L. C. Pauling -- three egregious errors in chemistry

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abstract

This essay discusses three of Pauling's flagrant and appalling errors in chemistry: in crystallography -- his refusal to accept the reality of quasi-periodic materials, in molecular medicine -- his insistence on the value of ascorbic acid in large doses with neither chemical basis nor experimental proof of its efficacy, and in discussing the chemical bond -- his amplitude functions chosen only in spherical polar coordinates are applicable to an atomic system of only rigorously spherical symmetry, hence with no other atom or external electric field in the system. When one takes account of the fact that a molecule in a quantum state has extension in neither space nor time, any justification of teaching quantum mechanics in undergraduate chemistry curricula is absolutely undermined.

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A statement [1] about Linus Carl Pauling as being the subject of a "general recognition as one of the two greatest scientists of the twentieth century" might not seem controversial, but, associated with a recent review [2] in *The New Atlantis - a Journal of Science and Technology*, there appears a suggestion that "in some projects ... the great scientist was given to naiveté and folly". Another view is that "Linus Pauling is one of the greatest chemists of the 20th century; he is also one of this century's most controversial scientists" [3]. That essay by Valiunas [2] concerns itself mostly with "the anti-war activism" and "his theorizing about vitamins". There exist other aspects of his undoubted naiveté and folly that impinge on science -- on chemistry in particular -- and that were excluded from that review that was designed for a general readership. The objective of this essay is to discuss three topics that illustrate a profound justification for an accusation of "naiveté and folly" in a chemical context and the implications for chemical education. We proceed in a reverse chronological order.

During the last decade of his life, 1984 - 1994, Pauling undertook a relentless crusade against quasi-crystals, or, more accurately, quasi-periodic materials. Solid matter in this form was first announced by D. Shechtman, whose account [4] is highly recommended for both the fundamental concepts of crystallography and the description of Pauling's tenacious opposition to the possibility of the existence of these materials. Pauling was first and foremost a chemical crystallographer: for his doctoral research project in chemistry in California Institute of Technology under the supervision of R. G. Dickinson, Pauling practised xray crystallography, to the extent that his first eight publications, during 1923 to 1925, were all concerned with the structures of various inorganic crystals derived from xray diffraction, and the associated technique. In particular, the second paper, published under his sole authorship, described the structure of an intermetallic compound, magnesium stannide [5]. Shechtman's discovery involved another intermetallic compound, of formula Al_6Mn, of which a tiny crystal violated two laws of crystallography that were at that time deemed to be sacrosanct: the crystal had no periodicity, and it exhibited a ten-fold rotational symmetry [4]. Two publications about this discovery, including theoretical aspects, occurred in late 1984 and mid 1985. In 1985 October, after Shechtman visited Pauling in his institute during the summer of that year [6], Pauling published a rebuttal of this thesis of quasi-periodic crystals [7]; he attributed the phenomenon to icosahedral twinning -- i.e. instead of one single crystal that diffracts xrays, joined crystals collectively diffract xrays to produce a pattern interpreted as indicating a quasi-periodic structure; Pauling invoked multiple twinning to explain the pattern. In succeeding years, Pauling published four papers in 1987, seven papers in 1988, two papers in 1989 and one each in 1990 and 1991 that attempted to bolster his view of the basis of an apparent quasi-periodic structure resulting from crystal twinning. Shechtman had clearly contravened the then current laws of crystallography, which some chemists viewed as a gross error. "During an American Chemical Society conference at Stanford, in front of thousands of scientists, Pauling proclaimed 'Danny Shechtman is talking nonsense. There is no such thing as quasi-crystals, only quasi-scientists'" [3]. Elsewhere [8], one can read "at a science conference in front of an audience of hundreds, Pauling ..." made the same claim. The definition of a crystal was subsequently revised to include any solid material having an essentially discrete diffraction pattern. In 2011 Shechtman became Nobel laureate in chemistry for his discovery and analysis of quasi-periodic materials. In his old age, Pauling was once again a crystallographer, amongst other pursuits, but his crystallography was conducted grossly in error.

