Are Orbitals Observable?

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Abstract: In this paper I discuss the question whether orbitals can be observed or not. I argue that the answer depends on how the terms 'orbitals' and 'observed' are understood. The fact that different authors take radically different stances on the issue is caused by their employing different uses of either of the two terms. I furthermore discuss a recent argument by Labarca and Lombardi to the effect that the orbital concept in chemistry is discontinuous with that in quantum mechanics. I argue that, quite to the contrary, there is continuity between the two.

Keywords: *Orbitals, observability, approximations, quantum mechanics.*

1. Introduction

Ever since the publication of an article in *Nature* entitled 'Direct observation of *d*-orbital holes' (Zuo *et al*. 1999) the issue of the observability of orbitals has been discussed by chemists and philosophers, Scerri in particular. In a number of publications he has argued that orbitals are unobservable in principle (Scerri 2000a, 2001, 2002).

Although according to Scerri, "there has been almost unanimous agreement among participants of several Internet discussion lists that orbitals cannot possibly be observed" (Scerri 2001, p. S78), several authors have put forward what appear to be completely different views on the issue. Both Ostrovsky (2005) and Schwarz (2006) maintain that orbitals can be – and in fact frequently are – observed.

The claims by Zuo *et al*. specifically, which sparked the debate in the philosophical literature, have been contested by several authors on various technical grounds (see for instance Wang & Schwarz 2000). In this paper, however, I will not be concerned with the specifics of the work by Zuo *et al*. but rather focus on the general question whether orbitals can be observed. I will argue that the controversy over whether they can be observed is to a large part due to different authors using the terms 'observable' and 'orbital' in different senses. I further reflect on two related issues: the approximate nature

of orbitals in many-electron systems and the question whether the two different orbital concepts that I distinguish are continuous with one another.

The paper is structured as follows. In sections 2 and 3, I discuss the meaning of 'observable'. I argue that whereas Scerri gives the term the specific meaning it has in quantum mechanics, both Ostrovsky and Schwarz appeal to the more general meaning of 'observation' in experimental science. In section 4, I consider Scerri's view that in many-electron systems, orbitals do not exist, which would imply their not being observable in any sense of the term. I counter that speaking of orbitals as either existing or not is an incorrect way of perceiving them and that orbitals can be observed when they give a good approximation to the system's state. In section 5, I discern a meaning of the term 'orbital' that differs from the quantum-mechanical one. I argue that this meaning is ubiquitous in chemistry and that under this meaning, orbitals are observable in both senses of 'observable'. Finally, in section 6 I discuss an argument by Labarca & Lombardi (2010) to the effect that the meanings of the term 'orbital' in quantum mechanics and in chemistry being different makes for a conceptual discontinuity between the two disciplines. I counter that, quite to the contrary, the two meanings of the term are continuous with each other.

I should make two preliminary remarks. First, although in the discussion on the topic the term 'visibility' and its cognates frequently pop up, the meaning of the term 'observable' in physics is entirely different from the one it carries in general philosophy of science, where it is close to the common sense meaning of 'visible'. In physics, an observable is a measurable physical quantity, and this has nothing to do with visibility. Second, I will take orbitals to be any one-electron functions. Among them, hydrogenic orbitals, which are the possible states of the electron in the hydrogen atom, are predominant both in chemistry textbooks and in the philosophical literature on orbitals. However, all arguments that I will consider in this paper apply to one-electron functions in general, not just to hydrogenic orbitals.

2. Observability in the strict sense

In physics, observables are measurable physical quantities. In classical mechanics, measurable quantities directly correspond with parameters in phase space or functions thereon, so that one can for instance track the trajectory of an object. In quantum mechanics, on the other hand, there is a fundamental distinction between states and observables. Quantum-mechanical states are given by wave functions, or, more formally, by vectors in a Hilbert space. Observables are not elements of a Hilbert space. Rather, with each observ-

able corresponds an operator that acts on the Hilbert space of the system, and the expected value of an observable O for a system in state ψ is given by $<\psi|O|\psi>$.

A quantity of particular interest to the topic at hand is electron density. It is an observable, which for a system in state ψ is given by ψ^2, a function on real space. Orbitals on the other hand are, in a rather trivial sense, not observable because they are states, not observables.

