

## Speculative Property

### INTRODUCTION

The later part of the nineteenth century was a period of consolidation in organic chemistry. Developments such as the publication of standardised melting and boiling points,<sup>1</sup> standardised reference materials,<sup>2</sup> and the increased use of standardised laboratory equipment (including glassware, thermometers, and scales) allowed chemists to exercise greater ‘control over experimental spaces’, which improved their ability to purify, characterise, and identify substances.<sup>3</sup> While patent law benefited from these changes, they did not really affect the way the two domains interacted. This is not the case, however, with a number of other changes that occurred in chemistry at the time; two of which stand out, namely, the development of structural theory and the standardization of naming practices. These changes, which were readily embraced by lawyers, patent attorneys, judges, and Patent Office officials, had a profound and lasting impact on the way that patent law interacted with chemistry. This is because it changed the way that patent law engaged with and thought about chemical subject matter.

As we saw earlier, in defining and demarcating the intangible property created by a chemical patent, nineteenth-century patent law relied on the tangible manifestations of the chemical invention. Whether directly, as with the use of chemical specimens, or more indirectly, as with the use of a compound’s physical witnessable properties, the tangible material aspects of a chemical compound were pivotal to the way the law engaged with chemical subject matter. The attention given to the material tangible dimension of chemical inventions was reinforced by the fact that patent law only dealt with chemical inventions at the level of the species (or variety); that is, patent law treated chemical subject matter as if it was a closed, singular, and material entity that was co-extensive with the chemical compound. The situation changed, however, around the turn of the century as patent law embraced structural theory.

<sup>1</sup> See Thomas Carnelley, *Melting and Boiling Point Tables* (London: Harrison & Sons, 1885).

<sup>2</sup> A job taken over by the National Institute of Standards and Technology beginning in 1905 with production of standard samples of iron but quickly spreading to other standardized samples.

<sup>3</sup> Catherine M. Jackson, ‘Chemical Identity Crisis: Glass and Glassblowing in the Identification of Organic Compounds’ (2015) 72 *Annals of Science* 187, 204.

## STRUCTURAL THEORY

As Alan Rocke said, the ‘dominating story of chemistry in the 1860s, 1870s, and 1890s was neither the periodic law, nor the search for new elements, nor the early stages of the study of atoms and molecules as physical entities’. Rather, it was ‘the maturation, and demonstration of extraordinary scientific and technological power of the “theory of chemical structure”’.<sup>4</sup> As with the rational formula that preceded them, structural theory grew out of the realisation that a simple understanding of the constitutive elements in a compound (provided by its empirical formula) was insufficient to account for the nature of chemical compounds.<sup>5</sup> In order to better understand chemical compounds, chemists realised that they needed to shift their focus of attention away from the composition of compounds to also include the compound’s constitution or inner organisation, that is, with the way that elements were organised within a compound, rather than merely the proportion and kind of elements that were in the compound.<sup>6</sup>

Scientific understanding of the internal shape of compounds began to take shape in the 1860s when chemists drew together experimental findings of previous decades to formulate several principals – which became known as structural theory – that ‘appeared to govern the internal architecture of organic chemical compounds in a way that accounted for different chemical phenomena and relationships’.<sup>7</sup> Loosely defined, structure theory was ‘a collection of principles for understanding the behaviour and relationship of organic compounds in terms of a ... model of their inner structure or “constitution”’.<sup>8</sup> That is, structure theory was a set of ideas that provided chemists with information about the way elements in a compound were joined (or bonded) together.<sup>9</sup>

In the early 1860s Alexander Brown developed ‘a style of graphic notation’ that translated this information into the now well-known structural formula (see for example Figure 4.1). These structural formula, which have been described as one of the trademarks of chemistry,<sup>10</sup> ‘expressed the constitution of compounds in accordance with the principles of structure theory’.<sup>11</sup> Structural formula built upon and extended the empirical formula that had been developed in the 1830s which, through the arrangement of letters and numbers, visually showed how elements

<sup>4</sup> Alan J. Rocke, *Image and Reality* (Chicago: University of Chicago Press, 2010), xx.

<sup>5</sup> Bernadette Bensaude-Vincent and Jonathan Simon, *Chemistry: The Impure Science* (2nd edn, London: Imperial College Press, 2012), 206.

<sup>6</sup> Alan J. Rocke, ‘Origins and Spread of the “Giessen Model” in University Science’ 50(1) (2003) *Ambix* 90, 93.

<sup>7</sup> Helen Cooke, ‘A Historical Study of Structures for Communication of Organic Chemistry Information Prior to 1950’ (2004) 2 *Organic and Biomolecular Chemistry* 3179, 3181–82.

<sup>8</sup> Evan Hepler-Smith, *Nominally Rational: Systematic Nomenclature and the Structure of Organic Chemistry, 1889–1940* (PhD Thesis, Princeton University, 2016), 12.

<sup>9</sup> Alan J. Rocke, *Image and Reality* (Chicago: University of Chicago Press, 2010), xx.

<sup>10</sup> Roald Hoffmann and Pierre Laszlo, ‘Representation in Chemistry’ (1991) 30(1) *Angewandte Chemie* 163, 164.

<sup>11</sup> Evan Hepler-Smith, ‘“Just as the Structural Formula Does”: Names, Diagrams, and the Structure of Organic Chemistry at the 1892 Geneva Nomenclature Congress’ (2015) 62 *Ambix* 1, 8.

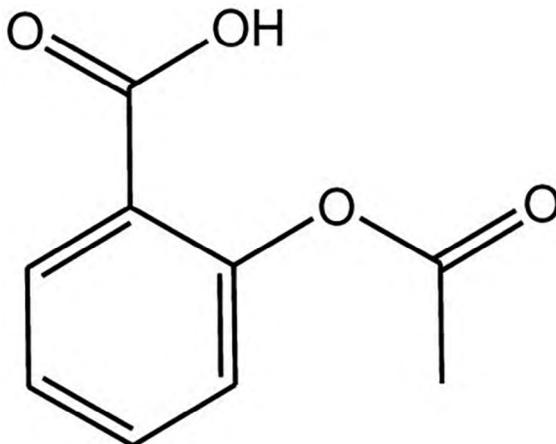


FIGURE 4.1 Modern structural formula for acetylsalicylic acid (Aspirin)

were combined with each other to display ‘chemical and spatial arrangements in an even more pictorial form’.<sup>12</sup> In this sense, structural formula’s diagrammatic representation of the internal structure of compounds marked a shift towards a more iconic mode of representation.<sup>13</sup> This is because while empirical formula only provided information about the nature and proportions of the components of a substance, structural formula also provided information about the way the elements in a compound were connected.

Structural formulas performed a number of different roles in organic chemistry. As well as providing information about the proportions of the elements in a compound, structural formulas also provided an ‘important insight into the details of molecular architecture in an invisibly small realm of nature’. Structural formulas also provided ‘heuristic guidance in the technological manipulation of those molecules, providing assistance in the creation of an important fine chemicals industry’.<sup>14</sup> In this sense, structural formulas were used as instruments of discovery to predict behaviour and to construct new compounds. That is they were used as tools that ‘could be manipulated on paper to create representations of a hidden scientific object’. Typically, structural formulas would begin their lives as informed speculations about the structure of a compound. Building on the principle of chemical valence, which was the idea that different elements can only form certain numbers

<sup>12</sup> Ursula Klein, ‘Not a Pure Science: Chemistry in the 18th and 19th Centuries’ (5 November 2004) 306 *Science* 981, 982.

<sup>13</sup> See Ursula Klein, *Experimental Models, Paper Tools: Cultures of Organic Chemistry in the Nineteenth Century* (Stanford: Stanford University Press, 2003).

<sup>14</sup> Alan J. Roche, ‘The Theory of Chemical Structure and Its Applications’ in (ed) M. J. Nye, *The Cambridge History of Science Vol. 5: Modern Physical and Mathematical Sciences* (Cambridge: Cambridge University Press, 2003), 255.

of bonds to other atoms – hydrogen (typically) to one; oxygen to two; nitrogen to three; and carbon to four – organic chemists worked backwards from chemical evidence to infer the way individual elements were linked to form molecules.<sup>15</sup>

In so far as structural theory established ‘relations between chemical substances, between reaction partners and reaction products connected by chemical transformation’,<sup>16</sup> it allowed chemists, more than ever, to draw inferences from existing compounds (or classes of compounds) to predict the existence of new compounds. On the basis that ‘relations between substances corresponded to relations between chemical structures’,<sup>17</sup> chemists could apply the rules of structural theory and systemic nomenclature to visualise or postulate the existence of undescribed or yet-to-be created compounds on an unprecedented scale.<sup>18</sup> Through the skilful interpretations of appropriate reactions based on structural theory, chemists were also able to discern patterns of atomic bonding which were then used to build a structural formula.<sup>19</sup> These initial speculations were then tested and retested until chemists were confident that the posited structural formula accurately reflected the inner makeup and shape of the compound in question.

Once a structural formula was firmed up and confirmed, its role changed. Once chemists were confident that a structural formula accurately represented the constitution of a compound, it could then be identified and classified.<sup>20</sup> Based on the idea that there was ‘exactly one characteristic chemical structure for every chemical substance’,<sup>21</sup> structural formula were used by chemists to identify, name, and single out the chemical compounds that the formula stood for. Structural formulas, ‘which told a concise story to the chemical reader’,<sup>22</sup> represented in two-dimensional form ‘a three-dimensional object for the purpose of communicating its essence to some remote reader’.<sup>23</sup> On

<sup>15</sup> Alan J. Rocke, *Image and Reality* (Chicago: University of Chicago Press, 2010), 67 ff.

<sup>16</sup> J. Schummer, ‘The Impact of Instrumentation on Chemical Substance Identity’ in (ed) P. Morris, *From Classical to Modern Chemistry: The Instrumental Revolution* (Cambridge: The Royal Society of Chemistry, 2002), 188, 196.

<sup>17</sup> *Ibid.*, 196.

<sup>18</sup> Eugene Geniesse, ‘Adequate Description’ (1945) 27 *Journal of the Patent Office Society* 784, 788. Structural theory allowed chemists to ‘theoretically name all the members of a broadly defined chemical genus that encompassed a large number of species.’ William D. Marsillo, ‘How Chemical Nomenclature Confused the Courts’ (1977) *Baltimore Intellectual Property Law Journal* 29, 30.

<sup>19</sup> Chemists could ‘explore the possibility of constructing molecules, in thought, following those valence rules. That is the essence of the theory of chemical structure’. Alan J. Rocke, *Image and Reality* (Chicago: University of Chicago Press, 2010), xiv.

<sup>20</sup> Structural formula functioned as instruments of classification, ‘as book-keeping devices for cataloguing chemical subunits’. Evan Hepler-Smith, ‘“Just as the Structural Formula Does”: Names, Diagrams, and the Structure of Organic Chemistry at the 1892 Geneva Nomenclature Congress’ (2015) 62 *Ambix* 1, 15.

<sup>21</sup> J. Schummer, ‘The Impact of Instrumentation on Chemical Substance Identity’ in (ed) P. Morris, *From Classical to Modern Chemistry: The Instrumental Revolution* (Cambridge: The Royal Society of Chemistry, 2002), 188, 193.

<sup>22</sup> Roald Hoffmann and Pierre Laszlo, ‘Representation in Chemistry’ 30(1) (1991) *Angewandte Chemie* 1, 13. Robin Findlay Hendry, ‘Structure as Abstraction’ (2016) 83(5) *Philosophy of Science* 1070.

<sup>23</sup> *Ibid.*, 6.

the basis that there was a 'one-to-one correspondence between compound and formula',<sup>24</sup> structural formulas operated like models that stood in for the compounds they represented.<sup>25</sup>

One of the notable things about structural formulas and a key reason for their success was that they were treated as if they were an accurate representation of a molecular reality. While there may have been some early doubts about the reliability of structure theory<sup>26</sup> and many users of 'structural formulas insisted that the diagrams were not meant to represent the physical microstructure of compounds', nonetheless chemists often 'thought about chemical phenomena as if the structural formulas did'.<sup>27</sup> Irrespective of 'their particular commitments with regard to epistemology and chemical theory, the majority of nineteenth century chemists took on' a position 'that asserts that chemical formula resemble reality'.<sup>28</sup> In structural theory, 'molecular structure were hypothetical entities whose ontological status each depended on the hypothesis of structure elucidation of the corresponding substance. The more this was supplemented by' experiment, the more chemists conceived 'of molecular structures as real entities. Thus, chemists no longer considered molecular structures simply as properties of chemical substances: instead, molecular species became ontologically on par with chemical substances'.<sup>29</sup>

Facilitated by improvements in printing technology that made it possible to include structural formulas in printed publications,<sup>30</sup> the development of conventions for the representation of structures,<sup>31</sup> and a growing realisation that structural

<sup>24</sup> *Ibid.*, 11.

<sup>25</sup> Manuel DeLanda, *Philosophical Chemistry: Genealogy of a Scientific Field* (London: Bloomsbury, 2015), 88.

<sup>26</sup> Evan Hepler-Smith, "'Just as the Structural Formula Does": Names, Diagrams, and the Structure of Organic Chemistry at the 1892 Geneva Nomenclature Congress' (2015) 62 *Ambix* 1, 8. 'Neither the three-dimensional nor the two-dimensional structural formula could correspond to molecular reality because the formulas were static representations of what must really be a phenomenon of dynamics' Mary Jo Nye, *From Chemical Philosophy to Theoretical Chemistry: Dynamics of Matter and Dynamics of Disciplines 1800–1950* (Berkeley: University of California Press, 1994), 100–01.

<sup>27</sup> Evan Hepler-Smith, "'Just as the Structural Formula Does": Names, Diagrams, and the Structure of Organic Chemistry at the 1892 Geneva Nomenclature Congress' (2015) 62 *Ambix* 1, 8.

<sup>28</sup> *Ibid.*, n 24.

<sup>29</sup> J. Schummer, 'The Impact of Instrumentation on Chemical Substance Identity' (ed) P. Morris, *From Classical to Modern Chemistry: The Instrumental Revolution* (Cambridge: The Royal Society of Chemistry, 2002), 188, 207.

<sup>30</sup> At the end of the nineteenth century when structural representations 'were being developed, engraving was the main means of typesetting drawings. This was an expensive process and even more so for lines drawn at an angle, hence three-dimensional structures were drawn in two dimensions'. Helen Cooke, 'A Historical Study of Structures for Communication of Organic Chemistry Information Prior to 1950' (2004) 2 *Organic and Biomolecular Chemistry* 3179, 3182. In 1890s there were problems in printing 'quasi-three-dimensional drawings' – while there were no problems in doing so on a blackboard, 'the printing media was not up to it, at least not at the budgetary levels appropriate to mass dissemination of a scientific journal ... engraving was the technique of choice for printing & it was expensive to set lines at an angle.' Roald Hoffmann and Pierre Laszlo, 'Representation in Chemistry' 30(1) (1991) *Angewandte Chemie* 1, 8.

