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A critique of Weisberg's view on the periodic table and some speculations on the nature of classifications

Eric R. Scerri

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Abstract This article carefully analyzes a recent paper by Weisberg in which it is claimed that when Mendeleev discovered the periodic table he was not working as a modeler but instead as a theorist. I argue that Weisberg is mistaken in several respects and that the periodic table should be regarded as a classification, not as a theory. In the second part of the article an attempt is made to elevate the status of classifications by suggesting that they provide a form of 'side-ways explanation'.

Keywords Mendeleev · Periodic table · Theory · Classification · Explanation · Models · Shapere

Comments on Weisberg's "Who is a modeler?"

In a paper published in 2007, Michael Weisberg sets out to answer the question of "who is a modeler?" (Weisberg 2008). His study presents a contrast between the work of Volterra's mathematical approach to the question of why there was an unusual shortage of fish in the Adriatic Sea shortly after the end of the First World War and Mendeleev's discovery of the periodic system in 1869. Weisberg claims that Volterra's work is a good example of scientific modeling and consequently that Volterra can definitely be said to be a modeler.

Weisberg then considers Mendeleev's discovery of the periodic system, and the subsequent use that Mendeleev made of his discovery, in order to argue that this was not an example of scientific modeling. Rather than being a modeler, Weisberg claims that

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E. R. Scerri (✉)
Department of Chemistry and Biochemistry, U.C.L.A., 607 Charles Young Drive East, Los Angeles, CA 90095, USA
e-mail: scerri@chem.ucla.edu

"…Mendeleev is a theorist", contrary to the account provided by Shapere among others (Shapere 1977).

In my own response I will have little to say about Volterra except to agree with Weisberg's assessment that this study was a good example of modeling. My critique will focus on the work of Mendeleev as described by Weisberg. Moreover, my concern will not be so much with whether or not Mendeleev was a modeler. It so happens that I also agree with Weisberg in denying that Mendeleev was acting as a modeler. My disagreement is with Weisberg's claim that, rather than being a modeler, Mendeleev was functioning as a theorist and that his periodic system can be regarded as a theory rather than as a model. My own suggestion is that Mendeleev provided a classification rather than a model or theory. Before returning to expand on this suggestion I would like to analyze Weisberg's statement about Mendeleev in some detail.

Mendeleev's predictions

Weisberg writes,

> Similarly, it has been argued that Mendeleev articulated an important classification system, but not a theory. For example, Shapere claimed that what Mendeleev discovered was an *ordered domain* and that '[o]rderings of domains are themselves suggestive of several different sorts of lines of further research' but not themselves theories (Shapere [1977], p. 534). I believe this view to be mistaken for several reasons. The first reason involves the remarkable predictions that Mendeleev was able to make on the basis of his Periodic System (Weisberg 2008, p. 213).

Weisberg continues by citing detailed evidence to show that three of Mendeleev's predictions, those of gallium, scandium and germanium were especially accurate.

Weisberg then writes,

> Mendeleev's predictions might look like trivial exercises, making inferences about missing 'books on the shelf' or filling empty slots. This underestimates the significance of the achievement: Mendeleev had no empirical knowledge that there were any empty slots to be filled (Weisberg 2008, p. 214).

I want to begin by exploring this last statement. I believe that, quite to the contrary, Mendeleev's basis for believing that there were slots remaining to be filled in the periodic table were *entirely* based on empiricism. After accommodating the 63 known elements into a two-dimensional grid it became glaringly obvious to Mendeleev that gaps remained to be filled.

Even if one considers just a one-dimensional ordering of the elements according to increasing values of atomic weights it is clear that gaps exist between zinc (65) and arsenic (75), as shown in Fig. 1, given that typical gaps between two consecutive elements involve lower atomic weight differences.[1] The necessity for such gaps becomes even clearer because of the second dimension of the periodic table, which is chemical similarity. This presents a further constraint, namely that other elements cannot be 'pushed' from side to side to avoid such gaps. That is to say, although there is a clear gap between the atomic weight values of zinc and arsenic, Mendeleev was not at liberty to move arsenic and

[1] Similarly the large gap in atomic weights between calcium (40) and titanium (48) led Mendeleev quite naturally to postulate the existence of an intermediate element to which he attributed the atomic weight of 44 as also seem in Fig. 1.

