## The History of the IUPAC Nomenclature of Organic Chemistry

*by Evan Hepler-Smith*

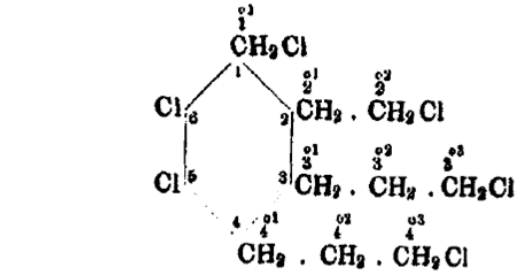
**For chemists and chemistry students around the world, "IUPAC" is synonymous with "nomenclature" – especially the nomenclature of organic chemistry. Generations of chemists have learned – sometimes grudgingly – to read and write systematic names for organic compounds using guidelines codified by the International Union of Pure and Applied Chemistry. [1,2,3] The prefixes, suffixes, numbers, and parentheses of IUPAC names put molecules in order: individually, by expressing the network of atoms and bonds that constitutes the structure of an organic compound, and collectively, by situating each compound among the tens of millions of known organic chemical substances. IUPAC names carry this order out of chemical journals and into such sites as patent records, customs lists, and environmental regulatory databases.**

The latest IUPAC *Nomenclature of Organic Chemistry* runs to 1,568 pages. [4] A curious reader thumbing through this volume might reasonably assume that systematic nomenclature is made by layering a verbal logic atop the ever-expanding variety of carbon compounds that nature and synthetic chemistry have devised. However, the drive for *rigor*—economical, categorical, logically consistent rules—is only a part of the story of systematic nomenclature. The making of the 1930 Liège Nomenclature, the foundation of official IUPAC organic nomenclature, also required *flexibility*—tolerance for carefully-curated variation and inconsistency among chemical names, in the service of making the nomenclature system easier to adopt and adaptable to a wider range of circumstances. Formed amidst the disordering aftermath of war as well as a disorderly chemical vocabulary, the Liège Nomenclature gained acceptance not only because of how it ordered molecules, but because of how it organized chemists.

The development of an international system of organic nomenclature began nearly three decades before the founding of IUPAC, at the Geneva Nomenclature Congress. During the late nineteenth century, as chemists synthesized more and more novel organic compounds, they often found it expedient to give each new compound a name that expressed their view of its chemical structure. However, since chemists turned to numerous conflicting conventions for doing so, such names threw the already disorderly nomenclature into further disarray. Over four days in April in 1892, thirty-four prominent organic chemists from across Europe gathered in Geneva to develop a system of nomenclature rules to put this confusion in order. [5]

The delegates to the Geneva Congress were presented with a choice between two ideas of how systematic nomenclature should work, each advocated by a leading chemist of the day. Charles Friedel, the Frenchman who organized the Congress, envisioned a flexible system of nomenclature that would allow chemists to use different sorts of trivial and systematic names adapted to their diverse needs and preferences. German luminary Adolf von Baeyer, in contrast, advocated a rigorous system of nomenclature rules. Such a system, Baeyer argued, could be an invaluable aid to chemical editors in the task of sorting an endless stream of organic chemical names into reliable subject indexes. Baeyer's plan won the day: the Geneva Nomenclature would generate a unique name for every organic compound, expressly for use in ordering and searching through the tens of thousands of entries in chemical handbooks and journal indexes.

That was the idea, anyway. In reality, generating unique names that clearly expressed the structure of organic compounds was no easy task. Most compounds of even moderate complexity – for example, anything containing more than one kind of functional group – fell outside of the scope of the rules that the Congress had been able to




Benzenchloromethyl-1-chloro-2-äthyl-2-chloro-3-propyl-3-chloro-4-propyl-4-dichlor-5,6.

