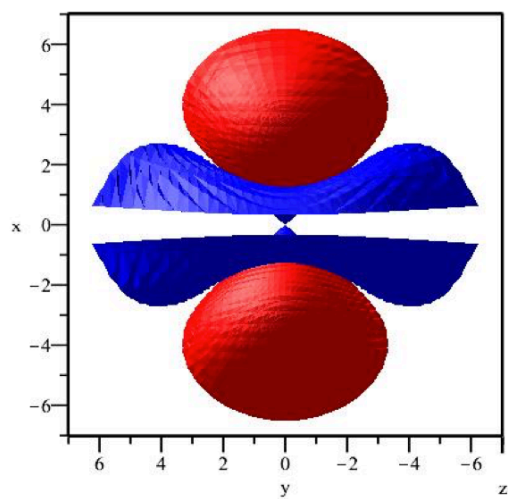


General Chemistry Without Orbitals



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• **ABSTRACT**

Orbitals are a standard component of explanations in general chemistry despite the confusion about these mathematical formulae. We illustrate the solutions of Schroedinger's equation for the hydrogen atom in coordinates of all four systems, and differentiate the applicability of orbitals in these four systems. After pondering typical queries from an instructor, we present reasons that future textbooks of general chemistry should exclude orbitals and discuss the teaching of general chemistry on this basis. The importance of the structure of molecules and materials from experiment, as defined by the observable total electronic density and its local maxima, is emphasized as an unobjectionable way to present the properties, reactions and applications of chemical substances and their mixtures. The incompatibility of molecular structure and quantum mechanics is discussed before a conclusion that quantum mechanics and its orbital artefacts are irrelevant for general chemistry.

• **KEYWORDS** Teaching general chemistry, orbitals, quantum mechanics, molecular structure

General Chemistry Without Orbitals

Science is concerned only with observable things. -- Dirac¹

• I INTRODUCTION

According to a reputable textbook² for general chemistry, "the solutions to Schroedinger's equation for the hydrogen atom yield a set of wave functions called **orbitals**". That definition is generally acceptable and approximately correct: the solutions number four sets³ rather than one; moreover, according to Schroedinger,⁴ these functions in any set independent of time are named amplitude functions, not wave functions, to which usage we accordingly conform.

At the outset we state no objection to the use of orbitals in basis sets for, or other uses in, actual calculations, even though they might be superfluous; for instance, calculations based on the amplitude function of James and Coolidge contained no orbital.⁵ Calculations according to density-functional theory can be made accurately with software for electronic structure free of orbitals^{6,7} -- no orbital is involved at any stage of the calculations, but the results for observable properties have accuracy comparable with that of alternative software for quantum chemistry. Quantum-chemical calculations are, however, irrelevant, and far remote from the teaching and practice of general chemistry; our concern is the suitability of invoking orbitals in teaching general chemistry to undergraduates in their first year of study after secondary school. Our content and arguments have, understandably, implications that are necessarily applicable to preceding and following instruction in chemistry.

The question at issue here is the use of orbitals in qualitative explanations of atomic and molecular structure and properties. Common textbooks of general chemistry customarily devote

much space and importance to orbitals as if they were somehow more, or other, than mere mathematical functions applicable to only the hydrogen atom, which is a logical fallacy. The incontestable principle according to which one must invariably abide is that electrons are fundamentally indistinguishable. The pertinent experimentally observable quantity is the total density of electronic charge in the vicinity of one or other atomic nucleus in a molecule or in a unit cell of a crystal. Any attempt to partition that density relies on arbitrary criteria and is thereby subject to error, invalid conclusions and refutable inferences.

Our purpose in this essay is first to define, objectively and comprehensively, orbitals according to their mathematical nature and algebraic form, then to diagnose the problems with their rampant qualitative use. Although no chemistry book known to the authors ever mentioned the fact that multiple sets of solutions to the Schroedinger equation for the hydrogen atom exist in disparate systems of coordinates, many textbooks of quantum mechanics in physics acknowledge the existence of a second set, resulting from Schroedinger's own solution in paraboloidal coordinates,⁴ but the facts of not only a third set but also a fourth set are still totally ignored.

In succeeding sections we summarise the orbitals according to the four systems of spatial coordinates in which they have been derived,^{8,9} accompanied in each case with an explicit single instance of an actual algebraic formula and its depiction as a surface of constant amplitude. We then undertake a critique of the nature of application of any such orbitals to describe or to explain the structure and binding within molecules and materials, before outlining how one can teach general chemistry effectively without invoking orbitals or analogous quantities, based on our actual experience in teaching general chemistry over the years.

We make no apology for presenting extensive algebraic formulae in section III -- orbitals are neither more than, nor less than, mathematical functions; each chemist must become reconciled to this fact of science.

• II SUMMARY OF THE TEACHING OF ORBITALS

There is a natural tendency for an experimental chemist to believe that orbitals are justified mathematically and for theoreticians to believe that orbitals are proved by experiment. A philosophical chemist might debate the existence of orbitals, and whether one should believe in orbitals.¹⁰ To continue to convey this model in introductory chemistry, a pragmatic chemist should, however, be convinced that orbitals are useful. The function of a model in science is to provide a rationale that unifies a series of apparently unrelated facts, but such a model must not violate fundamental chemical and physical laws. A student who is unable to understand or to apply the model to solve problems through prediction resorts to memorization, which is the state of teaching chemistry today.¹¹ Post described these models as ‘floating’ models, as neither are they derived strictly from theory nor are they based on experimental observation.¹² There is no experimental evidence for any explicit atomic orbital, and, as we show here, the theoretical basis of the use of orbitals is suspect.

How are orbitals taught and used in introductory chemistry? We list a few topics.

- 1) Electron configuration -- The orbital model for hydrogen serves as a rationalization of a supposed shell structure and subsequently the bonding between atoms of all elements.
- 2) Periodic table -- Atomic orbitals and the associated rules -- quantum numbers, Pauli principle, 'aufbau' principle, Hund's rule -- lend quantum credence to the organization of the periodic table.

- 3) Molecular structure --Authors of textbooks try to justify a structure (such as the angular shape of water) based on the orbitals of the constituent atoms.
- 4) Reactivity -- Some simple reactivity might be illustrated using orbitals to guide the student.

By far the most common use of orbitals is to bridge the concepts of bonding in molecules from two-dimensional Lewis diagrams to three-dimensional structures. The use of electron domains¹³ or a Coulombic model¹⁴ have been propounded as an ‘orbital-free’ model for three-dimensional structure. Jensen described this statement, however, as inaccurate.

“By the 1990s Gillespie was making the further dubious claim that the so-called ‘valence-shell electron domain’ or VSED model was in fact an alternative to orbital models, rather than a crude method for approximating localized MOs, and that the VSEPR approach itself did not require the use of any orbitals whatsoever for its theoretical justification... However, if it specifically refers to use of the VSED model as an alternative to orbitals, then there is a problem, since the division of the valence-electron density of molecules into spherical, nonoverlapping domains with integral populations consisting of pairs of electrons of opposite spins is identical – however you may choose to relabel it – to a use of the Kimball free-cloud model and definitely corresponds, despite claims to the contrary, to the use of an orbital model.”¹¹

There are other and less known uses of orbitals in undergraduate chemical education. For instance, orbitals have been used to describe the shape of isolated, gas-phase atoms, *i.e.* Mn atoms should be spherical whereas boron should be a prolate spheroid and carbon a oblate

spheroid.¹⁵ Such portrayal is devoid of both experimental and calculational evidence and must be considered untenable.

We show below that most confusion about orbitals is based on a long-held misconception that quantum mechanics provides a mathematically unique answer. In 1983 McKelvey asserted prophetically that some organic chemists would be upset to learn that aspects of Dirac's relativistic quantum mechanics -- quantum numbers, representation of orbitals, absence of nodes -- fail to show a correlation one to one with non-relativistic quantum mechanics.¹⁶ How do chemists feel when they realize that, even according to Schroedinger quantum mechanics, there are four variations on the theme of orbitals, as we proceed to demonstrate?