MENDELÉEFF'S TABLE I.—1871.

Series.	GROUP I. R_2O.	GROUP II. RO.	GROUP III. R_2O_3.	GROUP IV. RH_4. RO_2.	GROUP V. RH_3. R_2O_5.	GROUP VI. RH_2. RO_3.	GROUP VII. RH. R_2O_7.	GROUP VIII. RO_4.
1	H=1							
2	Li=7	Be=9.4	B=11	C=12	N=14	O=16	F=19	
3	Na=23	Mg=24	Al=27.3	Si=28	P=31	S=32	Cl=35.5	
4	K=39	Ca=40	—=44	Ti=48	V=51	Cr=52	Mn=55	Fe=56, Co=59 Ni=59, Cu=63
5	(Cu=63)	Zn=65	—=68	—=72	As=75	Se=78	Br=80	
6	Rb=85	Sr=87	? Y=88	Zr=90	Nb=94	Mo=96	—=100	Ru=104, Rh=104 Pd=106, Ag=108
7	(Ag=108)	Cd=112	In=113	Sn=118	Sb=122	Te=125	I=127	
8	Cs=133	Ba=137	? Di=138	? Ce=140	....	....	....	....
9	....	....	....	....	....	....	...	....
10	....	....	? Er=178	? La=180	Ta=182	W=184	....	Os=195, Ir=197 Pt=198, Au=199
11	(Au=199)	Hg=200	Tl=204	Pb=207	Bi=208	....	....	
12	....	....	....	Th=231	....	U=240	....	....

Fig. 1 Mendeleev's periodic system of 1871 accompanying the article in which he made detailed predictions on the properties of as yet undiscovered elements with atomic weights of 44, 68 and 72

selenium to the left, since doing so would destroy the vertical analogy between the chemical behavior of arsenic with phosphorus on one hand and selenium with sulfur on the other.[2]

I turn to the following passage from Weisberg's paper,

> His [Mendeleev's] task was thus not as simple as interpolating the properties of unknown elements on the basis of known elements. He first needed to hypothesize the existence of the missing elements by analyzing the theoretical structure he had created. Then he was able to use the trends posited by the Periodic Table to make predictions about the properties of the 'missing' elements. This prediction was a theoretical, not merely classificatory, achievement (Weisberg 2008, p. 214).

Unfortunately, Weisberg says nothing to support his claim that Mendeleev examined "the theoretical structure that he had created". This claim would need to be motivated by some reference to Mendeleev's own writings, although I do not think this will be possible from my knowledge of the Russian chemist's writings. I must therefore disagree with Weisberg and insist that Mendeleev's predictions were not a theoretical but a classificatory achievement. Nor do I regard the latter to be an achievement of the "merely" variety as Weisberg seems to suppose it would have been. I am interested in the fact that Weisberg seems to want to devalue the worth of classifications, an issue that I will return to in the second half of this article.

Returning to Weisberg's words,

[2] If the reader is wondering why authors before Mendeleev did not leave gaps and make predictions the answer is that several of them *did* do so contrary to the popular myth that only Mendeleev did (Scerri 2007). The fact remains however, that Mendeleev capitalized on gaps and predictions to a greater degree than the other discoverers of the periodic system.

> While I believe that Mendeleev's remarkable predictions are one sign that he had developed an important theoretical structure, this view is not uncontroversial (Weisberg 2008, p. 214).

Weisberg proceeds to a brief mention of the views of philosopher Dudley Shapere who is one of the few authors to have analyzed the philosophical status of the periodic system and who came to the conclusion that it was not of a theoretical nature but preferred to refer to it as a 'domain'. It might be added that no commentator from philosophy, history or the hard sciences has to my knowledge ever concluded that the periodic table should be regarded as a theory. Rather than being "not uncontroversial", I regard Weisberg's suggestion as *highly* controversial and one that has only ever been made by him. I agree with Shapere who writes that the fact that the periodic table led Mendeleev to make predictions does not render the periodic table a theory.

