

## Everything in Context: Two Episodes Relating Orbitals and Language

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### Introduction

I came to the field of literature and science (henceforth abbreviated L&S), about 20 years ago, from a career as a practicing scientist - an inorganic chemist, to be precise - and most of my efforts to date could be said to reflect that origin, directed mainly towards interpreting literature from a scientist's viewpoint. These include analyses of specific works with substantial scientific content, such as Richard Powers's novel *The Gold Bug Variations* (Labinger 1995) and Tom Stoppard's play *Arcadia* (Labinger 1996), as well as more general survey articles (Labinger 2002, 2010).

The complementary angle - examining scientific issues from the perspective of literary studies - is reflected in a question that has been occasionally posed to me by some of my scientific colleagues: how, if at all, does my interest in L&S affect the way I think about and practice science? This essay, which is intended to address that question, was inspired by two (reasonably friendly) arguments I have engaged in within the last few years. They both center on the topic of orbitals and bonding in chemistry, which is perhaps the closest thing to a physics-related subject on which I can speak with any authority at all; and they can both be related to the role of language in scientific discourse, although in rather different ways. Hence both individually and jointly they seemed to comprise particularly appropriate subject matter for the conference on whose proceedings this monograph is based.

The question of how language affects scientific thought and practice has been a common topic for L&S commentators. While I haven't done any thorough survey, I think one can safely say that their dominant view is that scientists pay insufficient (or no) attention to that issue: that scientists believe, whether consciously or otherwise, that an individual's ability to grasp an idea and successfully communicate it to others does not have to be complicated by the language in which it is expressed. This is not to say that any scientist would advocate carelessness in language usage, but rather that the effort of finding appropriate language is not inherently problematic. Roald Hoffmann, a Nobel Laureate and chemist who has thought about and written on such matters extensively, sums up this attitude:

In science, we think that words are just an expedient for describing some inner truth, one that is perhaps ideally represented by a mathematical equation. Oh, the words matter, but they are not essential for science. (Hoffmann 2012, 39)

To illustrate further, here are two brief extracts from L&S commentaries. The first is from an essay by Kate Hayles, a leading L&S scholar, discussing a text by biologist and science popularizer Richard Dawkins:

Dawkins, a skillful rhetorician keenly aware of the value of a good story, nevertheless espouses what might be called the giftwrap model of language. This model sees language as a wrapper that one puts around an idea to present it to someone else. I wrap an idea in language, hand it to you, you unwrap it and take out the idea [...] For example, at the critical juncture where the narrator is switching the unit of selection from the individual to the gene, we find this assertion. "At times, gene language gets a bit tedious, and for brevity and vividness we shall lapse into metaphor. But we shall always keep a skeptical eye on our metaphors, to make sure they can be translated back into gene language if necessary." (Hayles 2001, 147)

and the second, from a book on L&S by Ira Livingston:

[B]oth scientists and humanists tend to overstate the independence of language from the world. Each begins by treating words and things as separate and then offers to connect them, though in rather different ways. Science, one might say, offers to nail words to things [...] Ideally, language is conceived as a space of pure, undistorted reference to (or representation of) the world, rather like the controlled conditions of a scientific experiment [...] One might even argue that an inability to see beyond the referential dimension of language is an asset for scientists, one that makes it easier to sustain belief in the scientific enterprise. (Livingston 2006, 8)

It is striking, and more than a little ironic in a reflexive sort of way, that to address scientists' practices - including the use of metaphoric language - these two commentators employ metaphors that are almost perfect opposites! Hayles's scientist thinks words are readily detached from ideas, whereas Livingston's scientist wants them to be firmly nailed in place. Nonetheless, these apparently diametric opposites actually point in the same direction. Dawkins allows that metaphoric language has its place, to liven up a story; but it is mere window dressing that can be discarded at any time, leaving behind the completely unambiguous (in Dawkins's mind) "gene language," which constitutes an example of Livingston's "pure, undistorted reference to the world." Clearly both Hayles and Livingston, like many other L&S scholars, are dubious (to say the least) about such a straightforward view of the role of language in science. Livingston *does* appear to allow that practicing scientists may benefit from such a limited view (much as some horses race better with blinkers on, perhaps?).