• III SYSTEMS OF COORDINATES AND EXEMPLARY ORBITALS

In coordinates as spatial variables in exactly four systems, Schroedinger's partial-differential equation independent of time for the hydrogen atom becomes separable³ into three ordinary-differential equations that have unique solutions in well defined and explicit standard algebraic forms, as follows.

a) Spherical Polar Coordinates

The coordinates in this system,¹⁷ the only system known to almost all chemists, are conventionally named r , θ , ϕ ; a surface of constant r corresponds in Cartesian coordinates to a finite sphere of that radius with its centre at the origin of the coordinate system; a surface of constant θ corresponds to an infinite cone of circular cross section about axis z with angle θ from that axis and its vertex at the origin; a surface of constant ϕ corresponds to an infinite half-plane from axis z . These features are illustrated in Figure 1. Please be aware that, although one can

work directly with mathematical operations in various systems of coordinates, all pictorial representations must appear in Cartesian coordinates with which human eyes are familiar; advanced mathematical software (*Maple* for our work) readily fulfills these requirements. On this basis all our plots of orbitals are directly comparable.

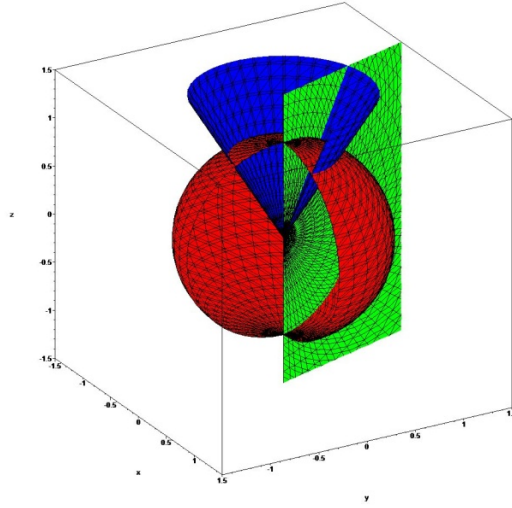


Figure 1 Definition of spherical polar coordinates: a sphere (red) of radius $r = 1$ unit with its center at the origin cut open to show the interior; a circular cone (blue) of constant θ at angle $\pi/6$ rad to axis z and with its vertex at the origin also cut open; a half-plane (green) of constant ϕ is at angle $3\pi/5$ rad to plane xz for which $y = 0$.

The solutions $\psi_{k,l,m}(r,\theta,\phi)$ to the Schrodinger equation independent of time in these spherical polar coordinates, *i.e.* the orbitals, are expressible as

$$\begin{aligned} \psi_{k,l,m}(r, \theta, \phi) = & \sqrt{\frac{Z \pi \mu e^2 k!}{\epsilon_0 h^2 (k+2l+1)!}} \left(\frac{2 \mu \pi e^2 Z}{(k+l+1) h^2 \epsilon_0} \right)^{(l+1)} r^l \\ & \text{LaguerreL} \left(k, 2l+1, \frac{2 \pi \mu e^2 Z r}{h^2 \epsilon_0 (k+l+1)} \right) e^{\left(-\frac{\pi \mu e^2 Z r}{h^2 \epsilon_0 (k+l+1)} \right)} e^{(im\phi)} \\ & \sqrt{\frac{(2l+1)(l-|m|)!}{(l+|m|)!}} \text{LegendreP}(l, |m|, \cos(\theta)) / (2(k+l+1)\sqrt{\pi}) \end{aligned}$$

In this equation that is deliberately expressed in terms of fundamental physical constants appear as parameters quantum numbers radial k , as first argument of generalised Laguerre functions denoted LaguerreL with coordinate r , azimuthal l as first argument of associated Legendre functions of the first kind and denoted LegendreP with coordinate θ , and equatorial m that is coefficient of equatorial angle ϕ and $i = \sqrt{-1}$ in an exponential function. Other symbols are atomic number Z , reduced mass $\mu = \frac{m_e m_p}{m_e + m_p}$ of the atomic system for which $Z = 1$ for H with a proton of mass m_p as atomic nucleus, electric charge $-e$ for an electron of mass m_e , Planck constant h and permittivity ϵ_0 of vacuum. In terms of quantum numbers specific for this coordinate system, energy quantum number n from experiment is equal to $k + l + 1$.

As that equation for an amplitude function as orbital comprises three independent variables -- r , θ , ϕ , as coordinates, and one dependent variable as amplitude ψ , a plot of such a function would require four spatial dimensions, which is impracticable. We hence show a surface of constant ψ at a value chosen to reveal the essential geometric features; the value of ψ is explicitly chosen, here and below, such that the surface of ψ^2 at that value would contain about 0.99 of the total electronic charge density. For quantum numbers $k = 0$, $l = 1$, $m = 0$, so $n = 2$, the amplitude function (commonly known as orbital $2p$) has this explicit algebraic form in terms of fundamental parameters:

$$\psi_{0,1,0}(r, \theta, \phi) = \frac{\sqrt{2} e^5 (\mu Z)^{\left(\frac{5}{2}\right)} \pi^2 r e^{\left(-\frac{\pi \mu Z e^2 r}{2 h^2 \epsilon_0}\right)} \cos(\theta)}{8 h^5 \epsilon_0^{\left(\frac{5}{2}\right)}}$$

A plot of the surface of this amplitude function or orbital, according to the stated criterion, appears in Figure 2. The surface comprises two separate hemispheres, of opposite phase on either side of plane xy for which $z = 0$, and with rounded edges; the overall nearly spherical shape is consistent with the fact that the Coulombic attraction between an electron and a proton has no angular dependence.

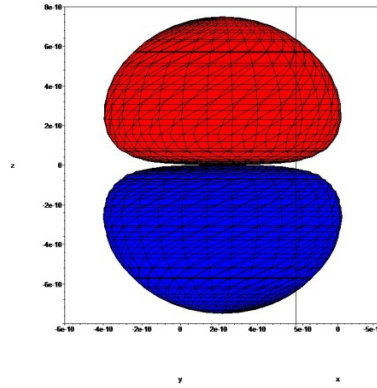


Figure 2 Surface of $\psi_{0,1,0}(r, \theta, \phi) = \pm 3.17 \times 10^{12} \text{ m}^{-3/2}$; the upper lobe (red) has a positive phase, the lower lobe (blue) has a negative phase. The length scale on each axis is in terms of metre consistent with the SI units of the plotted function.

b) Paraboloidal Coordinates

The spatial variables in this system¹⁸ are conventionally named u , v and ϕ : a surface of constant u corresponds to an infinite paraboloid, which is a parabola of revolution about axis z , opening downward and with its focus at the origin; a surface of constant v corresponds to an infinite paraboloid about axis z opening upward and with its focus at the origin; a surface of

constant ϕ again corresponds to an infinite half-plane from axis z . Figure 3 illustrates these features.

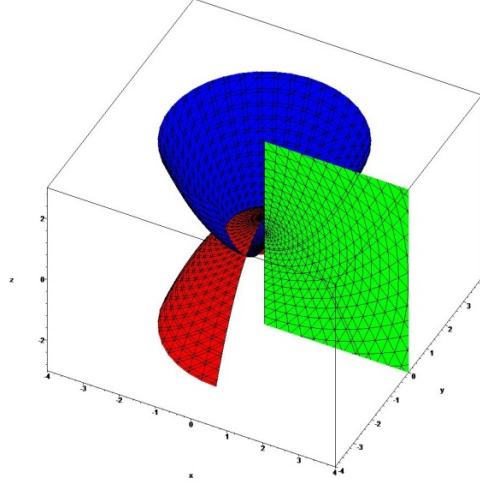


Figure 3 Definition of paraboloidal coordinates: a paraboloid (red) for $u = 1$ unit with its focus at the origin and opening downward, cut open to show the interior; a paraboloid (blue) for $v = 1$ unit with its focus at the origin and opening upward, likewise cut open; a half-plane (green) for $\phi = 0$ is, accordingly, in plane xz for which $y = 0$.