Notice that I have made a slight shift in wording – from an orbital not being *an* observable to it not being observable. In the discussion on the topic, 'observable' is taken by all authors to be a cognate of 'observe' and 'observation'. Hence the fact that an orbital is not an observable leads to the statement 'an orbital cannot be observed'. I will assume this to be unproblematic, with the notice that the meaning of any such statement is derived from the specific meaning of 'observable' in quantum mechanics. Henceforth I will refer to this sense of observability as the strict quantum-mechanical sense or simply the strict sense, to be contrasted with a broader sense later on.

The state-observable distinction is related to the idea that particles do not have definite values for quantities such as position. When a particle is in an eigenstate of the observable that is measured and hence has a definite value for that observable, the measurement is similar to a classical one in the sense that it merely reads off a value from the system's state. On the other hand, when it is not in an eigenstate of the observable and therefore does not have a definite value for it, the measurement is a truly 'quantum' one. It is in this connection that Scerri says that the reason that orbitals cannot be observed is that "according to quantum mechanics electrons may no longer be regarded as having definite trajectories or paths" (Scerri 2002, p. 310).

However, he goes on to add that Bohmian mechanics, which is a proposed alternative theory to quantum mechanics, does recognize particle trajectories. Although he does not say it explicitly, this suggests that if Bohmian mechanics were true, orbitals would be observable. But this is not the case. According to Bohmian mechanics, the states that quantum mechanics ascribes to systems are incomplete; to be added are particle positions. Thus the ground state of the hydrogen atom is given by *1s* plus a position which varies with time; it is 'guided' by the wave function 1s in the sense that the particle's momentum is a function of the value of the wave function at its position. The electron therefore has a definite trajectory, although this trajectory cannot be known, as due to the uncertainty principle any position measurement results in an uncertainty in the electron's momentum. However, whether or not electrons have trajectories does not bear on the conceptual role of 'orbital', which is the same in Bohmian mechanics and quantum mechanics. It is a state, not an observable.

This little excursion into Bohmian mechanics serves to make the claim that orbitals are unobservable in the strict sense stronger; it holds true even when Bohmian mechanics rather than quantum mechanics is true.

3. Observability in a broader sense

Both Ostrovsky (2005) and Schwarz (2006) have argued that contrary to Scerri's claims, orbitals can be observed. Schwarz points out that one can 'reconstruct' orbitals from measurement data. This is to say that when the state of a system is given by – or well approximated by – an orbital, one can infer from measurement data what orbital this is. He then writes that:

> The statement that some quantity has been 'measured' just means that it has been reconstructed from some measurements that were performed and analyzed on the background of conceptual and numerical approximations. [Schwarz 2006, p. 1515]

A number of things are outstanding in this quotation. First, Schwarz speaks of a measured *quantity*. Orbitals are not quantities, but I take it that Schwarz' use of the term is merely an instance of inattention and that nothing important depends on it. Second, Schwarz refers to the use of approximations. To this issue I will come back in section 4. Finally, Schwarz speaks of 'measurable' rather than 'observable', as he does throughout his paper. This already hints at his having a different understanding than Scerri of what it means to say that one has observed an orbital; and by stating that there is no in-principle distinction between 'reconstructing' an orbital and more directly measuring a physical quantity, he implicitly denies using the strict sense of 'observable'. What he seems to appeal to is the colloquial term 'observe' as it is used in science, which covers not only direct measurement results but also any useful information deduced from these results.

A similar view is brought forward by Ostrovsky (2005). He specifically refers to the reconstruction of a wave function from a measured electron density. The electron density is a function of the wave function, namely its square. The converse does not hold true, but different possible wave functions, given a measured electron density, differ only in their sign,[1] which can in principle be determined experimentally. Therefore, Ostrovsky points out, "the wave function can be fully restored from the observable charge density. This might be considered a *semi-direct* observation, albeit not a direct observation of [the orbital] in the strict sense" (Ostrovsky 2005, p. 116, emphasis added). As regards the observation not being a direct one, he goes on to add that "in modern experiments virtually nothing is directly observed and some

processing of raw data is always required" (*ibid.*). Ostrovsky does not mention the state-observable distinction in quantum mechanics and therefore apparently does not deem it relevant for the topic at hand. On the contrary, his remark that almost nothing is directly observed in experiments shows that he takes the case of orbitals to be not fundamentally different from other cases of inference from measurement data in science. Ostrovsky, like Schwarz, therefore has a notion of 'observable' that derives from the colloquial meaning of the term 'observation' in science and hence is different from the strict sense of the term. In this broader sense, orbitals are observable.