The connections between the two episodes I consider below are perhaps not immediately obvious. One shows an explicit example of a scientist's insistence on linguistic purity, while the other is more concerned with the relationship between language and pictorial representation. But I believe that both nicely illustrate, and support, what I take to be the L&S position summarized above: that scientific language does not - and should not - transcend features of "ordinary" language such as ambiguity, analogy and metaphor, and that better awareness of and appreciation of that fact by

scientists can be beneficial, particularly in the realm of education, by helping to focus on the goal of making scientific communication more contextually appropriate.

### Case Study 1: Can We “See” an Orbital?

The starting point for this first mini-debate was an article that appeared in the prestigious British journal *Nature*, reporting on an ultra-high resolution X-ray diffractometric study of cupric oxide (Zuo et al. 1999). X-ray diffractometry has been used to determine the structure of crystalline species since the 1910s, usually with the goal of mapping the atomic positions. However, since diffraction actually results from interactions of the X-rays with electrons, not nuclei, a study of sufficiently high quality can in effect “visualize” (that is, identify the location of) not just the atoms, but also the spatial distribution of electron density, both in bonds between atoms and surrounding the individual atoms themselves.

A brief reminder about atomic orbitals may be helpful. The concept, which dates back to Niels Bohr (in the 1910s, like X-ray diffraction), states that there is a set of mathematical functions that represent the spatial distribution of the electrons about an atom. Those functions can be converted into 2- or 3-dimensional pictorial representations; Figure 1 shows such a representation for a particular set of those, the so-called *d* orbitals. The authors of the *Nature* paper reported that their diffractometric study revealed patterns of electron density, centered around the copper sites in the crystal, that very closely resemble the calculated shape of the  $d_{z^2}$  orbitals:

The correspondence between our experimental map and the classical diagrams of  $d_{z^2}$  orbitals sketched in textbooks is striking. All our difference maps show strong non-spherical charge distributions around the copper atoms, with the characteristic shape of d orbitals. (Zuo et al. 1999, 51)

while the editors of the journal offered an even stronger claim of novelty and importance:

The classic textbook shape of electron orbitals has now been directly observed [...] For the first time the striking shape of some of the electron orbitals is revealed experimentally [...] The paper by Zuo et al. is remarkable because the quality of their charge-density maps allows, for the first time, a direct experimental ‘picture’ to be taken of the complex shape of the  $d_{z^2}$  orbital. (Humphreys 1999)

A number of equally or even more enthusiastic descriptions appeared in news sections of other journals and websites.

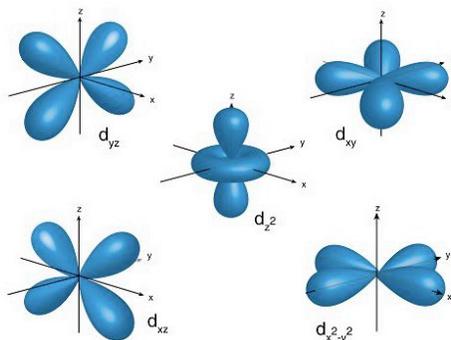


Figure 1. Images representing the spatial orientation of the five  $d$  orbitals.

Shortly thereafter a chemist, one who is also active in the field of philosophy of chemistry, objected strongly to these claims in an essay in the *Journal of Chemical Education* (Scerri 2000), as well as in a posting on a history of chemistry website (Scerri 1999). Even though it's not particularly my area of expertise, I found myself drawn into the ensuing online discussion.