The solutions $\Psi_{n_1, n_2, m}(u, v, \phi)$ to the Schroedinger equation independent of time in these paraboloidal coordinates, *i.e.* the orbitals, are expressible in terms of fundamental physical constants as

$$\begin{aligned}
\Psi_{n_1, n_2, m}(u, v, \phi) = & (-1)^{|m|} \sqrt{\frac{Z \pi \mu e^2}{\varepsilon_0 h^2}} \sqrt{\frac{2 n_1! n_2!}{(n_1 + |m|)! (n_2 + |m|)!}} \\
& \left(\frac{\pi Z e^2 \mu}{h^2 \varepsilon_0 (|m| + n_1 + n_2 + 1)} \right)^{(1 + |m|)} (u v)^{|m|} e^{\left(-\frac{\pi Z e^2 \mu (u^2 + v^2)}{2 h^2 \varepsilon_0 (|m| + n_1 + n_2 + 1)} \right)} e^{(i m \phi)} \\
& \text{LaguerreL} \left(n_1, |m|, \frac{\pi Z e^2 \mu u^2}{h^2 \varepsilon_0 (|m| + n_1 + n_2 + 1)} \right) \\
& \text{LaguerreL} \left(n_2, |m|, \frac{\pi Z e^2 \mu v^2}{h^2 \varepsilon_0 (|m| + n_1 + n_2 + 1)} \right) / (\sqrt{2 \pi} (|m| + n_1 + n_2 + 1))
\end{aligned}$$

In this equation appear quantum numbers n_1 , as first argument of a generalised Laguerre function denoted LaguerreL of which the spatial variable is u , n_2 as first argument of a generalised Laguerre function of which the spatial variable is v , and equatorial m that is again coefficient of equatorial angle ϕ and $i = \sqrt{-1}$ in an exponential function. Experimental energy quantum number $n = n_1 + n_2 + |m| + 1$, in terms of quantum numbers specific for this coordinate system. With the same criterion as for $\Psi_{0,1,0}(r, \theta, \phi)$ in Figure 2, we show a surface of constant $\Psi_{0,1,0}(u, v, \phi)$ at a value chosen to reveal the essential geometric features. For quantum numbers $n_1 = 0$, $n_2 = 1$, $m = 0$, so that energy quantum number $n = 2$, the amplitude function has this explicit algebraic form in terms of fundamental parameters:

$$\Psi_{0,1,0}(u, v, \phi) = \frac{Z^3 \mu^3 e^6 \pi^2 e^{\left(-\frac{Z e^2 \pi \mu (u^2 + v^2)}{2 h^2 \varepsilon_0} \right)} (\pi Z e^2 \mu v^2 - 2 h^2 \varepsilon_0)^2}{64 h^{10} \varepsilon_0^5}$$

A plot of the surface of this amplitude function. which is an orbital, according to the stated criterion, appears in Figure 4. The surface comprises two lobes, the upper one small, nearly ellipsoidal and of negative phase about axis z , the lower one large and of positive phase.

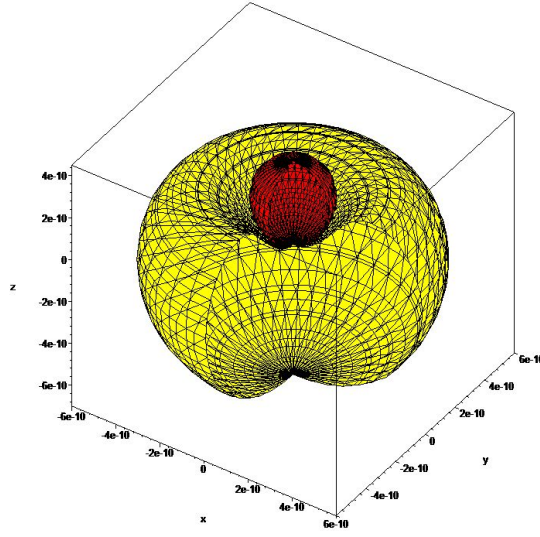


Figure 4 Surface of $\psi_{0,1,0}(u,v,\phi) = \pm 1.46 \times 10^{13} \text{ m}^{-3/2}$; the lower lobe (yellow) has a positive phase, the upper lobe (red) negative phase; both are cut open to reveal the details of the surfaces. The length scale on each axis is in terms of metres consistent with the SI units of the plotted function.

c) Ellipsoidal Coordinates

The coordinates in this system,¹⁹ also called prolate spheroidal, are conventionally named ξ, η, ϕ : a surface of $\xi = 2$ corresponds to a finite ellipsoid, which is an ellipse of revolution about axis z , with one focus at the origin and a second focus at $z = 2$; for $\xi = 1$ such an ellipsoid degenerates into a line along axis z from $z = 0$ to $z = 2$; for $\xi = a > 1$, the ellipsoid has axis z as its major axis and extends from $-a$ to $a + 2$ along that axis. A surface of constant η is an infinite hyperboloid coincident with axis $-z$ for $\eta = -1$ and its vertex at the origin, coincident with axis $+z$ for $\eta = +1$ and with its vertex at $z = 2$, and degenerating into a plane at $z = 1$ for $\eta = 0$; a surface of constant ϕ again corresponds to an infinite half-plane from axis z . Figure 5 illustrates these features.

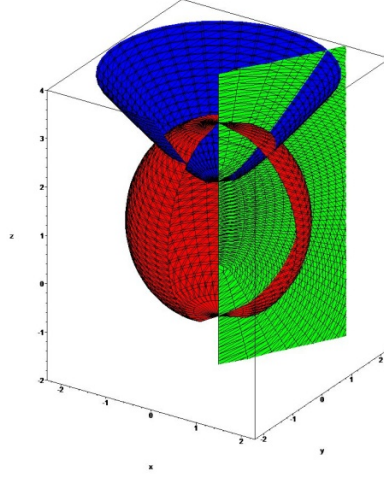


Figure 5 Definition of ellipsoidal coordinates: surfaces of an ellipsoid (red) with $\xi = 2$, an hyperboloid (blue) with $\eta = \pi/4$ rad, both cut open to reveal the inner details, and a half-plane (green) with $\phi = \pi/3$ rad. The axes are scaled in unit a_μ , which signifies a Bohr radius corrected for reduced mass μ of the system.

The solutions $\psi_{n,\lambda,m}(\xi,\eta,\phi)$ to the Schroedinger equation independent of time in these ellipsoidal coordinates, *i.e.* the orbitals, are expressible as

$$\begin{aligned} \psi_{n,\lambda,m}(\xi, \eta, \phi) = & N((\xi^2 - 1)(\eta^2 - 1))^{\left(\frac{|m|}{2}\right)} \mathbf{e}^{\left(-\frac{dZ(\xi+\eta+1)}{2a_\mu n}\right)} \mathbf{e}^{(im\phi)} \text{HeunC}\left(-\frac{2dZ}{a_\mu n}, |m|, \right. \\ & |m|, \frac{2Zd}{a_\mu}, \frac{m^2}{2} - \frac{Zd}{a_\mu} - \lambda(\lambda+1) + f_{n,\lambda,m}(d) - \frac{Z^2 d^2 n^2}{4a_\mu^2}, \frac{\xi}{2} + \frac{1}{2}\bigg) \text{HeunC}\left(-\frac{2dZ}{a_\mu n}, \right. \\ & |m|, |m|, \frac{2Zd}{a_\mu}, \frac{m^2}{2} - \frac{Zd}{a_\mu} - \lambda(\lambda+1) + f_{n,\lambda,m}(d) - \frac{Z^2 d^2}{4a_\mu^2 n^2}, \frac{\eta}{2} + \frac{1}{2}\bigg) / \sqrt{2\pi} \end{aligned}$$

In this equation that is expressed in terms of a_μ , which signifies a Bohr radius a_0 corrected for the

reduced mass of the system, $a_\mu = \frac{h^2 \lambda}{8 \pi^2 Z \mu e^2}$ with $a_\mu = \frac{m_e a_0}{\mu}$ for effective reduced mass μ of

the atomic system, appear normalising factor N and quantum numbers n , λ , and equatorial m that is again coefficient of equatorial angle ϕ and $i = \sqrt{-1}$ in an exponential function; the distance between the two foci of the ellipsoid is given symbol d , and all amplitude functions depend sensitively on the value of this parameter. Because Schroedinger's equation in these coordinates is a special case of Heun's differential equation, confluent functions HeunC naturally appear in the solutions. In this formula energy quantum number n appears directly, but, in an alternative and partial solution²⁰ in terms of variables ξ and η in separate series, $n = n_\xi + n_\eta + |m| + 1$.

