

A commentary on Weisberg's critique of the 'structural conception' of chemical bonding.

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1. Introduction

Chemical bonding has been described as one of the two big ideas in chemistry in response to some philosophers of physics who deny to the field of chemistry any form of philosophical importance (Scerri, 2020). Molecular structure and bonding are among the most quintessential topics that have been considered by the new wave of philosophers of chemistry that began to make itself known in the mid 1990s. It is therefore essential that such views be subjected to careful consideration in order to advance the burgeoning field further.

The purpose of the present article is to examine a paper on chemical bonding published by Michael Weisberg (Weisberg, 2008) which continues to be cited in philosophical articles about chemical bonding (Seifert, 2022). In addition, I will refer to an earlier article by Robin Hendry that appears to have served as the basis of some of Weisberg's views on chemical bonding (Hendry, 2008).¹

2. A brief history of the subject

The topic of chemical bonding has a long and complicated history, which begins with the work of chemist John Dalton at the beginning of the 19th century. As is well known, Dalton revived the atomic theory of the ancient Greek philosophers, some of whom held that matter was not infinitely sub-divisible but that division reached its

limit once one arrives at the atoms, or smallest components, of each of the elements (Greenaway, 1966).

Moreover, Dalton went on to consider the combination of atoms to form molecules such water, which he incorrectly believed to consist of one atom of hydrogen combined to one atom of oxygen. The nature of the attraction between these two kinds of atoms was a source of great difficulty for early chemists and in many respects the mystery remains up to the present time, although we now possess the means to carry out very accurate calculations on the properties of molecules both great and small. Nevertheless, the question of what chemical bonds actually are continues to pose problems and there are many remaining disagreements about how this issue should be approached among professional chemists (Malrieu, Guihéry, Jiménez Calzado, Angeli, 2006; Rzepa, 2009; Silvi, 2017).

Among the earliest views that were contemplated is one in which chemical bonds as physical links between the constituent atoms. These physical connections have variously been regarded as being stick like linkages or mechanical springs. Stated otherwise bonding was originally viewed in a naïvely realistic sense whereby bonds were regarded as physical objects just as much as the atoms that they were believed to connect together.²

In the early part of the 20th century great advances were made which resulted in the broad classification of chemical bonds into the categories of ionic and covalent bonding. Ionic bonding was postulated first to consist of an attraction between atoms, or more precisely ions, resulting from the complete transfer of electrons from metal atoms to atoms of non-metals. The ions formed in this way were understood as attracting each other to form three-dimensional crystal lattices such as in the typical example of sodium chloride (Kossell, 1916). Soon afterwards another kind of bonding was proposed by authors including G.N. Lewis in order to explain the existence of non-polar compounds, in which oppositely charged ions did not appear to play any role (Lewis, 1916). This other major form of bonding was called covalent bonding in order to reflect the notion that the constituent atoms were sharing electrons rather than transferring them entirely. Examples include such molecules as diatomic gases such as H₂, O₂, N₂ etc., CH₄ and so on. For about

100 years schoolchildren have been learning the basic distinction between these two kinds of chemical bonds right from the start of their chemistry classes.

However, as with all elementary facts in science, this simple picture must be increasingly qualified as instruction in the subject is taken to more advanced levels. Here then lies the first pitfall that philosophers of chemistry encounter, especially those with little training in advanced chemistry. Some of them discuss ionic and covalent bonding, as though they were of a radically different kind. This view should be tempered by the realization that the two forms are but extremes on a single continuous spectrum. It is more instructive to think of the two forms of bonding as being cases of approximately equal sharing of electrons in the case of covalent bonding, moving to very unequal sharing of electrons in the ionic case.³ Any philosophical analysis which is predicated on the characteristic difference between ionic and covalent bonding is therefore problematical from the outset, a feature which I believe has occurred in some of the recent discussion in the philosophy of chemistry community as I will attempt to show.