The main point the chemical philosopher/philosophical chemist made was that the term “orbitals” in no sense refers to any real physical objects. It refers only, in his view, to the mathematical wave functions calculated by quantum mechanics - even those are strictly valid only for the hydrogen atom, not for a multielectron atom - and hence orbitals are inherently not observable:

Let me now turn to the theoretical status and limitations of orbitals and why orbitals cannot possibly be observed. Atomic orbitals are mathematical constructs and strictly speaking are only genuine wave functions in one-electron systems such as the hydrogen atom. In many-electron atoms orbitals serve as a useful approximation [...] The orbital approximation is the basis of a great deal of the work conducted in quantum chemistry, but here it is recognized that orbitals are mathematical constructs and do not possess any independent physical status. (Scerri 2000, 1492)

I freely concede the importance of framing a discussion in terms of a very rigorous definition. But everything depends upon who is having the discussion! The meaning of “orbital” in the context of the quantum mechanical issues indicated in the above quote is unquestionably a topic of interest for philosophers of chemistry, who are concerned with the fundamental underpinnings of the science. One *might* argue further that practitioners of quantum mechanics should be aware of these issues too, although I doubt whether many of those actively engaged in computational chemistry pay much explicit attention to the strict meaning of “orbital,” or need to.

But Scerri carries his argument far beyond formal philosophical concerns to address pedagogical issues - as implied by his choice of venue, a journal devoted to chemical education. He urges educators strictly to observe his restricted usage of the word “orbitals,” even at the most basic levels:

Orbitals are part of the lingua franca of chemistry. They represent one of chemistry’s major paradigms, to use a much abused term. Surely it is essential that claims to having arrived at a new understanding of such a crucially important educational concept should be subjected to close scrutiny. It is also essential for chemical educators at all levels to take note of these developments in order to adjust their teaching accordingly if such adjustments are necessary. At the very least, educators should take some time to reflect on the meaning of such an important concept as an atomic orbital when it is claimed that, contrary to previous beliefs, they have now been observed for the first time [...] Just as the coordinate system of x, y, and z used to describe any particular experiment in classical physics is unobservable, so too atomic orbitals are completely unobservable even in principle. What can be observed, and frequently is observed in experiments, is electron density [...] My advice to chemistry educators is to avoid being seduced by the recent reports and not to revise their long-held view that atomic orbitals are just mathematical constructs. (Scerri 2000)

I completely disagree with this proclamation, whether it is meant to be taken as prescriptive or descriptive. Students, especially at elementary levels, will find the visual/mental picture of how electrons are distributed in space that is commonly associated with the concept of orbitals - which determines chemical bonding and thus molecular structure - *much* more valuable than any linguistic purification. It is certainly true that one observes electron density, not some abstract outline defined by a mathematical function. But what pedagogical purpose, outside of philosophy, would be served by admonishing a student, who is perhaps trying to account for the geometry of a molecule in terms of the spatial disposition and shape of orbitals, that no, you shouldn’t be talking about the orbital, but just the electron density? (If we do need a term that very precisely means the mathematical construct and nothing else, we have one: “wave function.”)

I also seriously doubt his claim that orbitals are really viewed as “just mathematical constructs” by many educators; I would wager a large sum that very few pay much if any attention to such linguistic niceties while teaching undergraduate students. (Figure 2 shows two important figures in 20<sup>th</sup>-century inorganic chemistry who apparently see the value of allowing orbitals to be contemplated as physical objects.)



Figure 2. Two leading inorganic chemists, Fred Basolo (left) and Ralph Pearson, manipulating three-dimensional models of  $d$  orbitals. Photo courtesy of Ralph Pearson.

Perhaps the most extreme statement of the position Scerri is staking out appeared not in the article, but in the online discussion:

Orbitals are mathematical constructs. In modern theory they are merely basis sets or a form of coordinate system used to express the wavefunction of any physical system. The claim that orbitals have been observed is tantamount to claiming that the x, y or z axis has been observed in any experiment in classical physics for example. What has been observed in the recent experiments is electron density. Any similarity to textbook  $d$  orbitals is either coincidental or due to somehow feeding  $d$  orbitals into the calculation which extracts the image. (Scerri 1999)

This comes across as a much stronger statement than just an argument against conflating the terms “orbital” and “electron density.” As I read it, he claims that the reported observations *can't be real* - that the similarity of the observed electron density distribution and the mathematical shape of the orbitals must be coincidental and/or artifactual. Why? Simply because if they *were* real, that would contradict his restricted usage of the word “orbital!”

