Bibliography

Books of mathematics for chemists

Chemical Calculations, Paul Yates, Chapman and Hall, London, 1997. This is Yates' first maths book. It is relatively short, and aimed at those with little or no maths. Yates' style is gentle and persuasive. It *encourages* the reader. He also employs a margin icon of a calculator, demonstrating its correct use at appropriate junctures.

Yates is a British physical chemist; the chapters of his book relate to a traditional course in physical chemistry (level I and some level II) so, within each chapter, Yates discusses the mathematics needed by a typical student. For example, Chapter 3 is entitled 'Solution Chemistry', Chapter 4 is 'Kinetics', and so on. This intelligent approach works well for students who struggle during a course in physical chemistry, but may not work so well for students on courses explicitly aimed at teaching mathematics. Yates himself must have felt the approach failed somewhat, because he includes an appendix of pure mathematics. Also, there is no logical progression from the mathematical fundamentals via symbols through to algebra, powers, etc.

Chemical Calculations at a Glance, Paul Yates, Blackwell, Oxford, 2005. This book represents a 're-statement' of Yates' earlier book *Chemical Calculations* (as above) since it covers the same material but is themed mathematically rather than according to the syllabus of a traditional course in physical chemistry.

The book is beautifully produced in A4 format, and shows a logical layout throughout, starting with notation and units, and moving eventually to calculus. The proportion of chemical examples is high. The number of worked examples is similarly higher than the average, although occasionally more detail would have helped. Nevertheless, it's a helpful tool.

The Chemistry Maths Book, Erich Steiner, Oxford University Press, Oxford, 1996. This book represents the 'Rolls-Royce' end of the market. Steiner is an inspiring and gifted teacher, and this book reflects that gift. It is beautifully written and well produced. The text is authoritative, comprehensive. It also has a good, long index. Furthermore, Steiner litters the text with clever quotes; most pages glisten with fascinating historical detail in a series of well-designed footnotes.

Maths for Chemists, Volume 1: Numbers, Functions and Calculus, Martin C. R. Cockett and Graham Doggett, RSC, Cambridge, 2003. This is a good book. It is well written and produced, as are all titles in the RSC's new 'Tutorial Chemistry Texts' series. The chapter on algebra is poor and far too short at 10 pages. There are no chemical structures, although to be fair the proportion of chemistry is pleasingly high. The index is short but better than average.

Maths for Chemists, Volume 2: Power Series, Complex Numbers and Linear Algebra, Martin C. R. Cockett and Graham Doggett, RSC, Cambridge, 2003. This book is the companion volume to the text immediately above. By 'linear algebra', the authors mean vectors, arrays, determinants, and the like. The book is very advanced, though its treatment of quite difficult topics is superb.

Beginning Mathematics for Chemists, Stephen K. Scott, Oxford University Press, Oxford, 1995. Chemistry staff like this book. Its approach is logical and gentle on the student. I like its principal titles 'warming up' and 'relaxing down', for example. The book is rather too short. Calculus occupies centre stage, with about 50 pages. Algebra occupies a mere 21 pages.

Essential Mathematics for Chemists, John Gormally, Prentice Hall, Harlow, 2000. The book is printed with two colours, and is visually appealing. Gormally arranges the seven short chapters into sensible and predictable groups, starting with 'handling numbers', then 'handling algebra'. It has separate chapters to describe differential and integral calculus. Its index is poor, but does include chemical terms as well as mathematics. The exercises are generally chemical, although almost all of these chemical terms relate only to physical chemistry.

Unfortunately, once more this book looks like a vehicle for mathematicians rather than for chemists. To the eye, its pages look to be crammed with equations. The number of figures is minimal, and there are no chemical structures.

Basic Mathematics for Chemists, Peter Tebbutt, Wiley, Chichester, 1994. The text is very traditional in style and content, with monochrome pages and narrow margins. It is slightly long. The overwhelming majority of the book represents mathematical content rather than chemistry.

Tebbutt's book contains more figures than those above, the majority of which are clearly of chemical origin, but, yet again, there are no chemical structures. The very short index includes chemical terms as well as mathematical terms. Most of these chemical terms relate exclusively to physical chemistry.

Calculations for A-Level Chemistry (3rd edn), E. N. Ramsden, Stanley Thornes, Cheltenham, 1994. This book was in print until quite recently, and some shops may still have copies. A revamped edition is expected soon.

The book contains a few chemical structures, and *all* examples derive from chemistry—and from all branches of chemistry, not just physical chemistry. No student could complain that this book was written for mathematicians.

The style is clear, concise, and constructive. Like Yates, Ramsden chooses to teach by chemical discipline rather than mathematical topic, which will preclude its use from most courses of 'Mathematics for chemists'. The intended audiences are students reading for pre-university qualifications, so its standard is only slightly above that of a modern HND.

