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# Chemical translators: Pauling, Wheland and their strategies for teaching the theory of resonance

BUHM SOON PARK*

> It was well said by Clerk Maxwell: 'For the sake of persons of different types of mind scientific truth should be presented in different forms, and should be regarded as equally scientific whether it appears in the robust form and colouring of a physical illustration, or in the tenuity and paleness of a symbolical expression.'
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> From N. V. Sidgwick's Presidential Address to the Chemical Society, London, 1937

During the years between 1930 and 1950, chemistry underwent a transformation that affected both research and education. New subdisciplines like chemical physics and physical organic chemistry emerged, encouraging an influx of ideas and experimental techniques from physics. X-ray crystallography and other spectroscopic methods became indispensable for determining structures of atoms, molecules and crystals; such chemical concepts as valence and bond were refined within a new explanatory framework based on principles of physics; and the study of reaction mechanisms and rates became closely intertwined with that of structures and properties of chemical compounds. In conjunction with these changes, introductory chemical textbooks began to shift their emphasis from thermodynamic equations and solution theories to three-dimensional arrangements of atoms in molecules and types of chemical bonds. There is no doubt that the most important impetus behind this transformation was the development of quantum mechanics in the mid-1920s, and the most prominent among those who applied it to chemistry was Linus Pauling.[1] And

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* Department of the History of Science, Medicine, and Technology, The Johns Hopkins University, 3400 North Charles Street, Baltimore, MD 21218, USA.

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[1] For the transformation of chemistry in this period, see John W. Servos, *Physical Chemistry from Ostwald to Pauling: The Making of a Science in America*, Princeton, 1990; Mary Jo Nye, *From Chemical Philosophy to Theoretical Chemistry: Dynamics of Matter and Dynamics of Disciplines, 1800–1950*, Berkeley, 1993; and William H. Brock, *The Norton History of Chemistry*, New York, 1992. For changing trends in chemical textbooks, see M. J. Nye, 'From student to teacher: Linus Pauling and the reformulation of the principles of chemistry in the 1930s', in *Communicating Chemistry: Textbooks and Their Audiences* (ed. Bernadette Bensaude-Vincent and Anders Lundgnen), forthcoming.

in Pauling's view, 'the principal contribution of quantum mechanics to chemistry' was the concept of resonance.[2]

The entry of resonance into chemistry, or the reception of the theory of resonance in the chemical community, has drawn considerable attention from historians of science. In particular, they have noted Pauling's flamboyant yet effective style of exposition, which became a factor in the early popularity of the resonance theory in comparison to the molecular orbital theory, another way of applying quantum mechanics to chemical problems.[3] To be sure, the non-mathematical presentation of the resonance theory by Pauling and his collaborator, George Wheland, helped to facilitate the reception; but this presentation was vulnerable to the confusion that arose among chemists owing to the similarity between resonance and tautomerism, or between foreign and indigenous concepts. The reception occurred at the expense of serious misunderstandings about resonance. This paper investigates the ways in which Pauling and Wheland taught, and taught about, the theory of resonance, especially their ways of coping with the difficulties of translating a quantum-mechanical concept into chemical language. Their different strategies for teaching resonance theory deserve a thorough examination, not only because the strategies had to do with their solutions of the philosophical question whether resonance is a real phenomenon or not, and whether the theory of resonance is a chemical theory or a mathematical method of approximation, but also because this examination will illuminate the role of chemical translators in the transmission of knowledge across disciplinary boundaries.

## VISUALIZING RESONANCE AND MYSTIFYING THE THEORY OF RESONANCE

By the spring of 1926, Linus Pauling (1901–94) had risen from a promising student of chemical engineering at Oregon Agricultural College to a newly minted Ph.D. of California Institute of Technology (Caltech) and a National Research Fellow studying X-ray crystallography and quantum theory. He had already started his prolific life of publication by writing more than a dozen research papers, and now hoped to learn quantum mechanics in Europe as a Guggenheim Fellow, having an eye on its application to the problem of molecular structure and chemical bonds.[4]

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[2] Linus Pauling, *The Nature of the Chemical Bond*, Ithaca, 1939, preface, and 'Modern structural chemistry', *Science* (1956), **123**, 255–8, on 256.

[3] The resonance theory is often called the valence bond theory. It is based on the assumption that the molecule is a composite of atoms. By contrast, the molecular orbital theory sees the molecule as a separate entity. These disparate viewpoints stem from different ways of approximating the Schrödinger equation, and lead to different interpretations of chemical valence. For the comparison of the two theories, see D. A. Bantz, 'The structure of discovery: evolution of structural accounts of chemical bonding', in *Scientific Discovery: Case Studies* (ed. T. Nickles), Dordrecht, 1980, 291–329; A. Russo, 'Mulliken e Pauling: Le Due Vie della Chimica-Fisica in America', *Testi Contesti* (1982), **6**, 37–59; Kostas Gavroglu and Ana Simoes, 'The Americans, the Germans, and the beginnings of quantum chemistry: the confluence of diverging traditions', *Historical Studies in the Physical and Biological Sciences* (1994), **25**, 47–110; K. Gavroglu, *Fritz London*, Cambridge, 1995, 38–95. For the reception of resonance theory in particular, see Thomas Hager, *Force of Nature: The Life of Linus Pauling*, New York, 1995.

[4] For biographical information on Pauling, see his 'Fifty years of physical chemistry in the California Institute of Technology', *Annual Review of Physical Chemistry* (1965), **16**, 1–13, and 'Fifty years of progress in structural chemistry and molecular biology', *Daedalus* (Autumn, 1970), 988–1014. See also Robert Paradowski, 'The

Arnold Sommerfeld's Institute for Theoretical Physics in Munich, where Pauling decided to begin his postdoctoral work, was one of the centres of the quantum revolution. For thirteen months, Pauling studied wave mechanics under the influence of Sommerfeld's practical and flexible style of mathematics, which placed emphasis on workable equations rather than logical rigour and philosophical argumentation.[5] Extending his fellowship period for half a year, he visited other centres, such as Niels Bohr's institute in Copenhagen, Max Born's in Göttingen and Erwin Schrödinger's in Zurich. During this period, Pauling enjoyed the opportunity to mingle with a number of young theoretical physicists, some of whom discouraged him 'a little' with their good basic training in mathematics and understanding of quantum theory.[6]

Pauling returned to Caltech in the autumn of 1927 to be an assistant professor of theoretical chemistry with a new vision and message in mind. As a convert from the old quantum theory to the new quantum mechanics and a witness of the men and institutions of the quantum revolution in Europe, he gave public lectures, which often sounded like sermons. At the Southern California Section of the American Chemical Society in April 1928, for example, Pauling compared the trail of quantum mechanics to 'a highway so well laid out and so well constructed that nearly every theoretical physicist traverses it with satisfaction, and is confident that it will serve to carry us far into the future'. Pauling then enthusiastically proclaimed that chemistry was taking its first drive on this highway.

> Theoretical chemistry, being more complicated and extensive, must necessarily follow theoretical physics in its development. It is, however, following closely; such advances have been made that we can now predict with a considerable measure of confidence the general nature of the future advances. We can say, and partially vindicate the assertion, that *the whole of chemistry depends essentially upon two fundamental phenomena*: these are 1) the one described in *the Pauli Exclusion Principle* and 2) *the Heisenberg–Dirac Resonance Phenomenon.*[7]

Besides the public lectures, Pauling's enthusiasm and optimism were visible everywhere. In some published papers, Pauling announced the advent of a new era in chemistry, reiterated the importance of resonance and Pauli's exclusion principle, and gave the impression that a detailed account of various chemical bonds was imminent.[8] His classroom notes for an

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Structural Chemistry of Linus Pauling', Ph.D. dissertation, University of Wisconsin, 1972; Judith R. Goodstein, 'Atoms, molecules, and Linus Pauling', *Social Research* (1984), **54**, 691–708; and Hager, op. cit. (3). For Pauling's relationship with A. A. Noyes at Caltech and his position in the history of physical chemistry, see Servos, op. cit. (1), ch. 6.

[5] For Sommerfeld's influence upon Pauling and Pauling's social life in Munich, see Hager, op. cit. (3), ch. 5.

[6] Robert C. Brasted and Peter Farago (eds.), 'Interview with Linus Pauling by David Ridgway', *Journal of Chemical Education* (1976), **53**, 471–6, on 472. See also Hager, op. cit. (3), 130.

[7] L. Pauling, 'The Nature of the Chemical Bond', talk at the southern California Section of the American Chemical Society, 6 April 1928, Linus Pauling Papers, Oregon State University (hereafter LPP), 274.5. See also Pauling, 'The Development of the Quantum Mechanics', talk at the San Bernardino Junior College, 21 October 1929, LPP: 171.20.

[8] L. Pauling, 'The application of the quantum mechanics to the structure of the hydrogen molecule and hydrogen molecular ion and to related problems', *Chemical Review* (1928), **5**, 173–213, and 'The shared-electron chemical bond', *Proceedings of the National Academy of Sciences* (1928), **14**, 359–62.

introductory course on quantum mechanics began with historical sketches, often accompanied with such imagery as political revolution and religious mysticism.[9]

In the course of the 1930s, Pauling's reductionism was qualified. He realized that solving the Schrödinger equation for molecules more complex than hydrogen was not only impractical but also almost impossible without introducing drastic approximations or employing experimental data.[10] Nevertheless, his confidence in quantum mechanics did not dwindle. It became more focused than before. In his 1936 lecture at Caltech, Pauling told students: 'About forty years ago Arthur Gordon Webster wrote that mechanics was the foundation of the modern physics of that day, which consisted in describing phenomena in terms of motion. We might say now that mechanics is the foundation of physics and chemistry; in as much as it is possible to refer *structure*, which is the soul of chemistry, to the motion of electrons in molecules.'[11]

At the same time, Pauling reinforced his intellectual ties with workers in structural chemistry. He even introduced himself as a legitimate student of G. N. Lewis's school, in his lectures at Berkeley where Lewis was head of the College of Chemistry.[12] Moreover, in his one-year course (1935–36) on the nature of the chemical bond at Caltech, Pauling regarded the subject as 'modern structural chemistry'. He spent the first lecture giving a brief historical survey of 'classical structural chemistry' that had culminated in Lewis's theory. 'The next step in the development of the theory of the chemical bond is to obtain an understanding of the way in which two shared electrons bind two atoms together', he argued. 'This step has been taken only in the last eight years, as a result of the application of the quantum mechanics. We shall discuss this subject in great detail, but without entering into the mathematical methods used.'[13]

Pauling's strong confidence in quantum mechanics and strategic alliance with chemists had a significant bearing on his teaching. He narrowed his audience to chemists, for whom he behaved like an authority in quantum mechanics or simply a quantum preacher. He picked up what he believed to be the most precious fruit from quantum mechanics and offered it to the chemists without mathematical details. That was the concept of resonance, the interpretation of which constituted an important part of his teaching.