I posted these thoughts on the website:

[Dr. Scerri's comments] seem to break into two distinct parts - the first, that observing patterns of electron density that match calculations does not mean we're actually seeing entities that we could call orbitals, and the second, that there is no significance to any such match - either it's an artifact of data processing, or a

coincidence. I can see a point to the first part, but I think it's more semantic than anything else - the term orbital certainly *does* refer to a mathematical construct, but if there are in fact these regions of electron density is it wrong to use the term to refer to them as well? (Should I look up in the sky and say, "Those aren't clouds I see, just regions of higher water vapor density"?) Maybe in some ideal philosopher's world every term has one and only one exact meaning, but that isn't the world we live in. As for the second part, for all I know (nothing) about the details of the experiment the patterns *could* be artifactual, but the fact that Eric also offers an alternative (coincidence) suggests that he doesn't have any particular grounds for proposing it; and falling back on coincidence to explain away an apparent similarity between observation and prediction suggests commitment to a philosophical position that is so strong as to rule out the possibility of an experiment that might shake it. (Labinger 1999)

and got this response:

I thank Dr. Labinger for his comments but would like to remind him that the attribution of a specific term to a particular entity is actually a form of scientific practice and not one solely confined to philosophers [...] Could it be that Dr. Labinger's increasingly public forays into the world of "Science and Literature" have led him to be far more liberal with language than he would have been in his more scientific past? (Scerri 1999)

Note how much this sounds like Livingstone: "nailing a word to a thing." My position (which, for the record, was no less liberal in my "more scientific past" before I was corrupted by "forays into the world of Science and Literature") is that trying to prevent a word such as "orbital" from referring to more than one thing - both a rigorous mathematical definition and a somewhat metaphorical but common physically real usage - is a hopeless project. Educators and students on all levels use the terms both ways and don't fret over it. Indeed, in most contexts such multiple reference is not just harmless, but productive: metaphoric usage in science encourages students and professionals alike to make useful connections between different concepts, and thus is both endemic and essential. That point was emphasized, with particular reference to atoms and orbitals, in Ted Brown's excellent discussion of metaphor in science:

[A]ny model we might use to characterize the atom is metaphorical, whether it be that of a billiard ball [...] or a densely mathematical description based on quantum theory [...] We don't ever "see" atoms [...] What we see are constructs that at their best represent reliable models of reality, with sufficient verisimilitude to serve as productive metaphors. They facilitate correlations, predictions, and interpretations of other data and stimulate the creative design of new experiments. That is all we can hope for. (Brown 2003, 99)

Case Study 2: Should We Draw a Bond? Who's Asking?



The molecule at issue in this argument,  $[\text{CpFe}(\text{CO})_2]_2$  (where Cp is an abbreviation for cyclopentadienyl, the  $\text{C}_5\text{H}_5$  group), comes from a class of compounds known as metal carbonyls, containing metal atoms and carbon monoxide molecules; much of the early work that established this field of research was carried out by Walter Hieber at the Technische Hochschule München starting in the 1930s. This particular example was first prepared (at Harvard: my own PhD institution!) and structurally characterized in the 1950s, and (as the above quote indicates) has virtually universally (in research and review articles as well as textbooks) been depicted in the VB mode of representation as shown on the left side of Figure 4, *with* an explicit bond drawn between the two Fe centers: a metal-metal (M-M) bond.

