The Avogadro Handbook

Carsten Niehaus

cniehaus@kde.org

The Avogadro Handbook

by Carsten Niehaus

Copyright © 2008 Carsten Niehaus

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.

Table of Contents

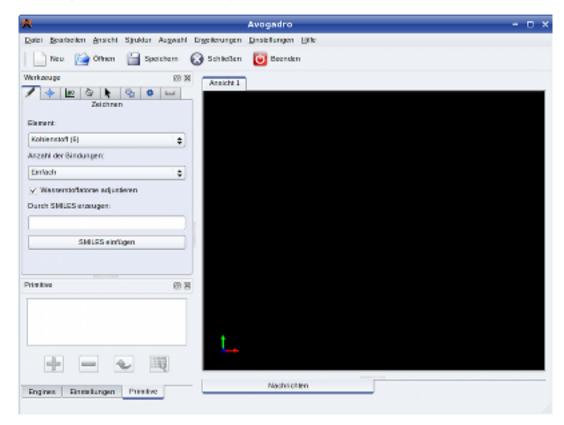
| 1. Introduction | 1 |
|-------------------------------|---|
| 2. Avogadro quick start guide | 2 |
| 3. Getting Involved | |
| 4. Credits and License | 4 |
| A. Installation | 5 |
| A.1. How to obtain Avogadro | 5 |
| A.2. Requirements | |

Chapter 1. Introduction

It is free and licensed under the GNU Public License. For more information, see the Homepage (http://avogadro.sourceforge.net).

Chapter 2. Avogadro quick start guide

Here is Avogadro looks like the first time you run it.



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 interesting in working on or with Avogadro please look at the Developer information that is available and subscribe to the mailinglist (http://lists.sourceforge.net/mailman/listinfo/avogadro-devel). 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.sourceforge.net/dev-api/).

Chapter 4. Credits and License

Program Copyright, 2006-2008 The Avogadro Team

Contributors:

- Donald <>
- Geoff <>
- Carsten Niehaus <cniehaus@kde.org>
- Marcus <>
- Benoît <>

Appendix A. Installation

A.1. How to obtain Avogadro

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

A.2. Requirements

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