For quantum numbers $n = 2$, $\lambda = 0$, $m = 0$, the amplitude function or orbital has this explicit algebraic form in terms of Bohr radius a_μ :

$$\psi_{2,0,0}(\xi, \lambda, m) = N e^{\left(-\frac{d Z (\xi + \eta + 1)}{4 a_\mu}\right)} \frac{\text{HeunC}\left(-\frac{Z d}{a_\mu}, 0, 0, \frac{2 Z d}{a_\mu}, -1 - \frac{Z d}{a_\mu} + \frac{d^2}{16 a_\mu^2} + \frac{\sqrt{\frac{d^2}{a_\mu^2} + 4}}{2} - \frac{Z^2 d^2}{16 a_\mu^2}, \frac{\xi}{2} + \frac{1}{2}\right)}{\sqrt{2 \pi} \text{HeunC}\left(-\frac{Z d}{a_\mu}, 0, 0, \frac{2 Z d}{a_\mu}, -1 - \frac{Z d}{a_\mu} + \frac{d^2}{16 a_\mu^2} + \frac{\sqrt{\frac{d^2}{a_\mu^2} + 4}}{2} - \frac{Z^2 d^2}{16 a_\mu^2}, \frac{\eta}{2} + \frac{1}{2}\right)}$$

With the same criterion as for $\psi_{0,1,0}(r, \theta, \phi)$ in Figure 2, we show in Figure 6 a surface of this amplitude function $\psi_{2,0,0}(\xi, \eta, \phi)$, at a value of d chosen to reveal the essential geometric features. The surface comprises two lobes, a small lobe nearly ellipsoidal and of negative phase along axis z , and a large lobe of positive phase. At distances $d < a_\mu/10$ the inner lobe begins as a sphere with its center at the origin (not shown) inside a concentric shell; with increasing d the lobe

assumes an ellipsoidal shape and moves upward along positive axis z and eventually separates from the large lobe as in Figure 4.

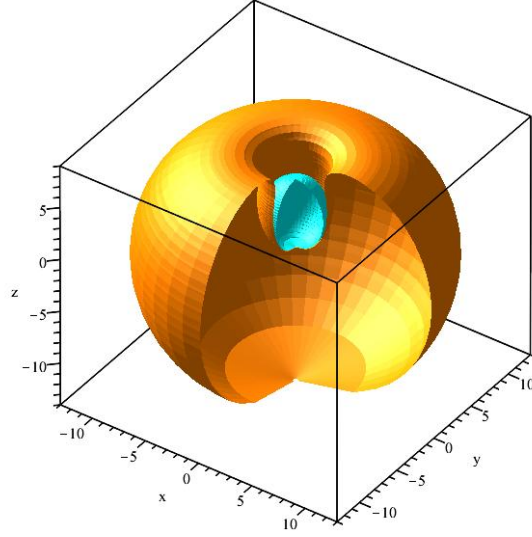


Figure 6 Surface of $\psi_{2,0,0}(\xi, \eta, \phi) = \pm 2.13 \times 10^{-4} a_\mu^{-3/2}$ at $d = 5 a_\mu$; the small lobe (light blue) of nearly ellipsoidal shape has a negative phase, the large lobe (coral) has a positive phase; both are cut open to reveal the inner details. The axes are scaled in unit a_μ .

d) Spheroconical Coordinates

The coordinates in this system,²¹ also called spheroconal, are conventionally named ξ , r , η : a surface of constant r corresponds to a finite sphere, as in spherical polar coordinates; a surface of constant ξ corresponds to an infinite double cone with its apices at the origin and oriented along axis z , whereas a surface of constant η corresponds to an infinite double cone with its apices at the origin and oriented along axis x . Each double cone has an elliptical cross section in any plane perpendicular to its axis. These features are illustrated in Figure 7.

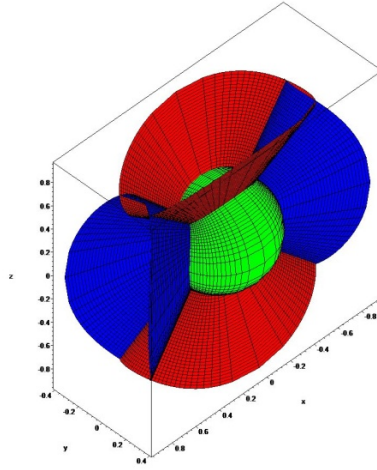


Figure 7 Definition of spheroconical coordinates: surfaces of a sphere (green) centered at the origin with $r = 2/5$ units, an infinite double cone (red) of elliptical cross section about axis z with $\xi = 1/4$, and a second infinite double cone (blue) of elliptical cross section about axis x with $\eta = 1/4$. The axes are scaled in unit a_μ .

The solutions $\psi_{k,l,\kappa}(\xi, r, \eta)$ to the Schroedinger equation independent of time in these spheroconical coordinates, *i.e.* the orbitals, are expressible as

$$\psi_{k,l,\kappa}(\xi, r, \eta) = N \sqrt{\frac{Z k! (2 + 2l + k)}{a_\mu (2 + 2l + k)!}} \left(\frac{2Z}{a_\mu (k + l + 1)} \right)^{(l+1)} r^l e^{\left(-\frac{Zr}{a_\mu (k + l + 1)} \right)} \\ \text{LaguerreL} \left(k, 2l + 1, \frac{2Zr}{a_\mu (k + l + 1)} \right) \text{HeunG} \left(-1, \kappa, -\frac{l}{2}, \frac{1}{2}, \frac{l}{2}, \frac{1}{2}, \frac{1}{2}, -2\xi^2 \right) \\ \text{HeunG} \left(-1, -\kappa, -\frac{l}{2}, \frac{1}{2}, \frac{l}{2}, \frac{1}{2}, \frac{1}{2}, -2\eta^2 \right) / (k + l + 1)$$

In this formula appear normalizing factor N and three quantum numbers, k and l that appear in associated Laguerre functions as for spherical polar coordinates, and κ that appears only in the two general Heun functions; the latter functions arise because the ordinary-differential equations for ξ and η after separation of the variables in Schroedinger's partial-differential equation in this system of coordinates are instances of Heun's differential equation. Energy quantum number $n =$

$k + l + 1$, in terms of quantum numbers specific for this coordinate system, so is independent of third quantum number κ . The most notable property of these amplitude functions in spheroconical coordinates is that, with N real, these orbitals have no complex character: there is no factor $e^{im\phi}$ in any amplitude function that might bestow some imaginary component, unlike the functions in the other three sets. This property warrants an expanded utilisation of these functions, but calculations with conventional quantum-chemical software involve no imaginary quantities in any case.

For quantum numbers $n = 1$, $l = 0$, $\kappa = 1$, the amplitude function has this explicit algebraic form in terms of Bohr radius a_μ , as above, with an explicit numerically derived normalizing factor. With the same criterion as for $\psi_{0,1,0}(r, \theta, \phi)$ in Figure 2, Figure 8 shows a surface of this amplitude function $\psi_{0,0,1}(\xi, r, \eta)$, according to the stated common criterion, to reveal the essential geometric features of this orbital. The surface comprises two lobes, a finite double conical lobe about axis x on either side of the origin with both apices at the origin, and a large torus of elliptical shape about that axis x and hence surrounding the cones near the origin.

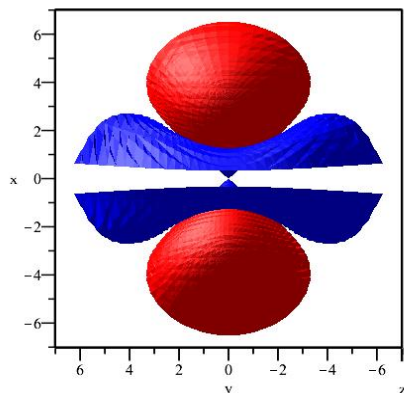


Figure 8 Surface of $\psi_{0,0,1}(\xi, r, \eta) = \pm 0.0041 a_{\mu}^{-3/2}$; the double conical lobe (red) with its apices at the origin has a positive phase; the torus (blue) about axis x has a negative phase. The axes are scaled in unit a_{μ} . The surface is cut open to show the interior.

e) Summary of Coordinate Systems

The impact of these eight figures on a reader should be that solutions to the Schroedinger equation for the hydrogen atom, and hence orbitals by definition, exist for coordinates in four distinct and independent sets. Each respective set of corresponding orbitals has its intrinsic three quantum numbers, not all common, and disparate shapes of surfaces of constant amplitude ψ . *There is no one and unique set of orbitals for the hydrogen atom.* Many further pictures of surfaces of amplitude functions in the four systems of coordinates are available elsewhere, with other properties and applications of these functions.^{17-19,21} Unless one is willing and able to treat orbitals in all these sets in general chemistry, it is unwise to waste time teaching the results of one set, only to teach subsequently that these results are not unique.