It was in Werner Heisenberg's helium paper of 1926 that 'resonance' was first used in

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[9] Pauling's Berkeley lectures in 1929 started with the following discussion: '[On the one hand]...the replacement of the old quantum theory by the quantum mechanics is not the overthrow of a dynasty through revolution, but rather the abdication of an old and feeble king in favor of his young and powerful son. It is true, on the other hand, that at times interpretations given the fundamental equations underlying a theory are later rejected completely in favor of alternative ones, and that especially the metaphysical ideas which develop with a physical theory fall often into complete disfavor. To this extent the development of the quantum mechanics was a revolution in physics.' His confidence in quantum mechanics was also displayed in a religious tone: 'This, then, is the quantum mechanics – the Cabala of the scientist, the mystic machine which, like the Oracle at Delphi, gives an answer to every question put to it, but which, unlike the Oracle, gives always the right answer', LPP: 243.l

[10] In his talk at the Southern California Section of the American Chemical Society on 7 February 1936, Pauling said that 'there is more to chemistry than an understanding of general principles'. L. Pauling, 'Recent Work on the Structure of Molecules', LPP: 274.14.

[11] Pauling's Caltech lectures in 1936–37 (Supplementary notes for use with textbook, L. Pauling and E. Bright Wilson, *Introduction to Quantum Mechanics*, New York, 1935), LPP: 172.12.

[12] Pauling's Berkeley lectures in 1931, LPP: 243.

[13] Pauling's Caltech lectures in 1935–36 on the Nature of the Chemical Bond, LPP: 173.6.

quantum mechanics. The problem of the helium atom, which had haunted theoretical physicists for a decade in the age of the old quantum theory, was indeed a touchstone for the new mechanical framework. And the unique difficulty of the helium problem lay in the physical explanation of its characteristic line spectrum, which had two different systems, one being singlet (parhelium) and the other triplet (ortho-helium). Heisenberg approached it first by supposing that there was no mutual interaction between two electrons of the helium atom, that is, a system degenerate in energy because of the indistinguishability of electrons. He then applied the interelectronic interaction as a perturbation to this degenerate system, and obtained a split of the energy level, which corresponded to the singlet–triplet separation. Finally, the consideration of electron spin accounted for the existence of the triplet and the singlet. The mathematical treatment of this problem was remarkably similar to that of the resonance phenomenon in classical mechanics, such as resonance in tuning forks or in coupled pendulums. Thus Heisenberg described the helium atom as a system showing resonance between the singlet and the triplet systems. More generally, he said: 'In quantum mechanics two atomic systems always enter – in harmony with general experience – into resonance, when the absorption frequency of one system coincides with the emission frequency of the other system, and vice versa.'[14]

Pauling unmistakably seized the meaning of resonance introduced by Heisenberg, teaching it as the energy transfer:

> *Meaning of Resonance Phenomenon*
> Heisenberg has discussed the coupled double harmonic oscillator, and has shown that the ordinary rules of quantisation lead to two non-combining sets of states, in one of which the electrons are in phase (→ ○ → ○) and in one out of phase (○ ← → ○). The energy of the system is successively transferred [*sic*] from one to the other – resonance! The frequency of this transfer is just the energy difference of the two states divided by *h*.
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> This is the interpretation in general.
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> If the two electrons are different the resonance phenomenon doesn't occur, for there then isn't degeneration.[15]

In his article published in the *Chemical Review* – the first synopsis of quantum mechanics for a general audience in chemistry – Pauling confounded this exposition with the visual description of the exchange of electrons, or the jumping of electrons between different atomic orbits. He based his explanation on the analysis of the mathematical term responsible for the energy split in helium. It was the integral ($H_{12} = \int \quad (1)\, \phi(2)\, (1/r_{12}) \quad (2)\, \phi(1)\, d\tau$, where (1) and $\phi(2)$ mean the description of electrons 1 and 2 with wave functions and $\phi$, respectively, and $r_{12}$ denotes the interelectronic distance), which came up during the calculation of a perturbation energy. Pauling explained that this integral had to do with the exchange of electrons: 'The added or subtracted term $H_{12}$ results from one electron

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[14] Werner Heisenberg, 'Mehrkörperproblem und Resonanz in der Quantenmechanik', *Zeitschrift für Physik* (1926), **38**, 411–26, on 416. On Heisenberg's interest in helium, which had begun in 1922, see Jagdish Mehra and Helmut Rechenberg, *The Historical Development of Quantum Theory: The Formulation of Matrix Mechanics and Its Modifications, 1925–1926*, New York, 1982, 282–301. See also Cathryn Carson, 'The peculiar notion of exchange forces – I: origins in quantum mechanics, 1926–1928', *Studies in History and Philosophy of Modern Physics* (1996), **27**, 23–45.

[15] Pauling's Caltech lectures in 1927–28, LPP: 172.11; and his Berkeley lectures in 1929, LPP: 243.

jumping from one orbit ( ) to the other (ϕ) at the same time that the other electron makes the reverse jump. For this reason $\pm H_{12}$ is called the interchange or resonance energy.'[16]

Although theoretical physicists including Heisenberg used the expression of 'exchange' or 'interchange', they did not give any physical meaning to this term as Pauling did. Walter Heitler, for instance, was agnostic about any attempt to interpret the exchange as the movement of electrons: 'I think…that the exchange is something typical for quantum mechanics, and should not be interpreted – or one should not try to interpret it – in terms of classical physics.'[17] For Pauling, however, the exchange of electrons and the energy split caused by it seemed to be a clue to a sharing process and the bond energy in Lewis's theory. In the hydrogen molecular ion ($H_2^+$), an electron appeared to be shared between the two nuclei, jumping from one nucleus to the other. Similarly, the hydrogen molecule ($H_2$) had two electrons exchanging their places, and its stability came from the resonance energy. This was the way Pauling read Heitler and Fritz London's paper on the hydrogen molecule, which he thought unveiled the mystery of the chemical bond.[18] He lectured: 'Whenever two electrons on different atoms interchange symmetrically we get a potential function leading to molecule formation. We shall see later that the requirement for this is that each electron be unpaired. Then they form an *electron pair – the Lewis electron pair*.'[19] To Pauling, the only remaining 'big' problem was that neither quantum mechanics nor the Lewis theory helped make a definite choice among alternative structures. Yet he maintained his optimism in that 'quantum mechanics at least holds out promises that it can be solved, for a knowledge of the mechanism of the formation of a shared electron pair bond should permit something quantitative to be said about it'.

In the early 1930s, Pauling completed the linkage of quantum mechanics and the Lewis theory, by suggesting that resonance should occur between several Lewis electronic structures. His often-used example was carbon monoxide. According to Lewis's scheme, this molecule could be drawn in either the double-bonded structure (:C::Ö:) or the triple-bonded one (:C:::O:). The data of interatomic distances and bond energies did not tell which structure was the right one: carbon monoxide had a shorter interatomic distance (1.15 Å) than the numerical mean of those of the two Lewis structures (1.28 Å and 1.13 Å, respectively); and its bond was stronger than either one. Thus he argued that carbon monoxide 'resonates between these structures, with the triple-bond structure somewhat more important than the other'.[20] In quantum-mechanical language, he taught that 'a hybrid function' ($a\ _{\text{double}}+b\ _{\text{triple}}$) with certain values of the coefficients *a* and *b* provided a better approximation than either a wave function of the double-bonded structure ( $_{\text{double}}$)

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[16] Pauling, 'Quantum mechanics', op. cit. (8), 184–5.

[17] Interview with Walter Heitler in the Archive for the History of Quantum Physics. Quoted in Gavroglu and Simoes, op. cit. (3), 64.

[18] Walter Heitler and Fritz London, 'Wechselwirkung neutraler Atome und homöopolare Bindung nach der Quantenmechanik', *Zeitschrift für Physik* (1927), **46**, 455–72. For Pauling's view of this paper, see 'The Hydrogen Molecule', LP Notes & Calculations Vol. III, 1926–1927, LPP: 241.

[19] Pauling's Berkeley lectures in 1929, pp. 84–5, LPP: 243. The emphasis is Pauling's.

[20] L. Pauling, 'Interatomic distances in covalent molecules and resonance between two or more Lewis electronic structures', *Proceedings of the National Academy of Science* (1932), **18**, 293–7. See also Pauling's Berkeley lectures in 1932 and 1933, LPP: 243.

or that of the triple-bonded one ( $_{\text{triple}}$) alone.[21] In such cases, the 'molecule could be described as fluctuating rapidly between the two electronic formulas, and achieving stability greater than that of either formula through the "resonance energy" of this fluctuation'.[22] Now there was no need to choose one among various structures, because the real one was a more stabilized 'resonance hybrid' of them. In this way, the language of chemistry and the symbolical representation of molecules were incorporated into the quantum-mechanical concept of resonance. Pauling provided a means by which resonance could be visualized with images and symbols familiar to chemists. As Per-Olov Löwdin said, 'chemical visuality' became striking in the theory of resonance, and the demand for a mathematical background was remarkably minimized.[23]

Pauling's research papers and lecture notes were elegantly synthesized in his masterpiece *The Nature of the Chemical Bond* (1939), which he began to write while visiting Cornell University as a George Fischer Baker Lecturer.[24] The book was the culmination of Pauling's attempts to bridge quantum mechanics and chemistry in a non-mathematical way. In the preface, he assured chemists that the ideas in this book required no more mathematical preparation than did the familiar concepts of chemistry: 'I formed the opinion that, even though much of the recent progress in structural chemistry has been due to quantum mechanics, it should be possible to describe the new developments in a thorough-going and satisfactory manner without the use of advanced mathematics.'[25] If that was the case, how could one understand new ideas like resonance without mathematics? Pauling's answer was practice and intuition: 'Some of [the ideas] may seem strange at first, but with practice there can be developed an extended chemical intuition which permits the new concepts to be used just as confidently as the older ones of the valence bond, the tetrahedral carbon atom, etc., which form the basis of classical structural chemistry.' Pauling expected the student of chemistry to be 'able to develop a reliable and useful intuitive understanding of the concept of resonance by the study of its application to various problems as described throughout this book'.[26] It is not surprising that he dedicated it to Lewis, rather than to his career's choreographer, A. A. Noyes of Caltech.

