Dietrich Klemm

Biochemical Principles and Mechanisms of Biosynthesis Biodegradation of Polymers

Edited by
Markus Stoeppler

Dietrich Klemm

Biochemical Principles and Mechanisms of Biosynthesis Biodegradation of Polymers

Organic Chemistry Nomenclature

Edited by
Markus Stoeppler

with the collaboration of
Gerard Böhm
Uwe Diderichsen

Third Edition

A Personal Foreword

The dilemma of rapidly emerging fields is that reviews are often outdated before they are printed. To make a contribution that would endure, we knew we had to go beyond a snapshot of the current state of fragment-based drug discovery and instead provide a framework for upcoming advances.

Basel, March 2006

Wolfgang Janke
Daniel A. Erlanson

Fragment-based Approaches in Drug Discovery. Edited by W. Jahnke and D.A. Erlanson

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Preface to the Third Edition

Here is preface to the current edition.

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Part I
Sample Part

1
Trust and Reputation For Service-Oriented Environments Technologies For Building Business Intelligence and Consumer Confidence

1.1
Section Title

Here is some text. Here is some text.

1.1.1
Subsection Title

Here is text in subsection. Here is text in subsection. Here is text in subsection. Here is text in subsection. Here is text in subsection. Here is text in subsection.

1.1.1.1 Subsubsection Title

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1.1.1.2 Subsubsection

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2
Sample Edited Book Chapter

Chapter Author[1)]

The first paragraph following the chapter title will not be indented. The first paragraph following the chapter title will not be indented.

2.1
Section Title[2)]

Wally Jumblatt, Stephen Queen[3)]

Here is some text. Here is some text.

2.1.1
Subsection Title[4)]

Glen Greenwald

Text in subsection. Text in subsection. Text in subsection. Text in subsection.

2.1.1.1 Here is a subsubsection

Formally, it is very simple to write down the electron density n in the conduction band. It corresponds to the integrated occupied density of states in the conduction band:

$$n = \frac{1}{V} \int_{E_{\mathrm{C}}}^{\infty} g_{\mathrm{C}}(E) f(E,T) \mathrm{d}E, \tag{2.1}$$

[1)] Chapter author footnote
[2)] Here is a section footnote
[3)] Section Author
[4)] Footnote in Subsection

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where $g_{\mathrm{C}}(E)$ is the density of states in the conduction band and E_{C} is the energy of the CBM. The density of missing electrons or holes in the valence band p can be calculated by an analogous formula:

$$p = \frac{1}{V} \int_{-\infty}^{E_{\mathrm{V}}} g_{\mathrm{V}}(E)[1 - f(E, T)]\mathrm{d}E, \tag{2.2}$$

with E_{V} being the energy of the VBM.

3
Nuclear Angular Momentum $\alpha\beta\Gamma\Delta 123$ and Magnetic Moment [1)]

Similarly to the moisture content, the enthalpy will not only change by the agglomeration of particles, but also by the size dependent heat and enthalpy transfer rates. The population balance approach can be used to model the combined processes of agglomeration and drying as

$$
\begin{aligned}
&\frac{\partial f\left(t,v,l,h\right)}{\partial t}+\frac{\partial G_l\cdot f\left(t,v,l,h\right)}{\partial l}+\frac{\partial G_h\cdot f\left(t,v,l,h\right)}{\partial h}\\
&= \frac{1}{2}\int_0^v\int_0^l\int_0^h \beta\cdot f\left(t,v-u,l-\gamma,h-\varepsilon\right)\cdot f\left(t,u,\gamma,\varepsilon\right)\mathrm{d}\varepsilon\,\mathrm{d}\gamma\,\mathrm{d}u \\
&- \int_0^\infty\int_0^\infty\int_0^\infty \beta\cdot f\left(t,v,l,h\right)\cdot f\left(t,u,\gamma,\varepsilon\right)\mathrm{d}\varepsilon\,\mathrm{d}\gamma\,\mathrm{d}u\,.
\end{aligned}
\tag{3.1}
$$

Again, f denotes the number density distribution. The advection terms on the left hand side of the equation represent the change of mass of liquid and enthalpy, respectively. The parameter G_l indicates the rate of change of liquid mass. Positive and negative values of G_l correspond to wetting and drying. The expression on the right hand side represents the birth and death of particles due to agglomeration. The triple integral explains that three independent particle properties are considered. The above equation provides the possibility to incorporate additional particle properties in the agglomeration kinetics β.