Schroedinger's equation independent of time is solvable²² also in cartesian coordinates x, y, z with also r as $\sqrt{x^2 + y^2 + z^2}$, but only a partial separation of spatial variables is practicable; as plots of the amplitude functions, with the same quantum numbers k, l, m as in spherical polar coordinates, show the same shapes and sizes of surfaces as the corresponding surfaces based on spherical polar coordinates, these cartesian amplitude functions must be considered merely a variant of the functions in spherical polar coordinates.

For the system of ellipsoidal coordinates, amplitude functions $\psi_{n_\xi, n_\eta, m}(\xi, \eta, \phi)$ exhibit limiting values that depend on distance d between the foci of the ellipsoid: as $d \rightarrow 0$, they become equivalent to amplitude functions $\psi_{k,l,m}(r, \theta, \phi)$ in spherical polar coordinates or linear combinations of these functions; as $d \rightarrow \infty$, they become equivalent to amplitude functions $\psi_{n_1, n_2, m}(u, v, \phi)$ in paraboloidal coordinates or their linear combinations, but at finite intermediate distance d these amplitude functions have characteristic shapes distinct from those of the limiting cases. One can readily recognize the similarity between Figure 6 as an intermediate case in relation to Figure 4 as a limiting case for these amplitude functions in ellipsoidal coordinates, such that $\psi_{0,1,0}(\xi, \eta, \phi) \rightarrow \psi_{0,1,0}(u, v, \phi)$ as $d \rightarrow \infty$; the other limiting case in this instance is $\psi_{1,0,0}(r, \theta, \phi)$ as $d \rightarrow 0$. For the ground state, $1^2S_{1/2}$, of the hydrogen atom, the surfaces of all respective amplitude functions are perfect spheres.

The amplitude functions in spherical polar and paraboloidal coordinates are presented above in terms of the fundamental physical constants and atomic parameters so as to provide, for a reader, a formulation of these functions alternative to what other reference sources⁸ typically present. For coordinates in the other two systems, the formulae become expressed more compactly with the use of Bohr radius a_μ corrected for reduced mass μ , but in all cases the

formulae are exact, within a context of the Schroedinger equation, and are exactly applicable to an atom of atomic number Z with only one electron, and the corresponding value of reduced mass μ for that atomic system. In no case is the quantum-mechanical nature of the atomic nucleus or its finite volume taken into account; the motion of the center of mass of the atomic system is assumed to be separated and treated appropriately. Apart from the latter qualm, the preceding information is precisely suitable for inclusion in a textbook of physical chemistry of which the authors might reasonably seek to present an unbiased treatment of the hydrogen atom according to wave mechanics, but is obviously unsuitable for introductory chemistry. Any responsible author of a textbook of general chemistry should nevertheless be aware of, and knowledgeable about, these fundamental aspects, namely the multiplicity of sets of orbitals, before embarking on a discussion involving orbitals in any manner, shape or form.

• IV ANALYSIS OF AMPLITUDE FUNCTIONS AS ORBITALS

There are several levels of consideration of orbitals in the context of general chemistry and in the light of the preceding discussion. We begin at the most superficial level and progress to more profound aspects relevant to the teaching of introductory chemistry.

a) In view of the multiple sets of orbitals according to the four systems of coordinates, which set should I use for teaching purposes?

Apart from the fact that this question supposes that teaching with orbitals is appropriate, which is negated at a further level of understanding, the properties involved in their derivation can enable a rational response to that question. The orbitals according to the separate sets of amplitude functions have clearly disparate shapes of their surfaces of constant amplitude ψ , as Figures 2, 4, 6 and 8 clearly demonstrate; typical qualitative applications of orbitals in general

chemistry rely on those shapes, even though the overall sizes do not vary markedly for functions corresponding to the same value of energy quantum number n . The amplitude functions in spherical polar¹⁷ and spheroconical²¹ coordinates are derived under conditions of *strictly spherical symmetry* -- no other atom in the system and no electric field; this condition logically precludes their use in discussing a bond between a hydrogen atom and another atom, contrary to practically universal practice in the former case. The amplitude functions in paraboloidal coordinates¹⁸ are suitable for use in the presence of an homogeneous electric field⁴ parallel to axis z , for instance, but that condition is far from applicable to the presence of another atom along that axis. In contrast, for amplitude functions in ellipsoidal coordinates, another atomic nucleus is perfectly acceptable at the otherwise vacant second focus of the ellipse; the atomic orbital of the former hydrogen atom then becomes a molecular orbital. This fact has been known since at least year 1930, in which Teller announced²³ that property based on his calculations of the dihydrogen molecular cation, H_2^+ , but chemists have ignored that wisdom. Any use of orbitals in spherical polar coordinates in relation to chemical bonds, as is common practice for instance, must hence be logically unacceptable.

b) Still under an assumption that teaching with orbitals is legitimate, can I justify the use of these orbitals in application to atoms other than hydrogen?

The derivation of the orbitals in all cases is based on a Coulombic attraction between a single electron, bearing a single negative electric charge, and an atomic nucleus, positively charged, which might possess multiple protons according to a variable atomic number Z , such as for He^+ , Li^{2+} , ... Factor Z in all general equations for amplitude functions in terms of coordinates in the four primary systems takes into account the fact that these functions are legitimately

applicable to any isolated atomic system involving one electron within the bound of a non-relativistic frame. The use of any such function for an atomic system involving more than one electron signifies an ignoring of the Coulombic repulsion between electrons at the same time that these electrons are subject to a Coulombic attraction to an atomic nucleus, in violation of the fundamental laws of physics. We reiterate that the use of orbitals as basis functions in proper quantitative quantum-chemical calculations is in no way contrary to this principle, because the repulsive effects are taken into account separately in a manner that is beyond the scope of qualitative arguments here or in introductory chemistry. In a discussion of the electronic structure of an atom other than the one-electron case, one should logically apply an amplitude function derived for that particular atom. For instance, for the helium atom or the hydride ion, either of which has two electrons associated with a single atomic nucleus, an exact amplitude function, implicitly in atomic units, for the ground electronic state near a point of coalescence is expressed²⁴ as follows in terms of distances r_1 and r_2 between one or other electron and that nucleus and distance r_{12} between the two electrons.

$$\begin{aligned} \psi = & 1 - Z(r_1 + r_2) + \frac{1}{2}r_{12} + \frac{1}{12}(4Z^2 - 2E + 1)r_{12}^2 + Z^2r_1r_2 \\ & + \frac{1}{6}Z(r_1^2 + r_2^2 - r_{12}^2)\ln\left(\frac{r_1 + r_2 - r_{12}}{r_1 + r_2 + r_{12}}\right) - \frac{1}{3}Zr_{12}(r_1 + r_2) \\ & + \frac{2}{3}(r_1^2 + r_2^2)\cos(\alpha)\operatorname{arctanh}\left(\frac{r_{12}\sqrt{1 + \sin(\alpha)}}{\sqrt{r_1^2 + r_2^2}\cos(\alpha)}\right) - \frac{2}{3}r_{12}\sqrt{r_1^2 + r_2^2}\sqrt{1 + \sin(\alpha)} \\ & - \frac{2}{3}(r_1^2 + r_2^2)\cos(\alpha)\operatorname{arctanh}\left(\frac{r_{12}(2r_1^2 + 2r_2^2 - r_{12}^2)}{(r_1^2 + r_2^2)\cos(\alpha)}\right) + \frac{2}{3}r_{12}\sqrt{2r_1^2 + 2r_2^2 - r_{12}^2} \end{aligned}$$

Here the atomic number is $Z = 2$ for He and $Z = 1$ for H^- ; E represents the energy of the ground state of the system; angle α denotes the value of $\arcsin(2r_1r_2 / (r_1^2 + r_2^2))$ subtended at the

nucleus. For a carbon atom there would be six distances r_j from the nucleus and fifteen distances r_{jk} between electrons; the resulting algebraic expression of an exact amplitude function would have intolerable length. Although the problem of many bodies interacting in a quantum-mechanical system is solvable in principle,²⁵ the result for even the He atom above is intractable for any practical purpose; an effort to produce a result for an atom with many electrons would be futile. These circumstances in no way excuse, however, a qualitative use of amplitude functions derived for the hydrogen atom, *i.e.* orbitals, in an application to an atomic system comprising multiple electrons.

c) How can I present theoretical predictions or justifications without the use of orbitals?