Pauling's appeal to chemical intuition had a significant connotation. Not only did it guide the readers of his book in solving problems without recourse to difficult mathematical details; it also mystified the quantum-mechanical origin of the resonance concept. While guaranteeing the solution of problems, Pauling asked students to follow him in the quantum-mechanical interpretation without questioning his authority. G. B. Kistiakowsky, a reviewer of *The Nature of the Chemical Bond*, saw both the success of Pauling's powerful

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[21] Pauling's Caltech lectures in 1935–36, pp. 8–9, LPP: 173.6.

[22] L. Pauling, 'The nature of the chemical bond III. The transition from one extreme bond type to another', *Journal of the American Chemical Society* (1932), **54**, 988–1003, on 997.

[23] I have adopted the term 'chemical visuality' from the Swedish quantum chemist Per-Olov Löwdin, who thought that the resonance theory had 'its great advantage in the close parallelism between the quantum-mechanical wave function and the corresponding chemical [structural] formula for the compound'. See P.-O. Löwdin, 'Present situation of quantum chemistry', *Journal of Physical Chemistry* (1957), **61**, 55–68.

[24] Pauling, 'Chemical bond', op. cit. (2).

[25] Pauling, 'Chemical bond', op. cit. (2), p. ix.

[26] Pauling, 'Chemical bond', op. cit. (2), 11.

theory and the excess of his authoritarian style: 'Dr. Pauling has been so successful in his attack upon many of the problems in the field that his advocacy of the doctrine of the infallibility of Pasadenean research and the somewhat pontifical style in which this book is written are understandable and should not be taken amiss.'[27] Robert S. Mulliken was more critical of Pauling than Kistiakowsky: 'Pauling was a much better showman.... [He] made a special point in making everything sound as simple as possible and in that way making it very popular with the chemists but delaying their understanding of the true [complexity of electronic structure]. He left them with a pretty crude idea and made them feel that that was satisfactory, whereas something better could have been done. So anywhere Pauling went, that became popular.'[28] As both men noticed, the popularity and power of Pauling's theory were intertwined with his style and method of presentation. Shrewdly developing the chemical visuality of resonance, and marshalling students and readers with his 'unquenchable self-confidence',[29] Pauling indeed maximized his influence upon chemists. His manner of presentation certainly contributed to the reception of the theory, but did not help remove a confusion about the meaning of resonance.

## RECEPTION AND CONFUSION: MESOMERISM, TAUTOMERISM AND RESONANCE

In the 1930s Pauling's efforts to build a bridge between quantum mechanics and chemistry attracted more audiences from the chemical community in Britain than in America or in Germany. This was closely related to differential national responses toward the Lewis theory in the previous decade.[30] Amongst the British chemists who recognized the value of

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[27] G. B. Kistiakowsky, 'The nature of the chemical bond', *Journal of the American Chemical Society* (1940), **62**, 457.

[28] Thomas S. Kuhn's interview with Robert S. Mulliken, in *Selected Papers of Robert S. Mulliken* (ed. D. A. Ramsay and J. Hinze), Chicago, 1975, 9. See also Mulliken's book review in *Journal of Physical Chemistry* (1940), **44**, 827–8.

[29] Pauling's self-assurance and self-confidence were well known. For example, James Watson vividly described his impression of Pauling's lectures as follows: 'There was no one like Linus in all the world. The combination of his prodigious mind and his infectious grin was unbeatable...Seeing Linus jumping up and down on the demonstration table and moving his arms like a magician about to pull a rabbit out of his shoe made them feel inadequate. If only he had shown a little humility, it would have been so much easier to take! Even if he were to say nonsense, his mesmerized students would never know because of his unquenchable self-confidence.' J. Watson, *The Double Helix*, New York, 1968, 35–6.

[30] For a differential reception of Lewis's theory across the national line, see Robert E. Kohler, Jr, 'The Lewis–Langmuir theory of valence and the chemical community, 1920–1928', *Historical Studies in the Physical and Biological Sciences* (1975), **6**, 431–68. Kohler concludes his paper with a perceptive note: 'The subsequent history of the nascent physical organic school and its relation to theoretical quantum chemistry is a separate story; but the emergence of quantum chemistry in the 1930's was profoundly influenced by the manner in which the Lewis–Langmuir theory was taken up by the chemical community in the 1920's' (p. 468). Whereas Kohler sees a direct link between the early reception of the Lewis theory in Britain and the early British leadership in physical organic chemistry, Martin D. Saltzman ascribes the slow and hesitant development of this discipline in the United States to the lack of an institutional base. M. D. Saltzman, 'The development of physical organic chemistry in the United States and the United Kingdom: 1919–1939: parallels and contrasts', *Journal of Chemical Education* (1986), **63**, 588–93.

the resonance theory was C. K. Ingold (1893–1970).[31] Ever since he set up his own research programme at the University of Leeds in 1925, Ingold's main interest was focused on the behaviour of electrons in chemical compounds during reactions. Not only did he undertake original experiments to elucidate reaction mechanisms; he also generalized results from previous experiments in organic chemistry, suggesting a new classificatory system of electron displacements. First, he distinguished two kinds of electronic mechanisms: a 'general inductive (*I*)' mechanism exerted in space like electrostatic induction; and a 'tautomeric (*T*)' mechanism relayed through carbon rings or chains. The former, represented by the arrow (→), had been indicated in the Lewis theory as a shift of the electron pair due to unequal sharing. The latter had been studied by British physical organic chemists including Robert Robinson who had called it a 'conjugative' effect and designated the curved arrow (↷) for it. In addition to this distinction, Ingold considered two kinds of electric states, permanent 'polarization' measured by dipole moments and transient 'polarizability' obtainable from molecular refraction. Consequently his system had four types of electron displacements: 'inductive' (a permanent effect by the *I* mechanism), 'mesomeric' (a permanent effect by the *T* mechanism), 'inductomeric' (a transient effect by the *I* mechanism) and 'electromeric' (a transient effect by the *T* mechanism). Alongside this classification, Ingold coined terms for two kinds of reagents, 'nucleophiles' (electron-releasing) and 'electrophiles' (electron-seeking). His research school flourished after he moved to University College London in 1930. And through his classic review essay of 1934, which he wrote during his leave at Stanford University, Ingold's new terminology and symbols reached an audience in America as well as in Britain.[32]

In 1933, while investigating the driving force behind the mesomeric effect or mesomerism, Ingold found that it had a similarity with resonance. He noted: 'this theory [of mesomerism] is developed in a very recent paper by Pauling and Wheland, who have employed an extremely interesting method of wave-mechanical calculation'.[33] The theory of resonance seemed to bolster his qualitative argument that 'the energy of degeneracy' was the source of energy of mesomerism; and for this reason, he called mesomerism 'valency degeneracy' or 'tautomeric degeneracy', to which he attributed the stability of aromatic molecules (benzene, pyridine, etc.). By 1938, Ingold became an ardent proponent of the theory of resonance. His article, 'Resonance and mesomerism',[34] revealed his understanding of resonance in quantum mechanics, his enthusiasm about it and his attempt to link it with his own mesomerism. He saw resonance as responsible for the energy-

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[31] For more details on C. K. Ingold's career and achievements, see C. W. Shoppee, 'Christopher Kelk Ingold', *Biographical Memoirs of Fellows of the Royal Society* (1972), **18**, 349–411; Nye, 'Chemical philosophy', op. cit. (1), ch. 8; K. Schofield, 'The development of Ingold's system of organic chemistry', *Ambix* (1994), **41**, 87–107; Brock, op. cit. (1), ch. 14; and Gerrylynn K. Roberts, 'C. K. Ingold at University College London: educator and department head', *BJHS* (1996), **29**, 65–82.

[32] C. K. Ingold, 'Principles of an electronic theory of organic reactions', *Chemical Reviews* (1934), **15**, 225–74. This review article had been used as a standard item in advanced organic chemistry courses in the United States in the 1930s until textbooks dealing with this topic appeared the next decade. See Saltzman, op. cit. (30), 590.

[33] C. K. Ingold, 'Significance of tautomerism and of the reactions of aromatic compounds in the electronic theory of organic reactions', *Journal of the Chemical Society* (1933), **136**, 1120–7, on 1127.

[34] C. K. Ingold, 'Resonance and mesomerism', *Nature* (1938), **141**, 314–18.

lowering of a system and thus 'fundamental to all valency theory': 'The one-electron bond, the ordinary two-electron bond, the double bond, the triple bond, van der Waals' forces, steric repulsion – all involve resonance.'[35] In comparison, mesomerism was a 'particular case of resonance', which arose when one could write several ordinary structural formulas, with the nuclei in fixed positions. As for the quantitative study of mesomerism, Ingold praised the Pasadena group: 'The most successful attempts to calculate the energy effect of mesomerism are those of Pauling and Wheland.'[36] By this time, the resonance concept became a part of Ingold's programme or systematization of reaction mechanisms.

Besides Ingold, the theory of resonance found its most effective, energetic spokesman in Nevil V. Sidgwick (1873–1952) of Lincoln College, Oxford.[37] Well-known for his study of organic chemistry of nitrogen, Sidgwick had been a great promoter of the Lewis theory. His influential classic, *The Electronic Theory of Valency*, capped the reception of the Lewis theory in Britain, and his rising international fame brought him a chance to lecture at Cornell University as a Baker Lecturer in 1931. On both sides of the Atlantic, Sidgwick incessantly stressed the unification of organic and inorganic chemistry and the cooperation of chemistry and physics.[38] In the 1930s he was at the peak of his scientific career, holding such important posts as chairman of the Chemistry Research Board, a member of the Council of the Royal Society, president of the Faraday Society and President of the Chemical Society. At that time, he was also a leading popularizer of the resonance theory in Britain.