<sup>31</sup> Helen Cooke, 'A Historical Study of Structures for Communication of Organic Chemistry Information Prior to 1950' (2004) 2 *Organic and Biomolecular Chemistry* 3179, 3189.

# UNITED STATES PATENT OFFICE.

BRUNO RICHARD SEIFERT, OF RADEBEUL, NEAR DRESDEN, GERMANY,  
ASSIGNOR TO DR. F. VON HEYDEN, NACHFOLGER, OF SAME PLACE.

## CARBONATE OF GUAIACOL AND CREOSOL.

SPECIFICATION forming part of Letters Patent No. 466,913, dated January 12, 1892.

Application filed December 17, 1890. Serial No. 374,981. (Specimens.)

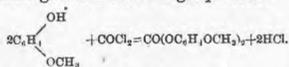
To all whom it may concern:

Be it known that I, BRUNO RICHARD SEIFERT, chemist, of Radebeul, near Dresden, in the Kingdom of Saxony, German Empire, have invented a new and useful Improvement in Medical Compounds, of which the following is a specification, reference being had to the accompanying drawings.

I have found that from guaiacol and its homologues—for instance, creosol contained in beech-wood tar—medical compounds may be obtained which are preferable to guaiacol, inasmuch as they are colorless, tasteless, and without effect upon the mucous membrane. These compounds are intended to be mainly used internally against tuberculosis and the diseases of the stomach and externally against the diseases of the skin and as an antiseptic.

Figures 1, 2, and 3 represent central vertical sectional views of three different forms of apparatus which may be employed in the manufacture of my compounds.

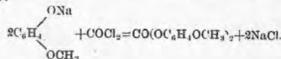
My new medical compounds are obtained by the action of phosgene on guaiacol or the homologue creosol. The reaction takes place according to the following equation:



In carrying out the process I proceed as follows: Two hundred and fifty kilograms of guaiacol and one hundred kilograms of phosgene are heated in a closed vessel. A temperature of about 100° centigrade is sufficient. After several hours the vessel is opened to allow the hydrochloric vapors to escape. The residual product is washed with water, or, if necessary, with an alkaline solution, and thereafter crystallized from alcohol. For this process I preferably use the apparatus Fig. 1, in which *a* is a closed vessel surrounded by a steam-jacket *b*, with the steam admission and outlet pipes *c* and *d*. *e* is an inlet-pipe for the phosgene, and *g* is an opening for the guaiacol to be put into the vessel *a*. This opening is provided with a suitable cover.

*f* is an outlet-pipe for the hydrochloric vapors to escape, and *h* is an outlet-pipe for the residual product to be drawn off.

Instead of guaiacol, a salt of it may be employed. In this case the reaction takes place, for instance, according to the following equation:



If a solid salt of guaiacol is employed, the apparatus Fig. 1 may be used; but I prefer to use an apparatus with an agitator. This apparatus is shown in Fig. 2, which is provided with or constituted of all the parts named in Fig. 1, and which are indicated in Fig. 2 by the same letters of reference; but this apparatus, Fig. 2, has, moreover, an agitator, which may be composed of an upright shaft *k*, with driving-gear *i* at top and with stirrers *l* within the vessel. If, however, a solution of guaiacol salt is employed, it is more simple and preferable to make use of an open vessel *a*—such, for instance, as Fig. 3—which is provided with agitator *i k l*, steam-jacket *b*, with pipes *c d*, phosgene-inlet pipe *e*, and draw-off pipe and cock *h*.

Of course the apparatus Fig. 3 may be used instead of Fig. 2, and the one shown in Fig. 2 instead of that in Fig. 3.

The mode of proceeding with salt of guaiacol is as follows: The vessel Fig. 2 or Fig. 3 is charged with solid or dissolved guaiacol salt, produced, for instance, from one hundred and twenty-five kilograms of guaiacol and forty and five-tenths kilograms of caustic soda. One hundred kilograms of phosgene are now admitted through pipe *e* until the contents of the vessel react neutral. This process is carried on at any desired temperature and pressure, all the while stirring by the agitator. The residual product is thereafter washed with water and crystallized from alcohol. The product resulting from such reaction consists of the carbonate of guaiacol. It is colorless, tasteless, and melts at about 85° centigrade. Its structural formula is

FIGURE 4.2 Early structural formula

Bruno Richard Seifert, 'Carbonate of Guaiacol and Creosol' US Patent No. 466,913 (12 Jan 1892). Courtesy of the National Archives at Kansas City.

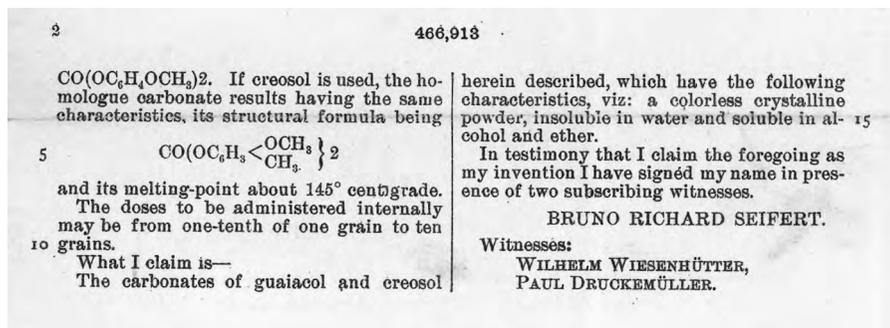


FIGURE 4.2 (cont.)

theory did what it promised, structural theory and the corresponding structural formulas were quickly adopted by organic chemists. By the end of the nineteenth century, structural formulas were 'by all measures the reigning doctrine of the science of chemistry, dominating investigations in both academic and industrial laboratories'.<sup>32</sup>

Structural formulas first began to appear in US patents in the 1890s.<sup>33</sup> As Helen Cooke has shown, there was little standardisation in the way chemical structures were represented in these early patents<sup>34</sup>, a problem compounded by the fact that printing technology at the time made it difficult to reproduce structural formulas in printed patents. An early example of the use of structural formulas is the 1892 patent for a new medical compound that was used to prevent tuberculosis, which was described as a carbonate of guaiacol and creosol with the structural formula set out in Figure 4.2.<sup>35</sup> As a result of advances in printing, by the turn of the century patentees were able to include more familiar representations of structural formula in their patents, such as in Julius and Reubold's 1900 patent for a new black sulphur

<sup>32</sup> Alan J. Roche, 'The Theory of Chemical Structure and Its Applications' in (ed) M. J. Nye, *The Cambridge History of Science Vol. 5. Modern Physical and Mathematical Sciences* (Cambridge: Cambridge University Press, 2003), 255; Helen Cooke, 'A Historical Study of Structures for Communication of Organic Chemistry Information Prior to 1950' (2004) 2 *Organic and Biomolecular Chemistry* 3179, 3189. Thinking in terms of molecular structures soon became, and 'remains today, the heart blood of chemistry.' Alan J. Roche, 'Ideas in Chemistry: The Pure and the Impure' (2018) 109 *Isis* 577, 582.

<sup>33</sup> Although typographical errors were said to be 'commonplace in formula and structure in patents' in the 1890s, this changed by 1895. Helen Cooke, 'A Historical Study of Structures for Communication of Organic Chemistry Information Prior to 1950' (2004) 2 *Organic and Biomolecular Chemistry* 3179, 3188.

<sup>34</sup> *Ibid.*, 3188.

<sup>35</sup> Bruno Richard Seifert, 'Carbonate of Guaiacol and Creosol' US Patent No. 466,913 (12 January 1892) (with specimen).

dye (Figure 4.3).<sup>36</sup> Given the advanced state of organic chemistry in Germany, it is not surprising that the structural formula first used in US patents were for German inventions, particularly in relation to dyes.<sup>37</sup> While structural formulas were used inconsistently across the 1890s and patentees were promiscuous in terms of the way they defined their chemical compounds (in the sense that they combined different modes of identification),<sup>38</sup> by the early twentieth century structural formulas were regularly being used by patentees, the Patent Office, patent attorneys, and the courts to identify, define, and demarcate chemical inventions. Indeed, on the basis that the chemical formula of a new product differentiated it from all other chemical products, Hugo Mock wrote in his 1911 *Handbook on Patents* that ‘necessarily the most satisfactory definition of a new product is its [structural] chemical formula’.<sup>39</sup>

The Patent Office also recommended that patentees use structural formulas where they were known because they offered the clearest and best way of describing chemical compounds.<sup>40</sup> The Patent Office’s adoption of structural formulas as the preferred way of identifying and describing chemical compounds was motivated by their efficiency and simplicity, by the fact that structural formulas offered, at least to a skilled reader, a quick and easy way of identifying and understanding the chemical compound in question. As the Commissioner of Patents said in 1923, ‘If an applicant is claiming a structure and claiming it so that any one skilled in the art may make and use it and his claims are phrased in an allowable form ... the Examiner should not waste Government time in compelling an applicant to draw fine distinctions with respect to the terminology of the materials used in his device, nor should he write a five-paper dissertation on the use of such expressions – particularly when he is about ten months behind with his work’.<sup>41</sup>

<sup>36</sup> Paul Julius and Frederick Reubold, ‘Black Sulphur Dye’ US Patent No. 650,327 (22 May 1900).

<sup>37</sup> Helen Cooke, ‘A Historical Study of Structures for Communication of Organic Chemistry Information Prior to 1950’ (2004) 2 *Organic and Biomolecular Chemistry* 3179, 3189.

<sup>38</sup> While the courts accepted that a ‘chemical formula may be the sole subject-matter of the claim’, (Richard Wirth, ‘The Framing and the Construction of US Patent Claims’ (1923) *Journal of the Patent Office Society* 155, 180) nonetheless patentees continued to hedge their bets by using a range of techniques to describe their inventions, including the ingredients and how they were mixed, the chemical formula as well as the defining characteristics of the resulting compound (such as melting and boiling point). In part this was because ‘the composition and formula of many simple organic substances remained unstable for much longer than is usually recognized’. Catherine M. Jackson, ‘The Curious Case of Coniine: Constructive Synthesis and Aromatic Structure Theory’ in (ed) Ursula Klein and Carstein Reinhardt, *Objects of Chemical Inquiry: The Synergy of New Methods and Old Concepts in Modern Chemistry* (Sagamore Beach, MA: Science History Publications, 2014), 61, 75.

<sup>39</sup> Hugo Mock, *Handbook of Chemical Patents: How Procured, Requisites of, and Other Information Concerning Chemical Patents in the United States and abroad* (Washington, DC: Mason, Fenwick, and Lawrence, 1911), 18. By 1911, patentees were being advised to define chemical compounds ‘in terms of its chemical formula or constitution, plus whatever chemical characteristics or properties may serve to identify the compound.’ Chester H. Biesterfeld, *Patent Law for Chemists, Engineers, and Students* (New York: J. Wiley and Sons, 1943), 44.

<sup>40</sup> *Report of the Executive Committee of the Patent Office Society* (1933) *Journal of the Patent Office Society* 842, 845 (recommendation 4:5).

<sup>41</sup> *Ex Parte Christian* (1923) 308 OG 231 (cited in Richard Wirth, ‘The Framing and the Construction of US Patent Claims’ (1923–24) 6 *Journal of the Patent Office Society* 155, 158).

# UNITED STATES PATENT OFFICE.

PAUL JULIUS AND FRIEDRICH REUBOLD, OF LUDWIGSHAFEN, GERMANY,  
ASSIGNORS TO THE BADISCHE ANILIN AND SODA FABRIK, OF SAME  
PLACE.

## BLACK SULFUR DYE.

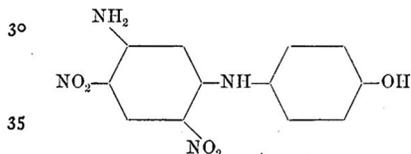
SPECIFICATION forming part of Letters Patent No. 650,327, dated May 22, 1900.

Application filed March 16, 1900. Serial No. 8,951. (No specimens.)

To all whom it may concern:

Be it known that we, PAUL JULIUS, doctor  
of philosophy, a subject of the Emperor of  
Austria-Hungary, and FRIEDRICH REUBOLD,  
5 doctor of philosophy, a subject of the King  
of Bavaria, both residing at Ludwigshafen-  
on-the-Rhine, in the Kingdom of Bavaria,  
Empire of Germany, have invented new and  
useful Improvements in Black Coloring-Mat-  
10 ters, of which the following is a specification.

Our invention relates to the manufacture  
of a new deep-black coloring-matter which  
directly dyes unmordanted cotton. It can  
be obtained from a certain diphenylamin de-  
15 rivative by treating the same with sulfur and  
sodium sulfid. The said diphenylamin de-  
rivative results from the condensation of one  
molecular proportion of symmetrical dinitro-  
meta-dichlor-benzene with one molecular pro-  
20 portion of para-amido-phenol in the presence  
of a substance that will bind the hydrochloric  
acid formed during the reaction, such as  
sodium acetate, and heating the condensa-  
tion product thus formed with ammonia un-  
25 der pressure, whereby dinitro-amido-para-  
hydroxy-diphenylamin is obtained, which,  
judging from the method of its formation,  
has the formula:



and this when treated with sulfur and so-  
dium sulfid in the manner to be described  
40 yields the coloring-matter which we desire  
to claim.

The following example will serve to illus-  
trate the manner in which our invention may  
be carried into practical effect and our new  
45 coloring-matter obtained. The parts are by  
weight.

*Production of a new black coloring-matter  
from dinitro-amido-para-hydroxy-diphenyl-  
amin.*—Prepare the required initial material  
50 by boiling in a reflux apparatus an alcoholic  
solution of one molecular proportion of dini-  
tro-dichlor-benzene and one molecular pro-  
portion of para-amido-phenol, with sufficient

sodium acetate to bind the hydrochloric acid  
formed during the reaction. Continue the  
heating until the dinitro-dichlor-benzene has  
practically disappeared. Isolate the dinitro-  
chlor-para-oxy-diphenylamin formed in any  
well-known manner. Heat seventy-five (75)  
60 parts thereof with one thousand (1000) parts  
of alcohol and five hundred (500) parts of an  
alcoholic solution of ammonia (containing  
about four and a half per cent. of  $\text{NH}_3$ ) for  
three hours at a temperature of about  $150^\circ$   
to  $160^\circ$  centigrade. Filter and precipitate  
65 the reaction product from the filtered solu-  
tion by the addition of water when cold.  
Mix together thirty (30) parts of the dinitro-  
amido-para-oxy-diphenylamin obtained as  
above described, one hundred and eighty  
70 (180) parts of crystallized sodium sulfid,  
and fifty (50) parts of sulfur in an iron vessel  
provided with a stirring arrangement and  
heat slowly up to  $140^\circ$  to  $150^\circ$  centigrade.  
Maintain the melt at this temperature until  
75 it has become dry. The powdered melt can  
be directly used for dyeing.