According to quantum mechanics, not only are all electrons indistinguishable but also all like nuclei, which are thus subject to permutational symmetry. The essential point to understand is that quantum mechanics is not a chemical theory, not even a physical theory, but a collection of methods of calculation, or algorithms, applicable to systems on an atomic scale;²⁶ wave mechanics with its Schroedinger equation implement only one such method, which has accordingly its intrinsic artefacts, such as orbitals. To understand this material one must have the mathematical skills and the determination to apply those skills.

In chemistry, the structure of molecules and materials in authenticated instances is an experimental fact, for which a theoretical prediction or justification is entirely redundant. For instance, consider this question. Why is methane tetrahedral? The tetrahedral geometric disposition of hydrogenic atomic centers about a carbon atomic center in a molecule of methane in the state of least energy is a matter of observation and scientific fact, first deduced from chemical evidence and subsequently abundantly confirmed with physical data -- there is no need

to justify this fact retrospectively. For a large system that imposes a severe limitation on the accuracy of the calculated results, the treated system is still an ideal prototype and must be of invariably questionable pertinence to the results of chemical and physical experiments on a real system on a macroscopic scale.

The incompatibility of molecular structure and quantum mechanics has been recognised for many years.²⁷ Apart from some perhaps esoteric aspects of this dichotomy, a simple understanding can be based directly on the fact that a calculation -- because quantum mechanics is a collection of methods of calculation -- in which the electrons and atomic nuclei are treated equitably, *i.e.* applying basis sets in wave mechanics to both electrons and nuclei and integrating over all coordinates, yields *no structure*; this effect is proved experimentally (computationally).²⁸ The exceptions are for diatomic molecules, for which a structure is trivial, and the simplest triatomic molecules, because nuclei are invariably distinguishable from electrons. Quantum-chemical calculations are valuable adjuncts for experimental observations, but such calculation is no component of introductory chemistry.

d) Could I use schemes of electronic structure other than orbitals to explain the structures and properties of molecules and crystals?

If one takes into account that the distribution of the density of electronic charge within a molecule or within a unit cell of a crystal is continuous and varies gradually in space in the vicinity of atomic nuclei, any classification of electrons becomes meaningless. Not only is there no $1s$, $2p$, ... electron, there is no valence electron, no lone pair and so forth, because electrons are *fundamentally indistinguishable*.

Both experimental measurement and accurate calculation that reproduce that measurement, either of which is subject to error, indicate that midway between the two protons in molecular $^1\text{H}_2$, at its equilibrium internuclear distance, the density of electronic charge is slightly -- less than 10 per cent, but significantly -- greater than would be the hypothetical case of two non-interacting ^1H atoms at the same distance.²⁹ Although that increased electronic charge between the two protons occurs at an expense of a slight depletion of electronic charge on the other side of each proton, the attribution of a chemical bond to a pair of electrons between the two atomic nuclei is clearly a gross exaggeration. The dihydrogen molecule, stable with respect to dissociation into two hydrogen atoms by about 4.48 eV, is an experimental fact; that dissociation energy is less than one third the ionisation energy of a hydrogen atom. For the dihydrogen molecular cation, $^1\text{H}_2^+$,³⁰ the dissociation energy is about 2.65 eV, slightly more than half the value for the neutral molecule. The dihelium molecule, $^4\text{He}_2$, is only weakly bound, but it exists and has a bound vibrational state. In contrast the dihelium cation, $^4\text{He}_2^+$, is strongly bound: its dissociation energy, about 3.1 eV, is similar to that of $^1\text{H}_2^+$.

For the next homonuclear diatomic molecule in order of increasing atomic number, dilithium $^7\text{Li}_2$, one might be tempted to insinuate a typical chemical bond involving two electrons, notwithstanding the caveat above; this species is stable to dissociation by 1.04 eV, whereas, for the diatomic molecular cation $^7\text{Li}_2^+$ for which only a one-electron chemical bond would seem to be possible, the dissociation energy is much greater, 1.4 eV.³¹ For the corresponding molecular anion, $^7\text{Li}_2^-$, the calculated dissociation energy is 0.86 eV, only slightly less than for the neutral molecule. If these ideas about an electron-pair bond fail in the simplest cases, quite apart from the complications for the boron hydrides, how can one have confidence that their more general application is worth the effort to rationalize these effects?

The idea of an octet of *valence* electrons that Abegg first reported³² was subsequently elaborated by Kossel³³ and by Lewis.³⁴ With the additional concept of electron spin dictated by the Pauli principle, that octet became viewed as four pairs of electrons, one electron of each spin within each pair. An alternative approach involved a double quartet of *valence electrons*, electrons in each quartet having the same spin and opposite the spin of electrons in the other quartet.³¹ In all three cases the indistinguishability of electrons, in differentiating valence electrons from other electrons, is contradicted. The extent of an orbital is infinite, even though there might exist surfaces of zero amplitude between regions of positive and negative phase, such as is discernible in Figure 2 for instance. One attempt to define a localised region of space in which an electron pair was likely to be found was implemented in a loge theory,⁵ so to partition the space surrounding atomic nuclei within a molecule into various loges. This endeavour seemed successful in the case of LiH but was increasingly unsatisfactory for BeH₂, BH₃ and CH₄; as those volumes designated as loges were in any case evaluated as a result of extensive quantum-chemical calculations, their applicability to explain molecular structure in general chemistry is minimal. Another region of space in the *valence shell* in which an electron pair is most probably to be found has been called an electron pair domain;³⁵ such a domain is based on an assumed electronic structure, and represents yet another circular argument. Any such partition of space surrounding atomic nuclei is based on arbitrary criteria, not subject to direct experimental confirmation.

Dirac stated that "science is concerned only with observable things".¹ The atomic centres in molecules are observable as local maxima of electronic density; orbitals are not observable. A molecule comprises a collection of atomic nuclei and their collective associated electrons; for this reason we refrain from referring to atoms in molecules. These locations of atomic centres

are most commonly defined in experiments on single crystals with the diffraction of X-rays, which, ironically, yield the locations of atomic centres, and hence the associated atomic nuclei therein, within a unit cell through the local maxima of electronic density, each attributed to an atomic nucleus. Hydrogen atomic centers are notoriously difficult to locate with X-rays because of the small scattering power of their electronic density, but diffraction with neutrons is highly successful for this purpose. As neutron diffraction is an uncommon practice, the relative positions of hydrogen atoms in many cases are imposed, based on expectations from known experimental data. The structures of molecules and crystals are hence the result of experimental determinations and should be taught from this point of view. Instead of electron configurations, the structures at the atomic (not sub-atomic) level, properties and reactions of chemical substances -- elements, compounds and their mixtures -- should be the main focus of attention in general chemistry.

• V ELIMINATION OF THE TRADITIONAL USE OF ORBITALS IN FUTURE TEXTBOOKS

Before 1957, most textbooks for introductory chemistry (with the exception of Pauling's textbook) included not 'Schroedinger' nor 'orbital' nor 'hybridization'.³⁶ Let us revisit the topics taught with orbitals in a textbook of the latter part of the twentieth century to investigate how a curriculum for the twenty-first century can be produced without orbitals.

- 1) Electron configuration: Of the electron configurations of gaseous atoms of the elements in their ground states, 27 per cent are anomalous in not obeying the combination of the aufbau principle and Hund's rule,³⁷ but we continue to show students and to test them on writing the electron configuration of the atomic elements and their ions (which have their

separate rules) as if there were an absolute pattern to this data. What do students learn from this exercise? Removing electronic configuration is one step to answer the query: “How many students (or even chemists) ever work with isolated atoms? A few spectroscopists certainly investigate samples in the gaseous phase, but nearly all experiments in general chemistry are implemented in aqueous solution. Nearly all industrial chemistry is done in condensed phases; nearly all organic chemistry is done in solution. Why do we waste time and effort teaching beginning students that neutral chromium atoms have $[\text{Ar}]3d^54s^1$ for an electron configuration?”³⁷

- 2) Periodic table: The original organization of the periodic chart of the chemical elements was based on observations of the recurring similarity of their chemical and physical properties. There is no quantum rationalization for this organization.^{38,39} Why should we not revert to the original meaning of periodicity?
- 3) Molecular structure: The atomic orbitals from the elements have been further applied to molecules. Consider a flow chart that we might ask students to follow to provide a three-dimensional structure of a molecule:⁴⁰

“In our current mode of pedagogy we ask our students to follow the path of memorization:

- (1) the ground state, gas-phase electron configurations of the atoms;
- (2) that electron promotion takes place;
- (3) that hybridization of the atomic orbitals occurs;
- (4) the shapes of the resulting hybrids;
- (5) the tenants of the Valence Shell Electron Pair Repulsion (VSEPR) model: and
- (6) that in trigonal-bipyramidal geometry the lone pairs of electrons go equatorial.