Sidgwick's 1936 presidential address to the Chemical Society was a memorable lecture on the history of structural chemistry in which he placed the theory of resonance as the latest development.[39] This emphasis on continuity was designed both to dispel 'false and pernicious' preconceptions about the progress of science and to reassure chemists of the benefits of the quantum-mechanical resonance concept. He began the lecture by criticizing those who held the view that a new discovery was made by negating previous conceptions. 'The progress of knowledge', he said, 'does indeed correct certain details in our ideas, but the main result of every great discovery is to establish the existing doctrines on a firmer foundation, and give them a deeper meaning'. He also argued against the view that science developed through increasing specialization, which meant 'knowing more and more about less and less'. The development of structural chemistry exemplified the advantage to be gained by attacking the same problem with different experiments on different kinds of properties. When structural chemistry was laid out in the 1850s and 1860s mainly through the work of Kekulé and Cannizzaro and extended to three dimensions by Van't Hoff and Le Bel in 1874, the molecule was simply assumed to be held together by links or bonds between atoms. The classification of bonds (single, double and triple) was proposed and

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[35] Ingold, op. cit. (34), 316.

[36] Ingold, op. cit. (34), 318.

[37] L. E. Sutton, 'Nevil V. Sidgwick', *Proceedings of the Chemical Society* (1958), 310–19; H. Tizard, 'Nevil Sidgwick', *Obituary Notices of Fellows of the Royal Society* (1954), **9**, 237–58.

[38] Nevil V. Sidgwick, *The Electronic Theory of Valency*, Oxford, 1927. According to Tizard, this book became an instant best-seller, selling some 10,000 copies. Sidgwick's Cornell lectures were published in 1933 as a book, *Some Physical Properties of the Covalent Link in Chemistry*, Ithaca, 1933.

[39] N. V. Sidgwick, 'Structural chemistry', *Journal of the Chemical Society* (1936), 533–8.

discussed, along with their spatial orientation and the maximum number of bonds atoms could have. However, no measurement was made as to physical properties (lengths, angles, heats of formation, electric and magnetic, etc.) of the bond, until various physical methods became available in the twentieth century.

To Sidgwick, the theory of resonance was an outcome of the recent cross-fertilization of physics and chemistry. He was, of course, aware that the full theoretical calculation of molecular properties by quantum mechanics was not yet possible except for a few of the simplest molecules. However, he believed that 'the progress of wave mechanics will give us new principles of structure and of reactivity which will be applicable even where a complete calculation cannot be carried out'. 'One such principle', he said,

> has already been discovered, and it constitutes the most important development of structural chemistry since the days of Van't Hoff. This is the principle of resonance, due originally to Hund [*sic*], but applied to organic chemistry mainly by Pauling and his school. The conclusions of this theory can only be reached by wave mechanics, but they can fortunately be expressed in very simple terms.[40]

This principle, he thought, provided a 'variety of approximations and short cuts' by which one could obtain something more than a qualitative solution of the structural problem and a physical picture for the sharing of electrons proposed by Lewis. Placing Pauling's historical position on a par with Van't Hoff's and higher than Lewis's, Sidgwick highlighted the significance of resonance theory and its continuity with old theories. His conclusion reiterated this point: 'I hope I have said enough to show that the modern development of the structural theory, far from destroying the older doctrine, has given it a longer and a fuller life; and further that the tendency of modern research is not to contract the scope of its material, but on the contrary to call in to its assistance an increasingly wide range of properties, and to bring to bear on its problems the results of every kind of physical and chemical investigation.'[41]

Sidgwick devoted his next presidential address of 1937 again to the popularization of the resonance theory, explaining that the 'modifications [in structural chemistry by it] are so important to all sides of chemistry that I think I cannot do better this year than say something more about them'.[42] In this address, he endeavoured to drive away some concerns raised by chemists about the mathematical nature of quantum mechanics in the theory. He advocated limited use of the technical language, as Pauling did.

> The general conclusions of the theory of resonance are of great practical importance, especially to the organic chemist. But it is not to be expected that more than a very few organic chemists will have either the time or the ability to master these mathematical operations. It is therefore obviously our duty to express – or to induce the wave-mechanicians to express – the results in the simplest terms that are possible, and this can really be done quite easily. The use of the technical language of wave mechanics for this purpose is quite unnecessary and in fact misleading, for it makes the non-mathematical reader think that as he can't understand the language he can't understand the conclusions either, which is quite untrue; and not commonly, I think, it leads the non-mathematical writer to believe that if he knows the technical terms he must understand their meaning, which is by no means always the case.[43]

[40] Sidgwick, op. cit. (39), 535. It is interesting that Sidgwick confused Heisenberg with Hund.

[41] Sidgwick, op. cit. (39), 538.

[42] N. V. Sidgwick, 'Hybrid molecules', *Journal of the Chemical Society* (1937), 694–99.

[43] Sidgwick, op. cit. (42), 694.

He then quoted Maxwell to emphasize that the scientific truth could be represented in different forms to persons of different types of mind and background.[44]

While the theory of resonance found a receptive audience in Britain because of its similarity with mesomerism and the possibility of non-technical representations, a terminological difficulty arose from the word resonance itself. This word undoubtedly suggested a rapid oscillation or vibration between molecular structures, an idea not foreign to chemists. It could be traced back to the 1870s, when Kekulé explained the non-existence of benzene isomers in terms of their fast oscillation. Years later, this idea was also applied to a case of reversible isomeric change, as in the interconversion of the keto- and enol-forms of acetoacetic ester, under the name tautomerism. Unlike Kekulé's inseparable benzene isomers, the tautomeric isomers turned out to be experimentally separable, implying that they were two different entities.[45] But this criterion of separability did not rule out the possibility that molecular oscillation could be an effective way of describing the structure of benzene. Thus it is not surprising that when the concept of resonance became available, many chemists tended to understand it as a kind of tautomerism having a very rapid interconversion.

As early as 1934, Ingold perceived a widespread misunderstanding of resonance, mesomerism and tautomerism. In a letter to *Nature*, he described the situation: 'The idea appears to have gained some ground that the conception of the mesomeric state is unnecessary, that the unperturbed structures [like the Kekulé structures of benzene] are all that exist, and that these pass into each other "like tautomerides but much more rapidly", the great frequency of interchange accounting for the energy effect.'[46] Although the expression of resonance was adopted from the mathematical analogy with classical mechanics, he found that chemists, following Pauling, tended to understand the term 'resonance' visually. To rectify this unfortunate situation, Ingold first clarified the meaning of tautomerism: 'It is a characteristic of tautomeric systems that forms exist which clearly correspond to separate molecular states, because each molecule spends the whole of its life partly in one form and partly in the other, and only a proportionately quite insignificant time in the actual process of transition.' In contrast, mesomerism or resonance meant a state where 'the frequency of interchange…is often so great as to require that the molecules must occupy their time in changing, and cannot remain quiescent for significant periods in either of the assumed states'. Therefore, Ingold stressed, the assumed structures were merely 'intellectual scaffolding'; and 'only the mesomeric state is real'. To minimize the confusion, he withdrew the expression 'valency tautomerism' that he had used for mesomerism before.[47]

Sidgwick was also worried about the misconception of resonance among chemists.[48] In his presidential addresses, he thus tried to make a distinction between resonance and tautomerism. In tautomerism, he explained, the substance was a chemical mixture of two

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[44] A quote I have used in the forefront of this paper. For this remark by Maxwell, Sidgwick drew on J. J. Thomson's *Recollections and Reflections*, New York, 1937, 392, rather than directly from Maxwell.

[45] John W. Baker, *Tautomerism*, London, 1934.

[46] C. K. Ingold, 'Mesomerism and tautomerism', *Nature* (1934), **133**, 946–7.

[47] Ingold, op. cit. (46), 947 n5.

[48] London to Sidgwick, 10 May 1934, in Nye, 'Chemical philosophy', op. cit. (1), 207.

kinds of molecules in equilibrium; thus the tautomeric system had no sign of greater stability, but rather the opposite. In resonance, by contrast, there was 'no chemical change, quick or slow'; and the occurrence of resonance necessitated an increase in the stability of the molecule.[49] He regretted that the 'bad' name resonance was more widely used than Ingold's mesomerism. Nevertheless, he urged chemists to accept the terminology of the physicists: 'It is however of little use for the chemist to adopt this [mesomerism] unless the physicists who are specially concerned with the problem will do the same.'

By the late 1930s, the resonance theory was more firmly entrenched in the British chemical community than its rival, the molecular orbital theory, even though the latter was not entirely neglected.[50] No doubt Ingold's systematization of reaction mechanisms provided the ground in which the theory of resonance took its root; in addition, Sidgwick's public advocacy of the resonance theory over the molecular orbital theory set the general atmosphere.[51] Two monographs in physical organic chemistry, William A. Waters's *Physical Aspects of Organic Chemistry* (1936) and Herbert B. Watson's *Modern Theories of Organic Chemistry* (1937), illustrate how chemists embraced the resonance theory. Waters, a protégé of T. M. Lowry of Cambridge University, structured his book around the old themes of organic chemistry, such as chemical affinity, valency, reactivity, unsaturation and acidity; and he explained how new ideas from physics had changed the study of those ideas. According to him, the concept of resonance had a wide range of applications, and its definition could be given in a phenomenological way: '[Pauling] has suggested that when one could assign to a molecule two alternative structures which have nearly the same energy content and a similar spatial arrangement, then a state of continuous and very rapid oscillation may occur between the two forms.' At the same time, he adopted the warning by Ingold and Sidgwick: 'a sharp distinction must be drawn between the concept of resonance as used by Pauling, and by Ingold, and the notion of "tautomerism"'.[52] Watson adopted a similar stance. As he said in his preface, 'the very fruitful alliance of organic chemistry with physics and mathematics' was made through the theory of resonance which expressed many earlier ideas in 'more definite and elegant language'. With this new, modern physical basis, Watson's whole book was centred around the exposition of Ingold's system and its applications. Furthermore, Watson explicitly declared his preference for the resonance approach: 'Both the electron pair [that is, resonance] method and the molecular orbital method are approximations, and the exact truth probably lies intermediate between them. The latter cannot be described as a wave-mechanical theory of valency, however, and the conception of the two-electron bond, as

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[49] Sidgwick, op. cit. (42), 695.

