Part IX

Reduction

The Limitations of Physics as a Chemical Reducing Agent

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Theories of chemistry have come to depend inescapably upon the frame-
work provided by atomic physics. This is a dependency which is anchored
upon the ability within quantum theory -- in particular since the
wave mechanics of Schrödinger -- to account for chemical bonding by the
pairing of electrons, the stability of their resulting structures, and
thereby to provide a basis from which to deal with chemical behavior
generally. The optimism generated fifty years ago by the initial at-
tempts to apply this framework[1] has bolstered the supposition, within
the sciences, that chemistry is exclusively an experimental science, it
has no theory except what it borrows from atomic physics. It seems to
have established, within philosophy, so secure an example of intertheo-
retic reduction that however often we hear it cited, it remains a case
rarely, if ever, examined.[2]

For all that, there are rather severe limitations on the extent to
which chemistry depends upon physics, limitations which undercut the
presumptive claims for reduction as explanation by deductive derivation.
To reconstruct the relationship between chemistry and atomic physics on
such grounds could only misconstrue chemists' original concerns for
'valence' and 'bonding', their own theoretical motivation to focus at-
tention upon 'structure' and 'stability', and would surely gloss over
the degree to which these concepts were already redirecting the thrust
of the whole problem of chemical bonding prior to the developments in
the late 1920's. But that historical episode is not what I wish to
examine here; rather I want to direct attention to the valence theory
of bonding as it has arisen in quantum chemistry over the last fifty
years.

C. A. Coulson has insisted ([2],p.259) that, "the first third of this
period was necessarily concerned with identifying the electronic nature
of the bond, and in escaping from the thought-forms of the physicist!"
Now surely Coulson cannot mean escaping from the framework of quantum
theory, but he apparently felt, and quite strongly, that there was not

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only a limit to chemistry's dependence but also a danger in borrowing too much. When L. Pauling published in 1939 the text which consolidated that first ten years of quantum chemistry, The Nature of the Chemical Bond, he forewarned the reader: "A small part only of the body of con- tributions of quantum mechanics to chemistry has been purely quantum- mechanical in character; only in a few cases, for example, have results of direct chemical interest been obtained by the accurate solution of the Schrödinger wave equation. The advances which have been made have been in the main the results of essentially chemical arguments." ([9],p.xi). In the 20 years or more after that remark was printed, techniques for approximating solutions to the Schrödinger wave equation were markedly improved -- not least from the increasing use of computers. But even then J. R. Platt has concluded: "...the most highly developed approaches to theoretical chemistry are failures as theories of chemistry. The ab- solute theories become computational nonsense when they try to go onto the chemical bonds commonly encountered in the laboratory. And many of the parametric theories are not scientific theories at all." ([10]; see also [11]).

At the very least these remarks suggest that the dependency of chem- istry upon physics is ill-suited to the schemas reductionists typically have in mind. If we can piece together some of the reasons why these "essentially chemical arguments" had to avoid the "thought-forms of the physicists" we may well find cause to doubt what E. Nagel, among others, still cite as: "the explanation (at least in principle) of chemical laws in terms of quantum theory." In fact we shall find that we cannot ex- pect, even in principle, to explain chemical bonding simply by its der- ivational reduction to (or deduction from) the quantum theory of atomic physics.

There are in the first instance some preliminary considerations about the reliance upon quantum theory about which we should be clear. When theoretical chemists purchase their "Schrödinger Wave Equation" from the quantum physicist, what they get for their money (or is it their soul?) is a framework within which a variety of things can be done in- cluding the possibility of altering the "frame" to their needs. It is not at all clear that it comes with instructions from the physicist as to how it is to be set up.