From all this we are now ready to state that, for example, the SF_4 molecule adopts a seesaw shape.”

We explain elsewhere that hybrids and hybridization models to explain molecular shapes are redundant.⁴¹ We provide there also a simple solution to the problem of explaining

molecular shapes -- remove the explanation and simply provide the three-dimensional structure as an experimental fact. Once the structure is shown, what can one predict from it? Would it not be preferable to show the experimental structure of a molecule in three dimensions with rotational capability on a computer screen or with a ball-and-stick physical model (for instance, SF_4 as a see-saw shape) and remove the unnecessary concepts, rules and the flow chart? From a three-dimensional structure we perceive the fundamental chemistry -- the properties and reactivity that are the interesting and powerful aspects of learning, and the applications that make chemistry the central science.

- 4) Reactivity: A discussion of reactivity free of orbitals might involve the use of maps of molecular electrostatic potential.⁴² We avoid a comparison of molecular-orbital (MO) theory versus valence-bond (VB) theory, also a comparison of canonical MO versus localized MO (LMO) versus hybridized atomic orbitals (HAO), as the conclusions remain the same: in introductory chemistry, all presentations of orbitals are unnecessary and can be eliminated without affecting the quality of the education, perhaps even improving that quality. Orbitals are neither necessary (intrinsic) nor essential (extrinsic) in introductory organic chemistry.⁴¹

• VI PREVIOUS DISCUSSION OF THE TEACHING OF ORBITALS

Various authors have presented overwhelming evidence in agreeing that orbitals and quantum chemistry are inappropriate for students of chemistry at high school (secondary education) level.⁴³⁻⁴⁸ The vague theory confuses the students and the mathematics are too advanced.⁴⁹⁻⁵⁰ Young adults must learn in secondary school the essential concepts that they can

apply in the world. “The course must be adapted primarily to the student who will not go farther into the subject. This type of student needs a course that will do two things. He needs first a ‘speaking acquaintance’ with the common, every-day facts, ideas and nomenclature of the subject in order to become conversationally intelligent regarding it. ... He needs, in the second place, to be able to apply the principles in the solution of everyday problems as they appear....It is the primary purpose of the high-school chemistry course to establish a familiarity with things chemical, and a comprehension of the governing laws and principles.”⁵¹ One might observe that the chemistry for secondary school based on suggestions of Bayles in 1930 was much more rigorous than today’s curriculum. As an analogy, the teaching of Boyle’s law is completely acceptable in secondary school but an explanation of gas laws based on the mathematics of statistical mechanics is not. This obvious perception seems less controversial than the quantum debate.

The discussion about quantum chemistry and orbitals in first-year university chemistry is complicated. Many chemical educators have clearly advocated against the teaching of orbitals until advanced chemistry courses.^{35,52-56} Gillespie strongly protested the inappropriate nature of quantum mechanics and orbitals in general chemistry.^{57,58} “If the authors of elementary textbooks do not understand quantum mechanics, how can we possibly expect students to understand the subject? All these difficulties could be avoided and a considerable amount of time could be saved if we were to abolish all this material from the curriculum of introductory courses. Quantum mechanics and quantum chemistry should, of course, be studied by all students of chemistry, but not until a later stage in their studies.”⁵⁹

A knowledge of quantum mechanics, or even its superficial trappings in the form of orbitals, has been suggested to be completely unnecessary for students (the majority) in first-year

chemistry who continue with biochemistry or engineering courses.^{60,61} One author labeled quantum mechanics as “Unteachable at the General Level”.⁶² Even Pauling wrote “Now in 1979, I would say that the first-year course in chemistry should give a student enough understanding of chemical structure and chemical properties to enable him to understand a good bit of molecular biology...I do not think that any of them would suffer from not having been exposed to molecular-orbital theory during their first year in chemistry.”⁶³

These voices against the teaching of orbitals in introductory chemistry have been lost or ignored. Part of the reality is that “...implicitly, many or most authors of textbooks and programmers of curriculum favour the use of orbitals to introduce chemical theory, as they include the issue not only in courses of college chemistry, but even in the (upper) secondary education in many countries. In our opinion, this acritical acceptance of the teaching of orbitals is just another consequence of the widespread ignorance of the complex status of quantum jargon within FMT [Folk Molecular Theory]. We think that for many chemistry teachers, and this is of course just a feeling with no empirical support, orbitals are simply necessary for the quantum [QC] description of a microscopic system. In this vision, there is no QC without orbitals.”⁶⁴ Moreover, all this discussion has proceeded in a complete ignorance of the fact that true orbitals exist in four sets, as outlined in section III, and in particular the invariant use of the least appropriate set of those orbitals.

With all the evidence presented in this paper, we strongly recommend the removal of orbitals from general chemistry. In a spirit of intelligent discussion, we present some arguments *for* the use of orbitals, and their critique.

In 1979, Morwick defended the teaching of orbitals in secondary school for two reasons.⁶⁵ First, the abstract concepts of orbitals and electron configuration are “indispensable

intellectual scaffolding” of further, more advanced topics. Morwick claimed that the language and images of orbitals should be taught in secondary school, with the anticipation of mathematical quantum theory at the university level (even though quantum mechanics is incompatible with molecular structure,²⁷ which is the main reason for invoking orbitals). Students in secondary school should be taught the shape of the orbitals (*s*, *p*, *d*, ...) and their energy levels ($1s < 2s < 2p \dots$), implicitly assuming spherical polar coordinates, leaving hybridization and anti-bonding orbitals as optional depending on the teacher. Second, as quantum chemistry is a “fundamental aspect” of chemistry, it should be introduced in secondary school with the other fundamentals,⁶⁵ despite the impracticality of solving partial-differential equations in that context.

As discussed in this article, the focus on only one ‘shape’ of orbitals (implied in the idea that there is only *one* Schrodinger equation for the hydrogen atom) is a common misconception. The conventionally taught orbitals are neither indispensable nor fundamental; every topic that might involve quantum mechanics can be alternatively presented and discussed, even at the introductory university level, without orbitals.

In 1988 Edmiston⁶⁶ refuted the arguments of Sanderson that chemistry can be taught without orbitals.⁵³ Edmiston provided several items in this refutation: orbitals give students insights into many properties of molecules; molecular-orbital calculations *ab initio* (and their visualization) are available; chemical bonding is better understood with orbitals; the reasons that molecules have their shapes can be rationalised. He recommended that localized molecular orbitals (LMO) corresponding to bonds, lone pairs and inner shells -- despite that electrons are all indistinguishable -- be shown to students and then form the delocalized spectroscopic MO as simple linear combinations of these LMO, and that what is needed is an improved presentation.

Molecular binding energies, especially in contrast to the method of Sanderson, are properties that he emphasised to be best explained in MO theory. “Binding effects result from the positive overlap of atomic orbitals to form bonding LMO, and antibonding effects result from negative overlap, causing MO nodes in ‘bond regions’. To ignore the teaching of these most basic ideas would deprive students of much important understanding.”⁶⁶

The use of quantum-chemistry software to determine molecular properties has altered the way that many chemists conduct their research. The tendency to include the latest research, while retaining all previous information, in chemistry textbooks has caused a large surge in the size and cost of these textbooks. In 1900 a chemistry textbook for a year course had about 200 pages;⁵⁹ today a typical textbook comprises more than 1200 pages. During the twenty-first century, it will be simply impossible to include all recent research into a curriculum for undergraduates. With a trend of reducing general chemistry to a one-semester course,⁶⁷ some topics must be eliminated, and orbitals are certainly dispensable. We hence contend that there is a great disparity between the use of quantum-chemical software for research and the presentation of quantum theory, in a superficial guise of orbitals, to provide an understanding of topics in first-year chemistry. We have no quarrel with the use of software to provide visualizations of molecules and their interactions; this visualization can be productively implemented without orbitals in an introductory course, without a complete (and unnecessary) understanding of how the software works.