> "From these experiments it is seen that both matter and radiation possess a remarkable duality of character, as they sometimes exhibit the properties of waves, at other times those of particles. Now it is obvious that a thing cannot be a form of wave motion and composed of particles at the same time - the two concepts are too different. ... The solution of the difficulty is that the two mental pictures which experiment lead us to form - the one of the particles, the other of the waves - are both incomplete and have only the validity of analogies which are accurate

[1)]Text for footnote.

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Fig. 3.1 (a) Sketch of the valence band and conduction band in the vicinity of the gap. The bands are described as parabolas with different curvatures (effective masses). (b) Even simpler picture in which valence and conduction bands are represented by single energy levels.

Fig. 3.2 Here is a caption that will fit in the width of the page so it will not wrap.

> only in limiting cases. ... Light and matter are both single entities, and the apparent duality arises in the limitations of our language.
>
> It is not surprising that our language should be incapable of describing the processes occurring within the atoms, for, as has been remarked, it was invented to describe the experiences of daily life, and these consist only of processes involving exceedingly large numbers of atoms. Furthermore, it is very difficult to modify our language so that it will be able to describe these atomic processes, for words can only describe things of which we can form mental pictures, and this ability, too, is a result of daily experience. Fortunately, mathematics is not subject to this limitation, and it has been possible to invent a mathematical scheme - the quantum theory - which seems entirely adequate for the treatment of atomic processes; for visualization, however, we must content ourselves with two incomplete analogies - the wave picture and the corpuscular picture." Heisenberg, 1930

Example 1 *Here is an example.* ■

Theorem 1 *Here is a theorem.*

Proof: Here is its proof. ■

Table 3.1 Binary Breakage with the finite volume scheme and $S(v) = v$, $t = 1000$

Grid Points, I	**Error, L_1**	**OC**
61	33.8559	-
122	8.8548	1.93
244[1)]	2.2363	1.98
488	0.5612	1.99[2)]

1) Here is a table note.
2) This is the second note.

Table 3.2 Again, Binary Breakage with the finite volume scheme and $S(v) = v$, $t = 1000$, and this time the caption is longer so it will wrap.

	Grid Points, I	**Error, L_1**	**OC**
Spring	61	33.8559	-
Summer	122	8.8548	1.93
Fall	244	2.2363	1.98
Winter	488	0.5612	1.99

Using `\useextraspace` for more vertical space between table lines. Bold column heads and bold line beginnings produced with `\tableboldfont`. `\boldmath` should be entered before math begins in column headers. Oddity, you need to surround `\boldmath` with curlys to avoid an error message when using `\midrule`, ie, `{\boldmath $\alpha\betat$ }`

Table 3.3 Effective masses for some semiconductors.

Material	$\boldsymbol{m_e^*/m_e}$	$\boldsymbol{m_h^*/m_e}$
Ge	0.60	0.28
Si	0.43	0.54
CdSe	0.13	0.45
GaAs	0.065	0.50

Here is some text. Here is some text. Here is some text. Here is some text. Here is some text. Here is some text.

> Note Bene
> ***Nota bene is a Latin phrase meaning "Note Well," coming from notare—to note.[1] It is in the singular imperative mood, instructing one individual to note well the matter at hand. (The plural form is notate bene.)***
> ***In present day English, it is used to draw the attention of the reader to a certain (side) aspect or detail of the subject on hand, translating it as "pay attention" or "take notice". It is often written in the abbreviated form: N.B.***

The following text is an example or a short quotation using the "quote" environment:

> *Human beings, who are almost unique in having the ability to learn from the experience of others, are al remarkable for their apparent disinclination to do so.* Douglas Adams

The "quote" environment is used for quotations that are only one paragraph long. For longer quotations, the "quotation" environment should be used instead, as we see here.

> "To be sure, it has been pointed out that the introduction of a space-time continuum may be considered as contrary to nature in view of the molecular structure of everything which happens on a small scale. It is maintained that perhaps the success of the Heisenberg method points to a purely algebraical method of description of nature, that is to the elimination of continuous functions from physics. Then, however, we must also give up, by principle, the space-time continuum.
>
> It is not unimaginable that human ingenuity will some day find methods which will make it possible to proceed along such a path. At the present time, however, such a program looks like an attempt to breathe in empty space." –Albert Einstein, *Out of My Later Years*

Text following the quotation should not indent.

The next example shows a marginnote, followed by some examples of listing environments using "itemize" and "enumerate".

