The Avogadro Handbook

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by Carsten Niehaus and Marcus Hanwell

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Avogadro is an advanced molecular editor designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It offers flexible rendering and a powerful plugin architecture.

The main concept behind Avogadro is to enable a strong framework for molecular visualization and editing. Each community has their own needs and goals for an ideal tool. So Avogadro seeks to allow users to easily provide their own plugins and scripts for rendering, tools, commands... etc. Avogadro is based on top of existing chemistry software, including Open Babel. In the future, it will offer strong scripting abilities to allow for automated demos, submission of calculations to local computational resources, and user-defined customization.

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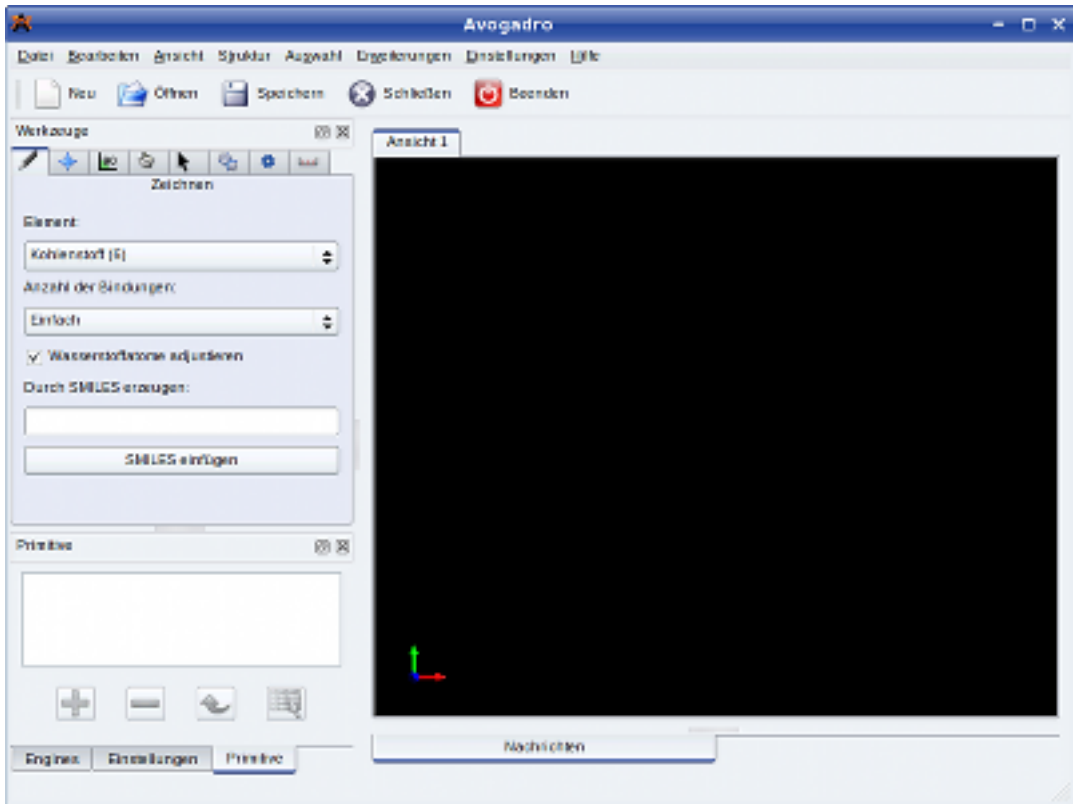
Chapter 1. Introduction

Avogadro is free, cross-platform and licensed under the GNU Public License. For more information, see the homepage (http://avogadro.openmolecules.net/).

Chapter 2. Avogadro quick start guide

This is what Avogadro looks like the first time it is run.



Chapter 3. Getting Involved

Avogadro has a very open and active development community. Currently there are more than 10 active developers and other various contributers. If you are interested in working on or with Avogadro please look at the developer information that is available on the wiki and subscribe to the mailing list (http://lists.sourceforge.net/mailman/listinfo/avogadro-devel). You could also join the IRC channel (#avogadro on irc.freenode.net) and talk with other developers. For information on the internals of Avogadro and LibAvogadro, review the avogadro developer API (http://avogadro.openmolecules.net/dev-api/).

Chapter 4. Credits and License

Program Copyright, 2006-2008 The Avogadro Team

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Appendix A. Installation

A.1. How to obtain Avogadro

Avogadro can be found on the Avogadro home page (http://avogadro.openmolecules.net/).

A.2. Requirements

Although Avogadro can work without any 3D-acceleration, an OpenGL capable card will vastly improve the user experience. At a minimum Avogadro requires a system capable of providing OpenGL software rendering. It is currently ported and tested on GNU/Linux, Apple Mac OS X and Microsoft Windows.

A.3. Building Avogadro from source

If you decide to build Avogadro from source, the following resources will be necessary:

- Git, to access certain code repositories
- CMake (>=2.6.0), the open-source build system
- Qt4 (>=4.4.0), the open-source application framework
- Eigen2, a library for linear algebra as a compile-time dependency of Avogadro
- OpenBabel (>=2.2.0), the chemistry toolbox

All of these programs and libraries are likely to be available through your distribution's repository.

Further information can be found on the Avogadro home page (http://avogadro.openmolecules.net/wiki/Compiling).