3. Weisberg's treatment of chemical bonding

Michael Weisberg begins his discussion cautiously by declaring that

Once one moves beyond introductory textbooks to advanced treatments, one finds many theoretical approaches to bonding but few, if any, definitions or direct characterizations of the bond itself. While some might attribute this lack of definitional clarity to common background knowledge shared among all chemists, I believe this reflects uncertainty or maybe even ambivalence about the status of the chemical bond itself. (Weisberg, 2008, 933).

I cannot share Weisberg's puzzlement of the lack of definitions of bonding in contemporary chemistry since the sheer variety of forms of bonding would preclude anything but the most general definition, even if one were to be attempted. Nor do I believe that the lack of any such definition betrays any form of uncertainty among the practitioners in the field. As I see it there is simply no need to provide a

sufficiently general definition of bonding, just like in the case of so many useful scientific terms that similarly resist precise definition. Moreover, contemporary chemists inhabit a world that is described by quantum mechanics, which, as is well known, defies all attempts at a common-sense understanding. There seems to be little reason why the notion of chemical bonding might be exempted from such problems?

Weisberg continues by writing,

This kind of ambiguity has led chemists to different conclusions. Most commonly, chemists adopt a pragmatic stance and simply demand that bonding theories be useful for making predictions and aiding in the synthesis of new molecules. The underlying ontological status of the bond holds little interest. Although useful to everyday chemical practice, this approach is deeply unsatisfying to the philosopher of chemistry because it leaves unanswered fundamental questions about the nature of the chemical bond. (Weisberg, 2008, 933).

In saying this Weisberg appears to be betraying something of a philosophical prejudice, since an anti-realist philosopher of chemistry might be perfectly willing to adopt the pragmatic view of bonding that he seems to attribute just to professional chemists. Still on the same general point, Weisberg writes,

Other chemists, including ones of deep realist commitment, draw a different and more skeptical conclusion from these facts. Robert Mulliken, a founder of quantum chemistry said, "I believe the chemical bond is not so simple as some people seem to think". (Weisberg, 2008, 933)

One cannot help wondering why the mere statement made by Mulliken, that the chemical bond is not as simple as people think, should be attributed any

particular philosophical significance. But be that as it may, Weisberg presses on while saying,

Whatever the ultimate verdict, entertaining Coulson's and Mulliken's skepticism raises many deep, philosophical questions about the nature of chemical bonds and molecular structure. These questions include the following: Are chemical bonds real? If so, should we think of them as entities? (Weisberg, 2008, 933).

I believe that this may be a case of question begging, since Weisberg is not telling us what he means by "real" in this or any other context for that matter. It also seems rather naïve to suggest that any chemists whatsoever continue to believe that bonds might qualify as entities, following the highly successful quantum mechanical account of chemical bonding that pervades all of modern chemistry. What I am driving at is that the debate and disagreement that Weisberg is pointing at, does not in fact exist, at least among professional chemists. No chemist seriously believes that bonds are "real" in the sense of being entities in spite of the historical heritage whereby they were once crudely conceived of as actual physical connections.

Weisberg then asks the further question,

If bonds are not real, is the phenomenon of bonding real? (Weisberg, 2008, 933).

The simple answer which I believe that a chemist would give is that 'bonding' is a chemical process rather than a physical entity in desperate need of being interpreted realistically. Some chemists might even venture to say that bonding is 'real' while still maintaining that chemical bonds as such are not real.⁴ Chemists can readily accept that one can have bonding without actual bonds. This would not seem to constitute any paradox that Weisberg seems to be implying. After these general remarks Weisberg gets down to the serious matter in hand by saying that his article,

...asks whether models of molecular structure endorse a structural conception of covalent bonds of the kind implicit in much of chemical practice (Weisberg, 2008, 934).

The approach that Weisberg chooses to use is one of a robustness analysis that he attributes to Levins and Wimsatt (Levins, 1966, Wimsatt, 1981). Briefly put, Weisberg sets out to identify elements of robustness in the quantum theories of chemical bonding by looking for any features that are common to the various approaches that have been developed.