Chemists interested in molecules are dependent upon what success phys- icists have had depicting atoms. However, it will come as no surprise that chemists can afford to be selective: they attend to electrons with some care, and to nuclei (though perhaps with less scrutiny), but the minions within the nuclear world they can afford to ignore. The fact that they are, and can in principle afford to be selective carries over to their specification of the Schrödinger Equation. It is set up so as to apply to systems of nuclei and electrons -- other particles need not be included more specifically. Moreover, the contribution to the energy of the system made by the movement of the nuclei can be ig- nored, simply because they are so slow compared with electrons. In a similar vein a variety of relativistic effects which pertain to such a system would alter the calculated results so slightly they can be

dropped as well. The overall result is that the Hamiltonian Operator is designed to include just those terms judged to be relevant to a chemical system at this scale of complexity and energy.

For most chemical applications the scale of complexity requires two or more nuclei and from two up to a large number of electrons. Since these must all be worked into the potential energy term of the Hamiltonian, the interdependency of the electron coordinates -- as in the classical 3-body problem -- keeps the equation from being soluable analytically. There are, of course, a wide range of numerical techniques which are capable of providing good approximations and it is upon these that quantum chemists depend almost exclusively.

I raise these two general points, the adaptation of the equation to each problem and the reliance upon approximations, not because either or both are sufficient to undercut reductionist claims but because they do forewarn us that reduction will not be accomplished in this case by simple, strict deduction from a given law of atomic physics, and also because they preview questions of adaptation and approximation which I shall argue in more detail.

Meanwhile, there remains a third general consideration that further complicates the reductionist's schema, which is that the Schrödinger Equation (that is the time-independent version) is not sufficient by itself. In the first place, the use of this equation ties the theoretical chemist not to "functions", in the manner in which philosophers have traditionally associated functions with scientific "laws", but is tied rather to "operators" (in this case the Hamiltonian) and their "eigenfunctions". That the equation restricts one to only certain functions associated with their "eigenvalues" accounts for its status and use within quantum theory, but this constraint (and other technical requirements such as "normalization", etc.) still permits indefinitely many eigenfunctions as solutions to the equation. Those which are of significance to the chemist, as with the physicist, follow from the auxiliary assumptions concerning the minimization of energy.[3]

In the valence theory of chemical bonding the fact that bonding occurs at all rests, finally, upon the stability a molecular system can achieve through minimization of energy, that is to say by a lowering in particular of its potential energy. Of course to suggest that the phenomena of bonding are explained by "low potential energy" is rather like saying we explain why ice floats by noting that it is less dense than its liquid phase. What the chemist wants to explain, however, is why it is that with water in particular its solid phase is less dense. Similarly, the task of the theoretical chemist is to say something about why this lowering of potential energy is correlated with specific, identifiable molecules, i.e., with systems of interacting atoms which exhibit a specifiable structure. It is for this correlation that the Schrödinger Equation has been so important, since its allowed wave functions can be interpreted in terms of spatial location and their associated eigenvalues provide for calculation of the system's energy. For this reason the relevant assumptions about "low potential energy" and the

Schrödinger equation, together, provide a framework currently necessary for the valence theory of bonding. But they are not of themselves suf-ficient.

And it is not as if, as in the deductive-nomological model of ex-planation, that these could stand as sufficient major-premiss-cum-auxiliary-hypotheses needing only particularizing circumstances (initial conditions or whatever) to provide a completed explanation of a speci-fic chemical phenomenon. At least to do so would miss the point. The pattern seems instead to be one of a general framework incorporating a few basic physical-mathematical assumptions which do little more than place certain general constraints upon what remains as indefinitely varied array of possible phenomena. Chemistry undoubtedly sits within the framework so far delineated, but the explanation of any one in-stance of chemical bonding requires a whole series of ever more specific constraints. And it is not clear that atomic physics can, even in prin-ciple, provide all of them.

If this sort of pattern of what is required for explanation is fruit-ful, and it can be shown that atomic physics cannot provide the suf-ficiency demanded by the derivational reduction of theoretical chemis-try, then this sort of insufficiency is not likely to be peculiar to quantum chemistry alone. Indeed, something of what I have in mind can already be seen to emerge for that level of phenomena, i.e., at a parti-cular scale of complexity and energy, very much at the borderline between atomic physics and chemistry.