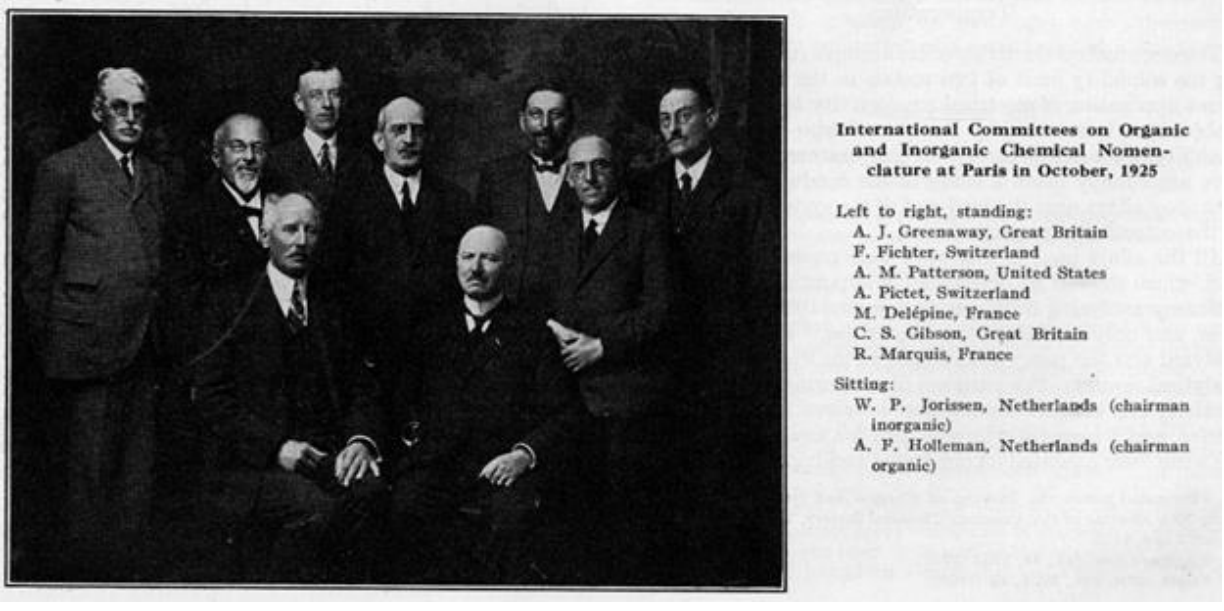
*German chemical lexicographer Max Moritz Richter, a colleague of Paul Jacobson, offered this example of the excessive complexity of some Geneva names. [Max Moritz Richter, "Ein Beitrag zur Nomenclatur," Berichte der Deutschen Chemischen Gesellschaft 29, no. 1 (1896): 603.]*

agree upon. To other compounds, the Geneva rules assigned names that seemed excessively complicated to chemical readers and authors alike. As a result, some of the editors for whose benefit the Geneva nomenclature had been created felt that they could not make use of it.

Foremost among these editors was Paul Jacobson. A young organic chemist of Jewish heritage, Jacobson had left a junior professorship in Heidelberg to become editor-in-chief of the publications of the German Chemical Society, an expanding collection of periodicals and reference works including the invaluable *Beilstein's Handbuch* [6] Jacobson considered the Geneva nomenclature to be a lost cause. In his publications, he shunned systematic nomenclature and alphabetized lists of names in favor of chemical indexes ordered by empirical formula. For the mammoth undertaking of compiling an entirely reorganized fourth edition of Beilstein, Jacobson and his deputy Bernhard Prager developed the elaborate classification of organic compounds that became known as the "Beilstein system."

Despite, or perhaps because of, his skepticism regarding the rigorous Geneva project, when another international project to reform organic nomenclature began to coalesce, Jacobson seized a leading role. At the first meeting of the International Association of Chemical Societies, held in Paris in 1911, Jacobson took the initiative to present a plan for the nomenclature work that the Association would undertake. [7] His approach was diametrically opposed to that of the Geneva Congress. Instead of prominent chemists, Jacobson advocated that the new nomenclature commission be made up of experienced editors and indexers. Instead of developing a rigorous system of nomenclature rules – or any system of nomenclature rules at all – he proposed that the commission merely evaluate novel nomenclature proposals and address specific instances of confusion among existing chemical names. Some of his fellow commission members had different ideas, but Jacobson managed to secure the chairmanship of the organic nomenclature commission. For an editor in the middle of a project as enormous as the fourth edition of *Beilstein*, it was a savvy move. By taking charge of nomenclature reform and shepherding it in the direction of flexibility, he could stave off any rigorous new rules that might interfere with his work in progress.