Returning to Weisberg's paper we find,

> Even if we grant Shapere's argument that prediction alone was not enough to make Mendeleev a theorist, we should note that Mendeleev *did* give explanations on the basis of his periodic system (Weisberg 2008, p. 214).

The first explanation, presumably of a theoretical nature, that Weisberg offers on behalf of Mendeleev is the following,

> One example of a trend Mendeleev explained using his system involves the oxides of the main group elements. For example, Mendeleev showed that the quantity of oxygen in the oxides was a periodic function of the element's group (column) on the Periodic Table. Group I elements (the alkali metals) formed oxides with structure R_2O, where R is a generic symbol of element. Group II elements (the alkaline earth metals) formed oxides as R_2O_2 and so on up to the halogens (R_2O_7) (Gordin [2004], p. 31). This can be accounted for by the Periodic Law, but would have remained mysterious otherwise (Weisberg 2008, pp. 214–215).

However, one can still argue that the formulas of these oxides remain mysterious even after they have been subsumed into the periodic law. There is nothing explanatory in the periodic law, which is a statement that the properties of the elements are a periodic function of their atomic weights.[3]

As I see it, this appeal to the formulas of oxides of the elements represents a rather circular argument and not the kind of deductive argument that Weisberg should be providing in order to ground his claim that Mendeleev gave theoretical predictions concerning the elements. I am trying to point out that if anything Mendeleev was led to constructing the periodic system because of the pattern of formulas for the highest oxides of the elements. Nowhere, however, is Mendeleev providing a deeper explanation for the occurrence of these formulas. All that one might say is that the periodic system is *consistent* with these patterns of oxide formulas, and not surprisingly since this kind of information was used to arrive at the periodic system. For an explanation to count as being theoretical it should be couched at a deeper or more abstract level. If the explanation is nothing but the periodic table which was partly devised to account for the data in question, I fail to see how it may be providing a theoretical account of that very data.

[3] Mendeleev wrongly believed that it was something about the property of weight that explained the periodic table. Mendeleev's periodic law was therefore not explanatory, even if modern accounts of the periodic law in terms of quantum physics do offer a causal explanation for the periodicity in elemental properties.

If the explanation is provided by the periodic *law*, something that Weisberg mentions in passing, this is already more convincing since there is a sense at least of a deduction from a more abstract level (Gordin 2004). In appealing to Gordin, Michael Weisberg seems to be equating scientific laws with theories. How else would the explanatory role of the periodic law, if indeed it had one, count in favor of the role of the periodic system qua theory?

But it should be noted that Gordin's detailed historical study of Mendeleev's work is concerned with how the periodic system gradually changed from a classification into the periodic law, at least as it was regarded by Mendeleev himself. It should also be realized that for all its historical value the question of whether Mendeleev believed that his system had become a law is of somewhat secondary value as Gordin duly notes. The more pressing question should be whether in fact it can be justly regarded as a scientific law and whether it provided any explanatory value over and above a phenomenological law that summarizes the observed regularities among the elements. But the true explanation for the occurrence of the various formulas, if anything, lies in the concept of valence of elements, not at the level of the periodic table, or indeed the periodic law, that summarizes the facts about formulas.

The putative theoretical explanation of the formulas of oxides of elements, that has just been discussed, would seem to be Weisberg's second of his claimed "many reasons" for believing that the periodic table should be regarded as a theory. I now move on to what appears to be his third reason in the course of which Weisberg already weakens his own position considerably,

> Although accounting for this trend did not give Mendeleev causal or mechanistic knowledge about the formation of oxides, it certainly allowed him to make contrastive explanations about the reactivity of different metals. It also brought a number of things previously accepted as brute facts into systematic unity. By the lights of many philosophers of science, these achievements count as explanatory ones and hence by Shapere's own standard, Mendeleev's system is a theory (Weisberg 2008, p. 215).