Our new coloring-matter is easily soluble  
in water with a green-blue color and dyes  
unmordanted cotton deep-black shades which  
80 are not essentially altered in appearance on  
treatment with bichromate, copper sulfate,  
and also with sodium peroxid. The aqueous  
solution gives on addition of hydrochloric  
acid a yellow-brown precipitate. 85

Now what we claim is—

The new coloring-matter which can be ob-  
tained from dinitro-amido-para-oxy-diphenyl-  
amin, sulfur, and sodium sulfid, which dis-  
solves in water with a green-blue color, dyes  
90 unmordanted cotton deep-black shades which  
are not essentially altered in appearance on  
treatment with potassium bichromate and  
copper sulfate, and also not on treatment  
with sodium peroxid, and which in aqueous  
95 solution, on addition of hydrochloric acid,  
yields a yellow-brown precipitate substan-  
tially as described.

In testimony whereof we have hereunto set  
our hands in the presence of two subscribing  
100 witnesses.

PAUL JULIUS.  
FRIEDRICH REUBOLD.

Witnesses:  
ERNEST F. EHRHARDT,  
JOHN L. HEINKE.

FIGURE 4.3 Structural formula for Black Sulfur Dye  
Paul Julius and Friedrich Reubold, 'Black Sulfur Dye' US Patent No. 650,327 (22 May  
1900). Courtesy of the United States Patent and Trademark Office.

## THE STANDARDIZATION OF CHEMICAL NAMES

The 1890s not only saw changes in the type of chemical formula that were used to describe chemical compounds, it also witnessed the move towards a more standardised way of naming chemical compounds. Over the course of the nineteenth century a range of different, often inconsistent, techniques were used to name chemical compounds. These included names based on the origin of the substance,<sup>42</sup> on a property of the compound,<sup>43</sup> or the name of the inventor of the compound. Unsurprisingly, these disparate naming practices created confusion and uncertainty: they made it difficult for chemists to communicate with each other, to compare experimental data, and to organise and classify compounds. In some areas, chemical nomenclature ‘was so dire that chemists could barely understand ... their varying claims regarding chemical composition, structure and behaviour’.<sup>44</sup> By the 1880s these problems had become acute. Concerned about the detrimental impact that this confusion was having, a series of international conferences were held in the 1880s and 1890s where chemists set out to formulate universal rules for the naming of organic compounds:<sup>45</sup> these culminated in the Geneva Congress of 1892, which laid the foundation for the system of chemical nomenclature that we have inherited today.<sup>46</sup>

One of the things that was agreed on by organic chemists at the end of the nineteenth century was that ‘every compound should bear a *systematic* name of such a character that it can at once be translated into the corresponding formula; and that, *vice versâ*, a name corresponding to any particular formula may be devised which we may count on finding in the *official* register, if the compound thought of have been described’.<sup>47</sup> It was also agreed that the way this was to be achieved was by breaking the structural formula down into parts that were each given individual names. Once this was done, the names of the parts were then reassembled to form the composite name of the chemical compound. While it was agreed that ‘a chemical name should uniquely express the structure of a compound’<sup>48</sup> and that this was

<sup>42</sup> Such as the use of the name ‘formic acid’ for the substance isolated from ants, *formica* being the Latin for ‘ant’. Evan Hepler-Smith, “‘Just as the Structural Formula Does’: Names, Diagrams, and the Structure of Organic Chemistry at the 1892 Geneva Nomenclature Congress” (2015) 62 *Ambix* 1, 6.

<sup>43</sup> Evan Hepler-Smith, *Nominally Rational: Systematic Nomenclature and the Structure of Organic Chemistry, 1889–1940* (PhD Thesis, Princeton University, 2016), 41.

<sup>44</sup> *Ibid.*, 39–40. Acetic acid had 18 different names in 1861. In 1859 Kekule identified 19 different formula for acetic acid (vinegar).

<sup>45</sup> Evan Hepler-Smith, “‘Just as the Structural Formula Does’: Names, Diagrams, and the Structure of Organic Chemistry at the 1892 Geneva Nomenclature Congress” (2015) 62 *Ambix* 1, 14.

<sup>46</sup> The Geneva Congress drew a distinction between a sphere of general usage (including trade names, trademarked names, well-established trivial names ‘to be left to its own devices’) and a ‘realm of official nomenclature, where each name was a precise and unique transcription of a structural formula diagram.’ *Ibid.*

<sup>47</sup> See, Henry E. Armstrong, ‘The International Conference on Chemical Nomenclature’ (19 May 1892) *Nature* 56, 57.

<sup>48</sup> Evan Hepler-Smith, *Nominally Rational: Systematic Nomenclature and the Structure of Organic Chemistry, 1889–1940* (PhD Thesis, Princeton University, 2016), 4. The rules fixed at Geneva Congress in 1892 demanded that the official name express the structure of the compound.

to be achieved by disassembling the compound into parts and reassembling them, the key issue was that chemists still needed to agree on how the disassembled parts were to be reassembled.

As Hepler-Smith has shown, in the lead up to the 1892 Geneva Congress, there were two competing views about the way structural formulas should be translated into words. One potential way of building the name of a new chemical compound, which did not prevail, was to organise the name of a compound around what it did and how it behaved. Under this approach, the functional groups in a compound are used as the starting point for determining the compound's name. The name of the compound was then built up around this functional core. For example, applying this approach the compound commonly known as *pinacone* was given the name *tetramethyl ethylglycol*. In this case, 'glycol' was selected as the root of the name 'to emphasise the compound's chemical function – a set of properties and characteristic chemical reactions that Friedel had established through painstaking experiment'.<sup>49</sup>

The alternate view, which eventually prevailed at the Geneva Congress, divorced the name of a compound from its function and properties to focus instead on the structure of the compound. Under this approach, compounds were 'divided ... into substituent radicals and a core corresponding to a parent compound'.<sup>50</sup> In order to develop an official name, a chemist would start with 'a compound's structural formula, reduce it to a carbon skeleton, identify the longest chain in that skeleton', which would be the foundation for the name to be given to the chemical compound. The chemist would then apply a series of rules that generated 'consistent unique names through the application of a consistent, even algorithmic procedure'.<sup>51</sup> Using these rules, *pinacone* is known as *2,3-dimethyl-2,3-butanediol*<sup>52</sup> (rather than *tetramethyl ethylglycol*, which was what the compound is called when a functional approach is adopted).<sup>53</sup>

The process of naming chemical compounds that was adopted at the 1892 Geneva Congress, which was embraced by organic chemists around the world, did not link the chemical name to chemical function nor to the properties of the compound. Rather, it tied the name of the compound to regularities in the structural formula. The Geneva Congress established a set of rules that systematically disassembled a structural formula into parts. The Congress also established rules that determined how the names of these parts were reassembled to form the composite name of the compound. Importantly this was done in such a way that 'the process could be reversed to regenerate the diagram from its official name'.<sup>54</sup>

<sup>49</sup> Evan Hepler-Smith, "'Just as the Structural Formula Does": Names, Diagrams, and the Structure of Organic Chemistry at the 1892 Geneva Nomenclature Congress' (2015) 62 *Ambix* 1, 19.

<sup>50</sup> *Ibid.*, 14.

<sup>51</sup> *Ibid.*, 19.

<sup>52</sup> Evan Hepler-Smith, "'Just as the Structural Formula Does": Names, Diagrams, and the Structure of Organic Chemistry at the 1892 Geneva, Nomenclature Congress' (2015) 62 *Ambix* 1, 19.

<sup>53</sup> *Ibid.*

<sup>54</sup> *Ibid.*, 22.

One of the consequences of applying this rule-bound approach to the formation of chemical names was that ‘each name was a precise and unique transcription of a structural formula diagram’.<sup>55</sup> That is, the rules ensured that each chemical compound had a unique chemical name corresponding in a precise rule-bound fashion to a particular structural formula.<sup>56</sup> Another consequence of the application of this rule-bound approach was that the resulting names were often very cumbersome and ungainly. For example, the black sulphur dye patented by Julius and Reubold in 1900 was called *dinitro-amido-parahydroxy-diphenylamin* (for the corresponding structural formula see Figure 4.3). For organic chemists, the unwieldy names were seen as a ‘necessary evil’ that had to be put up with in order to ‘identify and order chemical substances according to ... structural formula’.<sup>57</sup> Specifically, it was an evil that had to be lived with to ensure that compounds could be placed in alphabetically ordered indexes in chemical dictionaries, handbooks, tables, journals, reference books, and Patent Office catalogues.<sup>58</sup>

As with structural formula, patent law readily adopted the newly standardised chemical nomenclature. While structural formula and chemical names were inextricably linked, patentees adopted the new naming practices before they adopted structural formula. Indeed it has been suggested that in the 1890s, when empirical formula rather than structural formula were still commonly used in patents, structural information was often ‘conveyed through the ... names of compounds rather than the formula themselves, with reliance placed on the readers ability to translate such names into structures’.<sup>59</sup> While there was no formal requirement that patentees had to follow the Geneva rules when naming new chemical compounds, they were advised to do so not least because it left ‘less room for dispute than does the use of common words with their luscious accumulation of variant meanings’. The use of specialised technical terms was preferred by the Patent Office because it ‘renders the description concise and often conveys a better idea of the matter referred to than any other description of reasonable length’.<sup>60</sup> In line with this, patentees were advised that when ‘chemical substances are referred to the safest rule is to designate them by the correct chemical names ... If thus defined or designated, or the formula stated no question can thereafter arise as to what is meant’.<sup>61</sup> Patentees were also

<sup>55</sup> *Ibid.*, 25.

<sup>56</sup> While the basis of a name was the structural formula rather than the compound, as we will see, in patent law, at least, structural formula was treated as if they were coextensive with the compound.

<sup>57</sup> Seabury Mastick, ‘Chemical Patents II’ (1915) *The Journal of Industrial and Engineering Chemistry* 874.

<sup>58</sup> Evan Hepler-Smith, ‘“Just as the Structural Formula Does”: Names, Diagrams, and the Structure of Organic Chemistry at the 1892 Geneva Nomenclature Congress’ (2015) 62 *Ambix* 1.

<sup>59</sup> Helen Cooke, ‘A Historical Study of Structures for Communication of Organic Chemistry Information Prior to 1950’ (2004) 2 *Organic and Biomolecular Chemistry* 3179, 3182.

<sup>60</sup> Emerson Stringham, *Patent Claims: A Drafter’s Manual (Vol II)* (Madison: Pacot Publication, 1941), 839.

<sup>61</sup> A. M. Lewers, ‘Composition of Matter’ (1921–22) *Journal of the Patent Office* 530, 538. Seabury Mastick, ‘Chemical Patents II’ (1915) *The Journal of Industrial and Engineering Chemistry* 874.

advised in the Patent Office Style Guide to use the chemical spelling recommended by the American Chemical Society.<sup>62</sup>

#### THE IMPACT OF STRUCTURAL THEORY IN PATENT LAW

At the turn of the twentieth century, patent law was faced with two obvious choices when evaluating and dealing with chemical inventions. On the one hand, patent law could have focused on what a chemical compound did (its function). On the other hand, patent law could have ignored a compound's function and focused instead on the internal constitution or structure that was reflected in the compound's chemical name and formula. Unlike at the Geneva Congress where the delegates discussed the pros and cons of both approaches, patent law's decision to use structural formula and the newly standardised chemical nomenclature to identify and demarcate chemical compounds occurred with little fanfare or discussion. As was often the case with patent law's interaction with chemistry, the law simply passively accepted the changes that were presented to it, usually by patentees in their applications, which operated as syphers for the introduction of chemical innovations into the law.

Despite this, patent law's adoption of structural theory at the turn of the twentieth century fundamentally changed the way that the law dealt with chemical subject matter. This was particularly evident in the way that chemical compounds were identified. As we saw earlier, patent law relied on a mixture of factors to identify, demarcate, and distinguish chemical inventions prior to the uptake of structural formula. This included both the empirical formula of the compound (that listed the constituent elements) along with the compound's defining physical marks or traits such as how it smelt, what it looked like, and the temperature it boiled at. In many situations it also included the chemical specimens deposited with the application. One of the consequences of this was that the law treated chemical inventions as if they were tangible bounded individual entities. Because protection was limited to singular specific compounds, this meant that the law operated taxonomically at the level of the species rather than genus.

While patent law had previously relied on a mixture of factors to identify, demarcate, and distinguish chemical inventions (notably the empirical formula and the physical properties of the compound), this changed with the adoption of structural formula. This is because in the same way in which organic chemists came to visualize compounds in terms of their structural formula,<sup>63</sup> so too patent lawyers, judges,

<sup>62</sup> *Rules Governing the Printing of Specifications with a list of words and technical terms approved by the US Patent Office* (Washington: Government Printing Office, 1887), 28. The 1896 Patent Office style book *Rules Governing the Printing of Specifications* adopted the American Chemical Society's chemical spelling. K. P. McKelroy, 'Patent Office Chemical Spelling' (1931) *Journal of the Patent Office Society* 183, 184–85.

<sup>63</sup> E. A. Ustinov and O. V. Chelisheva, 'Are Markush Structures Matters of Chemistry and Law or Just Figments of the Imagination?' (1996) 18(1) *World Patent Information* 23, 24.

and Patent Office examiners also came to think about chemical compounds exclusively in terms of their structural formula and corresponding name.<sup>64</sup> Importantly, structural formulas and their associated names were not only treated as representational devices that stood in for the chemical compound, they also came to be treated as if they fully encapsulated the invention: a compound's function along with its physical features were no longer needed to identify a chemical compound. In this sense the 'description of a new compound by its formula or name in terms of standard nomenclature' was 'analogous to the description and drawing of a machine'.<sup>65</sup>

From the end of the nineteenth century, patent lawyers, examiners, and judges began to view chemical subject matter through the lens of structural formulas. Of particular importance was that chemical structures were used to identify and distinguish patented compounds.<sup>66</sup> For example, in the 1889 decision of *ex parte Latimer*, the Commissioner of Patents rejected an application for a patent for a fiber identified in the needles of the pine tree *Pinus australis*. This was on the basis that the 'pure fiber after it has been eliminated from the natural matrix of the leaf or stalk or wood is essentially the same thing and possesses the same construction. The chemical formula for this cellulose in all these variety of plants ... is the same'.<sup>67</sup> The important role that chemical structure played in the way that patent law thought about chemical subject matter was also reflected in the idea that a chemical invention only came into existence when the chemist 'had a mental picture of the structure of the chemical compound'.<sup>68</sup> In line with this, chemical inventions were classified in the Patent Office on the basis of their chemical structure and their elements, rather than in terms of what the compound did or the industry in which they were used.<sup>69</sup>

<sup>64</sup> While the decision of the Patent Office to refuse 'to issue a patent for a chemical compound if the chemical structure appeared anywhere in the published literature' was said to 'reflect the view of mechanical invention that if a drawing existed, an invention was unpatentable over the prior art' and was an 'illustration of the difficulty of attempting to fit chemical invention into the fixed confines of a body of law developed for mechanical invention', it is better seen as patent law following the lead of structural theory generally and the rules of chemical nomenclature established at the Geneva Congress more specifically. Jackie Hutter, 'A Definite and Permanent Idea - Invention in the Pharmaceutical and Chemical Sciences and the Determination of Conception in and Chemical Sciences and the Determination of Conception in Patent Law' (1995) *The John Marshall Law Review* 687, 720 n 232 (citing William D. Noonan, 'Patenting Medical Technology' (1990) *Journal of Legal Medicine* 263, 268–69 on the 'engineering bias in patent law').