Just as Jacobson's commission was beginning to get to work over the summer of 1914, the German army invaded Belgium. Like many other areas of international scientific cooperation, nomenclature reform came to a sudden halt. It remained suspended for the duration of World War I. Though dormant, the project was not forgotten; after the armistice, the members of Jacobson's commission sought to resume their prewar efforts. The conditions of international scientific relations had changed substantially. The International Association of Chemical Societies was dissolved in 1919, and the International Union of Pure and Applied Chemistry founded under the umbrella of the International Research Council (IRC). As with all the member unions of



**International Committees on Organic and Inorganic Chemical Nomenclature at Paris in October, 1925**

Left to right, standing:
A. J. Greenaway, Great Britain
F. Fichter, Switzerland
A. M. Patterson, United States
A. Pictet, Switzerland
M. Delépine, France
C. S. Gibson, Great Britain
R. Marquis, France

Sitting:
W. P. Jorissen, Netherlands (chairman inorganic)
A. F. Holleman, Netherlands (chairman organic)

*The members of the organic nomenclature working group, along with colleagues on an analogous group dealing with inorganic nomenclature (*Industrial & Engineering Chemistry *17, no. 12 (December 1, 1925): 1245.*

the IRC, a kind of scientific Treaty of Versailles established by representatives of the victorious Entente nations, Germans and German institutions were banned from membership in IUPAC. The landscape of organic nomenclature had changed as well. The initial volumes of the fourth edition of *Beilstein* had been published, as had another authoritative reference work, the first collective index to the American abstract journal *Chemical Abstracts*. Under these challenging conditions, and without the help of the German Jacobson, IUPAC took up the reform of organic nomenclature.

In 1921, the IUPAC Council established a Commission on the Reform of the Nomenclature of Organic Chemistry, composed of one representative from each of the Union's twenty-one member nations. (Parallel IUPAC commissions took up inorganic and biochemical nomenclature; the three commissions operated independently during the 1920s.) Over the following two years, several representatives proposed different starting points for the commission's work. One, for example, suggested picking up precisely where Jacobson's commission had left off; another advised portioning out the entire field of organic compounds and putting each commission member in charge of nomenclature within one such section. The commission met only at the Union's annual conferences, and chronic absenteeism among commission members left these meetings as *ad hoc* affairs offering little opportunity to reconcile the various proposals.

At the encouragement of the Union president, the commission decided upon a different way of advancing its work. The commission assigned responsibility for organic nomenclature reform to a working group made up of six members appointed by the editorial boards of leading American, British, Dutch, French, Italian, and Swiss chemical publications. Cutting through the Gordian knot of commission reports from before and after the war, the commission instructed this working group to base its discussions on the one concrete point of departure that could be identified without further discussion: the Geneva nomenclature.

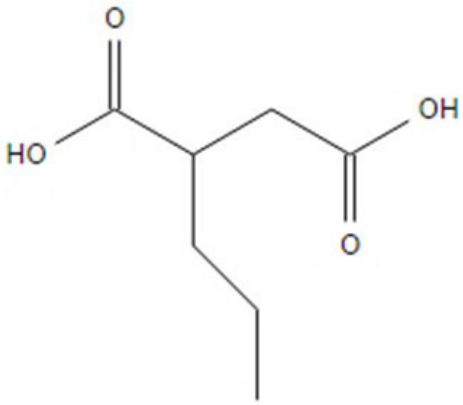
The working group took up this task in 1924, under the presidency of University of Amsterdam professor Arnold Holleman, a respected textbook author fluent in French, German, and English as well as his native Dutch. The American member, Austin Patterson, was regarded as the world's leading authority on organic nomenclature – outside of Germany, at least. Just as importantly, as the architect of the nomenclature used in *Chemical Abstracts*, Patterson could help ensure mutual understanding between the working group and this important publication. In order to establish a similar sort of relationship with Beilstein despite the IRC boycott of Germany, both Holleman and Patterson corresponded unofficially with Prager, the reference work's editor (Jacobson had died in 1923).