Between the early period of presumably competent crystallography and the late and incontestably erratic crystallography, and following a foray in 1930 into electron diffraction after xray diffraction, Pauling's attention became drawn to molecular biology [2], first to the structural and magnetic properties of haemoglobin and subsequently to the structure of proteins. Pauling favoured the structure of deoxyribonucleic acid as triply stranded, which he proposed in a paper in Nature in 1953, just before Watson and Crick in Cambridge proved that doubly stranded molecules were the correct explanation of experimental evidence available from xray diffraction. Pauling commented much later that he had overlooked the possibility that water was heavily incorporated in the samples with which he was able to work; the only way that he could account for the density of the crystal was to incorporate another strand of nucleic acids [9]. Pauling proceeded to speculate about the medical implications of his work [2].

The discovery of vitamins by F. G. Hopkins in Cambridge and the recognition that they are essential elements of a healthy diet were among the most important contributions to health ever made [2]. Vitamins are merely chemical compounds; some have large and complicated structures whereas others have simple structures, such as 3-pyridine carboxylic acid known as niacin and vitamin B_3, or are amenable to synthesis in the first laboratory courses in organic chemistry, such as ascorbic acid, vitamin C. Before his campaign against quasi-periodic crystals, Pauling embarked on a crusade to promote the consumption of vitamins in *megadoses*, in particular, vitamin C. A genuine medicine, rather than a placebo, is a chemical compound, or a mixture of such compounds, that is generally intended to react in a rather specific manner in some chemical conditions in a living organism. In 1973, Pauling established the Linus Pauling Institute of Science and Medicine that was dedicated to 'orthomolecular medicine', with major funding from a pharmaceutical company that produced much of the world's supply of vitamin C [10]. An anti-oxidant is a chemical substance found in foods that might significantly decrease the harmful effects of reactive species such as various oxygen and nitrogen compounds and free radicals that disrupt the normal physiological function at a cellular level in human beings. Apart from the general action of ascorbic acid and its salts as a dietary anti-oxidant, Pauling failed to demonstrate a particular molecular mechanism for vitamin C administered in massive doses. His enthusiastic advocacy of vitamin C in such substantial doses was an enormous boon to the health-food industry; his personal fame and scientific prestige assisted a campaign by that industry to weaken the protection of USA Food and Drug Administration against fraudulent claims for the nutritional benefits of many questionable products. Although in the second half of his life Pauling was able to publish papers in reputable scientific journals largely on the basis of his accumulated reputation, in the case of vitamin C he directly published five books promoting its use that were subject to no regular scientific scrutiny before promulgation. Pauling's extension of his chemical intuition into a biochemical area with no basis in experimental fact, whereas he should have proceeded to produce or to explain reproducible data from properly designed and controlled medical trials, has done great damage to human populations that are bombarded with false claims for purported nutritional products, which might be even counter-productive. Pauling's gross error was simply that he failed to apply the scientific method to a proposition that vitamin C in large doses might have significant salutary effects for human nutrition and against disease and morbidity; the victims of his error are the credulous customers and consumers of unhealthy 'health foods'. The nature of the targets of those dietary anti-oxidants is now itself suspect [11].

Of Pauling's awards of two Nobel prizes, one was for chemistry, "for his research into the nature of the chemical bond and its application to the elucidation of the structure of complex [sic, complicated] substances". Following the award of his doctoral degree for research in chemistry based on xray crystallography, with accompanying studies in mathematical physics, Pauling was awarded a Guggenheim Fellowship that enabled him to travel to and within Europe from 1926 March until 1927 September. He passed first some months in Munich in the vicinity of A. Sommerfeld, a period in Goettingen in the vicinity of M. Born and a further term in Copenhagen in the institute of N. Bohr, who were the leading physicists of that period but with whom Pauling had little or no direct contact. When Pauling became aware of an alternative development, by E. Schroedinger, of quantum mechanics in the form of wave mechanics, he applied for, and was granted, an extension of his fellowship. He then attended lectures of Schroedinger in Zurich; although Pauling attempted to meet Schroedinger privately for discussion, the latter denied him that privilege, indicating that Pauling's work was not interesting to him [6].