It would have been helpful if Weisberg had cited one or two examples of Mendeleev's giving "contrastive explanations" so that the reader might have had the opportunity to weigh up this further argument in favor of the periodic table being regarded as theoretically explanatory. Secondly, the fact that the periodic table brought about a great deal of unity, Weisberg's fourth reason, is quite undeniable but this does not necessarily imply that the periodic table was functioning as a theory. A system of classification, which the periodic table is usually regarded as being, is also quite capable of bringing about unification.

The final sentence in the above quotation is rather mysterious because even if other philosophers may regard the giving of contrastive explanations and unification to a body of knowledge as a mark of theoretical explanation, the simple fact is that Shapere is not among them, as he carefully points out in the course of his denial of a theoretical status to the periodic table (Shapere 1977). Providing explanations and unification are not the criteria which Shapere believes constitute a theory.

Let me move to the fifth and final reason why Weisberg seems to believe that the periodic table should be regarded as a theory and Mendeleev as a theorist.

> As Shapere further argued, Mendeleev's discovery of periodicity gives us a new fact that requires a further theoretical explanation. Periodicity is a phenomenon which is still not completely derivable from quantum mechanics (Scerri [2007]), although using semi-empirical methods, the trend can be derived (Levine [1991]). This is

another reason that some, including Shapere, have questioned whether the periodic system is a theory or that Mendeleev made a theoretical, as opposed to a classificatory, contribution to chemistry (Weisberg 2008, p. 215).

I think we should beware of conflating two distinct ideas, namely explanation of the periodic table and explanation from quantum mechanics. Moreover, Shapere's highly nuanced account seems to be treated far too briefly by in the above quotation. Weisberg seems to be willing to connect Shapere's account to the more recently discussed failure to fully reduce the periodic system to quantum mechanics that some authors have analyzed in the literature (Scerri 2007; Schwarz 2007). But Shapere's concern, as correctly reported in the first line of Weisberg's passage, is just that the periodic table, when first discovered, was in need of a theoretical explanation. Shapere continues by analyzing what kind of theoretical explanation was suggested and concludes that it was an atomistic explanation that was gradually taking shape in related fields such as statistical thermodynamics and spectroscopy. Nowhere does Shapere go on to discuss the eventual quantum mechanical explanation for the periodic system and certainly not the degree to which this explanation is successful or not.

So when Weisberg says in the last line of the previous quotation that the still current failure to fully explain the periodic system from quantum mechanics is another reason for Shapers' doubting the theoretical status of the periodic system he is erring for two reasons. First of all, Shapere did not comment on whether the periodic system had actually been explained from physics. Secondly Weisberg's analysis sets up a straw man position which does not necessitate the criticism that he proceeds to give when writing,

While it is true that Mendeleev's periodic system is in need of further theoretical explanation, the same could be said of any theory that is not a fundamental physical one. Everyone accepts classical thermodynamics as a theory, yet many would argue that core parts of it such as the Second Law themselves cry out for deeper theoretical explanation. Theories allow us to unify, make predictions, and frame explanations. It should not be required that they need no further explanation themselves (Weisberg 2008, p. 215).

Shapere is not asking whether the periodic system, qua theory, is fully explained by yet a deeper theory for the simple reason that he does not believe it to be a theory in the first place. Furthermore, it might even be said that if the periodic system did in fact have the nature of a theory it would have rendered its explanation by quantum mechanics a good deal easier. But if the periodic table's is regarded as a classification, this helps to explain why it is not even in a suitable form for reduction by a deeper theory. Indeed this may be one of the reasons why the reduction of the periodic system is problematic whereas the reduction of legitimate theories to deeper theories tends to be a more straightforward endeavor.

Weisberg concludes his section on the periodic table by saying,

Mendeleev's system clearly unifies, allows us to make predictions, and can serve as the basis for chemical explanations. Thus it ought to be considered a theory, and Mendeleev considered a theorist (Weisberg 2008, p. 215).