[50] For example, J. E. Lennard-Jones, who became the first holder of the prestigious Plummer Chair of Theoretical Chemistry at Cambridge in 1932, developed a strong research programme in the molecular orbital treatment of chemical problems. And the work of other molecular orbital theorists like Hund, Mulliken and Hückel was also introduced and discussed through the *Annual Report of the Progress of Chemistry*. See C. N. Hinshelwood, 'General', *Annual Report of the Progress of Chemistry* (1932), 13–21.

[51] In addition to his presidential addresses, see N. V. Sidgwick, 'The covalency rule', *Annual Report of the Progress of Chemistry* (1933), 110–16; 'The theory of resonance and the co-ordination of hydrogen', ibid., (1934), 37–43, and 'Wave mechanics and structural chemistry', *Nature* (1934), **133**, 529–30.

[52] William A. Waters, *Physical Aspects of Organic Chemistry*, New York, 1936, 113–14.

originally put forward by Lewis, still provides the most useful picture of the molecule for the purpose of interpreting chemical phenomena.'[53]

In America, Pauling's series of papers on the nature of the chemical bond, published in the *Journal of the American Chemical Society* and the *Journal of Chemical Physics* between 1931 and 1933, seemed to attract much attention from the chemical as well as physical community.[54] A systematic application of the resonance theory, however, did not immediately appear in the literature of organic chemistry beyond the work of Pauling's students and colleagues at Caltech. Perhaps Howard J. Lucas's *Organic Chemistry* (1935) was the first undergraduate textbook to introduce resonance.[55] Lucas, the lone organic chemist on the staff of Caltech, demonstrated in his book that the 'principle of resonance' could be applied to the study of reaction mechanisms, especially in connection with the stability of certain molecules. But Lucas's book was rather exceptional. Even at the advanced level, the theory of resonance was seldom discussed by organic chemists; and even if it was, the discussion did not go beyond the stage of introduction. For instance, most articles in Henry Gilman's *Organic Chemistry: An Advanced Treatise* (1937), written by leading American chemists, did not consider resonance at all, except the contributions by Pauling himself and by John R. Johnson of Cornell University.[56]

As in Britain, the reception of resonance theory was followed by the confusion between resonance and tautomerism. For example, Lucas's exposition of resonance was dependent on the idea of molecular oscillation: 'The molecule [$H_2^+$] is said to resonate between these two [structures, H· H and H ·H].' Lucas generalized from this case that 'when there are two equivalent states which an electron may occupy, it will resonate (or oscillate) between these states and act as a chemical bond'.[57] This definition did not prevent chemists from seeing resonance as a tautomerism of fast oscillation. A letter from J. B. Conant to Pauling in 1938 revealed the seriousness of this confusion. Conant wrote:

> With the aid of Dr. Tishler I am revising my text book of organic chemistry. In so doing I have had the pleasure of 'reading up' a bit on the application of resonance to organic chemistry. Your chapter in the Gilman has been most helpful. If I understand the subject correctly, however, the matter has been misunderstood by some organic chemists. I take it that resonating structures must all have the same atomic arrangement and can be connected one into another (on paper) without

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[53] Herbert B. Watson, *Modern Theories of Organic Chemistry*, Oxford, 1937, 14.

[54] Even before the publication of this series, Pauling had been coveted by Lewis of Berkeley and Conant of Harvard. In 1931, Slater offered Pauling a full professorship in physics, chemistry, or any combination of the two. See Hager, op. cit. (3), 149–59.

[55] Howard J. Lucas, *Organic Chemistry*, New York, 1935. For the role of Lucas in the development of physical organic chemistry in the United States, see Leon Gortler, 'The physical organic community in the United States, 1925–50', *Journal of Chemical Education* (1985), **62**, 753–7; and Saltzman, op. cit. (30), 590–1.

[56] L. Pauling, 'the significance of resonance and the nature of the chemical bond and the structure of molecules', in *Organic Chemistry: An Advanced Treatise* (ed. Henry Gilman), 2 vols., New York, 1938, 1850–90; John R. Johnson, 'Modern electronic concepts of valence', ibid., 1595–711. Johnson's article is interesting, because it suggests the existence of 'the dismay and confusion of many organic chemists' about the intrusion of quantum-mechanical ideas. While he welcomed the theory of resonance and Ingold's systematization of reaction mechanisms, he was concerned about organic chemists, who confronted with 'the serious problem of keeping abreast of the flood of speculative elaboration of electronic theories and seeking to understand and assimilate them'.

[57] Lucas, op. cit. (55), 25–6.

> shifting any atom or group. Therefore the tautomeric forms of urea, or the amides are not resonating structures. (The contrary statement I have met with in the literature) … I am sorry to trouble you, particularly at this time of year, but I would be deeply grateful if you could drop me a line. If I am right, it is important to set out the differences between the tautomerism in ring systems and resonance. Your reply will help.[58]

In his reply, Pauling confirmed Conant's understanding that a molecule resonating among several valence structures retained one equilibrium configuration of nuclei.[59] To make it clear that resonance was not identical with tautomerism, he provided a reason for the confusion between them in the minds of chemists: '[it] results from the fact that often the valence bond structures among which a molecule resonates are similar to the valence bond structure usually written for the individual tautomers'. Resonance was a victim of chemists' familiarity with tautomerism. While Pauling's strategy of depicting resonance in non-technical terms paid off in attracting the attention of chemists, it left much room for imprecise interpretation.

Since 1935, in fact, Pauling had been aware of this terminological problem raised by chemists.[60] Conant's letter might provoke him to discuss this problem in the final chapter of *The Nature of the Chemical Bond*. Surprisingly he acknowledged its subtle aspect: 'There is no sharp distinction which can be made between tautomerism and resonance; but it is convenient in practice to make a distinction between the two which is applicable to all except the border-line cases.'[61] The central issue of the problem was how fast the molecule oscillates between valence structures, the frequency of which is expressed in terms of the resonance energy divided by the Planck constant $h$. In the case of benzene, the resonance energy was so large (about 36 kcal/mol) that its frequency was a thousand-fold greater than the frequency of nuclear vibration. Hence resonance occurred in the time required for the nuclei to move an inappreciable distance (0.0001 Å), that is, in only one well-defined stable nuclear configuration. Neither two Kekulé structures nor other contributing valence structures could represent the nuclear configuration of benzene: the real one had an intermediate configuration among them. Therefore, it seemed to him that the comparison of the frequency of resonance and that of nuclear vibration, which would help determine the number of stable nuclear configurations, was a convenient and practical criterion for distinguishing resonance and tautomerism:

> When the magnitude of the electronic resonance integral (or integrals) and of the other factors determining the electronic energy function of a molecule are such that there are two or more well-defined stable nuclear equilibrium configurations, we refer to the molecule as capable of existing in tautomeric forms; when there is only one well-defined stable nuclear equilibrium configuration, and the electronic state is not satisfactorily represented by a single valence-bond structure, we refer to the molecule as a resonating molecule.[62]

The distinction between resonance and tautomerism was intertwined with the question of the reality of the constituent structures of a resonating system: if there is only one

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[58] Conant to Pauling, 29 August 1938, LPP: 13.7.

[59] Pauling to Conant, 2 September 1938, LPP: 13.7.

[60] Pauling's Caltech lectures on the nature of the chemical bond in 1935–36, 13, LPP: 173.6.

[61] Pauling, 'Chemical bond', op. cit. (2), 423–31.

[62] Pauling, 'Chemical bond', op. cit. (2), 427.

structure for benzene, are the constituent Kekulé structures real or imaginary? Some years earlier, Ingold had called these structures 'intellectual scaffolding', which implied their artificial status. Pauling's view appeared to be more abstruse. 'There is one sense in which this question may be answered in the affirmative; but the answer is definitely negative if the usual chemical significance is attributed to the structures', he said.[63] Pauling had in mind an operational definition of the molecule: if it is identified experimentally, it exists; if not, we cannot acknowledge its reality. In most cases, he argued, resonance is too fast to be detected by chemical experiments. And yet, when the frequency of resonance is smaller than that of nuclear vibration, an experiment can be devised to identify resonating structures. In this case, he said, 'the boundary between resonance and tautomerism is approached and passed'. The problem was only the difficulty of devising an experimental test that could be carried out quickly enough, not its impossibility. To Pauling, resonance and tautomerism differed only in degree, not in kind; the reality of the constituent structures was dependent on that degree. But Wheland, Pauling's collaborator, had a different view on how organic chemists should deal with this complicated subject.

## CONTROVERSY: A CONUNDRUM OF 'MAN-MADENESS'

By the early 1930s, Pauling's laboratory at Caltech had already become a magnet for postdoctoral researchers interested in the study of molecular structure and quantum chemistry. George W. Wheland (1907–72), who had obtained a doctoral degree at Harvard under Conant's tutelage, was one of those who opted for Caltech with a desire to work with Pauling.[64] During his postdoctoral period between 1932 and 1936, Wheland helped Pauling to develop the theory of resonance and to apply it to organic molecules. He co-authored three papers with Pauling, including the fifth of the series on the nature of the chemical bond.

Furthermore, Wheland made himself useful as a link between the Pasadena group of quantum chemistry and the London school of physical organic chemistry. In 1936, Wheland left Caltech for Britain to spend a year as a Guggenheim Fellow. Upon Wheland's arrival at University College London (UCL), Ingold was cordial enough to show him around the place and to help him get located. Wheland was also impressed by a large and well-equipped laboratory. 'In America we hear so much about Oxford and Cambridge that we are apt to overlook the fact that there are some other English universities, too, which do right well in their own way', he observed. The close contact with Ingold also gave him an opportunity 'to break into the English circle': he was invited to speak at the Chemical Society of London in November, where resonance in organic molecules was one of the session topics. On Ingold's suggestion, he discussed the effect of resonance on reaction

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[63] Pauling, 'Chemical bond', op. cit. (2), 428.

