

The IUPAC Orange Book—it's all about the journey

by Brynn Hibbert

The 20th century English conductor Sir Thomas Beecham is credited (probably incorrectly) with the advice: “Try anything once, except incest and Morris dancing¹”. After reading this, you may wish to add “editing IUPAC Color Books.” Or not.

The journey starts

The minutes of the Officers' meeting of the Analytical Chemistry Division (ACD) held in Beijing in November 2008 read “The officers discussed this issue [the lack of consistency of the 3rd edition of the Orange Book] at their meeting in Beijing, based on a report from the Secretary [D B Hibbert], and came to the conclusion that ACD should go for a complete updating of the Orange Book. This demanding task will involve all the division members. In particular, all the Titular Members will be involved in the revision of the Orange Book, each taking the responsibility for a sub-project.” This was confirmed at the General Assembly in Glasgow in 2009. As Secretary, and about to become Vice President, President and then Past President, it was thought that the six years of senior office would be more than sufficient to complete the project. (Ha, ha!)

IUPAC Color Books

To remind us, in addition to *Pure and Applied Chemistry* Recommendations, IUPAC has been publishing its terminology and nomenclature work as books for many years. The earliest appears to be the first edition of the Red Book (Inorganic nomenclature) in 1958. In 1987 it was decided to bring together terminology into a single text, called the Gold Book, not because of the importance of the colour, but after Professor Victor Gold, Daniell Professor of Chemistry at King's College London². The 1997 Gold Book was published as a series of pdfs 'on-line' in 2003, (<https://old.iupac.org/publications/compendium/>) and this gave the impetus for the xml Gold Book that became the signature version in 2006 until the latest 'Web 3.0' revision replaced it in 2019 (The IUPAC Compendium of Chemical Terminology, <https://goldbook.iupac.org>).

The first edition of the Orange Book was in 1977, and the 3rd edition in 1997. An on-line version which

¹ A kind of English country dancing involving bells tied around the legs and silly hats.

² And by curious coincidence the Head of Department when I was an undergraduate and postgraduate from 1969 – 1976. I never realised his IUPAC connections.

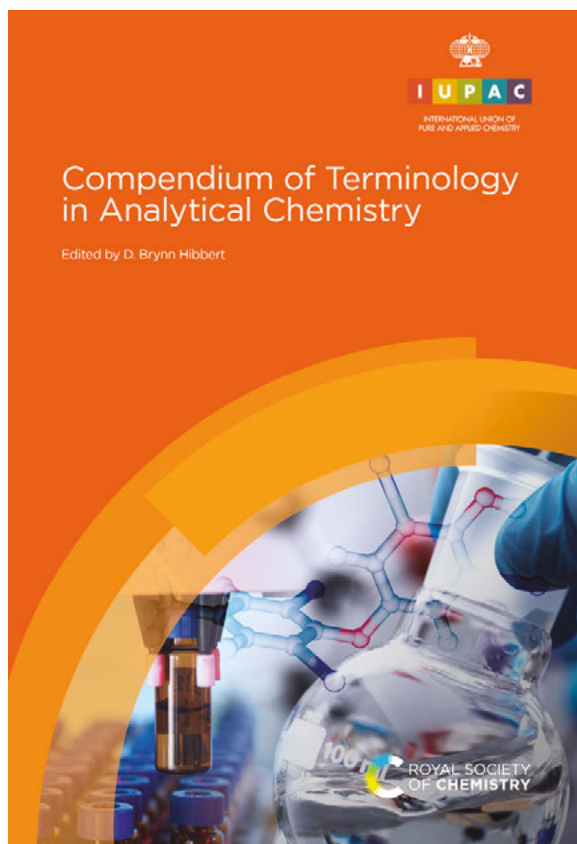


Figure 1: Front cover of “Compendium of Terminology in Analytical Chemistry, 4th edn” – “the Orange Book.” <https://iupac.org/what-we-do/books/orangebook/>

could be downloaded as a hyperlinked pdf was published in 2009, the year the decision was made to embark on the 4th edition [1].

The Orange Book to 2009

The First Edition was published in 1977 edited by the legendary H.M.N.H. Irving, H. Freiser and T.S. West. It was a collection of 23 reports published by IUPAC between 1960 and 1976. The Compendium was updated as the second edition in 1987 by the 11 reports published between 1976 and 1984.

Although mostly keeping the structure of the original editions, the 1997 third edition, edited by János Inczédy, was a major revision [2]. There were three new chapters: selections from the Green Book, [3] a chapter on quality assurance, and a chapter on applications. However, a report on the 3rd edition wrote:



The ACD Officers meeting in Beijing in November 2008: President Ales Fajgelj (4th from right), Vice President Walter Lund (3rd from right), Past President Ryszard Lobinski (at left or 1st from right), and Secretary Brynn Hibbert (5th from right). Among the hosts is Zhifang Chai (6th from right).