<sup>65</sup> Eugene Geniesse, 'Adequate Description' (1945) 27 *Journal of the Patent Office Society* 784, 787–88.

<sup>66</sup> 'A pure chemical compound such as nitroglycerine falls within the patentable class of "compositions of matter"'. 'In this case, the original ingredients have reacted so as to form an entirely new compound having distinct properties of its own. A composition of matter can thus be distinguished from others not only by its properties but also by its chemical structure'. Joseph Rossman, 'What the Chemist Should Know about Patents' (1932) 9(3) *Journal of Chemical Education* 486, 490.

<sup>67</sup> *Ex parte Latimer* (12 March 1889) 46 OG 1638, *Decisions of the Commissioner of Patents and of the United States Courts in Patent Cases* (Washington: Government Printing Office, 1890), 123, 125.

<sup>68</sup> *Amgen v. Chugai Pharma* (1991) 927 F.2d 1200, 1206 (treating the gene as a chemical compound).

<sup>69</sup> US Patent Office, *The Classification of Patents* (Washington: Government Printing Office, 1915), 26. Ridsdale Ellis, *Patent Claims* (New York: Baker, Voorhis and Co, 1949), 321.

The decision to treat structural formulas as if they were a definitive representation of the patented chemical compound was also evident in the way the courts approached the obviousness of chemical compounds. When considering whether a chemical invention was obvious, the courts focused on the similarities between the structure of the claimed compound and the structure of the compound disclosed in the prior art.<sup>70</sup> If a compound shared the same structural core as an existing compound, it was likely to be obvious. With structural obviousness, the properties of the compound were irrelevant. Instead, the question of whether a compound was obvious was determined by comparing the structures of the compounds.<sup>71</sup>

Another example of the way in which structural formulas were treated as definitive representations of chemical compounds was when compounds were evaluated to determine whether they were new and therefore potentially patentable. In this context, the mere appearance of a name or formula of a chemical compound in a printed form was sufficient to anticipate a claim to a compound and thus to render it unpatentable.<sup>72</sup> It did not matter whether the prior art disclosed what the compound did (its function) or what its properties were: all that mattered was that the prior art disclosed the internal structure of the compound either through its official name or its structural formula. This was made clear in the decision of *Von Bramer*, which concerned an application by Harold Von Bramer to patent a new and improved type of motor fuel; the key feature of which was that it contained the compound known as N-(primary alkyl) aminophenol, in which the primary alkyl group contained at least five carbon atoms. The question that arose in this decision was whether a pre-existing patent that specifically named N-butyl aminophenol anticipated Von Bremer's application. Importantly the prior art reference only named the chemical: it made no mention of its potential use in improving the quality of motor fuel. After the Primary Examiner and the Board of Appeal rejected the application on the basis of the prior art, Von Bramer appealed to the Court of Customs and Patent Appeals where he argued that it was not enough for the prior art merely to name the compound in question to anticipate. Rather, Von Bramer argued that a prior art reference could only be anticipatory if the chemical compound was described in one of two ways: either (1) by reciting a sufficient number of chemical attributes such as 'melting point, boiling point, color, crystalline appearance, solubility' and the like; or (2) by reciting a process which unquestionably produced the substance.

<sup>70</sup> William D. Marsillo, 'How Chemical Nomenclature Confused the Courts' (1997) *Baltimore Intellectual Property Law Journal* 29, 30.

<sup>71</sup> *In re Papesch* 315 F.2d 381 (CCPA 1963) (a compound and its properties were inseparable).

<sup>72</sup> Maurice W. Levy, 'Von Bramer: A Plea for Reorientation' (1951) *Journal of Patent Office Society* 401, 401-2. Emerson Stringham, *Patent Claims: A Drafter's Manual (Vol II)* (Madison: Pacot Publications, 1941), 853. A 'novel chemical compound was characterized by a unique feature: its structural formula.' E. A. Ustinoav and O. V. Chelisheva, 'Are Markush Structures Matters of Chemistry and Law or Just Figments of the Imagination?' (1996) 18(1) *World Patent Information* 23, 27.

The Court of Customs and Patent Appeals rejected Von Bramer's argument that a name without further description was insufficient to anticipate. This was because the N-butyl amino phenol mentioned in the prior art was 'more than a mere name of an individual substance, otherwise unrecognized'. Rather, as the Court said, it was 'a name according to a standard system of chemical nomenclature (Geneva system) whereby a chemical individual substance of definite chemical molecular structure is defined having generally predictable properties such as found for any similar N-alkyl amino phenol ... The use of a name falling in the standard chemical system by the patents is no accident because all of the many compounds named in [the earlier prior art disclosure] are deliberately named from this standard chemical system'.<sup>73</sup> On this basis the Court concluded that 'the naming of the reagents by the citations even though they are complex organic compounds and disclosed no further than by the customary chemical nomenclature is sufficient anticipation'. This was because the system of chemical nomenclature established at the Geneva Congress was 'sufficient to disclose the structure of the compound in detail. It is not believed relevant or necessary to determine possibility of preparing these compounds or degree of difficult involved'.<sup>74</sup>

The Patent Office and the courts quickly extended the logic of *Von Bramer* beyond chemical names to include structural formulas. This meant that the novelty of a chemical compound could be defeated merely on the basis of the prior existence of either the name or the structural formula of the compound whether in a chemical journal, an earlier patent, or in a book such as the *Beilstein Handbook of Organic Chemistry*.<sup>75</sup> It did not matter where the name or formula of a compound appeared: so long as the publication was available to the public, it would anticipate and thus undermine the novelty of the compound. This was the case even when the pre-existing name or formula was the result of a typographical error, was factually inaccurate,<sup>76</sup> or 'the reference contains only an inoperative method for producing the compound, or no method at all'.<sup>77</sup> It also did not matter if a compound had actually ever been made, if the investigator had access to the required ingredients, if the compound was part of the structure of another compound,<sup>78</sup> or if the prior art made no mention of what the compound did or what its properties were; all that mattered

<sup>73</sup> *In re Von Bramer* 127 F.2d 149, 152 (CCPA 1942).

<sup>74</sup> *Ibid.*, 151.

<sup>75</sup> The appearance of the name and formula of a compound in a publication was sufficient to anticipate subsequent patent applications, notwithstanding the fact that the investigator did not have starting material required for the process, nor did they produce the product. *Ex Part Signaigo*, Patent File 2,436,233/Case No 221) as cited in Maurice W. Levy, 'Von Bramer: A Plea for Reorientation' (1951) *Journal of the Patent Office Society* 401, 402.

<sup>76</sup> Maurice W. Levy, 'Von Bramer: A Plea for Reorientation' (1951) *Journal of the Patent Office Society* 401, 401-2.

<sup>77</sup> *Application of Charles F. Baranauckas and Eerl T McBee* 228 F.2d 413 (CCPA 1956).

<sup>78</sup> Maurice W. Levy, 'Von Bramer: A Plea for Reorientation' (1951) *Journal of the Patent Office Society* 401, 403.

was that the prior art disclosed a structure that was the same as the chemical compound being evaluated.<sup>79</sup>

#### TOWARDS A DEMATERIALISED CHEMICAL SUBJECT MATTER

Although patentees continued to use physical criteria to define their inventions, from the beginning of the twentieth century the Patent Office and the courts no longer used this information when interpreting chemical subject matter. Instead, they focused on the paper-based structural formula and name of the chemical compound. The willingness of the law to reduce a chemical compound to its structural formula and name meant that it was no longer necessary for patentees to deposit physical specimens of compounds as part of the application process. In line with this, the use of chemical specimens largely disappeared in the early part of the twentieth century. Indeed, by 1932 Rossman was able to write that it was rare that specimens of composition were required by the Patent Office during the prosecution of a patent.<sup>80</sup> The willingness to accept that a chemical compound could be identified solely on the basis of its structural formula and/or its associated name effectively decoupled chemical inventions from their physical material form. This had a profound and long-lasting effect on chemical subject matter.

As we saw above, prior to the adoption of structural theory it was common practice when describing their innovations for patentees to combine empirical formula that listed the proportion of elements in a compound, with the physical features of the resulting compound. The fact that the identity of a patented compound was inextricably tied to the compound's unique physical traits ensured that protection was limited to the specific compounds with those characteristics. The shift towards a paper-based subject matter that occurred at the turn of the twentieth century meant that the limitations that the physical features of a chemical compound imposed on the way the subject matter was construed no longer existed.<sup>81</sup> The fact that chemical patents were now decoupled (at least temporarily) from the physical compound meant that chemical inventions were no longer necessarily limited to individual

<sup>79</sup> This meant that to be valid, a patent had to define a difference in structure or composition: a mere statement of use was insufficient. P. W. Shepard and N. A. Asp, 'Claiming a New Use of an Old Substance' (1938) *Journal of the Patent Office Society* 912, 913. The idea that a chemical compound corresponded with (or was equivalent to) its chemical structure was also taken up in other areas of intellectual property. For example in an application in relation to register a trade mark for a medical compound, where questions about ownership arose, the Commissioner focused on the fact that the applicant was the 'owner or possessor of a formula for preparing a compound' as indicator of ownership of the compound *Richmond v. The Dr. S A Richmond Nervine Company* 52 OG 307 (21 June 1890), *Decisions of the Commissioner of Patents* 105. See also *Chadwick v. Covell* 51 OG 2087 (27 February 1890) (Supreme Judicial Court, State of Massachusetts) (*Decisions of State Patent Courts*).

<sup>80</sup> Joseph Rossman, *The Law of Patents for Chemists* (Washington, DC: The Inventors Publishing Company, 1932), 106.

<sup>81</sup> On the rise of 'paper-chemistry' see N. W. Fisher, 'Kekulé and Organic Classification' (1974) *Ambix* 29, 49.

(species-level) compounds that had a definite and verified physical form. In so doing, it created the possibility for change. And change it did. While patent law had previously only protected individualised chemical substances with a definitive and verified physical form, as a result of the acceptance of structural theory patent law now also protected families or classes of related compounds.

Across the nineteenth century, there was always a potential for class-based chemical patents. Thus, with recipe-based patents it was possible to claim, for example, ‘strong acids’ which covered the use of sulphuric acid or hydrochloric acids.<sup>82</sup> The situation was much the same when empirical and rational formula were used. Indeed, as we saw earlier, one of the problems with these formula was that it was possible for a single formula to apply to more than one compound (isomers). While there were exceptions, the potential for class-based claims did not eventuate. This was because it was common practice for patentees to combine chemical formulas with physical information about the compound such as melting and boiling points, how the compound looked, tasted, or smelt, and, in some cases, physical specimens. As a result, the potential that existed for broad class-based claims was ameliorated and protection was limited to single compounds.<sup>83</sup>

The situation began to change towards the end of the century. As Ruby complained when speaking of early twentieth-century chemical patents, while the composition of every true chemical compound was invariant, the composition ‘rarely defines unambiguously a true chemical compound’.<sup>84</sup> In some situations, this was a consequence of a decline in the use of specimens. In other situations, it was a consequence of the fact that instead of using ‘additional’ information such as melting and boiling points in combination with the chemical formula to define a single compound, patentees used the additional information to describe a specific example of one of the members of the class of inventions covered by the formula.

This subtle but important change in patent practice can be seen in US Patent Number 1,649,670 for hexyl resorcinol (an organic compound with local anaesthetic and antiseptic properties). Specifically the patent claimed: ‘New products as comprising hexyl resorcinols having the following formula:  $C_6H_3(OH)_2C_6H_{13}$ ’. While the patent only disclosed the production of one hexyl resorcinol of the given composition, ‘the formula  $C_6H_3(OH)_2C_6H_{13}$  represented two hundred and twenty two possible organic compounds’.<sup>85</sup> What made this class-based claim possible was

<sup>82</sup> Ridsdale Ellis, *Patent Claims* (New York: Baker, Voorhis and Co, 1949), 312–13.

<sup>83</sup> While it had been common practice for organic chemists to organise chemical compounds into classes or families of chemical compounds, for most of the nineteenth century ‘the basic species of chemistry were chemical substances.’ J. Schummer, ‘The Impact of Instrumentation on Chemical Substance Identity’ in (ed) P. Morris, *From Classical to Modern Chemistry: The Instrumental Revolution* (Cambridge: The Royal Society of Chemistry, 2002), 188, 207.

<sup>84</sup> Charles E. Ruby, ‘Are True Chemical Compounds, as Such, Inherently Patentable Subject Matter: Part II?’ (1941) *Temple University Law Quarterly* 321, 339–40.

<sup>85</sup> *Ibid.*

the fact that while the patent included additional information about how the new hexyl resorcinols were made and what their defining characteristics were, this was presented as a *specific example* of a class of compounds rather than the description of a singular patented compound.

While this change in patent drafting played an important role in shifting chemical patents towards class-based generic claims, the key reason for the move away from singular specific compounds was the rise of what were called '*general formula*': the key feature of which was that they applied to families or classes of compounds rather than to specific individual compounds.<sup>86</sup> Because general formula represent the composition of any member of an entire class of compounds, they were an effective and convenient way of representing very large classes of chemical compounds. Patentees first began to claim general formula claims in the early 1870s<sup>87</sup> and then more consistently from the 1890s.<sup>88</sup>

One of the notable things about general formula was that as well as using symbols that had an agreed chemical meaning such as O for oxygen or C for carbon, they also included non-chemical symbols that were only defined for the purpose of the particular formula where they were used: typically 'R',<sup>89</sup> but sometimes 'X', 'M', or 'H\*'.<sup>90</sup> Thus, in US Patent Number 623,638 (1899), whose generic claim 3 was directed to certain aminoanthraquinones with the amino groups -NH-R-X and -NH-R-NO<sub>2</sub> - 'R' was defined as an 'aromatic radical of the series homologous and

<sup>86</sup> Genus class-based applications took different forms. In some cases, instead of claiming a specific compound as an object in its own right (which had been the norm prior to the compound being decoupled from its physical form), patentees presented the individual compound in the patent application as an example of one of the members of the class of inventions covered by the formula. This subtle change in patent practice can be seen in US Patent No. 1,649,670 for hexyl resorcinol, for 'New products as comprising hexyl resorcinols having the following formula: C<sub>6</sub>H<sub>3</sub>(OH)2C<sub>6</sub>H<sub>13</sub>'. While the patent only disclosed the production of one hexyl resorcinol of the given composition, 'the formula C<sub>6</sub>H<sub>3</sub>(OH)2C<sub>6</sub>H<sub>13</sub> represented two hundred and twenty two possible organic compounds'. What made this class-based claim possible was the fact that while the patent included information about how the new hexyl resorcinol was made and what its defining physical characteristics were, the identified compound was presented as a member of a class of compounds, rather than the description of a singular patented compound. Charles E. Ruby, 'Are True Chemical Compounds, as Such, Inherently Patentable Subject Matter' (1941) *Temple University Law Quarterly* 321, 339-40.