4. Many-electron atoms and molecules

Another essential aspect of the controversy concerns the fact that describing many-electron atoms and molecules by (antisymmetrized) products of orbitals is strictly speaking incorrect, although it is common practice in chemistry to do so. The reason why it is incorrect is that one thereby ignores electron correlation. Because of Coulomb interactions between pairs of electrons, in many-electron systems the probability densities of the different electrons are not independent from each other. This electron correlation results in the wave function of the system being non-separable rather than a product of orbitals.

It must be stressed that representing the state of a many-electron system by a product of orbitals is incorrect for any one-electron functions, not just for hydrogenic or other 'simple' orbitals. After pointing out that states of many-electron atoms are nonseparable, Scerri makes the following remark:

> The continuing value of orbitals lies in their serving as basis sets, or a form of coordinate system, with which the wavefunction of an atom, ion, or molecule can be expanded mathematically. [Scerri 2001, p. S79]

Scerri here refers to the Hartree-Fock method in quantum chemistry. The outcome of a Hartree-Fock calculation, however, is a wave function composed of one-electron functions – orbitals – which are linear combinations of the orbitals in the basis set.[2] This wave function just as well fails to account for electron correlation.

Because many-electron states are nonseparable, they do not contain one-electron wave functions – orbitals. From this Scerri concludes that in many-electron atoms and molecules, orbitals *do not exist*:

> Quantum mechanics tells us that orbitals and configurations do not strictly exist, that is to say, they [do not] refer to real entities in the natural world. [Scerri 2000b, p. 420]

Since what does not exist cannot be observed, it follows that in many-electron systems orbitals cannot be observed.

Ostrovsky argues that although strictly speaking, Scerri is right, approximations are ubiquitous in science, in quantum mechanics no less than in other fields (Ostrovsky 2005, p. 111). In the case of orbitals, hydrogenic orbitals are not even the exact states of the electron in the hydrogen atom, for they are based on a model in which relativistic effects among other things are neglected. The approximation applied in many-electron systems is not qualitatively different, so if one is consistent one has to concede that orbitals are no more real in the hydrogen atom than they are in many-electron atoms and molecules. Of course one can go about maintaining that what is only approximate does not exist, but then one overlooks the fact that approximations carry a physical meaning. In most many-electron atoms, electron correlation is very weak, meaning that the motions of the electrons are largely independent of each other (*ibid.*, p. 112). There is therefore a physical reason why orbital wave functions can be good approximations to reality. For that reason, speaking of orbitals as not existing or non-referring is "hardly appropriate" (*ibid.*).

Schwarz is less cautious in countering Scerri's views. He flatly states that "the statement 'this object or structure exists' has the meaning that there is some objective structure in the real world that is satisfactorily described by the applied approximate concepts" (Schwarz 2006, p. 1512). By "satisfactorily" he refers to the fact that approximations can be better or worse. Therefore, Schwarz argues that orbitals can be said to exist in certain many-electron systems, namely those in which the model wave function that is a product of orbitals gives a good approximation. In this connection he points out that for instance for excited states, the approximation typically gives predictions that are off, in which case orbitals cannot be said to exist.

While Ostrovsky merely considers the statement that orbitals do not exist in many-electron systems inappropriate, Schwarz puts forward an instrumentalist view of existence, on which orbitals can be said to exist in certain systems. Both appeal to the fact that describing the wave function of a many-electron atom or molecule as a product of orbitals can be a better or worse *approximation*. I think they are right in emphasizing this fact. However, whereas Ostrovsky and Schwarz use it as an argument for some stance on the issue of *existence* of orbitals, I believe talk of existence or not of orbitals ought to be dropped altogether. As I have argued elsewhere (Mulder 2010), speaking of orbitals as either existing or not is an incorrect way of perceiving them. Orbitals are states, not entities. For entities there is a clear-cut distinction between existence or not; a cell, for example, either exists or it does not. Therefore, one can meaningfully ask whether the term 'cell' refers or not. With states, however, the situation is different. The question is not whether a

system such as an atom or molecule has a state or not, but rather: what is the determinate 'value' (the determinate functional expression) of the system's determinable state? When one assigns a certain determinate state ψ to a system, it is then not meaningful to say that ψ exists or not. To give an example, suppose one holds a stone in one's hands and makes an estimate of its mass and dimensions. These estimates will of course be off their real values. However, it is meaningless to say that these estimated values 'do not exist'. Similarly, when one assigns *1s* to an electron in the hydrogen atom – which, as I pointed out above, is an approximation – one does not thereby speak of a certain non-referring entity. Rather, it being an approximation means that the functional expression *1s* comes close to the real value of the system's state.