The author then draws on Robin Hendry's 'structural conception' of chemical bonding in order to see whether or not robustness exists. This conception is described by Michael Weisberg as follows,

Characterized in purely functional terms, the structural conception of bonding says that a covalent bond is a directional, sub-molecular relationship between individual atomic centers that is responsible for holding the atoms together (Weisberg, 2008, 934).

However, even in classical chemistry covalent bonding is not invariably directional and not is it necessarily sub-molecular although I will delay a fuller discussion of these points for the moment. Weisberg further writes,

In modern chemistry, it is completely uncontroversial to see electrons or electron density as what realizes the sub-molecular relationship. This leads to the following structural conception of bonding: a covalent bond is a directional, sub-molecular region of electron density located between individual atomic centers that is responsible for holding the atoms together (Weisberg, 2008, 934-5).

Why we should suddenly be limiting the discussion to just covalent bonding is not clear to the present reader, but let us not quibble too much.⁵ In any case, as I will be arguing, even if we do confine ourselves to covalent bonding this conception is somewhat flawed. The distinction between ionic and covalent bonding is something of an over-simplification. The modern study of chemical bonding frequently involves the application of the Schrödinger equation for the physical system in question and in so doing one does not pause to specify whether the bonding might be ionic or covalent. Give this state of affairs there would seem little point in attempting to specify the quintessential nature of just covalent bonding.

But let me return to what Hendry and Weisberg take to be the characteristics of covalent bonding. Weisberg proceeds to break down his, or rather Hendry's, three important characteristics of the structural conception.

First, it distinguishes covalent bonds from ionic bonds with the directionality restriction. Ionic bonds are omnidirectional electrostatic interactions between positively and negatively charged ions. Covalent bonds are regions of electron density that bind atoms together along particular trajectories (Weisberg, 2008, 935).

The second sentence would seem to imply that ionic bonds do not involve regions of electron density, which is surely not what these authors mean to say. As to the question of directionality, this characterization would seem to omit an entire class of covalently bonded compounds such as diamond or graphite in which bonding is multi-directional just as in classic cases of ionic bonding.

Weisberg, drawing on Hendry, continues by saying that,

Second, this conception says that bonding is a *sub-molecular* phenomenon, confined to regions between the atoms. This eliminates the possibility that bonds are a molecule-wide phenomenon (Weisberg, 2008, 935).

If this is intended as a further characteristic of just covalent bonding it is simply incorrect, since ionic bonding also occurs between atoms, or more correctly their ions. I am also puzzled by the apparent desire to exclude the possibility that bonds, or bonding, might be a molecule-wide phenomenon. Counter examples are easy to find. In addition to diamond and graphite, which are generally described as displaying giant covalent bonding, modern chemistry has revealed the frequent occurrence of delocalized bonding to occur in cases such as metals, conducting polymers, benzene and many other conjugated hydrocarbons. Moreover, delocalization of electrons is known to occur in many inorganic species such as oxyanions including the carbonate and sulfate ions. Bonding is indeed a molecule-wide phenomenon and delocalization is not confined to covalent compounds.

Here is the third feature of bonding as identified by Hendry and approvingly adopted by Weisberg,

Third, the region of electron density between the atomic centers has to hold these centers together, which I will interpret to mean that they are closer together than they would have been in the absence of the bond. In other words, bonds are a *stabilizing* force for the molecule, and this stabilization will manifest itself in the amount of energy required to separate the atomic centers (Weisberg, 2008, 935).

Unfortunately, this naïve characterization of bonding is rather inconsistent with the quantum mechanical view of chemical bonding as I will explain more fully in due course. To put it simply, for the time being, the highly influential molecular orbital approach to chemical bonding considers the stabilizing effect of the occupation of bonding molecular orbitals as well as the de-stabilizing effect of the occupation of anti-bonding molecular orbitals. To assert that bonding is simply a stabilizing force is to grossly oversimplify the situation.