After publication of five papers on sundry topics during 1925, Schroedinger published within 1926 another three papers on diverse topics and six papers on the wave mechanics that he began to develop in late 1925 in the light of the evolution of quantum mechanics in Goettingen under Born and in Cambridge under P. A. M. Dirac. In an authorised English translation, four of those six papers bore the title "Quantisation as a problem of proper values", and were collected in a book [12] with three related papers. Published in Physical Review [13], the tenth paper of 1926 was largely a partial summary of the content of papers published previously in periodicals in the German language. That book [12] contains also ten lectures delivered at the Royal Institution in London and elsewhere; the content of those lectures was likely similar to what Pauling heard in Zurich. In the first paper of the four under the specified title, Schroedinger presented a formal derivation of his temporally independent amplitude equation, produced amplitude functions in spherical polar coordinates -- which in Schroedinger's paper [11] are called simply polar coordinates -- for a hydrogen atom, and obtained a formula for the energies of its discrete states. Although this paper might be celebrated by some undiscerning persons as one of the most important achievements of physics in the twentieth century, and be supposed to have created a revolution in many areas of physics and chemistry, it was intrinsically a modest advance on existing science: those energy values, which had previously been derived by Bohr according to a completely incorrect theory, were inaccurate according to then known experiments, and those amplitude functions are merely parochial artifacts of the particular spherical polar coordinates in non-relativistic wave mechanics as one variant of quantum mechanics [14]. Regarding the energies, in 1924 G. M. Shrum in Toronto had already performed spectrographic experiments that proved the four separate spectral features in the Balmer series to be not single lines but multiplets [15]; Bohr's formula, and analogously Schroedinger's reproduction of it, were hence inadequate to express accurately the energies of the hydrogen atom in its discrete states, for which an improved derivation arose in Dirac's treatment with relativistic quantum mechanics in 1928 [16]. Schroedinger's second paper under the same title began with an analogy of the hamiltonian between mechanics and optics, and continued with applications of amplitude functions for a Planck oscillator, two rotors and a diatomic molecule as a non-rigid rotor. After two digressions to discuss the continuous transition from micro-mechanics to macro-mechanics and the relation between the quantum mechanics of W. Heisenberg, Born and P. Jordan and his own formulation of wave mechanics, Schroedinger continued the series with the third part; in a prodigious feat, he developed therein his perturbation theory, treated the hydrogen atom in paraboloidal coordinates and calculated the Stark effect on spectral lines in the Balmer series and, notably, their intensities and polarizations.

Heisenberg recognised that the observable properties of an atom are the frequencies and intensities of its spectral lines; his motive to develop quantum mechanics was to avoid the unobservable orbits of Bohr's theory. Neither Bohr nor his followers ever succeeded to calculate an accurate intensity of an atomic transition. Although Pauli had developed [17], before Schroedinger's first paper in the series, a symbolic approach to calculate the same inaccurate energies of discrete states of the hydrogen atom, he was likewise unable to cope with the intensities of spectral lines, which Schroedinger managed *at a stroke* in this third paper; the latter article contains also a mathematical appendix on Laguerre and Legendre functions and polynomials. In his fourth paper in the series, still in 1926, Schroedinger developed his temporally dependent partial-differential equation, having the form of a diffusion equation, and its solutions as "wave functions", in addition to considering a theory of perturbations that contain explicitly time, a theory of dispersion and the continuous spectrum, among other topics. To all this information Pauling must have been exposed during the latter part of his sojourn in Europe, before he joined the academic staff of California Institute of Technology in 1927 autumn, about the same time that Schroedinger transferred from Zurich to Berlin.

Despite his training in mathematical physics, Pauling practised an intuitive approach to his science and other pursuits [2,3]. Dismayed at the complicated nature of the mathematics involved in the quantum mechanics that was being developed in Goettingen and Copenhagen, he was immediately attracted to Schroedinger's approach that seemed to have a more physical basis. When he returned to California, Pauling was productive not only in his xray crystallographic experiments but also in calculations based on quantum-mechanical themes, particularly in relation to molecular structure and properties. For this purpose he adopted the results of Schroedinger in the dissatisfying first paper in the famous series, namely the solutions to the temporally independent equation in spherical polar coordinates for the hydrogen atom that are applicable to only a system with rigorously spherical symmetry. In so doing, he completely ignored the equally valid -- and much more useful -- solutions in paraboloidal coordinates in the third paper, although he cited the latter paper in various papers and in his book *Introduction to Quantum Mechanics with Applications to Chemistry*, with coauthor E. B. Wilson [18].