The case of electrons in many-electron atoms and molecules is merely quantitatively, not qualitatively, different. Therefore, talking about orbitals in terms of either existing or not is not just, as Ostrovsky sees it, less appropriate than in terms of being a better or worse approximation; it is mistaken. The upshot of this is that I substantially agree with Ostrovsky and Schwarz, although I believe their reflections on existence lead astray. Wave functions that are products of orbitals can be better or worse approximations to the exact wave function of an atom or molecule; and that is all there is to be said concerning the ontological status of orbitals in many-electron systems.

As regards observability, I see no principled reasons for denying that something that is a good approximation can be observed, in the broad sense. Whether orbitals can be observed in a certain atom or molecule therefore depends on whether the atom or molecule is well described by a wave function that is a product of orbitals, and this is an empirical question.

One might object that I have not defined what it means for something to be a 'good' approximation. This is true, but, as Schwarz (2000, p. 1508) has pointed out, scientists have reported observation of orbitals for decades, all of them of course being aware that orbitals give only approximate descriptions in many-electron systems. Having countered Scerri's arguments, I therefore believe the onus of proof rests fully with those who maintain that orbitals cannot be observed.

5. A second meaning of 'orbital'

In section 3, I pointed out that the statement 'orbitals are observable' is correct under an interpretation of 'observable' that is broader than the strict quantum-mechanical one. Similarly, the term 'orbital' can be understood in a broader sense. So far I have taken orbitals to be one-electron wave functions. The term 'orbital', though, is frequently used with a different meaning. With

each one-electron wave function comes a probability density function on real space for the electron's position. This is called electron density or charge density. This function in turn gives a region where the electron is likely to be found upon measurement, and it is this region that is then referred to as the orbital. Understood in this way, the concept of orbital is closely related to electron density; it is a region of high electron density. The only difference between the two is that in identifying a certain region of high electron density, one does not differentiate between electron densities within this region. When it carries this meaning, therefore, orbitals are experimental quantities.

It is in this sense that the authors of the by now infamous *Nature* paper spoke of having observed orbitals (Zuo *et al*. 1999). Although they do not say this explicitly in the publication itself, they do so in a response article (Spence *et al.* 2001, p. 87) to criticism by Scerri. In turn, Scerri (2002) replies that one should be cautious in using the term in the sense of 'electron density region' so as not to cause confusion. However, I believe Scerri underestimates how widespread this use of the term is. He charges Spence *et al.* for citing from the *New Shorter Oxford Dictionary* in defending their dual use of 'orbital', stating that there are "well-known distortions of scientific terms that occur in nontechnical dictionaries" (Scerri 2002, p. 310). Let me, however, give another citation: "Alternatively, the orbital can be thought of as an electric charge distribution." (Daintith 2004, p. 409) The citation is from the *Oxford Dictionary of Chemistry*. Indeed, in the balloon-like pictures of orbitals that one finds in any chemistry textbook, it is regions of electron density that are depicted, not wave functions.[3] It is in this light that Labarca and Lombardi assert that "in molecular chemistry the orbital of the hydrogen atom is understood as the region of space where the single electron of the atom is most likely to be located" (Labarca & Lombardi 2010, p. 154). This is perhaps a slight exaggeration, as a good many chemists will understand the dual meaning of the term. However, the point should be clear that the understanding of orbitals as regions of electron density is pervasive in chemistry.

Under this meaning of 'orbital', orbitals are observable – even in the strict sense, and even in many-electron systems. As I mentioned above, with each orbital is associated a certain charge density. When one models the wave function of a many-electron atom as a product of such orbitals, their charge densities add up, resulting in a total charge density of the atom – and remember that 'textbook orbitals' are regions of probability density, not wave functions, so this total charge density is a combination of 'textbook orbitals'. On the other hand, with the real, many-electron wave function of the atom comes the charge density that the atom in fact has. When the modeled and experimental charge densities are similar, it means that the first approximates the second to within a certain range, in which case it can be said to be observable.