<sup>87</sup> Adolph Ott, 'Improvement in Artificial Stones' US Patent No. 137,859 (27 March 1873) claimed a 'cement of the general formula: 10(SiO<sub>2</sub>.R<sub>2</sub>.O<sub>3</sub>)22CaO in which the letter R represents the aggregate quantity of alumina and oxide of iron contained in the cement); 'Improvement in Processes of Manufacturing Ammonia' US Patent No. 161, 137 (10 March 1875) used the general formula 2(MR<sub>x</sub>) + 2N + 3(H<sub>2</sub>O) = M<sub>2</sub>+ 6(RO) + 2(NH<sub>3</sub>) 'where M represents the triad or pentad element and R the oxidizable element; N, nitrogen; H, hydrogen; and O, oxygen'.

<sup>88</sup> Karl B. Lutz, 'Evolution of the Claims of US Patents' (1938) 20 *Journal of Patent Office Society* 457, 462.

<sup>89</sup> While it has been suggested that nineteenth century German dyestuff chemists and German patent attorneys devised the 'R' group definition in the US at least the R symbol was used first for inventions made in the US and France. Harold C. Wegner, 'The Right to Generic Chemical Coverage' (1978) 6 *APLA Quarterly Journal* 257, 261.

<sup>90</sup> John E. Gordon and Joyce Brockwell, 'Formalisation of the Language of Organic Chemistry: Generic Structural Formulas' (1983) 23 *Journal of Chemical Information & Computer Science* 117, 118.

analogous to 'phenyl'.<sup>91</sup> The use of these free-floating symbols, which allowed for structural variation in compounds, allowed patentees to claim even larger classes of compounds.<sup>92</sup> The structural and general formula claims that began to appear in patents in the later part of the nineteenth century often encompassed extremely large numbers of compounds. For example in *Hercules*, the court said that the formula in the patent potentially covered up to 100,000,000 compounds.<sup>93</sup> Similar figures appeared repeatedly in the literature.

Another notable feature of class-based general formula was that they typically included a mixture of chemical compounds that had already been created and tested in the laboratory, along with a range of compounds that had not yet been made. While the empirical nature of organic chemistry meant that chemists had long speculated on the possible existence of yet-to-be verified chemical compounds, this took on a new life with structural theory. This was because as a patent examiner wrote, in the field of organic chemistry 'theoretical, generalized knowledge has outstripped actual exploration in many respects. The subject matter is systematized and generalized by investigation of the behaviour of each of the commonly occurring functional groups. It is assumed that the same functional groups will similarly combine in the absence of other interfering groups'.<sup>94</sup>

Courts in the United States first accepted generic claims for mechanical inventions in *Ex parte Eagle*,<sup>95</sup> an 1870 decision that concerned the patentability of a 'box' with a 'follower'. Drawing on the fact that the application listed four different embodiments of the box, the examiner held that each of the four constructions of the box should be placed in separate applications (the generic use of the term 'box' covered all four of these constructions).<sup>96</sup> Commissioner Fisher overturned the Examiner's objection arguing that 'the applicant describes a new genus, to wit, a box provided with a follower. He may fairly describe several species of this genus, and may make any claim that is generic in its character and includes them all'.<sup>97</sup> In doing so, the Commissioner opened the door to the possibility of generic class-based claims for mechanical inventions.

There was widespread support for extending the logic of *Ex parte Eagle* to allow patentees to make generic claims for chemical inventions. As we have seen, the

<sup>91</sup> Harold C. Wegner, 'The Right to Generic Chemical Coverage' (1978) 6 *APLA Quarterly Journal* 257, 262. See M. Boniger, 'Yellow Azo Dye and Process of Making Same' US Patent No. 901,675 (20 October 1908) (where 'R' was used in a chemical formula as standing in for a methyl or carboxyl group).

<sup>92</sup> Helen Cooke, 'A Historical Study of Structures for Communication of Organic Chemistry Information Prior to 1950' (2004) 2 *Organic and Biomolecular Chemistry* 3179, 3182. 'X and M are fairly standard, nowadays R is frequently defined locally', *Ibid*.

<sup>93</sup> *Hercules Powder v. Rohm and Hass* 70 USPQ 297.

<sup>94</sup> Eugene Geniesse, 'Adequate Description' (1945) 27 *Journal of the Patent Office Society* 784.

<sup>95</sup> 1870 CD 137.

<sup>96</sup> This was made under Rule 41 'which limited applicants to one species claim'. Harold C. Wegner, 'The Right to Generic Chemical Coverage' (1978) 6 *APLA Quarterly Journal* 257.

<sup>97</sup> 1870 CD 137.

Patent Office first allowed generic claims for chemical inventions from the early 1870s. Judicial support for generic class-based claims, which first appeared in the 1903 decision of *Ex parte Dallas*,<sup>98</sup> was repeatedly reaffirmed, perhaps most famously in the *Markush* decision (which is often incorrectly seen as being the first decision to allow generic chemical inventions).<sup>99</sup>

While the process of extending patent law to allow for the possibility of generic class-based claims was relatively seamless, the idiosyncratic nature of chemical subject matter did create issues. Specifically, patent law had to deal with the fact that while patentees had begun to claim classes of chemical compounds that sometimes encompassed hundreds, thousands, or, in some cases, millions of individual compounds, patentees were not in a position where they could test all of the members of a class of compounds: primary because testing was prohibitively expensive, impractical, or overly time-consuming.<sup>100</sup> As one commentator noted, it was 'not possible in most cases to take the time and money to explore every possibility among the various compounds and groups to determine what is operative and what is not'.<sup>101</sup> As a result, patentees would frequently submit applications for very large classes of compounds even when they had only tested a small number of the compounds. Thus, for example, while the patent in *Matheson v. Campbell* for 'any sulpho acid of any radical' covered as many as 500 different sulpho acids, the applicant had only experimented with three or four compounds.<sup>102</sup>

In this situation, the law was faced with a choice. On the one hand, patent law could have limited protection to compounds that had actually been made and tested on the basis that the lack of chemical prevision meant that the only way of determining whether a given chemical was operative was to test it. If this had been followed it would have severely limited the protection available for patentees.<sup>103</sup>

<sup>98</sup> 106 OG 996 (CD 1903). On this see Harold C. Wegner, 'The Right to Generic Chemical Coverage' (1978) 6 *APLA Quarterly Journal* 257, 259.

<sup>99</sup> Harold Wegner spoke of the general myth that needed to be laid to rest that applicants were only permitted to claim generic chemical inventions since the decision of *Ex parte Markush* 1925 CD 126. Many '(if not the majority) of practitioners think of the *Markush* decision as being a decision of the Commissioner "permitting" structural formula type generic claims'. Instead he traces it back to *Eagle*. Harold C. Wegner, 'The Right to Generic Chemical Coverage' (1978) 6 *APLA Quarterly Journal* 257, 261. See also Robert I. Coulter, 'Markush' Claims' (1952) *Journal of the Patent Office Society* 901. Over time, *Markush* formulas became synonymous with generic formulas generally (despite the fact that the original *Markush* patent did not contain a generic formula in the claims), E. A. Ustinov and O. V. Chelishcheva, 'Are *Markush* Structures Matters of Chemistry and Law or Just Fignments of the Imagination?' (1996) 18(1) *World Patent Information* 23.

<sup>100</sup> Herbert H. Goodman, 'The Invalidation of Generic Claims by the Inclusion of a Small number of Inoperative Species' (1958) *Journal of the Patent Office Society* 745.

<sup>101</sup> Chester H. Biesterfeld, *Patent Law for Chemists, Engineers, and Students* (New York: Wiley and Sons, 1943), 36–37.

<sup>102</sup> *Matheson v. Campbell* 78 Fed Rep 910, 915 (2nd Circ, CCA 13 January 1897).

<sup>103</sup> Not least because it would have 'become very difficult for the inventor in the chemical field to frame a claim that would adequately cover the invention without incurring the risk of invalidity because of exceptions.' Chester H. Biesterfeld, *Patent Law for Chemists, Engineers, and Students* (New York: Wiley and Sons, 1943), 38.

The alternative option would have been to allow patentees to claim large classes of chemical compounds, even though they had only tested a small number of those compounds. With the exception of Charles Ruby, there was overwhelming support from legal commentators, lawyers, judges, and Patent Office officials in favour of allowing patents for classes or families of chemical compounds irrespective of whether or not they had been tested.<sup>104</sup>

Little explanation was given as to why patentees were allowed to claim broad classes of untested compounds. At best we were told that ‘in cases of doubt applicants should be permitted to claim the entire class. Only in that way can the inventor be made “secure” in his rights, as guaranteed by the US Constitution’.<sup>105</sup> In most cases, however, it was simply accepted that patentees should be able to patent their innovations. Thus we were told that as it was ‘not always possible to devote sufficient time and money in a research laboratory to examine all compounds that could possibly come within the scope of the invention’ that it was ‘necessary to indulge in a bit of speculation within reasonable limits’.<sup>106</sup> Or, as a Primary Examiner in the Chemical Division of the US Patent Office and later member of the Board of Appeals, Eugene Geniesse, said: while ‘it is desirable and customary ... for an applicant to include such information as he may have regarding those compounds he has actually produced and studied ... it is present practice to regard it as sufficient if a reaction product be described by its chemical constitution (i.e., name or formula) when it involves a definitive compound or class of compounds’.<sup>107</sup> Although the acceptance of class-based patents created exceptions to many of the doctrinal rules that had developed over the previous century, the changes went unacknowledged. Instead all Geniesse said was that he did know of any ‘authority which denies protection when [an] applicant may not have actually produced the compounds he claims as his invention and hence is not provided with information as to their properties, but which he has visualized as the reaction product of known materials’.<sup>108</sup>

Once it was accepted that patent protection included untested compounds, the nature of the subject matter inquiry changed. This was because while it may not have been necessary for a patentee to test all the members of a class, it was necessary for them to test a sufficient number of examples to justify protection. As a result, the subject matter inquiry changed from one where patent law merely asked whether the patent disclosed a composition of matter to become one where it was asked: *how many* compounds did a patentee need to test to justify grant of the class-based

<sup>104</sup> To be valid there needed to be some shared quality running through the members of the family or class of substances. See *Incandescent lamp Patent Case* 159 U.S. 465 (1895).

<sup>105</sup> Ridsdale Ellis, *Patent Claims* (New York: Baker, Voorhis and Co, 1949), 278.

<sup>106</sup> Chester H. Biesterfeld, *Patent Law for Chemists, Engineers, and Students* (New York: Wiley and Sons, 1943), 36–37.

<sup>107</sup> Eugene Geniesse, ‘Adequate Description’ (1945) 27 *Journal of the Patent Office Society* 784, 787–88.

<sup>108</sup> *Ibid.*

patent?<sup>109</sup> Unsurprisingly, a range of different answers were given to this factual question that varied from vague platitudes (patentees were required to test ‘sufficient numbers’ to ‘illustrate all ramifications of the class’,<sup>110</sup> or to ‘raise a presumption that the applicant number has really made a generic invention’<sup>111</sup>) through to equally unhelpful precise numbers.<sup>112</sup>

In part, the differing opinions about the number of compounds that an applicant had to test to justify protection for a class of compounds can be explained by the fact that the answer changed depending on the type of compound in question. In some cases the courts were more willing to allow claims for large classes of untested compounds on the basis of a small number of proven compounds. This was because as Wegner said, ‘knowledge in some areas of chemistry has become so advanced that decisions have accepted the existence of a high degree of predictability as to how certain changes are likely to affect structure’.<sup>113</sup> This was particularly the case with homologous compounds and isomers, that is with compounds that shared a similar core structure (but differed in terms of their properties).<sup>114</sup> As the Supreme Court said in *Brenner v. Manson*, ‘chemists knowing the properties of one member of a [homologous] series would in general know what to expect in adjacent members’.<sup>115</sup> The position was similar with isomers.<sup>116</sup> In other cases, however, the

<sup>109</sup> The converse question also arose: how many inoperative compounds were needed to invalidate a broad claim? Herbert H. Goodman, ‘The Invalidation of Generic Claims by the Inclusion of a Small number of Inoperative Species’ (1958) *Journal of the Patent Office Society* 745.

<sup>110</sup> Anon, ‘The Mortality of Chemical Patents in Court’ (1945–46) 34 *Georgetown Law Journal* 504, 510. For a more recent attempt to explain enablement see *Amgen v. Sanofi* 598 U.S. 594 (2023).

<sup>111</sup> Joseph Rossman, ‘The Rejection of Broad Chemical Claims’ (1932) *Journal of the Patent Office Society* 873, 874 (need for sufficient or reasonable number of species or members). Bert Russell, ‘The Improvements of Our Patent System’ (1933) *Journal of the Patent Office Society* 666, 672 (‘a reasonable number of species of the genus’).

<sup>112</sup> Bert Russell, ‘The Improvements of Our Patent System’ (1933) *Journal of the Patent Office Society* 666, 672.

<sup>113</sup> Helmuth A. Wegner, ‘Prima Facie Obviousness of Chemical Compounds’ (1978) 6 *American Patent Law Association Quarterly Journal* 271, 272.

<sup>114</sup> In 1944 courts were able to say that it was well understood by chemists that the ‘members of a homologous series of chemical compounds possessed the same principal characteristics ... and that knowledge of the properties and chemical behaviour of one of the members of the series suggest to the chemist the properties and chemical behaviour of the other members of the series.’ *In re Hass* 141 Fed Rep, 2d Series 122, 125 (CCPA 1944). See also Bruce M. Collins, ‘The Forgotten Chemistry of the Hass-Henze Doctrine’ (1962) *Journal of the Patent Office Society* 284.

<sup>115</sup> The Supreme Court defined a homologous series as a family of chemically related compounds in *Brenner v. Manson* 383 U.S. 519, 148 USPQ 689 (US Sup Ct, 1966). See Irving Marcus, ‘Chemical Product Patent Practice in the United States’ (1970) 52 *Journal of the Patent Office Society* 543, 545. *In re Hass*, 141 F.2d 122, 127, 139 (CCPA 1940) (prima facie obviousness was shown when chemical compounds ‘have similar structures that differ only in being adjacent homologs’).