4. Valence Bond Method

In the following two sections of his article Michael Weisberg explains the valence bond method which represents a formally equivalent quantum mechanical approach to chemical bonding to the molecular orbital method. Weisberg begins by considering a very simple approach for the diatomic hydrogen molecule. In this case each of the two nuclei is considered as having its own electron, such that a crude approximation for the molecular wavefunction is obtained by taking a product of the individual atomic wavefunctions. As the author correctly points out, such an over-simplified model predicts that the bond length should be 90 picometers and the bond energy 24 kJ per mole. Weisberg follows this statement by announcing that the experimental values are in fact 74.1 picometers for the bond length and 458.0 kJ per mole for the bond energy, while adding that,

We are in the right ball-park, but there is much room to improve our model (Weisberg, 2008, 937).⁶

In section 2.2 Weisberg moves on to considering a more accurate treatment that is afforded by the Heitler-London method. In this approach one no longer considers each electron to be localized around its own 'parent nucleus'. The first way in which this is carried out is to recognize the indistinguishability of electrons. The static view in which electron 1 is thought of as being associated with nucleus 1 and electron 2 with nucleus 2, needs to be modified to take account of the fact that the two electrons are not in fact distinguishable as number 1 and 2. This correction is carried out mathematically by a process of permutation of electrons such that the wavefunction becomes,⁷

$$\Psi = ca(1)b(2) + ca(2)b(1)$$

Weisberg interprets this expression to mean that the electrons have greater mobility but without much justification. I am not sure I agree with this claim. It does not necessarily follow that the permutation of electrons, which is a mathematical operation to reflect electron indistinguishability, can be physically interpreted to mean greater electron mobility.

Weisberg claims that,

By allowing greater electron delocalization, the model is brought into closer alignment with the experimentally measured values (Weisberg, 2008, 937).

I suggest that the author would have been better advised to write that the modified wavefunction achieves a closer agreement with experimentally measured values because it contains more mathematical flexibility.

5. Improving valence bond models

Weisberg proceeds to consider more accurate approaches within the valence bond method which consist in introducing what are generally known as ionic terms. These terms are intended to reflect the possibility of an unequal charge distribution such that one atom is depleted of electron density while the other one, in the case of a diatomic molecule, experiences an enhanced electron density. The result of such charge fluctuation would be surely to introduce greater localization of electrons and not greater delocalization as Weisberg again seems to think is the case.

Far from being an element of robustness across different bonding models, I claim electron delocalization is an unreliable way to characterize the improvement that one sees in progressing through these approaches.

6. Molecular Orbital Models

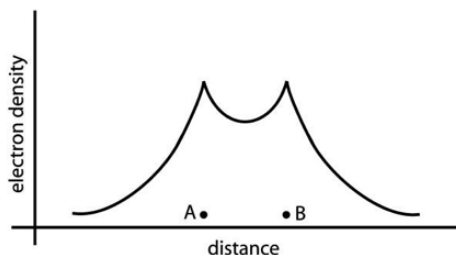
As is well known, the alternative approach to understanding chemical bonding using the valence bond/Heitler-London method is through the molecular orbital approach. In this approach one considers the interference of electron waves on adjacent hydrogen atoms, something that Weisberg fails to acknowledge incidentally. According to him one begins with the following trial wavefunctions,

$$\Psi_g = \Psi_A + \Psi_B$$

$$\text{and } \Psi_u = \Psi_A - \Psi_B$$

Although this is correct Weisberg does not explain that these two wavefunctions represent the simultaneous occurrence of in-phase or constructive wave interference in the first case, and out-of-phase or destructive interference in the second case. Weisberg then takes a combination of these two wavefunctions and concludes as follows,

Further, the electronic density is at its peak in the areas immediately surrounding the nuclear centers. Figure 1 is a cross section of the amplitude of the wave function of H_2 calculated from our model. We can see that the highest density is just around the nuclear centers, with considerable density in between the atomic centers...(Weisberg, 2008, 940).



Although this may be a correct description of the bonding orbital, which corresponds to the first of the trial functions mentioned above, chemical bonding results from the combined effect of both the bonding and anti-bonding orbitals, or in other words the combined effects of the two initially mentioned trial functions. What Weisberg has done is to select just one of these functions, presumably because it implies the build-up of electron density between the nuclei as shown in his figure 1 above.