To explain the tetrahedral disposition of hydrogen atomic centres about the carbon atomic centre in methane, Pauling invented *hybridisation*, as follows [19]. Three amplitude functions in spherical polar coordinates of the hydrogen atom with radial quantum number $k = 0$, azimuthal quantum number $l = 1$ and magnetic quantum numbers $m = 0, \pm 1$ yielded three real linear combinations from those one real and two complex amplitude functions; with a fourth real amplitude function with $k = 1$, $l = 0$ and $m = 0$, further linear combinations of those three real linear combinations yielded four real formulae of which the plots exhibited the desired spatial disposition to the corners of a regular tetrahedron. These linear combinations as tetrahedral hybrid functions he attributed to the carbon atom, although nobody before or since has derived directly such functions as explicit solutions of the Schroedinger equation for a carbon atom. This practice amounts to extrapolation from an atom with Z=1 and one electron, to an atom with $Z = 6$

and six electrons, i.e. extrapolation outward from a point. This production also amounts to a circular argument -- a logical fallacy: the tetrahedral hybrid real amplitude functions are formed to reproduce the tetrahedral structure of methane that motivated their construction. Pauling analogously announced other hybrid functions for the trigonal disposition of three atomic centres about each carbon atomic centre as in ethene, and for the digonal disposition of two atomic centres about each carbon atomic centre as in ethyne. The latter digonal hybrids involve two linear combinations of only real amplitude functions with $k = 0$, $l = 1$, $m = 0$ and $k = 1$, $l = 0$, $m = 0$, in terms of quantum numbers that are parochial to spherical polar coordinates. The objective of these efforts involving hybridisation was to generate amplitude functions with particular spatial dispositions, despite the fact that all resulting functions in spherical polar coordinates are still formally applicable to a hydrogen atom in a spherically symmetric environment. A further irony is that each such digonal hybrid function, constructed as a linear combination of direct solutions in spherical polar coordinates, is identical with a real amplitude function that arises directly in the solution of the hydrogen atom in paraboloidal coordinates, specifically those amplitude functions with $n_1 = 1$, $n_2 = 0$, $m = 0$ and $n_1 = 0$, $n_2 = 1$, $m = 0$; n_1 and n_2 are quantum numbers parochial to paraboloidal coordinates in the same way that k and l are quantum numbers parochial to spherical polar coordinates. Whereas the solution of the hydrogen atom in spherical polar coordinates is appropriate for a model as an isolated atom having rigorously spherical symmetry, i.e. with neither other matter nor electric field present in the system under calculation, the solution of the hydrogen atom in paraboloidal coordinates is appropriate for an atom in the presence of an isotropic electric field, which Schroedinger himself solved [9], or in a collision with an electron [20]. Of the two possible systems of coordinates known to a reader of either Schroedinger's papers or the specified book [12] for the solution of the hydrogen atom according to wave mechanics, Pauling chose the less appropriate system. In fact, for a hydrogen atom interacting with another atomic centre as in a diatomic molecule, amplitude functions in ellipsoidal coordinates are uniquely appropriate, as E. Teller recognised in 1930 [21] following Burrau and Wilson. One must understand that Schroedinger's partial-differential equation for the hydrogen atom, or atom with only one electron in general, is separable to enable exact algebraic solutions in coordinates in (at least) four distinct systems, namely the three mentioned above plus spheroconical coordinates [14]; for a particular application, calculations in one system might prove more convenient than in another, but an amplitude function expressed in coordinates in one system can become transformed into a corresponding amplitude function, or a linear combination thereof, in another system. Each system of coordinates has its associated amplitude functions characterised by quantum numbers in distinct sets and of which the surfaces have distinct shapes. At the time that Pauling embarked on papers in a series published under a general title "*The nature of the chemical bond*" from 1931 to 1933 [19], his arguments were based on amplitude functions expressed in an infelicitously chosen, and thus totally inappropriate, system of coordinates, apart from his brazen extrapolation from a point, which implies that electrons do not repel one another. His famous book of the same title [19] that appeared after several years and ran to three editions, was a significant part of the basis of his Nobel award in chemistry.