To summarize the discussion up until this point, let me address the question that is the title of this paper: are orbitals observable? The answer, I have argued, depends on how the terms 'orbital' and 'observable' are understood. Therefore the question is, in its generality, not meaningful. Orbitals can be taken to be either one-electron wave functions or their corresponding regions of high probability density, and observability can be understood both in a strict and a loose sense. Only when 'orbital' is taken to mean 'one-electron wave function' and 'observable' is meant in the strict sense are orbitals not observable.

6. A breach between chemistry and quantum mechanics?

In this final section I consider the relationship between the two meanings of 'orbital' distinguished in the previous section. Labarca & Lombardi (2010) have argued that the conception of the term 'orbital' in chemistry gives rise to a conceptual discontinuity between chemistry and quantum mechanics. In chemistry, in line with the meaning of 'orbital' explained in section 5, electrons are seen as "individuals located in a region of space close to the nuclei" (Labarca & Lombardi 2010, p. 154). This would be in conflict with two aspects of quantum mechanics: non-individuality and non-locality.

In quantum mechanics, particles cannot have definite values for all observables at a certain point in time.[4] On the basis of this fact, French & Krause (2006) have argued that the notion of individual does not apply to quantum particles, as individuality is conferred by the definite properties that an entity has. In chemistry, on the other hand, Lombardi & Labarca maintain, electrons are individuals, so there is a discontinuity with quantum mechanics. However, I believe Labarca & Lombardi's view is incoherent. This is because they maintain that in chemistry as well, electrons do not have definite trajectories, *i.e.* no definite positions at all times. On French & Krause's argument this is at variance with the supposition that they are individuals. What is more, it is by now well-established that individuality is undermined by another aspect of quantum mechanics, *viz.* entanglement.[5] Therefore, assuming that electrons have positions does not offer a way out; one has to accept that electrons are not individuals, whether in quantum mechanics or in chemistry.

Does this mean that chemistry is 'false' because it regards electrons as individuals? I think that one has to concede that to the extent that chemists speak of electrons as individuals, what they say is indeed not literally true. To assess the exact implications of this for the ontological status of chemistry would require a detailed study of chemistry's commitment to electrons being

individuals, which is beyond the scope of this paper. Let me however provisionally remark that the view that electrons are individuals seems, in the first place, to concern the pragmatic understanding that working chemists have. Therefore, individualism about electrons in chemistry is not on a par with non-individualism in quantum mechanics, where it is an insight obtained from a purely philosophical analysis of the mathematical formalism. This is not to belittle chemists, but to acknowledge the fact that quantum mechanics is notoriously hard to comprehend while at the same time scientists are in need of concepts and mechanisms that explain.

The second aspect under which Labarca & Lombardi maintain there is a discontinuity between quantum mechanics and chemistry is (non-)locality. In quantum mechanics, because of quantum non-locality atoms and molecules are correlated with all systems with which they have interacted in the past. In chemistry, on the other hand, these correlations are suppressed, leading to a conception of a molecule as something that "exists separately and independently in the sense that it can consistently said to 'have' certain properties, whether or not it interacts with anything else" (Woolley as cited in Labarca & Lombardi 2010, p. 154). In this context they also mention the Born-Oppenheimer approximation, which, as Woolley and Sutcliffe have argued, introduces molecular structure into quantum mechanics without there being a justification for this in quantum mechanics (see for instance Woolley 1976, Woolley & Sutcliffe 1977).

There has been extensive literature stretching out over the past few decades discussing the coming about of classical behavior from quantum mechanics, in the context of chemistry mostly concerning molecular structure. What is important in the present context is that if there is indeed any kind of "conceptual breakdown" (Labarca & Lombardi 2010, p. 155), it appears *within* quantum mechanics, equally affecting the quantum-mechanical and chemical meaning of 'orbital'. The very idea of a one-electron wave function requires both suppression of all interactions except those with the nuclei and relatively fixed nuclear positions.[6] Approximations are therefore made within quantum mechanics, as a result of which the quantum-mechanical concept of an orbital arises. Whether or not these approximations lead to a conceptual breakdown is therefore irrelevant for the relation between the quantum-mechanical and chemical meanings of 'orbital'; both would come after the breakdown, so to say. Indeed, the two meanings are far from discontinuous. As I pointed out in section 5, the meaning of 'orbital' as a region of high probability density follows quite straightforwardly from its meaning as a wave function; it is obtained by squaring the wave function and subsequently identifying the region in which the electron is highly likely to be found. The two concepts are therefore continuous with one another.