<sup>116</sup> The ‘broad concept of homology between next-adjacent organic compounds is well known to every chemist. Making another novel compound which differs only by close homology, isomerism, replacing oxygen by Sulphur, or by double bond shift, is just an exercise in manipulative chemical procedures’. E. S. Simmons, ‘Central Patents Index Chemical Code: A User’s Viewpoint’ (1984) 24 *Journal of Chemical Information and Computer Science* 10.

number of compounds a patentee was expected to test to prove the validity of a class of compounds increased. This was because ‘unless there is structural similarity as to suggest to those skilled in the art that the result would be substantially the same’,<sup>117</sup> it was well-established that ‘in chemical cases not to assume that untried chemicals will have the same effect as other’.<sup>118</sup> While the nature of the compound influenced the number of representative samples that a patentee needed to test to facilitate the patenting of a class of compounds, at the end of the day, however, it was ‘not easy to estimate with what degree of uniformity or certainty such rules as the foregoing may be applied; but it is easy to see that so elastic a tape can be stretched to conform to the whim of any authority having the last guess’.<sup>119</sup>

While the number of compounds that a patentee needed to test to prove the existence of a class of compounds may have been unclear, what was clear was that by allowing patentees to claim large numbers of untested compounds on the basis of a limited number of exemplary compounds that the nature of the subject matter inquiry changed. In particular, it became a quantitative, mathematical or, as one legal commentator preferred, an empirical exercise.<sup>120</sup> Allowing patentees to claim classes of untested compounds also impacted on chemical subject matter in other ways. This is because as Eugene Geniesse said, it allowed applicants to ‘base a patent application wholly on speculation (visualize) without doing any actual work or producing an actual result. Lack of description of the result is excused by lack of knowledge or merely *visualized* results. In layman’s language this means that a patent can be secured on mere supposition without having actually invented or discovered anything’.<sup>121</sup> That is, chemical subject matter became speculative.

While inventions are frequently never quite finished in the sense that there is often room for refinement and improvement, allowing patentees to make speculative claims for chemical compounds was different. This was because speculative paper-based patents, which protected ‘compounds claimed in specifications which have never been made or characterised which are being treated as real’,<sup>122</sup> allowed a patentee to make assumptions about the existence of things not yet tested or confirmed. And, unlike the case with the theoretical presumptions made about the

<sup>117</sup> *Ex parte Morris S. Kharasch* (1938) 19 USPQ 185, 186.

<sup>118</sup> *Ibid.*

<sup>119</sup> Bert Russell, ‘The Improvements of Our Patent System’ (1933) *Journal of the Patent Office Society* 666, 672. Faced with a patent which claimed ‘an enormous number of as yet non-existent compounds’ ... ‘to support a generic claim to a class of organic compounds’ a specification ‘should disclose specifically, a substantial fraction of the compounds in that class sufficiently diversified to illustrate all ramifications of the class’. Anon, ‘The Mortality of Chemical Patents in Court’ (1945–6) 34 *Georgetown Law Journal* 504, 510.

<sup>120</sup> Ridsdale Ellis, *Patent Claims* (New York: Baker, Voorhis and Co, 1949), 284.

<sup>121</sup> Eugene Geniesse, ‘Adequate Description’ (1945) 27 *Journal of the Patent Office Society* 784, 788.

<sup>122</sup> E. A. Ustinoav and O. V. Chelischeva, ‘Are Markush Structures Matters of Chemistry and Law or Just Figments of the Imagination?’ (1996) 18(1) *World Patent Information* 23, 24. Paper chemistry ‘degrades science and discredits the patent system’ (*ibid.*).

hidden chemical microworld that was beyond the reach of scientists, speculative claims were allowed not because it was not possible to visualise what happened beneath the surface of a compound; rather, they were allowed because it was not feasible to test them.<sup>123</sup>

Although it had no real impact on the way chemical patents were treated, class-based chemical inventions based on structural formulas did not fit comfortably with the distinction traditionally drawn in patent law between practical patentable results and non-patentable theoretical knowledge (or discovery). This was because, as one critic complained, 'a description of what may be "visualized" is not a description of an invention nor discovery'.<sup>124</sup> As a result, class-based chemical patents occupied 'a gray zone', which made them 'difficult to categorize'.<sup>125</sup> A key reason why chemical patents were so hard to categorise (at least according to traditional accounts) was because they represented the 'modern reunification of the theoretical and the experimental'.<sup>126</sup> That is, chemical subject matter brought together things that were, at least from a mechanistic understanding of patent law, meant to be kept apart. While in other contexts, this may have been problematic, this was not the case with chemical patent law, which was able to accommodate a hybrid subject matter.

The adoption of structural formula in patent law fundamentally changed chemical subject matter. Previously, patent law had identified and dealt with chemical subject matter in terms of the elements that were combined to form the compound (typically expressed by way of empirical formula), along with the defining physical traits of the resulting composition that had been tested and verified in the laboratory. Here, the intangible interest was not only inextricably linked to but also treated as if it was coextensive with the physical form (exemplified most clearly in the deposited specimen). As a result, chemical subject matter, which was limited to single individual compounds, operated at the level of the species. This is in marked contrast to subject matter post-structural formula. This is because by reducing the chemical subject matter to the structural formula and the corresponding name, the paper-based subject matter was detached from its physical form. This dematerialisation of the subject matter not only changed the way that the doctrinal rules were applied, it also paved the way for class-based claims. As a result, chemical subject matter moved from the level of species to that of genus: a process that also saw chemical subject matter become both quantitative and speculative.

While chemical subject matter changed considerably over the nineteenth and early twentieth centuries, one thing that remained consistent was patent law's reliance on chemistry in dealing with that subject matter. Organic chemistry not only

<sup>123</sup> It was possible to test the presumptions made about the existence of yet-to-be made compounds, but this had not occurred and, for various reasons, patent law was comfortable with this.

<sup>124</sup> Eugene Geniesse, 'Adequate Description' (1945) 27 *Journal of the Patent Office Society* 784, 789.

<sup>125</sup> Stanley H. Cohen and Charles H. Schwartz, 'Do Chemical Intermediates Have Patentable Utility?' (1961) *Journal of the Patent Office Society* 479.

<sup>126</sup> Roald Hoffmann and Pierre Laszlo, 'Representation in Chemistry' (1991) 30(1) *Angewandte Chemie* 1, 3.

consistently produced new objects for legal scrutiny, it also provided patent law with the means to deal with that subject matter. Patent law's willingness to use science when dealing with chemical subject matter was wholehearted, unreserved, and, for the most part, consistent. Not only was legal doctrine tailored to take account of the idiosyncrasies of organic chemistry, patent law and practice also relied on chemistry to identify, evaluate, and distinguish chemical subject matter. In some cases, the influence was indirect, such as with the standardisation of laboratory equipment. In other cases, however, the influence was more direct, such as with the use of structural formula to identify chemical compounds.

While a chemical understanding of the subject matter always had to be filtered through a legal lens, chemistry consistently provided answers to the legal questions being asked of the subject matter. In this sense, it is not a stretch to say that many legal questions were decided scientifically.<sup>127</sup> Indeed, one of the things that a history of patent law reveals is that the laws and procedures that were developed to deal with chemical innovations were a hybrid mixture of legal demands and chemical solutions. Whether in determining whether and if so when a compound had come into existence, or considering whether a compound was new, obvious, or useful, or in deciding if two compounds were the same or different, patent law consistently looked to chemistry for answers. This is not so much a case of the law looking outside of itself to external experts to provide answers to legal questions (which is one of the things that scholars of law, science, and technology have tended to focus on), so much as the products of that expertise becoming embodied or internalised within the law. Whether in patent documents, doctrinal rules, or Patent Office practice and procedure, chemistry was integrated into and became a part of patent law.

While the resulting 'judicial chemistry',<sup>128</sup> which was highly technical and specialised, allowed patent law to protect the outputs of organic chemistry, at the same time it also ostracised many academics, lawyers, and judges who found it difficult to comprehend chemical subject matter, which was 'at once both part of the patent-legal and scientific literature'.<sup>129</sup> Indeed, when called upon to decide the patentability of a patent for purified adrenalin in *Parke-Davis v. Mulford*, Judge Learned Hand complained about the 'extraordinary condition of the law which makes it possible for a man without any knowledge of even the rudiments of chemistry to pass upon such questions as these', because 'only a trained chemist is really capable of passing upon such facts, e.g., in this case the chemical character of Non Furth's so-called zinc compound or the presence of inactive organic substances'.<sup>130</sup> As a result, judges were left blundering and 'blindly groping among testimony upon matters wholly out of their ken'.

<sup>127</sup> At best, and comparatively rarely, the law was called upon to adjudicate on different scientific interpretations of scientific matters.

<sup>128</sup> R. Frankel, 'Chemists Should Read Patents' (1942) *Journal of the Patent Office Society* 565, 567.

<sup>129</sup> Edward H. Valence, 'Understanding the Markush Claims in Chemical Patents' (1961) 1 *Journal of Chemical Documentation* 87.

<sup>130</sup> *Parke-Davis v. Mulford* 189 F 95, 115 (CCSNY 1911).

## TOWARDS A MORE LEGAL SUBJECT MATTER?

As we have seen, patent law consistently relied on science to identify, demarcate, and classify chemical subject matter. Whether it was a mix of empirical formula and a compound's physical properties identified in a laboratory or, at the end of the nineteenth century, a compound's structural formula and/or its associated name (or a combination thereof), patent law routinely followed the scientific understanding of chemical subject matter. In these contexts, what the compound did – its function – was simply not relevant. The fact that utility was effectively guaranteed (because of the potential for compounds to be used to develop other compounds) meant that patent law focused almost exclusively on either the physical properties or the structure of the compound.

While patent law routinely internalised and followed the scientific rendering of chemical subject matter it was not all one-sided. The first crack in the unquestioned acceptance of a chemical understanding of the subject matter in patent law appeared in a series of cases at the turn of the nineteenth century where the courts adopted a more functional understanding of chemical compounds.<sup>131</sup> This can be seen, for example, in the 1896 decision of *Matheson v. Campbell*, which concerned a patent for a dye made from coal tar known as azo-black. The problem facing the patentee was that as azo-black dye had previously been imported into the United States, questions were raised about the patent's novelty and thus its validity. Because the patentee claimed azo-black as a product (rather than a process), it did not matter that the patented azo-black was made using mono-sulpho acid, while the imported azo-black had been made from di-sulphic acid. Instead, all that mattered was whether or not the imported dye was the same as the patented dye. In deciding whether the compounds were the same, the majority focused on a series of chemical tests that the patentee had included in the patent to identify the compound (including the fact that the resulting solution was very soluble in water, insoluble in spirit, dissolved in strong sulphuric acid with green colour, and so on). As the court said, the product 'answers all the tests of the patent, and other well-known tests not therein named, and that the azo-black is therefore the equivalent of naphthol-black and therefore anticipates it'.<sup>132</sup> On the basis that the products were chemically identical, the majority found the patent invalid for lack of novelty.

While the majority in *Matheson v. Campbell* relied upon the scientific tests of the subject matter set out in the patent, Judge Townsend (in dissent), ignored the scientific reading of the subject matter in considering whether the imported and patented dyes were the same. Instead, he compared the compounds in terms of

<sup>131</sup> It also occurred with the shift towards the quantitative evaluation of the subject matter that took place when determining the number of exemplary compounds that needed to be tested to prove the existence of a class of compounds. While chemistry may have provided some assistance, ultimately this was a legal question that required a legal solution.

<sup>132</sup> *Matheson v. Campbell* 7 Fed Reporter 280, 281 (Circuit Court, SD New York, 18 May 1896).

their effectiveness as dyes. As he said, ‘whatever may be the similarity or equivalency chemically, I do not understand that the azo-black was commercially or practically the same thing as the black of the patent in suit’.<sup>133</sup> The reason for this was that the imported dye was inferior to the patented dye (it rubbed off and was more expensive). For Judge Townsend, the ‘fact that the prior azo-black was sold in small quantities, at a high price to the public, whereas the complainant’s invention, a superior article is produced at a lower price, and is a marked commercial success, entirely replacing the original article in the market, is of much greater importance in the determination of the question of equivalency than are any mere chemical test, as to the sufficiency and effect of which experts differ and the court is in doubt’.<sup>134</sup> While chemical experts may have declared the patented azo-black and the imported azo-black to be chemically identical, the key factor for Judge Townsend was that they were not *practically* identical.<sup>135</sup>

One of the notable things about *Matheson v. Campbell* was that the imported dye had been described and named incorrectly. As the court noted, the imported dye was ‘now known to be in fact a naphthol-black’ rather than an azo-black dye.<sup>136</sup> While Judge Townsend was aware of this error, he did not challenge the accuracy of the scientific interpretation of the subject matter in reaching his decision. Instead, he simply shifted away from a scientific understanding of whether or not the two compounds were the same (the answer being yes) to focus on how the compounds functioned (the answer being differently).

The 1910 decision of *Kuehmed v. Farbenfabriken*, which concerned the validity of Felix Hoffmann’s patent for acetyl salicylic acid (aspirin),<sup>137</sup> is another situation where the courts were willing to ignore a scientific understanding of chemical subject matter. In his patent Hoffmann claimed acetyl salicylic acid as a new article of manufacture. After outlining the chemical formula, Hoffmann then described the physical traits of his invention including that when it was in a crystallized form it was easily soluble in benzene, alcohol, and glacial acetic acid, it was split by hot water into acetic acid and salicylic acid, and that it melted at about 135° centigrade. One of the notable things about the compound that Hoffmann had invented was that unlike previous products that were undesirable and unsafe, Hoffmann’s aspirin was both effective and safe.

The problem Hoffmann faced when he lodged his application in August 1898 was that in the 1859 edition of the leading journal of organic chemistry, *Annalen der Chemie und Pharmacie*, the German chemist Karl Kraut had not only disclosed a process for making acetyl salicylic acid, he also named and provided the structural formula for ‘acetyl salicylic acid’. As the compound disclosed in Kraut’s 1859

<sup>133</sup> *Ibid.*, 282.

<sup>134</sup> *Ibid.*, 284.

<sup>135</sup> *Ibid.*

<sup>136</sup> *Ibid.*, 281.