Table 1: IUPAC color books. (see also <https://iupac.org/what-we-do/books/color-books/>) Several color books have also been published on the web. The Gold Book has been web only since 2006. ¹ Pre-Green Book, “Manual of Symbols and Terminology for Physicochemical Quantities and Units”

Year	Book
1958	Red
1969	Green ¹
1973	Green ¹
1976	Green ¹
1977	Orange
1979	Blue
1987	Orange
1987	Gold
1988	Green
1990	Red I
1991	Purple
1992	White
1993	Blue
1993	Green
1995	Silver
1997	Orange
1997	Gold
2001	Red II
2005	Red
2006	(Gold online)
2008	Green
2009	Purple
2013	Blue
2016	Silver
2019	(Gold online)
2023	Orange
2023	Abridged Green

“Unfortunately, the Orange Book does not have a consistent structure. Some chapters are written like a textbook while others have a glossary format. In some cases, an alphabetical order of the terms is maintained within each paragraph.” (ACD Teamwork, March 2009, from <https://iupac.org/body/500>). This was the issue, along with the eleven-year gap, that triggered the discussion in Beijing in 2008.

Decisions, decisions

The overall stewardship of the project was given to me, but members of the Division Committee would be asked to look after particular chapters.

Having decided to more or less start from scratch with the 4th edition, two further decisions had to be made. First, what was to be included—and more contentiously—excluded. We were amazed that, in fact, analytical chemistry had moved a long way since 1997. Whole new areas such as statistics and experimental design needed inclusion, and traditional fields of spectroscopy (particularly NMR) and chromatography had burgeoned. Very quickly it was decided to stick to the terminology of principles and methods, and not have applications (as was found in the 3rd edition). There were simply not enough pages to include a sensible selection. So, in came a first chapter on

fundamental metrology and a last chapter on modern quality assurance. This added to a new chapter on chemometrics.

Secondly, the preparation of an entire book from scratch that would contain definitive terminology would have been a review nightmare. We therefore decided that each chapter would be prepared as a PAC Recommendation. The idea was that then the accepted and fully-reviewed terms could be easily moved into the Orange Book. This was a good idea and eventually saved the project from falling in a heap, but the execution of the transfer turned out to be a bit more complicated than we hoped.

Table 2 gives the published Recommendations (and one Technical Report). Two were published as separate projects outside the Orange Book; mass

spectrometry #7 and thermal methods #11. The remaining ten Recommendations appeared between 2016 and 2021.

Why did it take so long?

Zhifang Chai won the prize for being the first to submit his chapter on Radioanalytical methods to the Division in 2011. However, the Recommendation was not published until 2021, after some debate among different groups in the radioanalytical community. The first Recommendation actually published was Janusz Pawliszyn's paper on sample extraction in 2016 (and a Technical Report to go with it), closely followed by the chemometrics Recommendation. The rest dribbled in over the next five years. We had three deaths of people leading chapter projects, including Paul De Bièvre, to

Chapter	IUPAC Recommendation/ Technical Report
1, 13	Hibbert DB, Korte E-H, Örnemark U. Metrological and quality concepts in analytical chemistry (IUPAC Recommendations 2021). <i>Pure Appl Chem.</i> 2021; 93 (9):997–1048.
2	Hibbert DB. Vocabulary of concepts and terms in chemometrics (IUPAC Recommendations 2016). <i>Pure Appl Chem.</i> 2016; 88 (4):407–443.
3	Poole C, Mester Z, Miró M, Pedersen-Bjergaard S, Pawliszyn J. Glossary of terms used in extraction (IUPAC Recommendations 2016). <i>Pure Appl Chem.</i> 2016; 88 (5):517–558. Poole C, Mester Z, Miró M, Pedersen-Bjergaard S, Pawliszyn J. Extraction for analytical scale sample preparation (IUPAC Technical Report). <i>Pure Appl Chem.</i> 2016; 88 (7):649–687.
4	Camões M, F., Christian G, D., Hibbert DB. Mass and volume in analytical chemistry (IUPAC Technical Report). <i>Pure Appl Chem.</i> 2018; 90 (3):563–602.
5	Maryutina TA, Savonina EY, Fedotov PS, Smith RM, Siren H, Hibbert DB. Terminology of separation methods (IUPAC Recommendations 2017). <i>Pure Appl Chem.</i> 2018; 90 (1):181–231.
6	Infante, H. G.; Warren, J.; Chalmers, J.; Dent, G.; Todoli, J. L.; Collingwood, J.; Telling, N.; Resano, M.; Limbeck, A.; Schoenberger, T.; Hibbert, D. B.; LeGresley, A.; Adams, K.; Craston, D.: Glossary of methods and terms used in analytical spectroscopy (IUPAC Recommendations 2021). <i>Pure Appl Chem.</i> 2021; 93 (6):647–776.
7	Murray KK, Boyd RK, Eberlin MN, Langley GJ, Li L, Naito Y. Definitions of terms relating to mass spectrometry (IUPAC Recommendations 2013). <i>Pure Appl Chem.</i> 2013; 85 (7):1515–1609.
8	Pingarrón, J. M.; Labuda, J.; Barek, J.; Brett, C. M. A.; Camões, M. F.; Fojta, M.; Hibbert, D. B.: Terminology of electrochemical methods of analysis (IUPAC Recommendations 2019). <i>Pure Appl Chem.</i> 2020; 92 (4):641–694.
9	Chai Z, Chatt A, Bode P, Kucera J, Greenberg R, Hibbert DB. Terminology of radioanalytical methods (IUPAC Recommendations 2020). <i>Pure Appl Chem.</i> 2021; 93 (1):69–111.
10	Takeuchi T, McQuillan J, Shard A, Russell A, Hibbert DB. Glossary of methods and terms used in surface chemical analysis (IUPAC Recommendations 2020). <i>Pure Appl Chem.</i> 2020; 92 (11):1781–1860.
11	Lever T, Haines P, Rouquerol J, Charsley Edward L, Van Eckeren P, Burlett DJ. ICTAC nomenclature of thermal analysis (IUPAC Recommendations 2014). <i>Pure Appl Chem.</i> 2014; 86 (4):545–553.
12	Labuda, J.; Bowater, R. P.; Fojta, M.; Gauglitz, G.; Glatz, Z.; Hapala, I.; Havliš, J.; Kilar, F.; Kilar, A.; Malinová, L.; Sirén, H. M. M.; Skládal, P.; Torta, F.; Valachovič, M.; Wimmerová, M.; Zdráhal, Z.; Hibbert, D. B.: Terminology of bioanalytical methods (IUPAC Recommendations 2018). <i>Pure Appl Chem.</i> 2018; 90 (7):1121–1198.