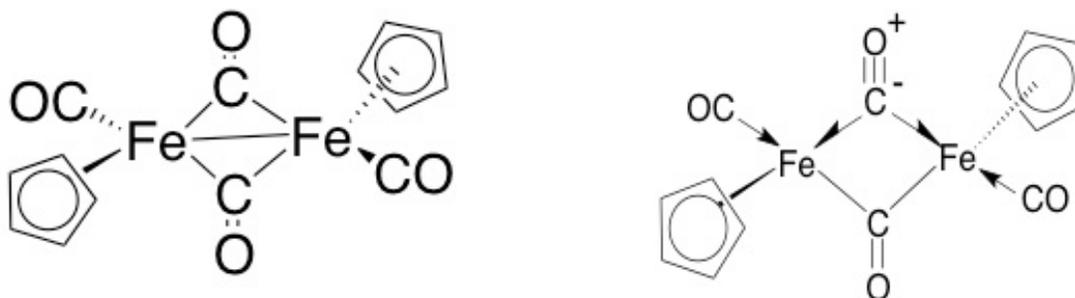


Figure 5. Photochemical cleavage of dimeric metal carbonyl complexes.

In contrast, Green et al. call the inclusion of an M-M bond a misrepresentation. Why? Because MO calculations do not show any significant electron density along the Fe-Fe axis, and therefore they feel the VB representation should not show a line there. Instead they draw the molecule as shown on the right side of Figure 4 (Green et al. 2012). (The detailed implications of their representation are complex and need not be considered here). My objection to their position is that it, in turn, misrepresents (or fails to represent at all) many features of the molecule that are arguably at least as important as the precise localization of electrons, especially its reactivity - which after all is the main thing that chemistry is all about! In particular, drawing a line between two atoms to represent a two-electron bond implies that at least in principle the bond could be split symmetrically to generate two odd-electron fragments. Indeed, as shown in Figure 5, under irradiation with light,  $[\text{CpFe}(\text{CO})_2]_2$  undergoes just such a fragmentation, as do other dimeric metal carbonyls. The latter clearly have a metal-metal bond: there is nothing else to hold them together! These compounds behave entirely analogously, and including the bond in the representation of  $[\text{CpFe}(\text{CO})_2]_2$  foregrounds that pattern of reactivity, while the alternate representation, without the bond, conceals it.