<sup>137</sup> Felix Hoffmann, ‘Acetyl Salicylic Acid’ US Patent No. 644,077 (27 February 1900).

publication and the compound disclosed in the patent were chemically identical, it potentially undermined the novelty and thus the validity of Hoffmann's patent. Aware of this, Hoffmann challenged the pre-existing disclosure arguing that Kraut had not in fact made the 'real' acetyl salicylic acid. As he said, 'the compound described by Kraut cannot be the real acetyl salicylic acid, but is another compound'. To prove this, Hoffmann included in the patent the results of a series of chemical tests he had conducted on the two compounds that showed that the compounds were different.<sup>138</sup> Specifically, Hoffmann distinguished his 'real' acetyl salicylic acid from Kraut's 'fake' acetyl salicylic acid in terms of (i) what happened to them when they were boiled with water (with Kraut's compound no acetyl salicylic acid was produced, whereas acetyl salicylic acid was produced with Hoffmann's), (ii) what happened when a watery solution of the compound was mixed with ferric chloride (Kraut's solution turned a violet colour whereas Hoffmann's did not) and (iii) if a melted solution of the compound was allowed to cool, the temperature at which it solidified (Kraut's compound solidified at 118° to 118.5° centigrade whereas Hoffmann's solidified at 'about 70° centigrade'). On the basis of these tests, Hoffmann said that the two compounds were 'absolutely different' and that 'the body obtained by means of my new process is undoubtedly the real acetyl salicylic acid [formula].<sup>139</sup> Therefore, the compound described by Kraut cannot be the real acetyl salicylic acid, but is another compound'.<sup>140</sup>

While the court ultimately agreed with Hoffmann that his patented compound was different to Kraut's, it used different reasoning to reach the same conclusion. While Hoffmann had taken the scientific route of testing the compounds in a laboratory to show that they were not the same, the court began by casting doubts over the accuracy of chemical formula generally, something that Hoffmann would have strongly disagreed with. As the court said, the 'fact that the formulae are identical cuts little figure. A chemical formula is simply the symbolic expression of the composition or constitution of a substance; as the formula for water is H<sub>2</sub>O'. The court continued in its attempt to undermine the accuracy of chemical formula arguing that '[c]ustomarily, chemists who intend to produce a combination of two substance write the formula of the product in advance of making it'. They continued in this vein saying that '[w]ithout doubt, processes have been described in chemical publications which give products differing somewhat in their chemical structure and name from which the writer supposed would be produced' or obtains a product that is not correctly represented by the structural formula or name given'.<sup>141</sup> In a statement that both misrepresents the nature of chemical formula and also confuses chemical compounds (such as H<sub>2</sub>O) with mixtures of

<sup>138</sup> Ibid.

<sup>139</sup> Ibid.

<sup>140</sup> Ibid. The 'responses to tests seems to be a fair method of determining the lack of identity of the product in suit.' *Kuehlmsted v. Farbenfabriken* 179 Fed 701, 707 (7th CCA 1910).

<sup>141</sup> Ibid., 703.

chemical compounds (such as sea water, which is made up of water (H<sub>2</sub>O) and other compounds including chloride, sodium, magnesium, and sulfate), the court went on to say that ‘assuming that the formula actually expresses the constitution of the substance chemically, the substance physically, and in consequences therapeutically, may be widely different, as, for instance, the water of the seas, differs, in its physical body from the water of certain springs, though the chemical formula for “water”, whether sea or spring, is H<sub>2</sub>O. That is to say the two substances, having the same chemical formula, may differ widely, as to impurities upon quantitative analysis’.<sup>142</sup>

After downplaying the usefulness of chemical formula as a way of identifying compounds, the court felt free to shift its attention to focus on what the compound did: its function. Ignoring the fact that the compounds had the same chemical name and formula (and were thus chemically the same), the court held that Hoffmann’s compound (which passed through the stomach to dissolve harmlessly in the intestine) was therapeutically different from Kraut’s compound (which broke down in the stomach causing harm to users). In so far as Hoffmann had produced a compound that was effective and safe compared to previous compounds that were ‘undesirable and unsafe’, the court held that Hoffmann had produced ‘a medicine indisputably beneficial to mankind – something new in a useful art, such as our patent policy was intended to promote’.<sup>143</sup> In the words of the lower court, Hoffmann took a comparatively worthless substance and changed it into something valuable.<sup>144</sup>

Unlike disputes over the patentability of aniline red dye in France in the early 1860s, where the push to look at dyes in terms of their functional properties rather than their structure was a consequence of scientific uncertainty (‘because “science” was far from reaching a definitive answer ... “practice” should have a much larger voice in the formation of judicial decision’ on patentability),<sup>145</sup> the decision to focus on a compound’s function in *Kuehmsted* was not so much the result of scientific uncertainty, so much as that the science was wrong. While it was rare for the courts to be confronted with such an obvious scientific mistake, these decisions were harbingers of an approach to chemical subject matter that was to reappear, albeit inconsistently and sporadically, in the future where the courts would ignore a chemical understanding of the subject matter that identified a compound by its chemical structure (sometimes referred to as ‘pure chemistry’)<sup>146</sup>

<sup>142</sup> *Ibid.*, 703–4.

<sup>143</sup> *Ibid.*, 705.

<sup>144</sup> *Kuehmsted v. Farbenfabriken* 171 Fed. 887, 890 (1909).

<sup>145</sup> Henk van den Belt, ‘Action at a Distance: A.W. Hofmann and the French Patent Disputes about Aniline Red (1860–1863), or How a Scientist May Influence Legal Decisions without Appearing in Court’ in (ed) R. Smith and B. Wynne, *Expert Evidence: Interpreting Science in the Law* (London: Routledge, 1989), 184.

<sup>146</sup> Anon, ‘The Mortality of Chemical Patents in Court’ (1945–46) 354 *Georgetown Law Journal* 504, 509 n 29 (neither court permitted the dust of the prior art relating to pure chemistry to obscure the issue).

to look instead at what the compound did or, as in *Park Davis*, what its therapeutic properties were.<sup>147</sup>

While these decisions were atypical in the sense that they remained exceptions to the general rule that patent law consistently looked to and followed a scientific understanding of the subject matter,<sup>148</sup> nonetheless they are still important in so far as they highlight an issue that the law has long struggled with: namely, faced with a hybrid subject matter that can be construed in different and sometimes inconsistent ways, how and why is one reading favoured over another? A recent example of this can be seen in the *Myriad* litigation (involving the patentability of gene patents) where the subject matter (isolated genes) was able to be construed either chemically (which led to a finding of patentable subject matter) or genetically (which led to a finding of non-patentable subject matter). This is an important issue that I will return to later.

#### MARKUSH CLAIMS AS SCIENTIFIC-LEGAL HYBRIDS

Another situation where patent law did not follow scientific practice was in situations where chemical nomenclature failed to provide the tools needed to adequately describe chemical inventions in a legal context. This was particularly evident in relation to Markush claims, which were approved by the courts in the 1924 decision of *Ex Parte Markush*.<sup>149</sup>

In 1923, Eugene Markush, the founder and President of the New Jersey Pharma Chemical Corporation that specialised in synthetic dyes, filed an application in which he made a series of alternative claims, namely for ‘a diazotized solution of aniline or its homologues or halogen substitutes’. While claims of this nature had been accepted previously, Markush’s claims were rejected in the words of the sub-committee on chemical practice of the Michigan Patent Law Association by an ‘overzealous’ examiner.<sup>150</sup> In response, Markush replaced his original alternate claims with the generic term ‘mono-amine’. The revised application was also rejected; this time on the basis that because it embraced material that was known to be inoperative, it was too broad.

The problem that Markush faced, which was increasingly common at the time, was that by claiming a very large classes of compounds there was a risk that the

<sup>147</sup> While *Parke-Davis* is usually seen as having laid the foundation for the product of nature doctrine, I prefer to look at it as an exception to the longstanding practice whereby legal questions about chemical substances were resolved using scientific criteria. For a history of the decision see Christopher Beauchamp, ‘Patenting Nature: A Problem of History’ (2013) 16 *Stanford Technology Law Review* 257.

<sup>148</sup> See also *Schering Corporation v. Gilbert* 153 F.2d 428, 435 (1946) (claim dismissed on the basis that it was ‘nothing but a chemical formula’). Or, as Judge Rich said, ‘a chemical compound and all of its properties are inseparable from the standpoint of patent law. The thing patented in a chemical compound is not the formula, which merely gives an identification, but the compound identified by it. What is critical is not the similarity of the formula to that of formulas of the prior art, but the similarity of the compounds and of all of their properties’. *In re Papesch* 315 F.2d, 137 USPQ 43 (CCPA 1963).

<sup>149</sup> *Ex parte Markush* 1925 CD 126 (Comm’r Pat. 1924).

<sup>150</sup> Sub-Committee on Chemical Practice, Michigan Patent Law Association, ‘Markush Claims’ (1955) *Journal of the Patent Office Society* 164, 166.

patent might inadvertently include individual compounds or groups of compounds that were inoperative (and invalid). While with mechanical inventions this was not an issue, it was with chemical inventions because the existence of even a small number of inoperative compounds could potentially defeat a generic claim.<sup>151</sup> The problems Markush faced were compounded by the fact that there was no readily available scientific term that he could use to describe his invention in a way that simultaneously captured both the breadth of the class of inventions and, at the same time, also excluded those individual compounds that were legally invalid. As a result, by 1925 'it was becoming extremely difficult for applicants to define their inventions adequately in terms of available, recognized generic expressions'.<sup>152</sup> The reason for this was that the 'existing nomenclature failed to supply a term commensurate in scope with the field which the applicant was entitled to cover'.<sup>153</sup> In this sense, science was not up to the demands that the patent system was making of it.

Markush responded to this dilemma by amending the scientific nomenclature to suit his legal needs. He did this by adding the expression 'material selected from the group consisting of aniline, homologues of aniline and halogen substitution products of aniline' to his generic scientific claim. After the revised hybrid claim was rejected by the examiner, Markush appealed to the Commissioner of Patents who allowed the revised claim saying: 'if there is no known sub-generic term' there was no reason why an applicant should not be able to be 'employ a generic term limited by explanatory terms in the absence of anticipating art'. So long as the modified claims did not do violence to the accepted principles of scientific classification, they were acceptable.<sup>154</sup> While these types of claims had been used for some time, *Ex Parte Markush* was the first decision to rule on such a claim. The hybrid claim, which became known as a Markush claim, were readily accepted by the Patent Office, the courts, and patentees.<sup>155</sup>

In essence, a Markush claim allows a patentee to claim material selected from a general class of compounds in an abbreviated way. The claims operate in situations

<sup>151</sup> The Markush claim was designed for 'emergency situations' such as where 'the genus is of vast extent and comprises substances of rare occurrence or not easily obtainable for experimentation'. The problem here was that there was a 'possibility that there may exist some little known substance within the genus which is inoperative in the applicants process (or composition) and which would consequently defeat a generic claim. It only seems fair to permit the use of a claim of the Markush type under such conditions. Such a 'Markush' claim must be restricted to the members of the generic class which applicants has shown in his application to be operative for this purpose'. *Ex parte Mayne* (PO Bd App) 59 USPQ 342. *Ex parte Dahlen* 21 USPQ 397, 1934 CD 9.

<sup>152</sup> Sub-Committee on Chemical Practice, Michigan Patent Law Association, 'Markush Claims' (1955) *Journal of the Patent Office Society* 164, 166.

<sup>153</sup> There was a 'lack of a suitable term or terms which will properly define the true scope of an applicant's invention'. *Ex parte Clark and Malm* 11 USPQ 52, 53.

<sup>154</sup> *Ex parte Dahlen* 1934 CD 9; 21 USPQ 397 (Comm December 1934) (cannot be so dissimilar that the grouping would be 'repugnant to accepted principles of scientific classification to associate them together as a generic if sub-generic group', *Ibid.*, 399).

<sup>155</sup> Manuel Rosa, 'Outline of Practice Relative to "Markush" Claims' (1952) *Journal of the Patent Office Society* 324.

where scientific nomenclature fails to provide an adequate term to describe the invention; they are used in place of the ordinary generic claim when no generic language is available to describe one of the features of the invention together with its stated equivalents.<sup>156</sup> As the Commissioner of Patents said, 'the paucity of the language may necessitate a waiver of the technical rules of this Office to the end that the applicant may properly protect his real invention.'<sup>157</sup>

In providing a solution to the problem created by the peculiarities of class-based generic chemical formula, the Markush claim is an interesting blend of the scientific and the legal. This was because the sub-group that was excluded from the generic class of compounds simultaneously shared scientific things in common with other members of the overarching class of compounds while, at the same time, it differed legally from the class as a whole. In this sense, the Markush claim offers an example of a situation where the law modified chemical practice to its own ends. Because, chemically speaking, the sub-class was grouped arbitrarily (which had to be taken from a 'natural genus'),<sup>158</sup> the Markush claim was recognized as an artificial genus that was designed to separate operative and inoperative compounds.<sup>159</sup> It was a novel legal-scientific taxonomic hybrid that was devised to afford patent protection for chemical inventions where the existing scientific nomenclature 'failed to supply a term commensurate in scope with the field in which the applicant was entitled to cover'.<sup>160</sup>

While the hybrid nature of the Markush claim, which merged scientific and legal nomenclature, successfully allowed patent law to accommodate class-based chemical inventions, it was criticised by both legal and scientific purists. In part this was because like so many things in chemical patent law, Markush claims required some familiarity with the science. While patent office examiners were comfortable in dealing with chemical nomenclature, the courts were often less so. This can be seen in the complaint made by the court in *In re Thompson* that 'there has never been any explanation by the Patent Office tribunals how it is determined that the substances in a Markush type claim possess or do not possess' the requisite qualities needed for them to be valid.<sup>161</sup> The legal nature of the Markush claim also occasionally attracted the ire of chemists who found them difficult to understand, 'baffling', and an 'seemingly absurd idiom', which was a product of the fact that the claims appear to be scientific but are not. At heart the complaint here was that the legal system was exceeding its authority not least because 'chemistry can only be described adequately by chemists'.<sup>162</sup>

<sup>156</sup> Robert F. Davis, 'Interpreting the Markush Decision' (1933) *Journal of the Patent Office Society* 187.

<sup>157</sup> *Ex parte Markush* 1925 CD 126 (Comm'r Pat. 1924).

<sup>158</sup> V. Richard, 'Infringement of a Markush Claim' (1941) *Journal of the Patent Office Society* 529, 531.

<sup>159</sup> Harold C. Wegner, 'The Right to Generic Chemical Coverage' (1978) 6 *APLA Quarterly Journal* 257, 261.

<sup>160</sup> *Ex parte Mayne* (PO Bd App) 59 USPQ 342.

<sup>161</sup> *In re Thompson* 61 USPQ 498 (1944).

<sup>162</sup> E. A. Ustinoav and O. V. Chelisheva, 'Are Markush Structures Matters of Chemistry and Law or Just Figments of the Imagination?' (1996) 18(1) *World Patent Information* 23, 24.