[64] Proud and confident of his former student, Conant wrote to Pauling: 'I am delighted to hear that Wheland is doing so well. If he can work hard and stick to this combination of quantum mechanics and organic chemistry for a few years, he ought to be a very outstanding man…I cannot tell you how pleased I am that he seems to have found the right line for his talent.' Pauling, as well, praised Wheland's talent for theoretical work. Conant to Pauling, 27 February 1933; Pauling to Conant, 25 September 1934, LPP: 13.7.

velocity, with special reference to aromatic substitution. His self-evaluation of the talk was modest, but he had a greater reputation in England than he thought.[65]

The correspondence between Wheland and Pauling shows how much Pauling was concerned about the English chemists' opinion of the theory of resonance and about their general research activities. Pauling was not surprised by Wheland's first impression of UCL, since he already regarded the London laboratory as 'the best one in England'. He wanted to hear more about the details of the chemistry department, such as funding and research interests.[66] By means of 'most tactful inquiries' among the graduate students and research fellows, Wheland was able to report that UCL was one of the best endowed in England, but that the chemistry department had recently been spending beyond its income.[67] As for the work in progress at the department, he commented on the research done by professors, among whom he believed Ingold was undertaking the most important work. Ingold had, in Wheland's expression, 'quite a number of different irons in the fire'. In addition to writing a series of eight articles on benzene, Ingold was interested in the exchange reactions involving deuterium and the mechanism of aliphatic substitution; and the relation between the Walden inversion and the reaction kinetics.[68] Most importantly, Pauling wished that their book-in-progress on the quantum mechanics of organic chemistry should satisfy English chemists. He said: 'have you anything to send to me? I am looking to you to learn the point of view of the English chemists thoroughly and to see that our book is written in a way that is satisfactory to them.'[69] Wheland also spent some months working with the physical chemist Cyril Hinshelwood at Oxford and taking opportunities to visit Sommerfeld in Munich, Erich Hückel in Stuttgart and J. E. Lennard-Jones in Cambridge.[70]

Returning to America in 1937, Wheland received several offers: a postdoctoral position at Pasadena; an assistant professorship at the University of California, Los Angeles; and a teaching position at the University of Chicago. Wheland decided to go to Chicago where a strong programme in physical organic chemistry was under construction.[71] Pauling foresaw a bright future in his career: 'Dr. G. W. Wheland is very well trained in organic chemistry in general, his knowledge of descriptive and theoretical organic chemistry being especially extensive. He has also a grasp of quantum mechanics comparable with that of the leading theoretical physicists. I feel that he is an outstanding man because of this combination of training and ability and that he will be an outstanding contributor to theoretical organic chemistry.'[72]

Like Pauling a decade earlier, Wheland was filled with optimism and had confidence in the application of quantum mechanics to chemical problems. If Pauling had been a

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[65] Wheland to Pauling, 29 September 1936, 29 November 1936; Pauling to Wheland, 30 October, 1936, LPP: 145.8.

[66] Pauling to Wheland, 30 October 1936, LPP: 145.8.

[67] The recent paper by Gerrylynn K. Roberts confirms Wheland's observation of Ingold's tactic of overspending. Roberts, op. cit. (31), 65–82.

[68] Wheland to Pauling, 29 November 1936, LPP: 145.8.

[69] Pauling to Wheland, 11 March 1937, LPP: 145.8.

[70] Wheland to Pauling, 11 May 1937, 7 June 1937, LPP: 247.6.

[71] Pauling to Wheland, 30 March 1937, 28 July 1937, LPP: 145.8.

[72] Pauling to H. I. Schlesinger, 23 December 1936, LPP: 145.8.

'quantum preacher', Wheland was a 'resonance preacher'. However, his close contacts with physical organic chemists led him to consider what kind of attacks could be made, theoretically and experimentally, on the theory of resonance, and how much the confusion between resonance and tautomerism retarded the correct understanding of the theory. Therefore, he sought to remove any source of misconception about resonance in his teaching, while furthering its application to organic chemistry. This effort was reflected in his book, *The Theory of Resonance and Its Application to Organic Chemistry* (1944), which grew out of his lectures for several years to the advanced undergraduate and beginning graduate students at Chicago.[73]

On the one hand, Wheland's book represented the growth of the theoretical study of organic chemistry in the United States. After Pauling's *The Nature of the Chemical Bond*, there was a surge of books dealing with organic chemistry from the new point of view. Louis P. Hammett of Columbia University wrote *Physical Organic Chemistry* (1940), which became a bible for organic chemists interested in reaction mechanisms and structure–reactivity relationships.[74] It was soon followed by Gerald E. K. Branch and Melvin Calvin's *The Theory of Organic Chemistry* (1941) and A. Edward Remick's *Electronic Interpretations of Organic Chemistry* (1943),[75] where the theory of resonance was introduced along with the symbolism and the language of the English physical organic chemists. The same trend was also found in the second edition of Henry Gilman's *Organic Chemistry* (1943).[76]

On the other hand, *The Theory of Resonance* was a continuation of Wheland's aborted project of writing a book with Pauling. Although this monograph did not include a detailed comparison of the resonance theory and the molecular orbital theory, which was originally to be Pauling's part in the project, it maintained the aim of structuring organic chemistry around the theory of resonance.[77] Pauling strongly recommended this book to the publisher: 'There is, I believe, no one who could do a better job of writing a book on this subject than Dr. Wheland…I believe that the book, despite its somewhat advanced character, will have a rather wide sale. It deals with a subject of interest to all organic chemists and to many physical chemists. In this respect it is similar to my own book, *The Nature of the Chemical Bond*, which has surprised both the Cornell University Press and me by selling very well. In understanding, too, that Branch and Calvin's book has sold pretty well, I believe that Dr. Wheland's book should be better.'[78] Wheland dedicated his book to Pauling.

Wheland's dilemma, like Pauling's a few years earlier, was where to strike a balance between the chemical and the mathematical exposition of resonance. He thought the

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[73] George W. Wheland, *The Theory of Resonance and Its Application to Organic Chemistry*, New York, 1944.

[74] For the profound influence that Hammett's book had upon the discipline of physical organic chemistry, see Gortler, op. cit. (55), 756.

[75] Louis P. Hammett, *Physical Organic Chemistry*, New York, 1940; Gerald E. K. Branch and Melvin Calvin, *The Theory of Organic Chemistry*, New York, 1941; and A. Edward Remick, *Electronic Interpretations of Organic Chemistry*, New York, 1943.

[76] Gilman, op. cit. (56), 2nd edn, 4 vols., New York, 1943.

[77] Several chapters of the unpublished book, 'Quantum Mechanics of Organic Molecules', mostly written by Wheland, are in LPP: 443 and LPP: 444.

[78] Pauling to W. Bradford Wiley, 11 May 1943, LPP: 145.8.

resonance theory should be presented in terms familiar to organic chemists, since this theory had its most interesting application and greatest value in their field. However, it was difficult to ignore the fact that the basis of the theory was in the mathematical depth of quantum mechanics. His teaching experience showed that 'often more difficulties are created than are avoided if the attempt is made to ignore entirely the underlying physical basis of the theory'. No doubt the theory of resonance could be presented precisely and completely 'only in highly mathematical language'. Finally, he made 'some sort of working compromise' in favour of the more qualitative, descriptive and non-mathematical approach.[79] In this regard, Wheland followed the path Pauling had taken.

However, Wheland was more concerned about the confusion between resonance and tautomerism, and was less authoritarian than Pauling. Wheland warned his readers: 'resonance is a man-made concept in a more fundamental sense than most other physical theories. It does not correspond to any intrinsic property of the molecule itself, but instead it is only a mathematical device, deliberately invented by the physicist or chemist for his own convenience.'[80] To Wheland, there were obvious elements of arbitrariness in it: the selection of resonating structures for a molecule was purely arbitrary; and moreover, the resonance theory was but one quantum-mechanical approach to chemical problems, given the existence of the molecular orbital theory. To be sure, Wheland shared Pauling's view by claiming that 'these facts in no way detract from the usefulness of the concept from a practical point of view'. But he also asserted that '[t]hey do require us, however, always to bear in mind that resonance has meaning only with reference to a *particular* method of *approximating* the actual situation, and constantly to be on guard lest we assign to the various resonating structures a physical significance which they do not possess'.[81]

Wheland introduced an analogy to eliminate the image of fast oscillation in resonance:

> The significance of the above distinction between tautomerism and the newer concepts can be made clearer with the aid of an analogy. A mule is a hybrid between a horse and a donkey. This does not mean either that some mules are horses and the rest are donkeys, or that a given mule is a horse part of the time and a donkey the rest of time. Instead, it means that a mule is a new kind of animal, neither horse nor donkey, but intermediate between the two and partaking to some extent of the character of each.[82]

Likewise, he argued, the resonance theory pictured the benzene molecule as having 'a *hybrid* structure, not identical with either of the Kekulé structures, but intermediate between them'. It was a mental picture, rather than a real one. In addition to this analogy, Wheland developed a set of rules that the chemist could use to distinguish easily between tautomerism and resonance.[83]

*The Theory of Resonance* was well received among chemists. One reviewer noted that Wheland achieved a good measure of his purpose, recommending that 'the book should

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[79] Wheland, op. cit. (73), p. iii.

[80] Wheland, op. cit. (73), 28.

[81] Pauling did not like Wheland's special emphasis on the 'man-made' nature of resonance. See Wheland to Pauling, 20 January 1956, 4 February 1956; Pauling to Wheland, 26 January 1956, 8 February 1956, LPP: 145.8. See also Gavroglu and Simoes, op. cit. (3), 91–4.

[82] Wheland, op. cit. (73), 3.

[83] Wheland, op. cit. (73), 6–18.

certainly be in the hands of all organic chemists working in any field involving resonance interpretations'.[84] Its usefulness in teaching and research was also appreciated: 'The book will undoubtedly find a large audience, by no means restricted to organic and physical chemists, and it should be required reading for anyone teaching an advanced course in physical organic chemistry and for the research worker in the field.'[85] In short, it was 'a volume of which both Pauling and Wheland may well be proud'.[86] But no one foresaw that Wheland's special emphasis on the man-madeness of resonance would become the target of criticisms in the Soviet Union.

