

# Groovy Cheminformatics...



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## Keywords

Cdk, Java, Cheminf, Cdkbook

## Abstract

Update: the fourth edition is out.

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**Update:** the [fourth edition](#) is out.

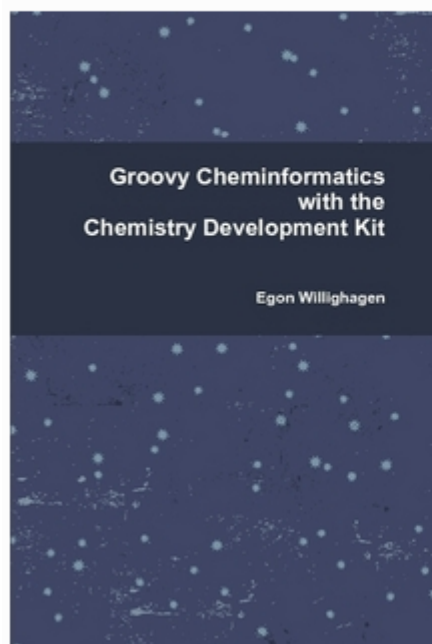
Some project are never finished. Neither is this one, but it is never too late to change how things work, so, taking advantage of publishing-on-demand, here I introduce the release-soon, release-often equivalent of cheminformatics books, my [Groovy Cheminformatics with the Chemistry Development Kit](#) book:

## Groovy Cheminformatics with the Chemistry Development Kit

By Egon Willighagen

Paperback, 72 pages ★★★★★

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**Ships in 3–5 business days**

This book introduces the reader to the wide variety of functionality available in the Chemistry Development Kit (CDK) library. It will discuss parts of the data model, basic cheminformatics algorithms, chemical file formats, etc. It discusses bits of chemical graph theory, computer representation, etc. But the goal of this book is not to provide an introduction into cheminformatics. However, this book does require a basic chemical education. It assumes that you know what atoms are, how they are connected by chemical bonds, and it assumes some basic computer knowledge. This book is about learning how to perform cheminformatics tasks using the CDK. But to keep the required knowledge to a minimum, the examples will be pretty verbose. The book details the CDK data model, discusses input and output, atom types, graph properties, missing information, and substructure searching. It demonstrates the CDK library with 75 code examples.

With a serious discount for just being the first edition (1.3.8-0), but still counting at 72 pages with 75 code examples, this edition marks a personal milestone (and probably not much more than that). There remains much to do, but I promised a release by tomorrow, so here it is. Next releases will contain more code examples, more functionality descriptions, and more literature reviewing where such code is used in science. The plan is to make new editions with each new [CDK](#) release, as well as new editions when I added a new chapter, section, or just paragraph. But, there will not be a Nightly build service anytime soon.

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Now, the book content is **not** open content. However, it contains nothing that is not available in other means. It's just the compilation that makes this book interesting, as well as that I put effort in ensuring the code examples remain working. For that, I ask a minor financial contribution.