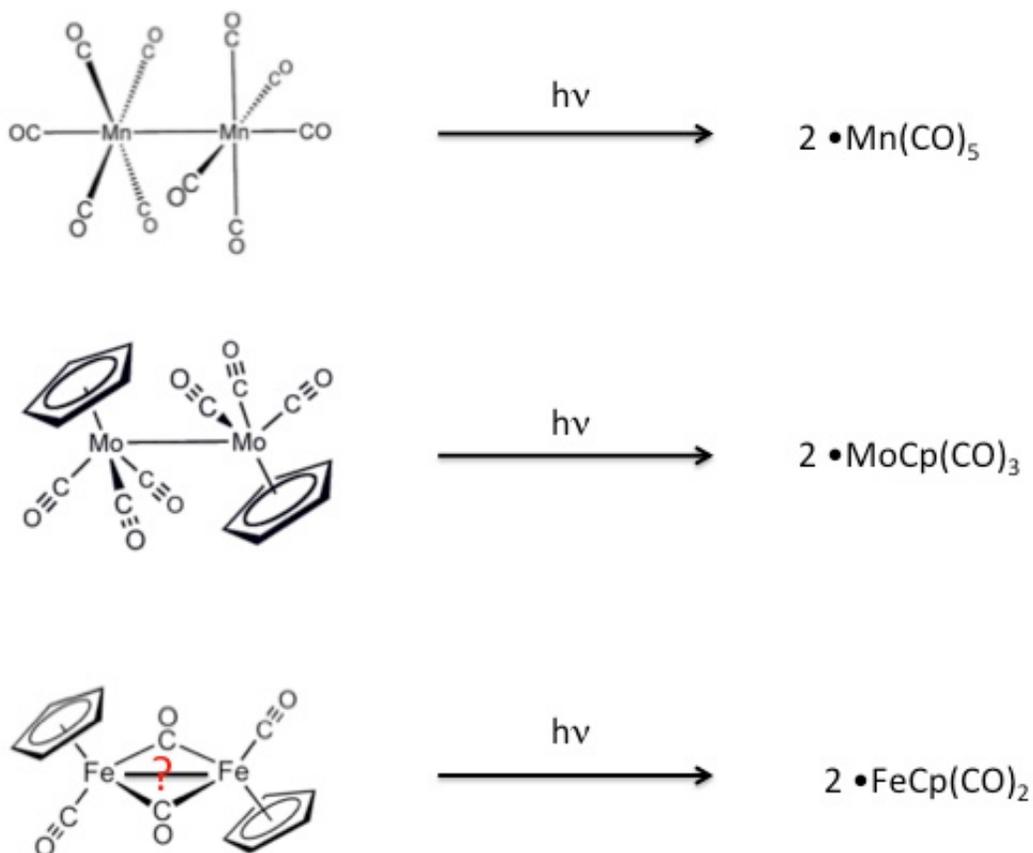


Figure 5. Photochemical cleavage of dimeric metal carbonyl complexes.

Arguments can thus be made for either of the alternative VB representations in Figure 4. Can we decide which is better? I think the answer must depend upon which aspect(s) of the molecular description are most important to us. If the distribution of electron density is of prime importance, then the no-bond version might be considered a more accurate depiction. But, as noted above, we only know that distribution by means of an MO calculation, so an MO representation would seem to be much more appropriate in that case. Several different forms of such representations are shown in Figure 6. They are not so readily amenable to visualization, are they? Those of us who are not completely comfortable with these highly mathematical representations would prefer to convert them to a more easily grasped pictorial (VB) form; and as we've seen (Figure 4), we have (at least) two different ways to do that. So the question of which representation is better becomes a question of how best to effect that conversion.