On 15 July 1951, the *New York Times* brought news of a controversy brewing in the Soviet Union: 'About two years ago Soviet Russia decided that the quantum theory... is nothing but bourgeois mysticism. Now comes an attack on the chemical theory of resonance as it has been set forth by Dr. Linus Pauling of the California Institute of Technology.'[87] The *Chemical and Engineering News*, weekly magazine of the American Chemical Society, dubbed the controversy a chemical version of Lysenkoism. It maintained that the resonance theory, though 'now an accepted part of chemistry', was under attack because it apparently violated the materialistic outlook of Soviet scientific policy-makers.[88] Pauling himself counter-attacked the Soviet blast by emphasizing the value of resonance theory in teaching and research, and other chemists lamented this controversy as 'the most shameful event in the history of science and mankind forever'.[89]

However, the resonance controversy was more than a confrontation between science and ideology in the Soviet Union. For it was deeply associated with the confusion about the nature of resonance, as one can see in the response of G. M. Kosolapoff, a chemist from Auburn, Alabama. Kosolapoff claimed, in a letter to the *Chemical and Engineering News*, that the opposition from the East was 'quite apart from any political reasons that may have spurred the rift'.[90] Rather, he argued, it had grown because of a misunderstanding of the resonance concept, and this misunderstanding was occasioned by Western chemists who regarded it as a 'static', 'mental' superposition of resonating structures. Unless he was 'completely wrong in interpretation of the lucid writing of Dr. Pauling', he maintained, it should be regarded as a system of 'dynamic' equilibrium, *à la* Kekulé. Ironically, Kosolapoff's viewpoint illustrated both how influential Pauling's book was among

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[84] M. Calvin, 'The theory of resonance and its application to organic chemistry', *Journal of the American Chemical Society* (1945), **67**, 1043.

[85] F. C. Nachod, 'The theory of resonance and its application to organic chemistry', *Chemical and Metallurgical Engineering* (1945), **52**, 241.

[86] C. D. Hurd, 'The theory of resonance and its application to organic chemistry', *Chemical and Engineering News* (1945), **23**, 578.

[87] 'Soviet dispute a chemical theory', *New York Times*, 15 July 1951, E9. The resonance controversy in the Soviet Union has been analysed in detail by Loren R. Graham, 'A Soviet Marxist view of structural chemistry: the theory of resonance controversy', *Isis* (1964), **55**, 20–31, and *Science*, *Philosophy*, *and Human Behavior in the Soviet Union*, New York, 1987, ch. 9.

[88] 'Soviet blast Pauling, repudiate resonance theory', *Chemical and Engineering News* (1951), **29**, 3712–14.

[89] The News Bureau of the California Institute of Technology, 'Resonance Controversy', 1 September 1951, LPP: 261.11. For other chemists' responses, see A. Taurin to Pauling, 24 November 1951; and Irving S. Bengelsdorf to Pauling, 13 December 1951, LPP: 261.15.

[90] G. M. Kosolapoff, 'On "nonresonance" between East and West', *Chemical and Engineering News* (1952), **30**, 2474.

chemists and at the same time how easily his account of resonance could mislead them. Furthermore, the resonance controversy was a philosophical debate about the ontological status of resonance. In 1953, for example, the New York Chapter of the National Council of Arts, Sciences, and Professions proposed a symposium for a three-sided written debate among N. D. Sokolov of Moscow, C. A. Coulson of Oxford and Pauling of Caltech.[91] Although this symposium did not happen, the suggested questions reflected the philosophical aspects of the resonance controversy:

1. What is the resonance theory?
2. What is the evidence in proof or disproof of the resonance theory?
3. Is the convenience of the theory a proof or corroboration of the theory?
4. Is the resonance theory essentially a theory with physical meaning, or a mathematical technique, or both?
5. Has the resonance theory a basis in related sciences, such as physics?
6. Is the resonance theory applicable in all aspects of chemical valence, or only in special cases?
7. Is the resonance theory equivalent to other theories of valence, or is it in conflict?[92]

The resonance controversy and the lingering confusion between resonance and tautomerism concerned Wheland. He countered Kosolapoff's view right away, strongly arguing that Kosolapoff not only completely misinterpreted the resonance concept but also completely misunderstood the Russian criticisms.[93] Furthermore, Wheland made a serious effort to eliminate the imprecise and misleading use of terminology in his revised book, *Resonance in Organic Chemistry* (1955).[94] In fact, he was not alone in this effort. Even before the eruption of resonance controversy, Coulson scrutinized the meaning of resonance in quantum chemistry, and argued that despite its splendid applications in chemistry, resonance was not a real phenomenon.[95] However, no chemist was more careful in the semantics of resonance to meet 'customer complaints' than Wheland.[96] First, he tried to weed out any implication that the molecules of a resonance hybrid were oscillating back and forth between valence structures and hence that these structures were real physical entities.[97] He thus proposed not to use such common statements as 'the hybrid *resonates* among the structures'; 'the structures *resonate* with one another'; and 'the bond (or charge) *resonates* around the molecule, or among various positions'. Because these statements gave a 'quite erroneous impression' that resonance had a real physical significance, he carefully avoided using the verb 'resonate' throughout his revised edition. The statement that 'resonance *occurs* among a set of structures' was also problematic, for it gave the impression that there was some sort of action that the molecule was performing. He thus wanted to use the more precise statement that 'the substance of interest *is being*

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[91] Murray Vernon King to Pauling, 23 January 1953, 27 July 1953, LPP: 261.17.

[92] King to Pauling, 9 February 1954, LPP: 261.17.

[93] G. Wheland, 'Resonance again', *Chemical and Engineering News* (1952), **30**, 3160.

[94] G. Wheland, *Resonance in Organic Chemistry*, New York, 1955, p. vii.

[95] C. A. Coulson, 'The meaning of resonance in quantum chemistry', *Endeavor* (January 1947), 42–7.

[96] S. D. Silver, 'Resonance in organic chemistry', *Journal of the American Chemical Society* (1956), **78**, 2344.

[97] Wheland, op. cit. (94), 7–8.

*regarded as a resonance hybrid*', or simply that 'resonance *exists*', or that '*there is* resonance'. All this care in the choice of words was an attempt not to speak of resonance as a phenomenon. As one reviewer of his book said, Wheland was 'a master at intricate argument and the critical examination of assumptions'.[98]

While making the terminology of resonance clearer, Wheland also abandoned his mule analogy. Since the donkey and horse were as real as the mule, this analogy might mislead chemists by implying that the individual structures of a hybrid molecule had a physical significance. For this reason, he discarded it and introduced the analogy of a rhinoceros.

> We may imagine that a medieval traveler, in the course of his wandering, saw a rhinoceros; and that, after his return to his home, he attempted to describe this strange beast to his friends. A convenient way for him to convey an approximately correct idea of the animal's appearance would be to say that the rhinoceros is intermediate between a dragon and a unicorn; for, as we may assume, the people to whom he was talking would have fairly clear ideas of what these two latter purely mythical creatures were supposed to look like. Similarly, a convenient way to give an approximate description of the true structure of benzene is to say that it is intermediate between the two purely imaginary Kekulé structures.[99]

Just as the fictitious dragon and unicorn called forth clear pictures to medieval men and women, the equally fictitious Kekulé structures would evoke a picture of benzene to modern organic chemists. In each case, 'the unfamiliar reality [wa]s explained by reference to a familiar fiction'.

Still the rhinoceros analogy was not perfect. Like the mule analogy, it suggested that resonance must always involve exactly two structures, and hence that the resulting hybrid must always be exactly halfway between them. In resonance, however, any desired number of structures could be included. Therefore, instead of extending the rhinoceros analogy to cover this aspect, he adopted a third one.

> The best way to describe a man's personality is frequently by means of a comparison with familiar characters of fiction. For example, if we say that a certain actually existing man, John Doe, is a cross between Sherlock Holmes and Don Quixote, we give a fairly clear picture of the real John Doe, even though neither Sherlock Holmes nor Don Quixote ever lived. Moreover, if we now add that John Doe is more like Sherlock Holmes than he is like Don Quixote, and that he has also a slight resemblance to Sir Galahad, we make the picture still more definite.[100]

In the analogy of John Doe, there was no restriction either on the total number of the individual fictional characters or on the relative weight that is assigned to them. In the theory of resonance, likewise, there was an arbitrariness in selecting imaginary structures. By employing analogies, Wheland reiterated his previous conclusion that resonance was fundamentally a man-made concept.

In the aftermath of the resonance controversy in the Soviet Union, Pauling expressed reservations about Wheland's way of teaching resonance. 'In the description of the theory of resonance in chemistry there has been a perhaps unnecessarily strong emphasis on its arbitrary character', he said in his 1954 Nobel Lecture.[101] Instead, he suggested that this theory should be valued on the basis of its great usefulness and convenience, which made

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[98] 'Earmarking the role of resonance', *Chemical and Engineering News* (1956), **34**, 2600.

[99] Wheland, op. cit. (94), 4.

[100] Wheland, op. cit. (94), 5.

[101] Pauling, 'Chemical bond', op. cit. (2), 255–8.

the disadvantage of the element of arbitrariness of little significance. In this regard, Wheland's *Resonance in Organic Chemistry*, though dedicated again to Pauling, did not please him but provoked his complaint:

> At the bottom of page 28 you describe resonance as a man-made concept in a more fundamental sense than most other physical theories. Do you think that there is any difference at all, in this respect, between the theory of resonance and the ordinary structure theory of organic chemistry? Is a Kekulé structure for benzene…any more of a man-made concept than the carbon–carbon double bond? The answer that I have given to this question is No. I think that the theory of resonance is exactly equivalent to the ordinary structure theory – the difference between writing two structures involving single bonds and double bonds, and writing one structure is very small.
>
> On page 29 you mention that if the quantum mechanical problem could be solved rigorously the idea of resonance would not arise. I think that we might also say that if the quantum mechanical problem could be solved rigorously the idea of the double bond would not arise.[102]

Interestingly, the viewpoint that Pauling criticized was nothing new: exactly the same sentences he quoted were also in Wheland's previous book.[103] This shows that the resonance controversy in Russia exposed dormant differences between Pauling and Wheland regarding how to teach the theory and what to emphasize.