Books describing the mathematics

The 'teach yourself' series of books are generally excellent. For example, each of the following is superb and highly recommended:

- *Teach Yourself Mathematics*, Trevor Johnson and Hugh Neill, Hodder and Stoughton, London, 2003.
- *Teach Yourself Algebra*, Paul Abbott and revised by Hugh Neill, Hodder and Stoughton, London, 2003.
- *Teach Yourself Trigonometry*, Paul Abbott and revised by Hugh Neill, Hodder and Stoughton, London, 2003.
- *Teach Yourself Calculus*, Paul Abbott and revised by Hugh Neill, Hodder and Stoughton, London, 2003.

Mathematics support

There are several good websites that support a course of 'Mathematics for chemists'. One of the best is the page of 'Mathematics Support Materials' at the University of Plymouth:

http://www.tech.plym.ac.uk/maths/resources/PDFLaTeX/mathaid.html (accessed 12 May 2005), which hosts pdf files of high quality.

Books describing physical chemistry

Most of the chemistry in these pages comes from the physical branch. Some may see this weighting as unfortunate, but Physical chemistry is generally mathematical.

The physical chemistry in these pages is adequately described in straightforward books on physical chemistry. For example, the best-selling textbook of physical chemistry in the world is undoubtedly Atkins' *Physical Chemistry*. The latest edition is the seventh, by P. W. Atkins and Julio de Paula, Oxford University Press, Oxford, 2002. Many students will find it rather mathematical, and its treatment is certainly highbrow. Its 'little brother' is *Elements of Physical Chemistry* (4th edn), P. W. Atkins, Oxford University Press, Oxford, 2005, and is intended to overcome these perceived difficulties by limiting the scope and level of its parent text. Both are thorough and authoritative.

Several texts approach the topic by means of worked examples. *Physical Chemistry*

(2nd edn), C. R. Metz, McGraw-Hill, New York, 1989, is a member of the 'Schaum Out-line Series' of texts, and *Physical Chemistry*, H. E. Avery and D. J. Shaw, Macmillan, Basingstoke, 1989, is part of the 'College Work-out Series'. Both books are crammed with worked examples, self-assessment questions, and hints on how to approach typical questions. Avery and Shaw is one of the few general textbooks on physical chemistry that a non-mathematician can read with ease.

Monk has tried to get away from a traditional approach in his *Physical Chemistry: Understanding our Chemical World*, Wiley, Chichester, 2005. In this book, the examples take centre stage, and the theory is deduced from these examples. The mathematics is explained in minute detail, but without any loss of rigour.

Books describing analytical chemistry

The following contain sufficient material to explain the analytical chemistry described in these pages: *Statistics and Chemometrics for Analytical Che*mistry (5th edn), J. N. Miller and J. C. Miller, Pearson, Harlow, 2005, is well written and offers a well-balanced approach. While the book *is* mathematical, the maths is not overbearing. Alternatively, *Analytical Chemistry* (5th edn.), G. F. Christian, Wiley, New York, 1994, is fairly comprehensive and will cover some of the material covered here. *The Elements of Analytical Chemistry*, S. P. J. Higson, Oxford University Press, Oxford, 2001, is part of the 'Oxford Primer' series, so will be cheap and affordable.

Books describing electrochemistry

Many of the examples come from electrochemistry, which is a notoriously mathematical discipline. Without doubt, the best 'all round' book for the electrochemist, and already regarded as a modern classic, is *Electrochemical Methods* (2nd edn), A. J. Bard and L. R. Faulkner, Wiley, New York, 2005. Its treatment is generally very mathematical.

Alternatively, *Fundamentals of Electroanalysis*, P. M. S. Monk, Wiley, Chichester, 2001, is written as part of a distance-learning package, 'Analytical Texts in the Sciences'. It is therefore brimming with worked examples and illustrations.

Examples cited in the text

Chapter 2

Worked example 2.10:
For full details of the reaction, see: J. Cordaro, J. McClusker, and R. Bergman, Synthesis of mono-substituted 2,2′-bipyridines, *J. Chem. Soc., Chem. Commun.*, 2002, 1496.

Chapter 6

Worked example 6.11:
The fascinating topic of the relationship between the Golden Ratio and τ is described in the web page, *www.austms.org.au/Modules/Fib/fib.pss* (accessed 10 June 2004). Alternatively, see:

http:www.maven.smith.edu/~phyllo/About/fibogolden.html
(accessed 8 July 2005).

Chapter 13

Worked example 13.4:
The adsorption of methyl viologen on platinum is described in the paper by K. Kobayashi, F. Fujisaki, T. Yoshimina, and K. Nik, An analysis of the voltammetric adsorption waves of methyl viologen, *Bull. Chem. Soc. Jpn*, 1986, **59**, 3715.

Worked example 13.5:
An accessible introduction to magic-angle NMR may be found in C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy* (4th edn), McGraw–Hill, Maidenhead, 1994, pp. 274–6.

Chapter 14

Additional problem 14.3:
The data for this example come from *Physical Chemistry: A Molecular Approach*, Donald A. MacQuarrie and John D. Smith, University Science Books, Sausalito, CA, 1997, p. 954.

Additional problem 14.5:
The temperature dependence cited relates to the electron mobility due to ionized-impurity scattering; see *The Physic and Chemistry of Solids*, Stephen Elliott, Wiley, Chichester, 1998, p. 510.