The working group faced a conundrum. Under Jacobson's watch, international work on organic nomenclature had shifted decisively in the direction of flexibility, and the further entrenchment of the nomenclature systems used in *Chemical Abstracts* and *Beilstein* seemed to make such flexibility all the more important. At the same time, the working group had been charged with building rules based on the rigorous Geneva nomenclature.

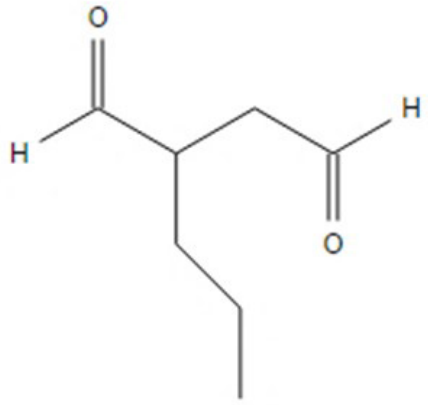
Holleman's solution was to adopt the content and form of the Geneva rules, but to subtly reshape them according to the spirit of Jacobson's flexible approach. During five meetings over the course of two and a half years, Holleman led the working group step by step through the official text of the Geneva nomenclature. By 1927, Holleman's group had agreed upon a set of sixty-eight rules. These rules covered nearly the same ground as the sixty-two Geneva rules, sanctioning most of the same prefixes and suffixes. However, when it came to general matters, the working group took a much more flexible approach, tolerating variation and preserving well-established trivial names where the Geneva rules had assigned exclusively unique, systematic names. Where the Geneva Congress had codified a rigorous approach to organic nomenclature, and Jacobson had resisted the codification of any such system, the working group's nomenclature codified a *systematically flexible* approach to organic nomenclature.

Satisfied that they had discharged their duty, the working group submitted these rules for affirmation by the organic nomenclature commission. One commission member, though, stood ready to defend the rigorous spirit of the Geneva Nomenclature. Victor Grignard, who represented France on the commission, saw the flexible approach embodied in the working group's rules as an abdication of the consistency and logic achieved by the Geneva Congress. His opinion mattered more than most; Grignard was a Nobel laureate and one of the most famous chemists in France. Speaking from a position of scientific prestige akin to that of Friedel and Baeyer in 1892, Grignard advocated instead addressing the shortcomings of the Geneva rules by developing an alternative but no less rigorous system.

At the 1927 IUPAC conference, Grignard laid out this critique for his fellow commission members. His eloquent appeal to the logic of Geneva – and surely also his scientific reputation – convinced the commis-




Geneva: 3-methyl-1,3[1]-hexanedioic acid
WG: 1,2-pentanedicarboxylic acid
propylsuccinic acid




Geneva: 3-methyl-1,3[1]-hexanedial
WG: propylbutanedial
propylsuccinaldehyde

***Naming a diacid and its corresponding dialdehyde according to the Geneva rules and the rules proposed by the working group in 1927. The Geneva rules assign systematic names to each compound using a consistent logic. These names are cumbersome, but they express the structural relationship between the two compounds unambiguously. The working group's rules address each compound using a different approach; the resulting names are easier to read, but they do not capture the structural similarity of the compounds as precisely. The working group's approach also permitted the use of the established trivial names* succinic acid *and* succinaldehyde. *(Neither system considered stereochemistry.)***

sion to defer its approval of the working group's rules. Over the subsequent year, Grignard had his critiques printed and distributed, seeking to generate enough opposition to the rules to stave off their acceptance once more.