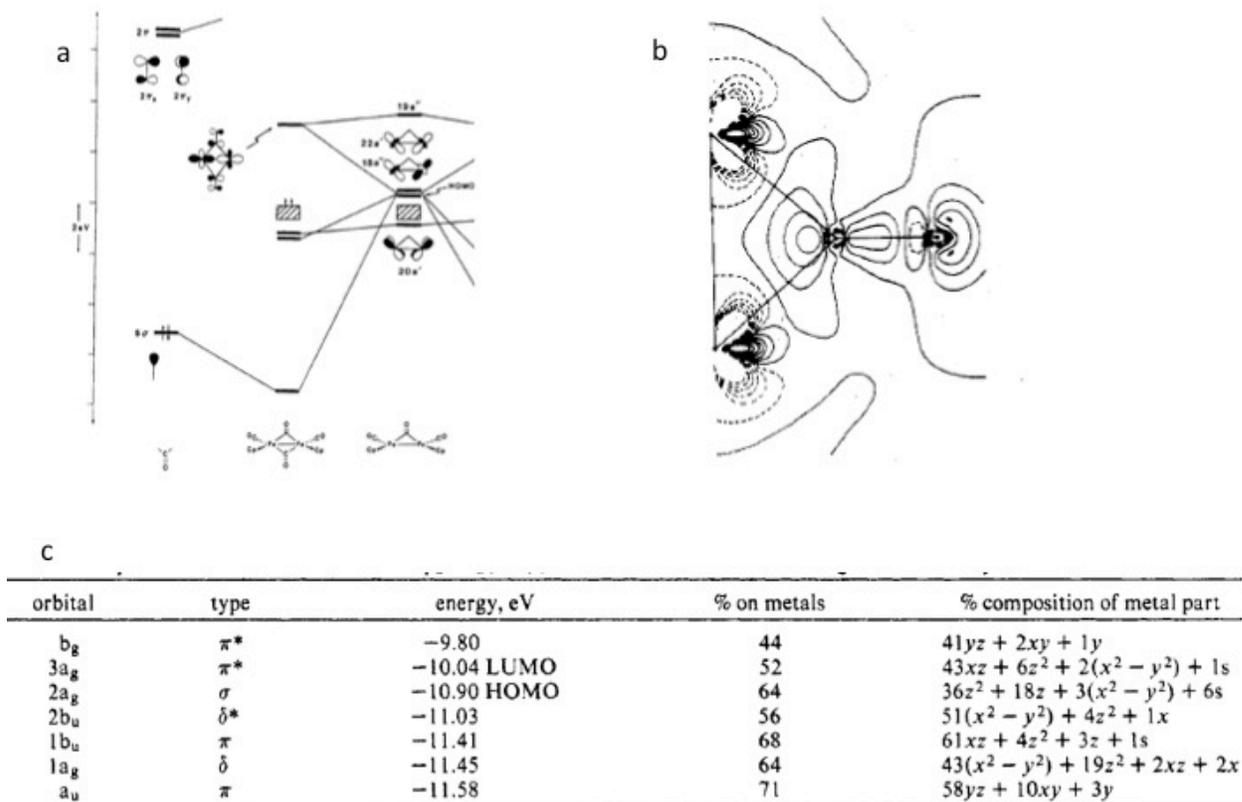


Figure 6. Three different MO representations of dimeric metal carbonyl complexes. Reprinted from a) B. E. Bursten, R. H. Cayton, *J. Am. Chem. Soc.* 108 (1986) 8241-8249; b) M. Bénard, *Inorg. Chem.* 18 (1979) 2782-2785; c) E. D. Jemmis, A. R. Pinhas, R. Hoffmann, *J. Am. Chem. Soc.* 102 (1980) 2576-2585. Copyright American Chemical Society.

This is where literature (finally!) comes in. Galileo famously proclaimed that “the book of nature is written in the language of mathematics” (more or less: this is the most common, but not the only possible, English version of the Italian original). Not all of us are perfectly fluent in the language of mathematics! I propose that we should think about VB and MO as two different languages that we use to talk about molecular structure, and recognize that it is often necessary to “translate” from one to the other. This seems to me a highly useful analogy, because the process of converting MO to VB raises the same sorts of issues that are common in literary translation. And literary translation is almost *never* straightforward: there are always choices to be made.

As it happens, a few years ago I was present at a panel on literary translation, at which one of the panelists - a translator from Italian – discussed several recent translations of Dante’s *Divine Comedy*. Afterwards I asked him what he thought of the (much older) version I knew from my college days, and was rather taken aback when he proclaimed it *completely unacceptable!* Why? Here are the first couple of stanzas of the original Italian and the translation in question, in which the fatal deficiency is already apparent:

Nel mezzo del cammin di nostra vita  
mi ritrovai per una selva oscura,  
ché la diritta via era smarrita.

Ahi quanto a dir qual era è cosa dura  
esta selva selvaggia e aspra e forte  
che nel pensier rinnova la paura!

(Dante Alighieri 1317)

Midway in our life's journey, I went astray  
from the straight road and woke to find myself  
alone in a dark wood. How shall I say

What wood that was! I never saw so drear  
so rank, so arduous a wilderness!  
Its very memory gives a shape to fear.

(Ciardi 1954, 28)

The panelist's sole objection arose from Ciardi's choice not to follow the exact rhyme scheme Dante devised for the Comedy, called *terza rima*: the first and third line of each stanza rhyme with each other and the second line of the previous stanza (ABA BCB CDC ...). As can be seen, Ciardi doesn't *quite* manage that. In his translation the first and third lines of each stanza do rhyme with each other, but not with the second line of the previous stanza (ABA CDC EFE ...). For the panelist, that choice was enough to invalidate the whole translation.