While I agree that Mendeleev's system unifies, classifies and allows us to make predictions, this is not sufficient to conclude that it should be considered as a theory. What is lacking is the fourth quality that Weisberg is attributing to the periodic system, namely the ability to serve as the basis for chemical explanations. If it does give any form of explanation it is not of the deductive theoretical kind that Weisberg is alluding to but more in the form of a bootstrapping explanation which shows *consistency* with the chemical facts. As I conceded earlier, I accept that the periodic *law* does provide some form of deductive explanation but I claim not a very successful one. As I also stressed earlier, in many cases it was the chemical facts that led to the discovery of the periodic system rather than the periodic system explaining the chemical facts.

It would appear that for Weisberg there exist just two main options, namely models and theories. He wishes to deny that the periodic system is a model and so is compelled to argue that it must be a theory. In doing so Weisberg shows an unusual reductionist bent, given that the overwhelming tendency in the philosophical study of models in recent decades has been a move towards claiming that models, rather theories alone, explain scientific phenomena. What Weisberg seems to miss is the possibility that the periodic system, qua classification system, is also capable of a form of explanation, albeit a different form of explanation than one obtains from theories. It is to this issue that I would like to turn in the second part of this article.

Do classifications provide explanations and if so what kind of explanations?

Classification is a basic human activity which we all perform hundreds of times a day. We sort objects into appropriate piles, and we even arrange our thoughts before an important encounter. We classify new people we meet after a few instants in order to cope better with any ensuing interactions. If I meet a child of 5 years old I draw on my store of knowledge and classify the child with other 5 year olds I may have encountered because this act of classification allows me to act accordingly.

This kind of activity is not usually regarded as providing any form of explanation but I want to propose that in many ways it may represent explanation, albeit of the non-deductive kind. It is a form of explanation that functions by accommodating new data among the already known store of data that we possess. It is a form of explanation which provides insight by establishing consistency with previously encountered information. It can be called a form of bootstrapping explanation.

Classification is highly devalued in the sciences. Rutherford famously declared that the only true science was physics while all the rest were just forms of stamp collecting. Authors like Weisberg who acknowledge the predictive power of the periodic classification are apparently obliged to try to elevate the periodic system into a form of theory because they believe that the only forms of valid explanation are bottom–up deductive explanations which appeal to theories. But these days there is a move in the philosophy of science towards claiming that it may be models rather than theories that are the agents of explanation (Cartwright 1999). However, this kind of license has never been extended to classifications as far as I am aware.

Mendeleev himself tried to justify the predictions and accommodations he made concerning various elements by declaring that he had discovered a periodic law. But his discovery was not strictly a law since the periodicity in the property of the elements is not exact and there are numerous exceptions. In addition his newly claimed law did not provide any form of explanation since it was merely a statement of the fact that chemical behavior recurs after regular intervals.

Another blemish in Mendeleev's periodic law, although not discovered until later, was that the period length before repetition occurs is not constant, although this feature can be explained by recourse to quantum mechanics. Last but not least, Mendeleev's periodic law

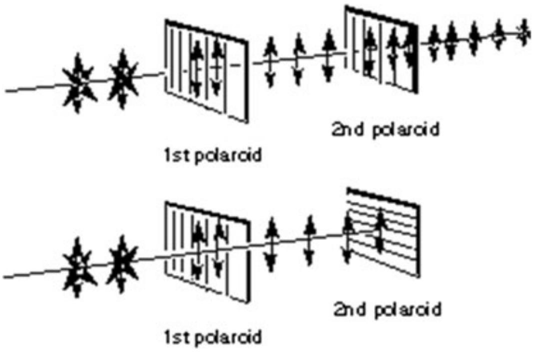

Fig. 2 Proposed analogy. Non-polarized light (*on left*) is analogous to multi-directional explanation while plane-polarized light (after passage through first polarizer) is analogous to uni-directional or conventional explanation

was actually incorrect because chemical periodicity is a periodic function of atomic number rather than atomic weight. For example, Mendeleev's insistence on using atomic weight led him to predict that iodine had to have a higher atomic weight than tellurium, which it does not (Scerri 2007).