## LEGAL INFLUENCES ON CHEMICAL INFORMATION

Another situation where patent law's relationship with science was less one-sided was in terms of the way chemical information was organised and the role that patent law played in this process. (It seems that patent law also played a role in standardising drawing practices for chemical publications).<sup>163</sup> Chemical information, which was pivotal to the success of organic chemistry, took many forms including journal articles, patents, reference works, and textbooks.<sup>164</sup> One of the challenges that organic chemistry continually faced was ensuring that this ever-expanding corpus of information was able to be used.<sup>165</sup> Over time, a range of different methods were used to organise chemical literature to make it more accessible. These included the development of abstract journals, digests, and specialist bulletins such as the National Research Council's *Bibliography of Bibliographies in Chemistry and Chemical Technology* (1900–1924) and Marion E. Spark's *Chemical Literature and Its Use* (1921).<sup>166</sup> While these are important, I wish to focus here on the efforts of Edwin A. Hill, who after working as a lawyer and civil engineer for various railway companies 'switched gears' to undertake a PhD in chemistry at George Washington University where he subsequently become a professor of chemistry and his attempts to organise and catalogue chemical substances for use by the Patent Office.

One of the requirements for a patent to be valid is that the invention must be novel or new: that is, the invention must not have been available in the public domain previously. When examining a patent application, patent examiners search the prior art to determine whether the invention is in fact new. In many ways, the effectiveness of the examiner's search is largely dependent on the way that the prior art is organised and classified and whether it is legible to patent examiners. One of the challenges that the Patent Office faced when examining applications for chemical patents was the sheer size of the chemical prior art and the fact that much of it was chaotic and disorganised. As a result 'anything like a complete search' was 'rendered practically impossible'.<sup>167</sup> One of the

<sup>163</sup> Patent Office rules that specified how chemical inventions were to be represented in patents were used as part of the platform to standardise drawing practices for chemical publications. N. Edward and M. Hoshall, 'Chemical Drawing' (1934) *Journal of Chemical Education* 21, 27.

<sup>164</sup> Anon, 'Utilization of Chemical Literature' (15 March 1941) *Nature* 310. Patents were particularly useful source of chemical information in so far as they were up to date and also because they often were the only source of information for some compounds.

<sup>165</sup> In order to 'avoid priority struggles and parallel research one needs a powerful classification system, based on established criteria of species identity and able to incorporate indefinitely many new species.' J. Schummer, 'The Impact of Instrumentation on Chemical Substance Identity' in (ed) P. Morris, *From Classical to Modern Chemistry: The Instrumental Revolution* (Cambridge: The Royal Society of Chemistry, 2002), 188, 195.

<sup>166</sup> See Ivan P. Tashof, 'Prior Art Investigations' (1925–26) 8 *Journal of the Patent Office Society* 432.

<sup>167</sup> Edwin A. Hill, 'Chemical Patent Searches and the Chemical Card Index' (1923–24) *Journal of the Patent Office Society* 506, 508.

consequences of this was that 'the validity of chemical patents was more or less in doubt' because 'a five-line paragraph in the files of some little known chemical journal ... would be sufficient if cited in court to invalidate the granted patent'.<sup>168</sup> To address this problem, in 1899 the US Patent Office commenced work under the guidance of Edwin A. Hill to develop a bibliographical card index of chemical substances for use in its official work. As Hill said, the Patent Office needed the index for the same purpose as the scientific or practical chemist; to 'obtain references to the literature concerning definitive chemical bodies, where either the name or the chemical composition or both is given'.<sup>169</sup>

As we have seen, one of the notable things about chemical substances is that they can be represented in a number of different ways, notably in terms of their official scientific names, as well as their empirical and structural formula. In putting his index together, Hill was faced with a decision as to which of these modes of representation he was going to use to organise chemical substances. For Hill, chemical names were not an option, not least because they were often unclear and changing. This was because as Hill said in an address to the Washington section of the American Chemical Society in 1900, 'most bodies known to chemists have more than one name, many have several, and the names approved in prior decades are generally not the names on highest repute to-day; nor is it likely that the names now in use will in all or even in most cases, remain in future years'.<sup>170</sup> One of the consequences of this was that it made a dictionary approach to the ordering the chemical prior art, which arranged chemical compounds alphabetically by name problematic. These problems were compounded by the fact that many chemical bodies were unnamed, which made a dictionary-style approach even more problematic.

Hill also rejected the use of structural formula to organise the card index. This was because he was guided by the principal that a 'reference index or digest should in no way depend upon any theory subject to future changes with advancing knowledge'.<sup>171</sup> The reason why he wanted to avoid theory-based representations of compounds (such as structural formulas) was because there was always a chance that if the theory changed, the structural formula would also change. The decision to avoid using any theoretical information in organising chemical compounds meant that Hill could not use structural formulas in developing his alphabetical list. As Hill

<sup>168</sup> *Report of the Taft Commission on Classification of Patents and Printed Publications*, as cited in J. Harold Byers, 'A Chemical Patent Index' (1934) *Journal of the Patent Office Society* 36.

<sup>169</sup> Ever 'since chemists started to represent chemical substances by means of names, formulae, and symbols, there was the need to find information about specific compounds, and this was primarily through the use of indexes where names would have to be searched for in the same way as other topics'. Helen Cooke, 'A Historical Study of Structures for Communication of Organic Chemistry Information Prior to 1950' (2004) 2 *Organic and Biomolecular Chemistry* 3179, 3189.

<sup>170</sup> Edwin A. Hill, 'On a System of Indexing Chemical Literature: Adopted by the Classification Division of the US Patent Office' (1900) *Journal of the American Chemical Society* 478, 479.

<sup>171</sup> *Ibid.*

said, the ‘indexing, and conversely, the finding of the body in the index’ should be rendered ‘absolutely independent of any theories of constitution [or structure] whatsoever.’ This meant that the index needed to be ‘independent of any changes in the formula consequent upon future changes of view with reference to constitutional [structural] formulas and other matters of theory’.<sup>172</sup>

Instead of using scientific names or structural formulas to organise the *Card Index to Chemical Literature*, Hill decided to use empirical formula as the basis for indexing and digesting chemical literature. This was because while names and structural formula may change, one thing that did not change – ‘the one unchangeable mark of identification of the substance’ – were the elements in a compound, which were represented by its empirical chemical formula.<sup>173</sup> As Hill said, the ‘kind and number of the component atoms of a chemical compound’ which are set out in an empirical formula’ are its most unvarying characteristic, and are subject only to errors of chemical analysis’.<sup>174</sup> By focusing on the empirical formula of a compound, Hill could say that ‘the use of the digest is as far as possible independent of all theory, and founded only on unchanging facts.’<sup>175</sup>

With this decided, the next question that arose was how the empirical formula should be translated into an alphabetical list. As Hill said, the ‘simplest, most certain and most direct system would be to recast the empirical formulas of the compounds, writing the atoms in the alphabetical order of their chemical symbols and them to arrange the formula on an alphabetical basis.’<sup>176</sup> The problem with this, however, was that as most organic compounds contain ‘C’ and ‘H’, if a straightforward application of the alphabetical organisation was used, it would have created problems in so far as it would have separated compounds that should have been grouped together. To avoid this, Hill proposed that the alphabetical approach should be modified so that the number of C atoms should be written first, the number of H atoms should be written second, and the remaining elements should be arranged alphabetically by their symbols.<sup>177</sup> The revised and rewritten formula were then arranged alphabetically. As Hill said, the rewritten formula was an ‘arbitrary arrangement’ that ‘unerringly indicates one, and one only, definite and specific place in the index where we are to look for all references with a certainty that no other character, name or tile of the body can afford’.<sup>178</sup>

From three to six workers supervised by Hill worked continuously on the card index from 1900 to around 1920 (when it was suspended due to cost). The index

<sup>172</sup> *Ibid.*, 483.

<sup>173</sup> Edwin A. Hill, ‘Chemical Patent Searches and the Chemical Card Index’ (1923–24) *Journal of the Patent Office Society* 506, 509.

<sup>174</sup> Edwin A. Hill, ‘On a System of Indexing Chemical Literature: Adopted by the Classification Division of the US Patent Office’ (1900) *Journal of the American Chemical Society* 478, 479.

<sup>175</sup> *Ibid.*, 488.

<sup>176</sup> *Ibid.*, 479–80.

<sup>177</sup> *Ibid.*, 480.

<sup>178</sup> *Ibid.*, 492.

## ONE FORMULA CARD :

$C_{12}O_{18}Fe_2O_{12}$  or  $(CH_3.CO_2)_6Fe_2$ .  
 Ferric Acetate ; Acetate of Iron ;  
 Klapproth's Iron Tincture; Tinctura  
 Ferri Acetatis ; Iron Tincture,  
 Klapproth's.

See A Treatise on Chemistry. By H. E.  
 Roscoe and C. Schorlemmer, Vol. 3, Or-  
 ganic Chemistry, Part I, Page 505.

## ONE POLYMER OR MULTIPLE FORMULA CARD :

$C_6H_9FeO_6$  Polymer Class 2.  
 See  $C_{12}H_{18}Fe_2O_{12}$  or  $(C_6H_9FeO_6)_2$   
 Ferric Acetate.

## TWO CLASSIFICATION CARDS :

Acetates  
 Ferric.  
 See  $C_{12}H_{18}Fe_2O_{12}$  or  $(CH_3.CO_2)_6Fe_2$ .

Iron  
 Acetate of.  
 See  $C_{12}H_{18}Fe_2O_{12}$  or  $(CH_3.CO_2)_6Fe_2$ .

## FOUR SUBJECT-MATTER OR TITLE CARDS :

Ferric Acetate  
 See  $C_{12}H_{18}Fe_2O_{12}$ .

Klapproth's Iron Tincture  
 See  $C_{12}H_{18}Fe_2O_{12}$ .

Iron, Klapproth's Tincture of  
 See  $C_{12}H_{18}Fe_2O_{12}$ .

Tinctura Ferri Acetatis  
 See  $C_{12}H_{18}Fe_2O_{12}$ .

FIGURE 4.4 Library Bureau Card for Ferric Acetate  
 United States Patent and Trademark Office, Chemical Index.

was prepared and placed on a 7½ by 12½ cm Library Bureau card (see Figure 4.4). The rearranged formula of the compound was placed at the top of the card above a ruled blue line. Below the line, all of the given names of the compound were listed along with reference to any works indexed. By 1907, the card index included nearly

500,000 cards.<sup>179</sup> By 1923 the card index had increased to over one million cards in 1040 drawers.<sup>180</sup>

The completed card index, which was described as a ‘national monument to chemical literature’,<sup>181</sup> was placed in the Patent Office Library where it was made available for use by patent examiners, patent lawyers, chemists, and scientific workers (all free of charge). While the card index was used ‘enthusiastically’ during the war by the Chemical Warfare Service<sup>182</sup> and was popular with members of the public, Hill complained that the index was not used much by patent examiners primarily because it was located ‘far away from the examining divisions’ in ‘cramped, narrow and ill lighted quarters’.<sup>183</sup> Despite repeated recommendations from a range of quarters that the indexing work should be continued, a lack of funding meant that by 1934 Hill’s card index at the Patent Office was obsolete.<sup>184</sup>

While Hill’s card index may have run its course at the Patent Office by the 1930s, nonetheless it had an important and long-lasting impact on the way chemical information was organised outside of the legal system. This was particularly the case in relation to the efforts undertaken by the American Chemical Society to shape chemical literature. ‘Faced by the unwieldy chaotic mess of rapidly accumulating chemical facts and chemical theories’ the American Chemical Society established the magazine *Chemical Abstracts* in 1907 to ‘collect, condense and then publish it in an abstract of every worthwhile article on chemicals and chemistry appearing in the current scientific magazines in every language.’<sup>185</sup> By 1921, abstracts were taken of articles from over 738 periodicals and from US and select foreign patents.<sup>186</sup>

To improve access to information on compounds, in 1920 *Chemical Abstracts* decided to publish a formula index. While there were various scientifically driven indexes that could have been used, the index system adopted by the American Chemical Society in *Chemical Abstracts* was the system that Hill had developed for use at the Patent Office.<sup>187</sup> Hill’s system of organisation was chosen in preference to

<sup>179</sup> Edwin A. Hill, ‘The Chemical Card Index of the Patent Office’ (1907) 29 *Journal of the American Chemical Society* 936.

<sup>180</sup> Edwin A. Hill, ‘Chemical Patent Searches and the Chemical Card Index’ (1923–4) *Journal of the Patent Office Society* 506, 508. There were 1,200,000 cards by 1912: Edwin A. Hill, ‘The Card Index to Chemical Literature of the United States Patent Office’ (1912) 34 *Journal of the American Chemical Society* 416.

<sup>181</sup> L. H. Baekeland, ‘The Index to Chemical Literature’ (1913) *The Journal of Industrial and Engineering Chemistry* 534.

<sup>182</sup> Edwin A. Hill, ‘Chemical Patent Searches and the Chemical Card Index’ (1923–24) *Journal of the Patent Office Society* 506, 510.

<sup>183</sup> J. Harold Byers, ‘A Chemical Patent Index’ (1934) *Journal of the Patent Office Society* 36.

<sup>184</sup> *Ibid.*

<sup>185</sup> Edward Thomas, ‘Computing Progress in Chemistry’ (1936) *Journal of the Patent Office Society* 357.

<sup>186</sup> Frank E. Barrows, *Investigations of the Chemical Literature* (New York, 1921), 20.

<sup>187</sup> J. Harold Byers, ‘A Chemical Patent Index’ (1934) *Journal of the Patent Office Society* 36.

other chemical indexing systems such as Richter's Lexikon because of its simplicity and the speed and ease by which compounds could be located.<sup>188</sup>

As well as informing the way that *Chemical Abstracts* were indexed and the related Chemical Abstract Services (CAS) Number – which is the permeant, unique and unambiguous numerical identifier given to every chemical substance that is widely used by scientists and patentees today to define and describe chemical substances<sup>189</sup> – were organised, the Hill system was widely adopted and used within chemistry. Indeed it has been said that it is now the most commonly used system to sort lists of compounds in chemical databases and printed indexes.<sup>190</sup> What we see here is that as well as forming part of the chemical prior art, patent law also helped to shape the way chemical information was organised and classified. While in other contexts, patent law willingly followed the lead of chemistry, the roles were reversed when it came to the chemical public domain.

<sup>188</sup> William A. Noyes, 'Presidential Address: Chemical Publications' (1920) *The Journal of the American Chemical Society* 2017. The editors of the Chemical Abstracts 'gratefully acknowledge their indebtedness to Dr Edwin A. Hill for the opportunity and privilege of using his admirable system of arrangement'. American Chemical Society (December 1920) 14 *Chemical Abstracts* 4559.

<sup>189</sup> Chemical Abstracts Service, *A National Historical Chemical Landmark* (Chemical Abstracts Service, 14 June 2007), 2.

<sup>190</sup> Gary Wiggins, *Chemical Information Sources* (New York: McGraw Hill, 1991), 120.