Table 2: Chapters of the Orange Book and their Recommendations

whom the Orange Book is dedicated; one member of the Division committee (I shall not name him) totally withdrawing after several years of coming to meetings saying his chapter was nearly finished—any day soon; and a couple of chapters that lingered in the PAC editorial system perhaps a tad longer than necessary. With the impending completion of all Recommendations a contract was signed to deliver a manuscript to the RSC in 2021. This happened on April 1st to be followed by a retraction because not all chapters had been appropriately reviewed. Careful and quick work by the Division, and an equally speedy and thorough, review by ICTNS, allowed a second submission of the manuscript on 19th May 2022. There followed rounds of proofs and some discussion, with the final file sent to the publishers on 25th October 2022. The Orange Book was published on 27th January 2023.

So what took so long? Nothing really—this is how long these kinds of projects take.

Editors ... and editors

It might be thought that the job of an editor is to collect the chapters, make sure they are sensible and bring them together in a nice order for publication. This turns out not to be the case for a Color Book. Even with a published Recommendation the order of terms might need amending, duplications (surprisingly many) must be resolved, introductions to chapters harmonized and finally an index of terms and symbols created. Learning a lot about writing terminologies, I found myself a co-author on eight Recommendations in addition to writing the Recommendation for Chapter 2, so here the title 'editor' covers a bit more than usual.

What next?

There is life after a Color Book—another Color Book. For me, it is working with Stuart Chalk on the massive Gold Book project. The Orange Book and its Recommendations came at a good time to try out the

new Term Review System (TRS) for transporting entries into the Gold Book. This, like the Orange Book, will take as long as it takes, but when it is finished IUPAC will be the better for it, and will have fulfilled its mission to be “the world authority on chemical nomenclature and terminology.”

Acknowledgements

The list of 57 people who contributed to the Orange Book may be found in the front matter of the book. To this must be added the IUPAC secretariat and new friends in the RSC. Some have contributed more than others, and have been thanked, but the Orange Book was a team effort and the winner is IUPAC.

References

1. The “Orange Book” Online”, *Chem Int*, vol. 24, no. 5, 2002, p. 19; <https://doi.org/10.1515/ci.2002.24.5.19a>
2. J. Inczedy, T. Lengyel, A. M. Ure. *IUPAC Compendium of Analytical Nomenclature. Definitive Rules 1997, IUPAC Orange Book, 3rd edition*. Blackwell Scientific, Oxford (1998).
3. E. R. Cohen, T. Cvitaš, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Tamaki, A. Thor. *Quantities, Units and Symbols in Physical Chemistry, IUPAC Green Book, 3rd edition*. The Royal Society of Chemistry, Cambridge, UK (2007).
4. IUPAC. *Compendium of Chemical Terminology, IUPAC Gold Book, 2nd edition. Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997); Web 2.0 version by Stuart Chalk 2019. <http://goldbook.iupac.org> accessed 10/10/2022.*

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<https://iupac.org/what-we-do/books/orangebook/>
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Preparation, formatting and review of IUPAC Technical Reports and Recommendations, IUPAC-sponsored books, or other items carrying the IUPAC label

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All guidelines proposed by the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) for the preparation, formatting and review of IUPAC documents have been reviewed and compiled in one single document now directly available in PAC: <https://doi.org/10.1515/pac-2022-1106> (*Pure Appl. Chem.*, vol. 94, no. 11-12, 2022, pp. 1257-1267)