Among the other restrictions provided by quantum physics, one cannot describe the trajectory of an electron, nor can one distinguish one electron from another (nor let one's mathematical formalism do so). Consequently, the wave function can only be interpreted as representing an _orbital_ and pictured in terms of the area within which there's a high probability of one being located -- or as is more typical within chemistry as a cloud of charge of specifiable dimensions. Therefore, the only properties which can be attributed to an electron must be attri-buted to this "area", delimited as one permissible "state" of the system. Its dispositions are characterized not only by its Coulombic charge but by the size and shape of the boundary contour within which it is largely contained.

One basic consequence which we have already noted is that only certain distinct orbitals are allowed. As an additional postulate, the Pauli Exclusion Principle, exactly two electrons are permitted of opposite spin within each orbital. With these constraints on the system, the re-sults of interaction even between orbitals could presumably be specified according to what allowed "states" achieve a minimum of potential energy.

For an isolated atom this "minimum" applies only to the "ground" state, and the indefinitely many other orbitals represent all possible "excited" states. But a new feature emerges here; what are called "p" orbitals represent 3 orthogonal wave functions which all are associated

with the <u>same</u> level of energy. Placing electrons in these orbitals two by two fits remarkably well with the "aufbau" of atoms represented in the Periodic Table, but it also reaches a theoretic insufficiency. At the next allowed level of energy there is a 5-fold degeneracy, but it is clear which set of 5 orthogonal wave functions represent these in an isolated atom. More that one set is mathematically feasible and so long as the atom is taken to be in isolation, which is the "correct" set is <u>under</u>determined. As soon as the case includes consideration of, say, a magnetic field then a choice can be rationalized. Note that the "underdetermination" here is not concerned with the location of a <u>particle</u> (and the whole train of philosophic debate which has arisen to interpret that) but the lack of determination for a particular wave function or set of them. We will find this typical of the problems the quantum chemist must face.

The chemist, of course, especially when confronting the problem of chemical bonding is never concerned with atoms in isolation, but with the prospect of low potential energy due to orbital interaction. There is, however, a conceptual problem here typical of the difficulties of interpretation with which quantum theory is fraught.

If the agency which orbital interaction represents is taken as "casual", we tend to slip rather too easily into the habit of speaking as if -- conceptualizing as if -- this casual influence were a "force". Coulombic forces are, indeed, involved (not as Coulomb might have envisaged, but as "fields") but they are not, in a very real sense, responsible for either the stability or structure of a molecule. The effect produced is not the classical conception of atoms <u>forced</u> to remain together. The agency in quantum chemistry results, if anything, from the extra freedom of the electrons involved and the <u>limitations</u> placed upon their mutual Coulombic repulsions, both of which are possible only under the umbrella of the Exclusion Principle.

In calculating these effects, the changes which effect bonding have come to be associated with the "exchange" of electrons and the "correlation" among them. "Exchange" has the effect of an <u>attractive</u> force, but it is between electrons which normally repel, and only misleadingly can be referred as a force since it arises because of our manipulation of the formalisms so as to maintain the indistinguishability of electrons -- that is, within the same orbital as allowed by the Exclusion Principle. "Correlation" has the effect of a repulsive force, but it is due to the exclusion demanded by this same principle between electrons of like spin, and is much stronger -- in energetic <u>effect</u>, it not being a "force" -- than Coulombic forces.[4]

The <u>structure</u> of a molecule, therefore, results from the Coulombic forces between nuclei and between electrons but especially from their "correlation". These provide for the localization of charge clouds which produce an overall configuration. The countervailing influence is due to electron "exchange", and since this manages to lower the potential energy twice as much as this combination of effects raises the kinetic energy it provides for a system which is <u>stable</u>.