Classification as sideways explanation

I want to now return to Weisberg's statement, quoted above, concerning the oxides of elements and their formulas and my saying that I believed that there was a grain of truth in Weisberg's analysis. While I denied that the periodic system could be regarded as providing a deductive explanation, which would have allowed us to bestow the honorific label of 'theory' to it, I have claimed that there is nonetheless a form of bootstrapping explanation or explanation by virtue of displaying overall consistency with the facts. It is this form of explanation that I will term sideways explanation to distinguish it from bottom–up explanation that theories provide. Classifications to the extent that they explain at all, do so in a sideways fashion but not in a deductive fashion. I believe that it is this intuition that is guiding Weisberg but that he lapses into saying that such consistency relationships represent a form of bottom–up explanation from a theory.

As Shapere and others have pointed out, the periodic system has been described as a classification, a model and an ordered domain but very seldom as a theory either by the discoverers of the periodic system or by later commentators. In a later article I will explore the notion of sideways explanation as distinct from bottom–up (deductive) or top–down type explanations. The uni-directionality of explanations, whether bottom–up as traditionally conceived or top–down as discussed by some emergentists, is seldom questioned (McLaughlin 1992). Here I am proposing a widening in the way that we regard explanation.[4] I propose that explanations may occur in a multi-directional sense and that joint explanations may frequently be operating at once.

Finally, I propose to represent the comparison of sideways explanation on one hand with the conventional view of explanation on the other, by considering an analogy with plane polarized light. Plane-polarized light relative to non-polarized light is like conventional or unidirectional explanation is to multi-directional explanation (Fig. 2). In order to obtain a

[4] Many other authors have proposed similar schemes in which causation is not necessarily directed either upwards or downwards. See for example the work of Denis Noble as summarized in his recent book, *The Music of Life*.

richer, and more general, understanding of explanation we need to widen our view of these topics. We need to, as it were, remove the polarizing film and need to revert to a multi-directional non-polarized view of these issues.

Just as accommodation is traditionally devalued in the assessment of scientific discoveries, so is sideways explanation. This is not so surprising as sideways explanation is a form of accommodation of data. I propose that the properties of an element can be regarded as explained in a sideways fashion if its properties are accommodated by the constraints that exist from surrounding elements on each side as they appear on a periodic table.[5] It is suggested that removing the 'filter' which biases out all but vertical explanations might provide a richer understanding of scientific explanation. Such a general proposal for explanation of a lateral form is not altogether original and has been discussed by systems biologists in particular (Noble 2006).

Return to elements

What causes germanium to have a valence of 4? According to a bottom–up explanation, it is due to atoms of germanium having four outer-shell electrons which can be shared. Of course what Mendeleev termed his periodic law could not explain this fact since electrons had not yet been discovered.

In addition to this explanation is the fact that germanium lies between gallium and arsenic which have valences of 3 and 5, respectively which causes it to have a valence of 4 since this valence represents a stepping stone from that of gallium to that of arsenic. Similarly, the properties of germanium can be predicted from those of the two adjacent elements, gallium and arsenic, since its properties are constrained by these flanking elements. When Mendeleev predicted the properties of gallium he was using the periodic system which in the sense I am suggesting provides a sideways explanation for the properties of this element.

It is possible that this new view of classification providing explanation in a side-ways fashion can cast new light on the much debated question of the relative value of prediction and accommodation by scientific developments. The form of side-ways explanation that I am proposing is closely related to accommodation by scientific theories or scientific developments in general.[6] The fact that bottom–up explanation has been universally favored over sideways explanation, is similar to the notion that prediction from a theory should be favored over accommodation. It is due perhaps to the lingering influence of the logical positivist approach to philosophy of science and the belief that explanations must be of the reductive or top–down variety in which everything is ultimately deducible from physical theory.

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[5] Of course the constraints can be provided from the elements above and below in a group of the periodic table or even elements placed diagonally. This will still be regarded as sideways explanation although it may not be literally sideways on a two-dimensional periodic table.

[6] Recall that the periodic table which has been the subject of a good part of the recent prediction—accommodation debate is not a theory, at least for the vast majority of authors.

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