Schaefer defended the presentation of quantum mechanics in general chemistry by proclaiming “Quantum mechanics is arguably the most significant intellectual achievement of the twentieth century. Furthermore, quantum mechanics has been foundational to why chemistry is understood in a much more profound manner than was the case in 1926. Whether one likes it

or not, orbitals have become the *lingua franca* of chemistry since the 1963 paper of Woodward and Hoffmann."⁶⁸

We refute the statement that orbitals are the *lingua franca* of chemistry, once again citing the multiplicity of sets of amplitude functions for the hydrogen atom; one can acknowledge the great achievement of quantum mechanics in physics while searching for alternative approaches for chemical education in the twenty-first century. According to our experience, chemistry has become more difficult to teach and less understood by the public, in large part due to the complications of orbitals.

Astonishingly, we could find no reference after 1997 discussing the inclusion or exclusion of orbitals in the curriculum for general chemistry. It seems that the dice had been cast. It is time to reopen the discussion about what to include in the curriculum and provide all evidence in favor or against.

In 2011, orbitals gained the imprimatur of the American Chemical Society Examinations Institute (ACS-EI) with their content map of anchoring concepts for general chemistry.⁶⁹ The concepts presented here are designed to span the content that routinely appears in examinations of general chemistry produced by ACS.

The quantum model of the atom is capable of explaining many observations, and it organizes electrons into “orbitals”, which are wavefunctions that are identified using quantum numbers.

a. The quantum mechanical model of the atom introduces the concept of orbitals, including atomic orbitals.

b. Quantum numbers specify the wavefunctions that are the orbitals.

The occupation of atomic orbitals by electrons is summarized in the electron configuration, and this tool is helpful in understanding which atoms form chemical bonds, what type, and how many bonds they form.

a. Electron configuration is a shorthand notation that summarizes the orbital occupations of electrons in an atom or ion.

b. Electron configuration notation for transition metal ions reflects that they can differ slightly from the patterns observed for main group ions.

c. Electrons will occupy atomic orbitals following both the aufbau principle and Hund's rule.

Valence bond theory describes bonds in terms of overlap of electron waves.

a. The concept of atomic orbital overlap leading to chemical bonding as embodied in valence bond theory represents a useful tool for understanding the basic components of the quantum mechanics of bonding.

b. Sigma and pi bonds are a key way to distinguish chemical bonds obtained from valence bond theory.

A theoretical construct that describes chemical bonding utilizes the construction of molecular orbitals for the bond based on overlap of atomic orbitals on the constituent atoms.

1. Molecular orbital theory describes chemical bonds via molecular orbitals derived from atomic orbitals.

a. In the quantum model of atoms and molecules, the combination of atomic orbitals leads to the formation of bonding and antibonding molecular orbitals.

b. Bond order can be defined in terms of the occupation of bonding and antibonding orbitals by electrons.

c. Hybrid atomic orbitals are useful in describing bonding, particularly for organic molecules.

In view of our discussion above, we of course consider unnecessary the explanations that orbitals, quantum numbers, electron configuration, MO and VB theory provide for a student who is learning the basic themes of chemistry and lacks the required mathematical understanding.

Instead of discussing the necessity of orbitals, a series of articles has been published in the twenty-first century lamenting the difficulty of teaching quantum mechanics and orbitals or the (understandable) confusion that students show when tested on quantum-mechanical principles.

What do first-year undergraduate students actually learn about quantum mechanics and orbitals? The research states 'not much'. Tsaparlis wrote that Greek undergraduate students in chemistry lack a clear understanding of the concepts of atomic and molecular orbitals.^{70,71} Nakiboglu noted that Turkish undergraduates that proceed to become teachers of chemistry in secondary school show serious misconceptions about orbitals.⁷² Conceicao used computer software to alleviate partially the problems that USA students have with the concept of orbitals.⁷³

Taber noted that further research is required to eliminate the misconceptions of students about orbitals at Cambridge.⁷⁴ Chamizo *et al.* lamented that ideas such as orbitals are unconnected to their utility or practical use and that they are presented to Mexican students with no experimental evidence⁷⁵ -- because there is none. Bouayad *et al.* emphasized the confusion of Moroccan students and directly connected quantum mechanics as an impediment to deep understanding.⁷⁶ Lima and Silva observed the lack of clarity and knowledge of quantum matters in Brazilian students.⁷⁷ Internationally, students have the same difficulties; internationally, orbitals are the problem! Considering that orbitals have been ‘forced’ on first-year chemistry students for more than 60 years and that there still are problems in their pedagogy, should we not rethink the strategy?

We leave the last words in this section to Gillespie: “Concepts such as hybrid and molecular orbitals and the equations of thermodynamics are too abstract and too difficult for an introductory course. Moreover, they are unnecessary... at best students acquire only a very superficial understanding that often involves misconceptions that need to be unlearned if the student continues in further chemistry courses. And at worst students just memorize the appropriate jargon needed to pass tests and examinations and they understand and remember almost nothing.”⁵⁹

• VII TEACHING GENERAL CHEMISTRY WITHOUT ORBITALS

We have shown to the pragmatic chemist that teaching and learning of general chemistry is practicable without orbitals. We envision a future in which the content is divided into modules, each linked to another, that focus on learning chemistry in a more practical way: the importance of chemistry to industry, medicine and the environment. ‘How’ questions should be the focus of

the modules to be able to predict properties and reactivity, with ‘what’ questions providing descriptions. Hence, ‘How can the elements be organized in a periodic chart?’, ‘How can organic molecules be organized with functional groups?’ ‘How does the molecular structure affect the physical properties of a substance?’

‘Why’ questions (such as why is the structure of a water molecule angular?) can be dismissed completely. Pragmatic science teaching does not concern itself with why.

The principal emphases of introductory or general chemistry might be epitomised to be stoichiometry and chemical equilibrium, especially ionic equilibria in aqueous solution that is the basis of not only traditional analytical chemistry but even life itself. A standard precept in the effective teaching of experimental science is that there should exist a strong correlation between the lecture and laboratory components of a particular course or subject. Any discussion of atomic orbitals in lectures hence violates this precept because orbitals, as indisputable artefacts of not just one particular method of quantum mechanics but also a selected coordinate system (as delineated in section III), are not observable quantities subject to experimental verification. The presentation of chemical and physical equilibria and associated thermodynamic and kinetic aspects provides little or no legitimate occasion for an involvement of electron configurations or orbitals but profound opportunity for experimental practice without major equipment and cost, other than for chemicals consumed.

After conventional preliminary topics up to and including the stoichiometric trends of simple compounds based on the periodic chart of the chemical elements, a discussion of structure at a microscopic level begins, naturally enough, with the structures of simple crystals. The discussion of structure proceeds with other simple binary compounds, including others containing carbon as a basis of organic chemistry.

• VIII CONCLUSION

We end as we begin, by recalling Dirac's perceptive dictum, "science is concerned only with observable things".¹ Orbitals are not observable; hence leave these mathematical functions to the physicists, if they want.⁷⁸ In a chemical context, electrons might be tangible things, but individual electrons, or even purported electron pairs, are not observable -- only the total density of electronic charge in the vicinity of atomic nuclei. What are observable, and on which the entire edifice of chemistry is based, are the atomic centers in a molecule or material, each comprising an atomic nucleus of positive electric charge embedded within its associated environment of continuous negative electronic charge density.

As a basis for the properties, reactions and applications of chemical substances and their mixtures, the structure of molecules and materials is the primary focus of chemistry. "Syntheses, reactions, and commercial processes, physical properties, phases at various temperatures and pressures, structures, habits and solubility behaviors that we can see, smell, touch and even hear - this is material that is eminently memorable. Indeed, this is the stuff the students remember all their lives and whose immediacy can capture their imaginations."⁴⁰ As quantum mechanics is anathema to molecular structure,^{27,28} forget about quantum mechanics and its orbital artefacts; apply instead the quantum laws or laws of discreteness⁵⁴ that suffice for accurate explanations of atomic and molecular spectra across many frequency ranges. For many common purposes of calculations one can apply methods of molecular mechanics, with no quantum-mechanical provenance whatsoever, instead of methods of quantum chemistry; such calculations yield results of acceptable accuracy, and likely at a great economy of computing duration,⁷⁹ but this calculating activity is still alien to general chemistry.

If instructors of chemistry genuinely understood the mathematics underlying the production and application of the algebraic functions defined as orbitals,² such as we have summarised above, they would not teach such irrelevant material; although we concur with Gillespie⁵⁹ on this matter, our conclusion is based on undeniable mathematical fact and profound understanding, not merely intuitive feeling. It is timely to jettison the ponderous yoke of orbitals and to redirect the attention of students of introductory chemistry to the reality of the structure of molecules and materials as a product of scientific experiment based on chemical and physical principles.

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