Although some textbooks of physics treat cursorily the hydrogen atom in paraboloidal coordinates, no known textbook of chemistry even mentions their existence, despite extensive coverage of amplitude functions in spherical polar coordinates in both explicit algebraic form and graphical depictions of mostly lesser accuracy. This lacuna is undoubtedly due to Pauling, who wielded an enormous influence on chemists during the middle decades of the twentieth century, and whose influence continues to thrive because, according to Mulliken, Pauling was "a master salesman and showman" [22] or, according to Valiunas, "a 'showman' who dazzled the credulous masses -- that sad benighted chemistry professoriate -- with beguiling simplifications..." [2], from which rehabilitation has yet to occur. That "benighted chemistry professoriate" is hereby awakened. Such a deliberate failure to acknowledge, and to comprehend the fundamental significance of, the existence of multiple coordinate systems for an exact solution of Schroedinger's equations for the hydrogen atom [14], and in particular to understand the molecular application of ellipsoidal coordinates, is Pauling's gross error; the victims are gullible chemists who have been deceived about the nature of the mathematical basis of the chemical bond and molecular structure for many decades. Two authors have recently published books on the topic *where physics went wrong* [23, 24]; here we identify where chemistry went wrong, and the man mostly responsible for this debacle was Pauling.

To progress from this unhappy malaise in the understanding of molecular structure, and of its explanation in chemical education, one must recognise and accept the following truths. Electrons are fundamentally indistinguishable: there is no *s*-electron, no *p*-electron, ... no σ-electron, no π-electron, no bonding electron, no lone pair ...; there are only electrons. The measurable quantity is the total density of electronic charge in locations near atomic nuclei within a chemical sample, whether a molecule in the gaseous phase or the content of a unit cell of a periodic crystal. Amplitude functions of an atom with one electron, commonly called orbitals, are the results, or *output*, from a calculation such as Schroedinger demonstrated in both spherical polar and paraboloidal coordinates [12]; not only the algebraic formulae and the shapes of surfaces of these orbitals under specified conditions but even the associated quantum numbers in particular sets depend on the selected coordinate system [14], and are hence parochial to that system. Although some such formulae might legitimately serve in basis sets for a useful calculation of atomic and molecular properties with quantum-chemical programs, one must distinguish meticulously between those orbitals -- the *output* from one calculation, and the constituents of basis sets -- the possible *input* into other calculations. Such quantum-chemical calculations do not even require basis sets composed of orbitals: calculations with density functionals free of orbitals yield satisfactory results for many purposes [25]. The results of observable quantities from appropriately performed quantum-chemical calculations have no dependence on the particular basis set, whether composed of functions resembling orbitals or other. Molecular structure is a classical concept, alien to quantum mechanics: according to quantum mechanics, a molecule in a quantum state has extension in neither time nor space, hence no structure [26], although appropriate expectation (or average) values of distances between particles of particular types might be estimated. The application of quantum mechanics in any form to explain molecular structure is hence a logical fallacy. What matter for chemists are the quantum laws, or laws of discreteness [27], not quantum theories. Although Pauling lived 18 years beyond that recognition, long overdue, by Woolley [26] of the incompatibility of quantum mechanics and molecular structure, Pauling never recanted his folly. His gross and appalling errors continue to exert a severely deleterious influence in chemical education.

One might suppose that the other of the two "greatest scientists of the twentieth century" [1], from a point of view in USA, would be A. Einstein. His work was confined to merely the first half of that century, and his total achievements might compare unfavourably with those of either Born or, especially, Dirac. Einstein's first successes in 1905 were highly significant, but must be recognised to have consisted of incremental advances on existing themes, on which he built subsequently in developing general relativity. The scope of Born's research was broader than that of Einstein; for instance, the term quantum mechanics itself appeared first in a paper by Heisenberg and Born, 1924; that theory originated in the work of his research assistant, Heisenberg. Born had to place Heisenberg's calculations on a rigorous mathematical basis to become matrix mechanics. Both Einstein's and Born's achievements pale before the postulate of the quantitative existence of anti-matter -- the positron, which was implicit in Dirac's relativistic quantum mechanics in 1928 [16]; a subsequent momentous achievement was his quantum electrodynamics. The triumphant scientific activities and careers of both Born and Dirac were undertaken in a European context during difficult historical periods, which might have made them less visible in a setting of general thinking in USA. The scientific impact of the work of Born, Dirac, Einstein and Heisenberg maintains its currency, but much of Pauling's work and his ideas lack enduring scientific value and are worthy of abject rejection. Pauling's motive to provide a mathematical basis for an understanding of molecular structure might have been commendable, but his methods were critically flawed: the end does not justify the means.

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