There are of course many criteria one might use to assess a translation - especially of verse. They range from obvious ones such as faithful representation of meaning, rhyme, meter, etc.; down to much more subtle aspects, such as keeping content correlated with position. (Note that Ciardi doesn't do that either: the first half of the first line of the second stanza in the original is transposed to the first stanza in the translation. Should we care?) To disqualify it on the grounds of just one - any one - is to make an extremely strong value judgment about the relative importance of those criteria.

Furthermore, considering how impoverished English is in rhyming opportunities compared to Italian, it's far from clear to me that rhyming *should* be the number one criterion. In fact, according to Wikipedia (2014) there have been many more than 100 translations of the *Commedia* into English over the years, only about a quarter of which even try to employ *terza rima*. Here are a couple of examples. The first (a recent one) is in strict *terza rima*, but completely abandons Dante's regular meter; the second (a 19<sup>th</sup> century version by Longfellow) is entirely unrhymed, but fairly faithful to the rhythm:

In the middle of our life's way  
I found myself in a wood so dark  
That I couldn't tell where the straight path lay.

Oh how hard a thing it is to embark  
Upon the story of that savage wood,  
For the memory shudders me with fear so stark  
(Zimmerman 2003)

Midway upon the journey of our life  
I found myself within a forest dark,  
For the straightforward pathway had been lost.

Ah me! how hard a thing it is to say  
What was this forest savage, rough, and stern,  
Which in the very thought renews the fear.  
(Longfellow 1865)

Which should we prefer? I happen to like the second – it sounds much better to me - but I certainly wouldn't pretend to have an argument that could convince everyone to agree with me. Maybe we should abandon *both* rhyme and rhythm as top priorities in favor of a hyper-literal rendering of the meaning? That was argued by Nabokov in the preface to his translation of *Eugene Onegin*:

In transposing *Eugene Onegin* from Pushkin's Russian into my English I have sacrificed to completeness of meaning every formal element save the iambic rhythm [...] in the few cases in which the iambic measure demanded a pinching or padding of sense, without a qualm I immolated rhythm to reason. In fact, to my ideal of literalism I sacrificed everything (elegance, euphony, clarity, good taste, modern usage, and even grammar) that the dainty mimic prizes higher than truth. (Nabokov 1964)

but his position, I believe, received little support from translators and readers alike.

Issues such as these seem to me closely akin to those that arise in deciding how best to portray a molecular structure. How shall I “translate” the mathematical representation of my molecule into a pictorial representation? It really depends on who is asking - that is, on what aspects I am most concerned with portraying. In Figure 4 the with-bond version on the left tells us about reactivity, while the no-bond version may more accurately locate electron density. Different people can quite legitimately have different preferences, as they can for translations. What is to be avoided, in my opinion, is dogmatism: one should *not* proclaim one or the other a “misrepresentation,” just as one should not proclaim a translation unacceptable because of a choice that doesn't happen to agree with one's needs or preferences.

## Conclusion

I believe that these two case studies, highly specialized and limited in scope though they may be, are quite relevant to much more general considerations of the role of language in science. I would emphasize three points: 1) The polysemous, metaphor-laden nature of language is productive in science just as in all realms of communication; it is by no means something that we should try to purify out of scientific discourse. 2) The problematics of translation between languages apply to science just as they do to literature. 3) Most importantly, keeping those considerations from literature somewhere near the forefront of one's mind can have a significant and beneficial impact on scientific practice, even in such a "hard" scientific area as physical chemistry. As two thoughtful chemists have expressed it:

[T]here is no single correct analysis of the complex entities of chemistry expressed in a single adequate language, as various reductionist scripts require; and yet the multiplicity and multivocality of the sciences...do not preclude but in many ways enhance their reasonableness and success [...] We understand the reality whose independence we honor as requiring scientific methods which are not univocal and reductionist precisely because reality is multifarious, surprising, and infinitely rich. (Grosholz and Hoffmann 2012, 223)

Surely, in such a reality, literature and science should not be separate pursuits; indeed, they have great potential for being mutually supportive.

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