Notice:
Here is text in the margin, pointing out an issue here that needs to be remembered.

Numerical results The following problems have been considered for the comparison

– binary breakage, $b(u, v) = 2/v$ with selection function, $S(v) = v$, and

– binary breakage, $b(u, v) = 2/v$ with selection function, $S(v) = v^2$.

- First subitem.
- Second subitem.

In both problems, mono-disperse particles with size unity are taken as initial data. For numerical computation, the volume domain has been divided by the rule $x_{i+1/2} = 2^{1/q}x_{i-1/2}$. **Caution!**

1. This is the first item in the numbered list.
2. This is the second item in the numbered list. This is the second item in the numbered list. This is the second item in the numbered list.

I. This is the first item in the itemized list.

II. This is the first item in the itemized list. This is the first item in the itemized list. This is the first item in the itemized list.

Text following itemize or enumerate should not indent. User should be sure not to leave a blank line after these environments.

3.1 Discussion and Problems

3.1.1 Discussion

1. What is the difference between a metal, a semiconductor, and an insulator?
2. How does the resistance of a semiconductor (typically) change as a function of temperature and why?
3. In an intrinsic semiconductor, the chemical potential lies in the middle of the gap for low temperatures. Why?
4. Explain the difference between "electrons" and "holes."
5. How many mobile electrons and holes do you have as a function of temperature for an intrinsic semiconductor?

3.1.2 Problems

1. *Nondegenerate semiconductors*: Derive the simplified expressions for the Fermi function (Eq. 11) and (Eq. 12), assuming that the chemical potential is situated approximately in the middle of the gap.

2. *The chemical potential in metals*: In Chapter 2, we have simply identified the chemical potential μ in a metal with the Fermi energy E_{F} and stated that this is a good approximation for all temperatures, that is, that the chemical potential is independent of the temperature. Use the charge-neutrality arguments introduced in this chapter to show that this is indeed a justified approximation.

3. *Doped semiconductors*: Consider a nonionized phosphorus donor atom in a Si crystal. (a) What is the "Bohr radius" of the resulting "atom"? (b) How many Si atoms are contained within this "Bohr radius"? (c) Estimate how high the concentration of impurities would have to be for the "Bohr radii" to overlap and what would you expect to happen in this case?

$$R_{\mathrm{H}} = \frac{E_{\mathrm{H}}}{Bj_x} = \frac{p\mu_{\mathrm{h}}^2 - n\mu_{\mathrm{e}}^2}{e(p\mu_{\mathrm{h}} + n\mu_{\mathrm{e}})^2}. \tag{3.2}$$

The crucial difference between a metal and a semiconductor is that the carrier concentration for the former can increase very strongly as the temperature is raised whereas it is constant for the latter.

In a very simple picture, this leads to the conclusion that semiconductors become more conductive at higher temperature whereas metals become less conductive. The decrease in the conductivity of a metal is due to a stronger scattering of the electrons from phonons. This process is also present for semiconductors but unimportant compared to the increased number of carriers. But is this really always the case, in particular, for doped semiconductors? Consider for example the carrier concentration in Fig. 2.3 around $T = 300\,\mathrm{K}$. Speculate how the conductivity would change around this temperature.

Chapter Appendix: Luminousity of Beams of Particular Particles

Here is where an optional chapter appendix should appear.

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Part II
End of Book Environments

Glossary

GaAs Gallium Arsinide. For similar device sizes GaAs transistors have three to five times greater transconductance than those of of silicon bipolar and MOS transistors.

VLSI Very Large Scale Integration. Since the mid-1970s VLSI technology has been successfully used in many areas, but its effect on computers of all shapes and sizes has been the most dramatic. Some of the application areas got boosts in performance while others became feasible.

Luminosity A number describing how intense the beam(s) of particles are before (while) they interact with each other (with a target). It is measured in $cm^{-2}*sec^{-1}$ and is related to the intensities of the beams. Multiplying the luminosity by the cross section results in the event rate which is the what is directly measured.

Quantum Mechanics Theory describing how things work at small distance scales from atoms on down to quarks. Quantum mechanics describes a duality where particles can be viewed as having a wave function but also letting light (energy) have a particle or localized aspect. It introduces uncertainty into measurement of a physical system such as not being able to measure exactly and simultaneously the position and momentum of an electron. It is also responsible for the quantizing of energy levels of the atom.

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A
This is an Appendix

A.1
Here is a section

$$\alpha\beta\Gamma\Delta \tag{A.1}$$

Here is text.

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