Acknowledgements

Notes

[1]   Wave functions can furthermore differ in their phase factor, but in the case of stationary states, which are assumed in all discussion on the topic at hand, this is irrelevant.

[2]   Modeling the wave function of a many-electron atom as a product of *hydrogenic* orbitals amounts to ignoring all interactions between electrons. In the Hartree-Fock method, the interactions are dealt with, but only in an average way, by taking each electron to move in the main field of the other electrons.

[3]   As Wang & Schwarz (2000) have stressed, 'textbook orbitals', *i.e.* the graphic depictions of orbitals in textbooks, are not all too accurate representations of reality. In particular, orbitals are made 'slimmer' in regions where they overlap with other orbitals. This is for instance the case with the *p*-orbitals, which are depicted as being very narrow close to the nucleus, whereas in reality they are rather broad there, making for significant overlap with one another. However, this leaves unaffected the fact that textbook orbitals depict regions of probability density, albeit in a not so literal sense.

[4]   Labarca & Lombardi refer to this as 'contextuality'. The latter term, however, has a somewhat different meaning, *viz.* that in any hidden-variable extension of quantum mechanics, the definite properties that particles have cannot be intrinsic, but rather are dependent on the measurement context. Particles necessarily having indefinite properties is a facet of quantum mechanics itself, which is expressed in the uncertainty relations that obtain between non-commuting observables.

[5]   See Ladyman & Ross, pp. 132-40 for an overview of arguments surrounding the issue.

[6]   The motions of an electron in an atom are correlated with those of the nucleus, but the latter can be factored off. This allows for instance for the Hamiltonian of the hydrogen atom to be exactly solvable.

References

Daintith, J.: 2008, *Oxford Dictionary of Chemistry*, Oxford: Oxford University Press.

French, S. & Krause, D.: 2006, *Identity in physics: A historical, philosophical, and formal analysis*, Oxford: Oxford University Press.

Labarca, M. & Lombardi, O.: 2010, 'Why orbitals do not exist?', *Foundations of Chemistry*, **12**, 149-57.

Ladyman, J. & Ross, D.: 2007, *Every thing must go: Metaphysics naturalized*, Oxford: Oxford University Press.

Mulder, P.: 2010, 'On the alleged non-existence of orbitals', *Studies in History and Philosophy of Modern Physics*, **41**, 178-82.

Ostrovsky, V.N.: 2005, 'Towards a philosophy of approximations in the 'exact' sciences', *Hyle: International Journal for Philosophy of Chemistry*, **11**, 101-26.

Scerri, E.: 2000a, 'Have orbitals really been observed?', *Journal of Chemical Education*, **77**, 1492-4.

Scerri, E.: 2000b, 'The failure of reduction and how to resist the disunity of science in chemical education', *Science and Education*, **9**, 405-25.

Scerri, E.: 2001, 'The recently claimed observation of atomic orbitals and some related philosophical issues', *Philosophy of Science*, **68**, S76-S88.

Scerri, E.: 2002, 'Have orbitals really been observed?' (author reply), *Journal of Chemical Education*, **79**, 210.

Schwarz, W.H.E.: 2006, 'Measuring orbitals: Provocation or Reality?', *Angewandte Chemie International Edition*, **45**, 1508-17.

Spence, J.C.H.; O'Keeffe, M. & Zuo, J.M.: 2001, 'Have orbitals really been observed?', *Journal of Chemical Education*, **78**, 877.

Wang, S.G. & Schwarz, W.H.E.: 2000, 'On closed-shell interactions, polar covalences, d shell holes, and direct images of orbitals: The case of cuprite', *Angewandte Chemie International Edition*, **39**, 1757-62.

Woolley, R.G.: 1976, 'Quantum theory and molecular structure', *Advances in Physics*, **25**, 27-52.

Woolley, R.G. & Sutcliffe, B.T.: 1977, 'Molecular structure and the Born-Oppenheimer approximation', *Chemical Physics Letters*, **45**, 393-8.

Zuo, J.M.; Kim, M.; O'Keeffe, M. & Spence, J.C.H.: 1999, 'Direct observation of d-orbital holes and Cu-Cu bonding in Cu_2O', *Nature*, **401**, 49-52.

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