extra dependency.
  - Pre-compiled for a lot of Operating Systems.
  - Used by a lot of scientific softwares:
    - open source, like ITK, the Insight Segmentation and Registration Toolkit for image analysis
    - free software, like VMD, Visual Molecular Dynamics for molecules visualization.
- CONVIVIAL runs on Win32 (XP,Vista,7), Linux, Solaris, \*BSD, MacOSX.
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