I do not take "exchange" and "correlation" as examples of the "thought-forms" Coulson tells us chemists had to escape. But I suspect the interpretation just given of them was not simply borrowed from physics (theoretical chemists do not talk, for example, of the "virtual exchange of particles") but arose as jargon pertinent to the chemist's own context -- his own domain -- though such concepts are very much at the mercy of the mathematics devised to deal with each specific problem. The key difficulty, rather, seems to be that the energetic advantage a molecule has over its component atoms is an amount of energy very small compared to their total electronic energy (the ratio in H_2 is 1/7, Li_2 is 1/14, CH_4 is 1/38, and so on). But as the comparative magnitude of the bonding energy gets smaller and smaller the difficulty in devising methods of approximation grows. In addition, there is not one typical method of approximation but a great number of them with a multitude of variations all of which makes interpreting from the mathematics what is happening chemically itself problematic. Indeed, for the first 10-15 years of quantum chemistry, it was very much the chemists' intuition of what must be happening which determined what approximatory approach to take -- what further constraints to add.[5]

The simplest example is the simplest molecule, diatomic hydrogen. The first step is to rely upon the physicists' wave function for the electron in each isolated H atom. If it is presumed these do not interfere with each other one can simply rely upon one wave-function for each atom to construct a wave function for the molecular system. The eigenvalue associated with this molecular wave function actually shows an energetic advantage at a specifiable distance between nuclei, but it is much too small. This result can be interpreted as showing that the Coulombic forces alone which are exerted between all the particles at this distance is responsible for only the slightest advantage -- the electrostatic attraction gained by both electrons being attracted to both nuclei accounts for only 1/4eV of the 4 3/4eV observed. Heitler and London, whose work in 1927 represents the first excursion into quantum chemistry, found a means of representing within the formalism the "exchange" phenomenon mentioned above (this constraint peculiar to quantum mechanics in which the Pauli Exclusion Principle is brought to bear) with the result of improving the energy calculated to over 3eV. In 1928 Wang raised that figure to 3.78 by also including the suspicion that the electrons when located between the nuclei would screen their mutual repulsion. When in the early 1930's the effect of momentary polarizations etc. were included, the calculations finally climbed to 4eV and over. Since then further refinements have been worked into an appropriate Hamiltonian and an appropriate approximation of the wave function, which (especially with the aid of computers) has produced results exactly in line with experimental measurements -- at least for H_2.[6]

These results are possible given the whole series of constraints devised for this problem. Since the case of H_2 lies too close to the border (or in a region of overlap) between the domains of chemistry and atomic physics there is little that was exclusively chemical about the intuitions which suggested these refinements. But these constraints are not readily generalizable, and in more complex examples chemical

intuition has had to "escape the thought-forms of the physicist."

When we turn to molecules of at least three atoms, for example, the possibility of different structures arises. The chemical problem had been not just to distinguish which triatomic structures are manifested, but to explain why for example CO_2 is linear and H_2O is not. The more general constraints within quantum theory provided one ready response. The differentiation of electron orbitals on the grounds of spectroscopic evidence already included, for any atom with five or more electrons, "p" orbitals in three perpendicular versions. Consequently, it could be supposed that the valence electrons of boron, carbon, and on across the Periodic Table, had directional dispositions which one would expect to result in molecules in which the angles of different bonds on the same atom would likewise be perpendicular. That fits CO_2 well enough having a bond angle of 180°, but not H_2O with an observed bond angle of over 104°.

The solution proposed by L. Pauling and widely used since, was to "superpose" the "s" and "p" orbital functions associated with oxygen's valence electrons and thereby form "hybridized" orbitals. Such orbitals can be interpreted as representing the localization of charge density in just those directions which their structural arrangement requires. But let me emphasize that there are a wide array of "superpositions" which are equally good solutions to the equation, and in complex molecules the energetic advantages between many such linear combinations is very slight in face of the difficulty of approximation. At the time "hybridization" was proposed and first extensively used, it was not as the conclusion to an atomic physicist's argument. What is more, the particular variations on hybridization which represent the well known tetrahedral structures typical of carbon are not even energetically feasible until the constituent atoms interact through excited states of their valence electrons.