He was perhaps more successful than he intended. When the organic nomenclature commission assembled once again in 1928, Grignard's impassioned campaign and the Union's lax approach to commission participation combined to turn the meeting into a free-for-all. Grignard and his sympathizers once again spoke out against the working group's rules, as curious delegates wandered into and out of the meeting room at will. A few of these visitors volunteered off-the-cuff ideas that had nothing to do with either the rules or Grignard's critiques. With tempers flaring among commission members, Holleman adjourned the meeting early, though not before Grignard had rallied a majority to vote down the working group's rule for naming carboxylic acids. Still, Holleman did not back down from his commitment to flexibility. Instead of replacing the working group's rule with Grignard's preferred approach, he retained the former as an acceptable alternative.

At the insistence of the IUPAC Council, Holleman scheduled his rules for a definitive vote at the 1930 conference in Liège. While Grignard carried on his attempts to rally chemical public opinion, Holleman worked to shore up his support among influential editors. At Patterson's request, Holleman agreed to suppress a rule that might have led to conflicts with the nomenclature used in *Chemical Abstracts*. After revisions in IRC and IUPAC bylaws opened the way for Germany to join the Union, Holleman met with German editors in Berlin. There, he allowed Prager to attach a rider to the working group's rules, stipulating that they were not to be taken to interfere with naming practices in the two preeminent reference works.

Holleman's painstaking revisions made the working group's rules more flexible and less rigorous – a change in the opposite direction as that sought by Grignard and his fellow critics. However, they secured the support of the editors of Beilstein and Chemical Abstracts. Holleman no doubt reminded the commission members of the importance of this support when he solicited their votes – this time, before they assembled at the conference.

The appeal succeeded. Even Grignard conceded the fight, though not the argument, acknowledging that the nomenclature practices of the reference publications presented, in his words, "nearly insurmountable difficulties" for one aiming to bring rigorous no-

menclature into an international setting. [8] When the nomenclature commission met in 1930, the working group's rules were approved without debate, and became the Liège Nomenclature.

In recent years, the focus of IUPAC nomenclature work has turned to the development of unique identifiers for organic compounds, in the form of "preferred" IUPAC names (PINs) and computer-readable notation (InChI). [4,9] Such projects are driven by the demands of a new technological context – the wholesale shift from print to a variety of computer-based resources for handling chemical information. But their fundamental aim is neither entirely new, nor even the next step in a progression of increasingly rigorous ways of naming and ordering chemical compounds. Rather, the InChI and PIN projects are the latest episodes in a long history of competing demands for flexibility and rigor in organic nomenclature, a history whose product is IUPAC nomenclature itself. Today's efforts to develop nomenclature and notation standards are related by both analogy and genealogy to decisions taken in 1892, the 1920s, and since. The more we understand about how chemists have confronted the challenges that the making of systematic nomenclature has presented over the past century and a quarter, the better we can equip those who develop and use chemical information systems to deal with these challenges, now and in the future.

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## Notes, References, and Further Reading


1. Verkade, Pieter Eduard. *A History of the Nomenclature of Organic Chemistry*, trans. S. G. Davies. Boston: Reidel, 1985.
2. Fennell, Roger. *History of IUPAC, 1919-1987.* Boston: Blackwell Science, 1994.
3. For more information on current IUPAC nomenclature activities, see the webpage of the Chemical Nomenclature and Structure Representation Division. www.iupac.org/body/800
4. Favre, Henri A. and Warren H. Powell, eds., *Nomenclature of Organic Chemistry: IUPAC Recommendations and Preferred Names 2013.* Cambridge: Royal Society of Chemistry, 2014.
5. Hepler-Smith, Evan, "'Just as the Structural Formula Does': Names, Diagrams, and the Structure of Organic Chemistry at the 1892 Geneva Nomenclature Congress," *Ambix* **62**(1): 1-28, 2015.
6. Founding editor Friedrich Beilstein transferred responsibility for his *Handbuch* to the German Chemical Society during the late 1890s.
7. Van Tiggelen, Brigitte and Danielle Fauque, "The Formation of the International Association of Chemical Societies," *Chemistry International* **34**(1):9–11, 2012.
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9. Heller, Stephen, et. al., "InChI - the Worldwide Chemical Structure Identifier Standard," *Journal of Cheminformatics* **5**:7 (January 24, 2013).