Pauling's letter, in fact, gave rise to an intense debate with Wheland about the nature of the theory of resonance. Wheland did not disagree with Pauling either that the theory was very useful and convenient for organic chemists, or that a double bond was a man-made concept. To Wheland there seemed to be no real conflict between the two men: if anything, they were just 'emphasizing different aspects of the complex problem'.[104] What he wanted to stress was that resonance in benzene was more man-made than the double bond in ethylene; and furthermore that the theory of resonance was more man-made than the ordinary structure theory of organic chemistry. In anthropomorphic terms, he argued, 'the molecule does not know about the resonance in the same sense in which it knows about its weight, energy, size, shape, and other properties that have what [he] would call real physical significance'. The double bond in ethylene, albeit man-made, could be regarded as an 'indirect approximate description of such real properties as interatomic distance, force constant, charge distribution, chemical reactivities and the like'; in contrast, the benzene molecule did not know about its resonance energy, since it was either calculated as the difference of energies at two arbitrarily chosen levels, or experimentally determined as the difference between a predicted energy and the true energy. In essence, resonance was not a real phenomenon; nor was resonance energy an intrinsic property of the molecule. By maintaining a quantitative difference of man-madeness between the resonance theory and other structure theories, Wheland hoped to counter 'the wide-spread view that resonance is a real phenomenon with real physical significance'. He wrote: 'It has been my experience that most misunderstandings of the theory are in the last analysis based on just this misapprehension, and I hoped that, if the man-made character of resonance were sufficiently emphasized, a lot of the nonsense that (especially) the organic chemists have been putting in the literature could be avoided.'[105]

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[102] Pauling to Wheland, 16 January 1956, LPP: 145.8.

[103] Wheland, op. cit. (73), 28.

[104] Wheland to Pauling, 20 January 1956, LPP: 145.8.

[105] Wheland to Pauling, 20 January 1956, LPP: 145.8.

Pauling was adamant. He did not see why one could not make use of the resonance structure of benzene to explain such properties as the hexagonal symmetry and the interatomic distance in the same way as one could make use of the double bond to explain certain properties of ethylene. He felt that Wheland had done 'an injustice to resonance theory by overemphasizing its man-made character'.[106] Wheland's next letter in reply did not change his stance.[107] To persuade Pauling, Wheland employed a comparison of the theory of resonance to the study of temperature variations using the Fourier series, whose mathematical components, sines and cosines, do not directly correspond to any physical reality. However, the more Wheland tried to enlarge upon the quantitative difference of man-madeness between the resonance theory and other structure theories, the more strongly Pauling made an alliance between them. Finally, Pauling severed the theory of resonance from its quantum-mechanical root: '[it] is independent of the valence-bond method of approximate solution of the Schrödinger wave equation for molecules. I think that it was an accident of development of the sciences of physics and chemistry that resonance theory was not completely formulated before quantum mechanics.'[108] At this point, Pauling portrayed it as a chemical theory, having an essentially empirical, inductive basis, not as a deduction from the first principles of quantum mechanics. This tactical move was made public in his article, 'The nature of the theory of resonance',[109] which was inserted into the third edition of the *Nature of the Chemical Bond* in 1960. To Wheland, the theory of resonance was a mathematical method of approximation that turned out to be useful for chemists.

However, Pauling and Wheland did not differ substantially as to the meaning of resonance. In the final chapter of *Resonance in Organic Chemistry*, where he discussed the mathematical basis of resonance, Wheland mentioned a subtle aspect of the issue of man-madeness: 'Throughout this book, we maintained that the individual structures which contribute to the state of a resonance hybrid are merely intellectual constructions, and hence that they do not correspond to any actual molecules. The situation is, however, too complicated to be rigorously described by such a simple statement.' Wheland considered three possible cases: that of benzene, where the resonance energy was large enough to say that resonating structures were indeed imaginary and that only the hybrid existed; that of lactic acid, where the energy was so small that the hybrid was the fiction and only the individual structures (tautomers) described real molecules; finally, that of ammonia, where it had an intermediate value, making the question of physical significance difficult to answer.[110] Consequently, he concluded, 'the statement that the contributing structures are merely intellectual constructions is correct only if the substance of interest belongs to the first one of the three types'. And it was the case where the resonance concept was chemically useful. On these what he called 'fine points', Wheland echoed Pauling's exposition of resonance and tautomerism in 1939. As Wheland said in his letter to Pauling,

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[106] Pauling to Wheland, 26 January 1956, LPP: 145.8.

[107] Wheland to Pauling, 4 February 1956, LPP: 145.8.

[108] Pauling to Wheland, 8 February 1956, LPP: 145.8.

[109] L. Pauling, 'The nature of the theory of resonance', in *Perspectives in Organic Chemistry* (ed. Alexander Todd), New York, 1956, 1–8.

[110] Wheland, op. cit. (94), 612–13.

they differed only with respect to 'a value judgment', which was 'more of a philosophical question than a scientific one'; and their debate was largely concerned with 'matters of personal taste'.[111]

## CONCLUSION

> I am well aware how very hard it is
> To bring to light by means of Latin verse
> The dark discoveries of the Greeks. I know
> New terms must be invented, since our tongue
> Is poor, and this material is new.
>
> Lucretius, *The Way Things Are.*

All the difficulties that Pauling and Wheland found when easing the entry of resonance into chemistry may be compared to difficulties of translation of language from one culture to another, such as putting Greek science into Latin Christendom, or Western science into China.[112] When translators cannot find an exact analogue for the word they are translating, they face a dilemma: whether they should give the meaning of it in terms appropriate to the intended audience or in terms faithful to its original usage. To translate the word in terms familiar to the intended audience has the advantage of fostering communication at one level; but at another level it is difficult to handle misunderstandings by such a translation. Pauling and Wheland had the same kind of dilemma, and when they chose to teach the theory of resonance in a language that most chemists could understand, several misunderstandings ensued. Wheland's teaching diverged from Pauling's on the point of how to solve the problem of misunderstandings. While Pauling stressed the intuitive understanding of resonance by solving chemical problems, Wheland emphasized its man-madeness and portrayed it as a mathematical method of approximation. These two translators had the same understanding of resonance at the level of its quantum-mechanical basis. But they developed different strategies of teaching and characterizing the theory of resonance for a general audience in chemistry.

Of course, the metaphor of translation has limitations in recounting all aspects of their contributions to twentieth-century chemistry: for Pauling and Wheland were undoubtedly more original thinkers than mere translators. Nevertheless, it has merit in describing how

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[111] Wheland to Pauling, 4 February 1956, LPP: 145.8.

[112] For the difficulties of perfect translation between specialists of different scientific communities, see Peter Galison, 'Computer simulations and the trading zone', in *The Disunity of Science: Boundaries, Contexts, and Power* (ed. P. Galison and David J. Stump), Stanford, 1996, 118–57; and *Image and Logic: A Material Culture of Microphysics*, Chicago, 1997. According to Galison, the specialists develop an intermediate language, a 'pidgin', to communicate and handle negotiations in a 'trading zone', where radically different activities can be 'locally' coordinated. My case is similar to Galison's in that the non-mathematical exposition of resonance by Pauling and Wheland can be considered to be a pidgin language that expedited the communication between physicists, physical chemists and organic chemists. However, this communication was made possible through devoted translators like Pauling and Wheland, rather than through local coordination of activities in a trading zone like Los Alamos. Helge Kragh and Stephen J. Weininger's paper on the entry of entropy from physics to chemistry also shows the difficulty of translation across the disciplinary line. H. Kragh and S. J. Weininger, 'Sooner silence than confusion: the tortuous entry of entropy into chemistry', *Historical Studies in the Physical and Biological Sciences* (1996), **27**, 91–130. In particular, they illustrate how many writers of chemical textbooks taught the second principle of thermodynamics without an explicit use of the entropy concept for a while.

they narrowed the gulf between physics and chemistry, and how they thereby helped transform chemistry and chemical education.

When Wheland died in 1972, his colleagues established the George Willard Wheland Medal in memory of his leading role in the development of theoretical organic chemistry.[113] They valued his critical scholarship, which was 'to rationalize, explain, put chemistry in order, and to do so in terms readily intelligible to the organic chemist'. As a lecturer and teacher, he was also remembered for 'great clarity of presentation spiced with dry humor, and characterized by scrupulous fairness'. Moreover, his books, including *Advanced Organic Chemistry*,[114] were hailed as the ones that 'radically altered education in chemistry': they 'initiated the pattern of integrating quantum mechanical interpretive theory and experiment which is seen in so many current texts. Taken together, these books can be seen to have greatly influenced how we think about and how we teach organic chemistry.' Yet perhaps Pauling's influence was more far-reaching than Wheland's. His lucid writing and theatrical teaching performance commanded a wide range of audience in many subdisciplines of chemistry. His monograph, *The Nature of the Chemical Bond*, soon became a standard text at most of the leading universities not only in America but also in many other countries, and it also became a basis for his popular undergraduate textbooks, *General Chemistry* and *College Chemistry*.[115] In 1979, Derek Davenport epitomized Pauling's contribution to chemical education: 'most of us merely teach students, a few are teachers of their peers, and the greatest are teachers to their science. And so I give you the greatest teacher to the science of chemistry of the last fifty years – Linus Pauling.'[116] Chemistry, to be sure, was not fully reduced to physics, nor had it become completely mathematical. None the less, chemists could make use of quantum mechanics in their language, thanks to chemical translators like Pauling and Wheland.

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[113] 'George Willard Wheland Medal: An Appeal for Funds', Mulliken papers: 41.12, University of Chicago Library.

[114] G. Wheland, *Advanced Organic Chemistry*, New York, 1946, 1949 and 1960.

[115] L. Pauling, *General Chemistry: An Introduction to Descriptive Chemistry and Modern Chemical Theory*, San Francisco, 1947, and *College Chemistry: An Introductory Textbook of General Chemistry*, San Francisco, 1950. For the importance of Pauling's *The Nature of the Chemical Bond*, see Hager, op. cit. (3), 216–18.

[116] Derek A. Davenport, 'Linus Pauling – chemical educator', *Journal of Chemical Education* (1980), **57**, 35–7, on 37.