With the oft cited case of "benzene", the problem is not only to account for its structure (a chain of six carbon atoms linked to form a ring) for the hybridization is sufficient to account for the requisite bond angles, but also with the peculiar stability of this overall structure and its disposition toward substitution at preferred sites. The answer seems to be provided by the "Molecular Orbital" approach which portrays a "sigma" bond lying directly between each carbon nuclei and with the spare "p" orbitals a "pi" bond which is delocalized all around the ring. There seems to be an extra gain in stability through thus delocalizing certain electrons (at select energy levels) around the molecule as a whole.

It is not my intention to counter reductionist claims simply by the "emergence" of hybrid orbitals. Rather I am trying to illustrate that theoretical chemistry operated from within a very loose framework, not by deduction. The minimization of the system's potential energy can be accomplished in an indefinite number of ways, just as the mathematical techniques called upon can approximate proper wave functions in indefinitely many ways. Within this framework chemical results are left under-

determined by atomic physics. Only the particular chemical context can suggest what sort of "superpositions" might be appropriate, and only experimental measurements can specify when enough mathematical terms have been added. The point is, that once it was clear that via wave mechanics the effect of orbital interaction could be calculated, it was still on chemical grounds that specific techniques were worked out for each special circumstance. As a contemporary text insists: a whole set of such treatments is required, "at least one for each important type of molecule!"[7]

It is at any rate considerations of this sort that Pauling and Coulson seem to have in mind when they suggest that chemists were forced to do their own theorizing. But I think there is the kernel here of something more. It is not just that the proper series of constraints has to be worked out with chemists' help, that deductions can only be erected in hindsight, or that the reduction of chemistry is only a philosopher's reconstruction. It is rather that the constraints sufficient to account for various cases of bonding and chemical reactivity generally are peculiar to this scale of complexity and energy.

In the first case, it is a well known frustration of quantum theory that the formalisms do not admit of easy interpretation. What observables can be associated with the Schrödinger Equation and its solutions chemists have learned to interpret in their own way: they pay lip service to "probability" but what they use is charge density, i.e., real spatial distribution of charge! And there are good reasons for them doing so. Wave/particle choices, and most of the dilemmas philosophers have posed because of them, evaporate in the domain of the chemist as a feature of the spatial-temporal magnitudes over which he is concerned. Chemical reactions have not to do with the interaction of electrons as particles simply because reactions are too slow. They occur as they do because of the relationships (structural and energetic) between charge clouds -- hence it is the wave mechanics of orbitals rather than strictly the quantum mechanics of electrons. Bonds are the localized (increased) density of electron charge, not the link between electrons. They result from the most efficient combination of "exchange" and "correlation" phenomenon under the circumstances, not because of specific particle interactions nor coulombic forces. This is, at any rate, how theoretical chemists articulate their domain.

Hence we can both say that a bond contains nothing other than electrons interacting and that it is not simply identifiable with the electrons depicted in the laws of atomic physicists. As soon as a physicist approaches the magnitude of the chemist's domain, he must conclude that the "electron" of a hydrogen atom is to be identified with a specifiable "orbital". When two hydrogen atoms bond their electron orbitals change -- both in energy and distribution. Now we can say there remains nothing in diatomic hydrogen but those two electrons, but at the level of hydrogen atoms actually bonded there is a new and different orbital. One of the requirements recognized by reductionists is that the terms of the one theory be identifiable (contingently and referentially) with terms in the other. But if we "reconstruct" the theories of chemist and

physicist in question, we find that the term 'electron' must be replaced with 'orbital' and that between hydrogen atom and hydrogen molecule the referent changes. It is not the same orbital. Our temptation to say it's still the same pair of electrons fails to recognize what the quantum theory demands at this scale of time.[8] Dispositions can only be determined in context.

