chem-bla-ics

Groovy Cheminformatics 3rd edition

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Update: the fourth edition is out.

I am starting to get the hang of this publishing soon, publishing often thing, and just uploaded edition 1.4.1-0 of the Groovy Cheminformatics book. The cover is the same (with one typo fix), and the content is 20 pages thicker. True, six of those pages are isotope masses of all natural isotopes. That leaves 14 pages with this new content:

- Section 2.7 on line notations with 2.7.1 about reading and writing SMILES
- Section 6.3 about Sybyl (mol2) atom types
- Section 7.4 on atom numbering with 7.4.1 on Morgan atom numbers, and 7.4.2 on InChI atom numbers
- Chapter 9 on molecule depiction with the new rendering code, with
  - Section 9.1 on drawing molecules,
  - Section 9.2 on rendering parameters, and
  - Section 9.3 on the generator API and how to add custom content
- Section 11.4 on calculating aromaticity
- Appendix A.2 listing all Sybyl atom types
- Appendix B listing all naturally occurring isotopes

Features requests most welcome.