Had he also considered a similar diagram for the other function he would have been forced to acknowledge that the anti-bonding orbital results in a decrease, instead of an increase, of electron density between the hydrogen nuclei. Rather than considering the combination of the two trial functions as he claims to do, the author is selecting just the expression that happens to correspond to an increase in electron density between the nuclei.

On the question of directionality, it seems rather odd that the author has chosen to discuss the diatomic hydrogen molecule since in this case directionality only exists in the trivial sense, since the molecule is linear. Any meaningful discussion of directionality should therefore have been carried out with at least one example of a non-linear polyatomic molecule. Furthermore, as Hettema has correctly pointed out in an excellent earlier commentary on Weisberg's article, the most elementary way that directionality has been recovered in quantum mechanical calculations of chemical bonding has been through Linus Pauling's notion of orbital hybridization (Hettema, 2008). Neither the name of Pauling nor his hybridization procedure are mentioned in the article that the present comment is directed at.

7. Modern Molecular Orbital Models

Weisberg continues his survey of molecular orbital models by briefly discussing more advanced approaches such as the Hartree-Fock method. As in his previous sections the author insists that the inclusion of greater electron delocalization is the essential feature that allows one to obtain greater agreement with experimental values of bond energies and similar molecular properties.

Without attempting to distinguish between different kinds of electron correlation,⁸ Weisberg equates this effect in a naively realistic fashion to mean that it can be accounted for by allowing a greater extent of electron delocalization and that it therefore reinforces his notion that the robust aspect of bonding that survives across all these approaches is electron delocalization.

Unfortunately, this view is incorrect, since electron correlation counteracts the effect of electron delocalization. Furthermore, electron correlation takes place in atoms as well as molecules and, as a consequence, cannot be a characteristic of chemical bonding in the manner that Weisberg implies it to be. This is especially relevant in view of Weisberg's statement that

We have now come to the conclusion of our whirlwind tour of molecular models, searching for the robust properties of chemical bonds. (Weisberg, 2008, 943).

8. Conclusions section

Weisberg argues that the naïve notion of electrons being shared between two atoms is definitely not robust across modern models of chemical bonding.

The structural conception does not demand that electrons are shared or even fully located in the region between the atoms. Indeed, it only demands that bonds can regularly be identified as directional, sub-molecular regions of electron density (Weisberg, 2008, 944).

What is robust across models of chemical bonding for Weisberg is the delocalization of electrons, a feature that he believes weakens the structural conception.

Weisberg writes,

The second robust feature of the models is that greater electron delocalization leads to stabilization. When we moved from the simple valence

bond model to the Heitler-London model, we saw considerable stabilization. This accompanied relaxing the restriction that pinned electron 1 to nucleus A and electron 2 to nucleus B. We further improved that model by adding terms to the basis function that allowed greater flexibility to the resultant wave function, which has the physical significance of allowing greater delocalization...(Weisberg, 2008, 944).

However, as I have pointed out above, interpreting the introduction of greater flexibility in the wavefunction of molecules as necessarily indicating the introduction of ever greater electron delocalization is itself a form of realism that is not sanctioned by quantum mechanics. It would appear that Weisberg's critique of the structural conception, which he takes from Hendry, is predicated on an incorrect conflation of flexibility in wavefunctions with the delocalization of electrons. Furthermore, in attempting to criticize the notion that bonds are 'real' Weisberg appears to be reifying some mathematical procedures such as the introduction of an increasing number of terms into molecular wavefunctions. This is to say nothing of whether or not Hendry's structural conception succeeds in identifying the essential features of covalent bonding which, as I argued at the outset, I do not consider it to do. I do not believe that the analyses of chemical bonding that Hendry and Weisberg have proposed bring us any closer to clarifying the question of whether bonds or even 'bonding' should be interpreted realistically or not. Having said this, it should be noted that Hendry remains agnostic as to whether the structural or energetic view of chemical bonding should be considered as a more correct account. On the other hand, the entire thrust of Weisberg's article would seem to be that the energetic view of bonding is somehow superior to the structural view given that he titles his article as "A challenge to the structural view".