There is a real danger in any attempt to argue strictly from the "hybridization" or "localization" of electron orbitals which is possible only at the level of the chemical domain, for it is difficult to say to what degree these are artifacts of the particular mathematical technique applied.

Since the 1940's the major theoretical differences between various approaches have been minimized (especially the valence bond and molecular orbit approaches) in an effort to provide calculations ab initio which include just as large a linear combination as required to give rigorous results. But it is just this effort which has run into the failure mentioned by Platt. Such calculations are based upon orbital functions chosen because they are amenable to rigorous calculation not because they represent anything chemically significant. They may result in accurate calculations of total energy, but at the cost of representing anything significant concerning the system's bonding or overall structure. (You've thrown in every conceivable configuration just to get a solution). One is faced with what has been called [12]: "the conceptual dilemma of quantum chemistry: agreement with experiment demands more rigorous theory, yet in more rigorous theory the conceptual structure of chemistry is not readily apparent." The problem of bonding by electron pairs, i.e., the localization of charge density, evaporates in a model mathematized so that each electron participates in the interaction between any pair of nuclei, where all electrons are represented only in the sense that some orbital basis has been chosen which is all inclusive.[9]

What the chemical theoretician faces are just those circumstances in which a comparatively minor amount of energy is associated with the most significant features, the structure and reactivity of molecules. External influences and internal interactions which are capable of no particular effect on component atoms (since we tend to identify them with their nuclei) can have what appears as a dramatic effect on structural arrangement and subsequent behavior -- over the whole molecular system. There is a sensitivity or susceptibility which is peculiar to this scale of complexity, and it is not just an artifact of one mathematical technique. Chemical bonding represents a step up in complexity compared with the domain of the atomic physicist and a step down in magnitude of stabilizing energy.

For this reason chemical theoreticians seem to be caught: if they provide the accuracy required to match and even anticipate such slight variations in energy, they must call upon approaches which obliterate much of what little is open to interpretation. If they set it up so

354

that interpretation is comparatively straightforward, they are forced
to depend upon the sort of constraints suggested only on chemical
grounds. In either case, it would seem peculiar to describe this
dependency upon the framework of quantum theory as a deductive deriva-
tion.

Notes

[1] The development of quantum theory was such that by 1929 P. Dirac
could declare ([5],p.714): "The general theory of quantum mechanics is
now almost complete ... the underlying laws necessary for the mathema-
tical theory of a large part of physics and all of chemistry are thus
completely known."

[2] E. Nagel first suggested requirements for this standard portrayal of
reduction in [8]. He explicitly cited as an example, p. 362, the "cer-
tain parts of nineteenth century chemistry (and perhaps the whole of this
science) is reducible to post-1925 physics." In 1970, in [7], Nagel
still cites "the explanation (at least in principle) of chemical laws
in terms of quantum theory." By this he means: "the macroscopic (or
higher level) regularities found in chemical interactions are reducible
to the microscopic statistical regularities formulated by quantum
theory."

[3] It is this assumption which suggests reliance upon the Variational
Principle in a wide range of approximatory procedures for constructing
a viable wave function.

[4] See the explication of "exchange" and "correlation" provided by Sir
John Lennard-Jones in [6]. Although it would seem "correlation" in
particular results only from the effect of the Pauli Exclusion Prin-
ciple with regard to electron orbitals (i.e., only in such systems), I
am not basing my arguments on the mystification which might be induced
by these concepts. They might well be altered or replaced by advance-
ment in quantum theory, but even so, such conceptual changes would little
affect the limitations I am posing. To quote C. A. Coulson from his
inaugural address to the new chair of Theoretical Chemistry in Oxford,
"Theoretical Chemistry: Past and Future": "The time may come when some
even more abstract and fundamental theory will replace wave mechanics
and the quantum theory. It has not yet come, nor at the moment is there
any sign of it. Further, when it does come, it will be of only secon-
dary interest to the chemist unless, as seems rather unlikely, it deals
with atoms and electrons. For these, and not neutrons or quarks, are
the entities with which chemistry is concerned."