Additional problem 14.5:
The effective potential is described in Atkins, *Physical Chemistry*, p. 369.

Additional problem 14.7:
The expression is given in Atkins, *Physical Chemistry*, p. 738. Scattering in general is discussed from p. 736.

Additional problem 14.8:
Virial coefficients and other alternatives to the ideal-gas equation are discussed in Atkins, *Physical Chemistry*, p. 17.

Additional problem 14.9:
These aspects of molecular interactions may be found in Atkins, *Physical Chemistry*, p. 699.

Additional problem 14.10:
The form given to b here may be found in Atkins, *Physical Chemistry*, p. 842. (Atkins symbolizes it as B.)

Chapter 15

Additional problem 15.9:
The equation for ϕ comes from *Physical Chemistry: A Molecular Approach*, Donald A. MacQuarrie and John D. Smith, University Science Books, Sausalito, CA, 1997, p. 413. In this text, it is symbolized as ϕ_{1s}^{STO}.

Chapter 16

Additional problem 16.2:
The expression is given in Atkins, *Physical Chemistry*, p. 738.

Additional problem 16.3:
Lasers are discussed in Atkins, *Physical Chemistry*, p. 553ff. Non-linear effects and frequency doubling are discussed on p. 559.

Additional problem 16.4:
An accessible introduction to magic-angle NMR may be found in C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy* (4th edn), McGraw–Hill, Maidenhead, 1994, pp. 274–6.

Additional problem 16.7:
The equation for ϕ comes from *Physical Chemistry: A Molecular Approach*, Donald A. MacQuarrie and John D. Smith, University Science Books, Sausalito, CA, 1997, p. 413. In this text, it is symbolized as ϕ_{1s}^{GF}.

Additional problem 16.8:
The example is amended slightly, from *Physical Chemistry* (2nd edn), C. Metz, Schaum Outline Series, McGraw-Hill, New York, 1989, p. 296.

Additional problem 16.9:
The expression linking λ and θ is given in *Physical Chemistry: A Molecular Approach*, Donald A. MacQuarrie and John D. Smith, p. 540.

Additional problem 16.10:
The expression linking λ and θ is explored in *Physical Chemistry: A Molecular Approach*, Donald A. MacQuarrie and John D. Smith, 1197.

Chapter 17

Worked Example 17.4:
The equation comes from C. N. Banwell, *Fundamentals of Molecular Spectroscopy* (3rd edn.), McGraw-Hill, Maidenhead, 1983, p. 157.

Additional problem 17.4:
Shielding and screening are discussed in Atkins, *Physical Chemistry*, p. 261.

Additional problems 17.6, 17.7:
The derivation of these expressions is available in *Physical Chemistry: A Molecular Approach*, Donald A. MacQuarrie and John D. Smith, University Science Books, Sausalito, CA, 1997, pp. 972, 973.

Additional problem 17.8:
The coiling of polymer chains is discussed in Atkins, *Physical Chemistry*, p. 721.

Additional problem 17.10:
The Eyring equation is discussed in Monk, *Physical Chemistry: Understanding Our Chemical World*, pp. 416–20. The Eyring equation is poorly treated in many books of physical chemistry, and may appear differently than here.

Chapter 19

Probably the first person to develop the mathematics of integration was English mathematician, physicist, and philosopher Sir Isaac Newton (1642–1727). However, our current notation (dy/dx for a derivative and the so-called **script-S** for an integral) is that of Gottfried Leibniz (1646–1716). The 'script S' was used merely as an abbreviation for 'sum'. Its calligraphic style followed contemporary handwriting. For more information on Newton and Liebniz, see the website:

http://www.bbc.co.uk/history/historic_figures/newton_isaac shtml

For more information on writing styles, see the interesting detail at:

http://www.waldenfont.com/public/dhmanual.pdf

(both sites accessed 31 March 2004).

Additional problem 19.2:
This temperature relationship between C_p and T is discussed in Atkins, *Physical Chemistry*, pp. 50 and 105.

Additional problem 19.3:
The temperature dependence between C_p and T at very low temperatures is mentioned in Atkins, *Physical Chemistry*, p. 51.

Additional problem 19.4:
The temperature dependence of this phase boundary is given in *Physical Chemistry: A Molecular Approach*, Donald A. MacQuarrie and John D. Smith, University Science Books, Sausalito, CA, 1997, p. 951.

Additional problem 19.5:
For more information, including a full derivation of A, see *Physical Chemistry* (3rd edn), Gilbert Castellan, Addison-Wesley, Reading, MA, 1983, p. 671.

Chapter 20

Additional problem 20.1:
This derivation of an expression for ΔG from the appropriate Maxwell relation is discussed in Atkins, *Physical Chemistry*, 128ff., and Monk, *Physical Chemistry: Understanding our Chemical World*, p. 154ff.

Chapter 21

The term 'standard deviation σ' causes much confusion, in part because some workers use different terms to mean σ, and the same terms to mean different statistical parameters. The web page:

http://mathworld.wolfram.com/StandardDeviation.html

has a concise but useful summary of the different usages (page accessed 28 April 2005).