To end on a more positive note, the question of chemical bonding does indeed deserve far greater scrutiny from philosophers of science since it is one of the main characteristic features of chemistry and perhaps even the biggest idea in this much neglected branch of science. Although I do not propose to advance this question much further in the present article, I would like to indicate the general

direction in which I believe such questions should be regarded.⁹ Contrary to Weisberg, who wants to assert some weaknesses in the structural view, and more in keeping with Hendry who presents the two views as being equally viable, I believe the question boils down to one's views on reduction.

I do not regard the two views that have been discussed as presenting any form of tension. The structural and energetic view of bonding are rather the views that a typical working chemist and working physicist respectively would tend to hold. Said otherwise, to a chemist operating at the level of molecules and images of their structures it is perfectly reasonable to consider bonds as being directional and in some general sense as being 'real'. For a physicist however, the reality of bonding, or perhaps the view of bonds as substantial entities, would tend to give way to a mathematical description for the molecules in question or perhaps via a density functional approach to the problem. What is real to the chemist may not be real to the physicist. There is no preferred level which gives us access to the ultimate reality, unless one is a naïve reductionist in which case only the view from physics would count as the real one.

However, the reality or otherwise of chemical bonding needs to be viewed in a wider context. The philosophy of chemistry has witnessed a similar debate as to whether atomic orbitals are real or not (Ogilvie, 1990, Pauling, 1992, Scerri, 1991). To chemists they are regularly pictured in textbooks and chemical explanations and can be justifiably be considered as being real entities. To the physicist, atomic orbitals are anything but real, since they consist of complex mathematical functions rather than ones involving real numbers. The discussion concerning the ontological status of atomic orbitals was also revived in 1999 when it was reported that atomic orbitals had been directly observed for the first time (Zuo, 1999; Scerri, 2001, Mulder, 2011, Schwarz 2006). Indeed, an analogous, although less vivid form, imaging of chemical bonds is obtained via the now well-established method of atoms in molecules pioneered by Richard Bader (Bader, 1994; Bader, Matta, 2013).

Notes

¹ The articles by Hendry and Weisberg that I am referring to were first presented as part of a symposium on the philosophy of chemistry at the PSA meeting of 2008.

² To the extent that atoms were regarded as real physical entities, a view that was by no means universal among chemists such as Mendeleev and many others, especially in the 18th and 19th centuries.

³ This point was already emphasized by G.N. Lewis almost exactly 100 years ago.

⁴ Robin Hendry makes the same point in the article to which Weisberg was responding. (Hendry, 2008).

⁵ In any case, as hinted in my introduction, modern chemistry does not put too much store in the simplistic distinction between ionic and covalent bonding. The modern study of any chemical compound consists in the application of Schrodinger's equation in order to calculate the structural features of a compound such as bond lengths or bond angles in some cases. None of this activity depends on whether the compound might be ionic or covalent.

⁶ It is rather perplexing that a calculated energy of 24 kJ per mole, as compared with an experimental value of almost twenty times this amount, could be regarded as being in the "right ballpark". To say that a numerical quantity is in the right ballpark, at its most charitable, is generally meant to say that the values being compared lie within the same power of ten, something that does not apply in this case.

⁷ In fact, the valence method requires the inclusion of a further term consisting of $\Psi = ca(1)b(2) - ca(2)b(1)$. This term is due to the anti-symmetry requirement of wavefunctions which in turn is demanded by the Pauli Exclusion Principle. In fact it was only after the incorporation of such an electron exchange treatment that Heitler and London succeeded, for the first time, in accounting quantitatively for chemical bonding in a quantum mechanical manner. This feat was simply impossible in the absence of anti-symmetry.

⁸ Electron correlation is a non-visualizable quantum mechanical effect that cannot be interpreted in the way that Weisberg attempts to (Lowdin, 1959).

⁹ The wider question will be the subject of a later article that is currently in preparation.

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