[5] In [3], p. 113, Coulson insists: "these operations are not merely
mathematical; each represents the introduction of some aspect of chem-
ical intuition and experience. It is not unfair to say that in this,
as in practically the whole of theoretical chemistry, the form in which
the mathematics is cast is suggested, almost inevitably, by experimen-
tal results."

[6]See Coulson's [3] for details of this development and its impact.

[7]Cotton and Wilkinson's [1]:   "In principle, the best approach--one that would supercede all others if it could be carried through system-atically--should be a comprehensive and numerically accurate ab initio MO treatment ...or, rather, a whole set of such treatments, one at least for each important type of molecule. It must be stressed that in order to predict molecular geometry reliably, the calculation would have to be far more vigorous....would have to be carried out over a whole range of configurations in order to search for the configuration of lowest energy." ([1], p. 137).

[8]As Nagel suggests in [8] and [7] reductive derivation is typically reconstructed in terms of chemical "laws". It is not at all easy, how-ever, to specify what these are, and chemists' usage is less than con-sistent. To suppose each universal descriptive counts as a law lead to the highly questionable supposition that the Periodic Table is/was a chemical "theory". The valence theory of bonding would be a more fea-sible example, but has only served as a theory since the late 1920's. A closely associated correlation (between energy and distance) called the Lennard-Jones Potential might better serve as the relevant chemical law, though chemists have never referred to it as more than a descriptive correlation of information. One might even contrive to deduce it from the Schrödinger Equation in some sense, but the "law" and the means for its deduction have developed concomittantly, and not within atomic physics. If this "law" be explained, then it is so not by atomic phys-ics or even quantum theory so much as the conservation of energy.

[9]Since the late 1940's with the increasingly widespread use of Mole-cular Orbital formulations, and the advent of computers, ab initio cal-culations have been carried out for a wide range of molecules. More recently, however, there has arisen sharp criticism of the bold assump-tions required and the degree to which it undercuts the conceptual needs of the chemist. See G. Del Re's [4] and the papers by K. R. Roby and R. Daudel in [12].

References

[1] Cotton, F.A. and Wilkenson, G. Advanced Inorganic Chemistry.
     3rd ed. New York: Wiley and Sons, 1972.

[2] Coulson, C.A. "Recent Developments in Valence Theory." Pure
     and Applied Chemistry 24(1970): 257-287.

[3] ------------. Valence. 2nd ed. London: Oxford University
     Press, 1961.

[4] DelRe, G. "Current Problems and Perspectives in the MO-LCAO
     Theory of Molecules." Advances in Quantum Chemistry 8(1974):
     95-136.

[5] Dirac, P. "Quantum Mechanics of Many-Electron Systems."
     Proceedings of the Royal Society. A 123(1929): 714-733.

[6] Lennard-Jones, Sir John. "New Ideas in Chemistry." Scientific
     Monthly 80(1955): 175-184.

[7] Nagel, E. "Issues in the Logic of Reductive Explanations." In
     Mind, Science, and History. Edited by H.E. Keifer and M.K.
     Munitz. Albany: SUNY Press, 1970. Pages 117-137.

[8] --------. The Structure of Science. New York: Harcourt, Bruce
     and World, 1961.

[9] Pauling, L. The Nature of the Chemical Bond. Ithaca, NY:
     Cornell University Press, 1939.

[10] Platt, J.R. "The Chemical Bond and the Distribution of Electrons
     in Molecules."

[11] ----------. "Properties of Large Molecules That go Beyond the
     Properties of Their Chemical Sub-Groups." Journal of Theoretical
     Biology 1(1961): 342-358.

[12] Price, W.C., Chissick, S.S., and Ravensdale, T. (eds.). Wave
     Mechanics: The First Fifty Years. London: Butterworth, 1973.