Finding causal structure

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The periodic table of elements represents and organizes all known chemical elements on the basis of their properties. While the importance of this table in chemistry is uncontroversial the role that it plays in scientific reasoning remains heavily disputed. Many philosophers deny the explanatory role of the periodic table, while insisting that it is "merely" classificatory (Shapere 1977, 534-5) (Scerri 1997a, 239). In particular, it has been claimed that the table doesn't figure in causal explanation because it "does not reveal causal structure" (Woody 2014, 143). This paper argues that the modern periodic table does reveal causal structure in the sense of containing causal information that figures in explanations in chemistry. However, this analysis suggests that the earliest versions of the table did serve more of a classificatory role, as they lack the causal structure present in modern versions.

1 Introduction. To the extent that there is a trademark figure for the field of chemistry it is surely the periodic table. Considered by many to capture the "essence" of this scientific domain, the periodic table represents and organizes all known chemical elements on the basis of their properties (Scerri 2007, xiii). While the importance of this table in chemistry is uncontroversial, the role that it plays in scientific reasoning remains heavily disputed. Many suggest that this table serves as a helpful tool for classifying chemical substances, while denying that it figures in scientific explanation (Shapere 1977, 534-5). The periodic table is said to resemble classifications such as Linnaean taxonomy and the Dewey decimal system, which organize phenomena on the basis of various features without explaining them (Scerri 1997a, 239). More specifically, it has been claimed that the periodic table does not figure in causal explanation because it "does not reveal causal structure" (Woody 2014, 143).[1] Typically, causal explanations involve explaining some outcome by appealing to its causes. If the periodic table lacks causal information or causal structure this would indicate its inability to participate in such explanations.

When these claims are examined in the context of chemists' discussions and use of the periodic table they raise a number of puzzles. First, chemists claim that the table allows them to explain particular properties of the elements and the periodic nature of these properties (Chang 2007, 326) (Myers 2003, 66) (Weller, Overton, Rourke, and Armstrong 2014, 273). Second, they often invoke information in this table in ways that suggest it has causal implications. The table contains information about atomic structure, which they claim "determines," "dictates," and "is responsible for" properties of the elements in a way suggesting causal responsibility (Myers 2003, 44, 66, 85). These puzzles lead to a number of questions. If the table is "merely" a classification device why do scientists seem to invoke it in explanations these phenomena? If the table lacks causal structure, why does it figure in explanations that appear to be causal in nature? Furthermore, what exactly does it mean to say that a figure has or "reveals" causal structure as opposed to capturing some non-causal classification?

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[1]Even those philosophers who ascribe some explanatory status to the periodic table deny its role in causal explanation (Kitcher 1989, 428-9) (Woody 2014, 143).

In this paper, I argue that the modern periodic table does reveal causal structure in the sense of containing causal information that figures in causal explanations in chemistry. I provide an analysis of what it means for a figure to reveal causal structure where this analysis relies on an interventionist account of causation. This analysis suggests that the earliest versions of the table served more of a classificatory role, as they lack the causal structure that has been incorporated into modern versions. The rest of this paper is organized as follows. Section 2 reviews background leading up to the development of the modern periodic table. In section 3 the interventionist account is introduced and used to specify a set of criteria for causal structure. These criteria are used to examine the table in the latter half of section 3 and in section 4, where information relevant to the explananda and explanantia are examined, respectively. Section 5 clarifies differences between the modern periodic table and systems that are "merely" classificatory, such as Linnaean taxonomy and the Dewey Decimal system. Section 6 concludes.

2 The periodic table: some background. The modern periodic table originated with developments in the mid-19th century. Soon after the acceptance of a standardized set of atomic weights published by Cannizzaro from 1858-1860 it was discovered that many chemical and physical properties of the elements are a periodic function of their atomic weight (Moeller, 1980 p. 23) (Scerri 2007, 66). Properties such as atomic volume were shown to increase in repeated intervals among elements serially ordered by atomic weight, as shown in Meyer's graph in figure 1 (Meyer 1870). For example, the repeating peaks in figure 1 correspond to elements that share the property of large atomic volume (Li, Na, K, Rb, Cs), while the valleys correspond to elements with low atomic volume (B, Al, Co, Rh). Attempts to clearly capture this pattern led to a number of representational formats, including some of the earliest periodic tables. Mendeleev produced some of the most well-known examples of these tables where he ordered elements of increasing atomic weight in columns from top-to-bottom and left-to right, such that their chemical similarity or "family resemblance" was captured along a horizontal dimension, by rows (Mendeleev 1869) (Scerri 2007, 125).[2] This can be seen in figure 2 where, for example, the 14th row from the top identifies elements (Li, Na, K, Rb, Cs, Tl) with the shared properties of large atomic volume and a valence (or combining power) of 1. The consistent periodic relationship between an element's properties and atomic weight led Mendeleev to use this "periodic law" to make a number of predictions about the behavior of undiscovered elements of particular atomic weights (Moeller, Bailar, Kleinberg, Guss, Castellion, and Metz 1980, 158). Some of these predictions would be confirmed in later work and they are represented by various question marks in his table.[3]

While many chemical and physical properties were shown to follow a periodic pattern, ordering the elements on the basis of atomic weight sometimes produced inconsistencies in this pattern. For example, although Tellurim (Te) should be ordered after Iodine (I) due to its higher atomic weight, reversing their order placed both in horizontal rows among similar elements. Mendeleev's careful studies of chemical properties (and his conviction that they should approximate periodicity) led him to attribute these inconsistencies to incorrectly measured atomic weights (Scerri 2007, 125-126) (Scerri and Worrall 2001, 435).[4] While the atomic weights of some elements would be adjusted

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[2]Meyer and others produced similar tables, with horizontal similarities. Mendeleev had other non-tabular representations of chemical periodicity.

[3]For example, the question marks "?=68" and "?=70" represents such predictions.

[4]He claimed that the correct weight of Tellurium was less than Iodine, which restored the periodic pattern. Mendeleev's reversal of these elements can be seen in figure 2.
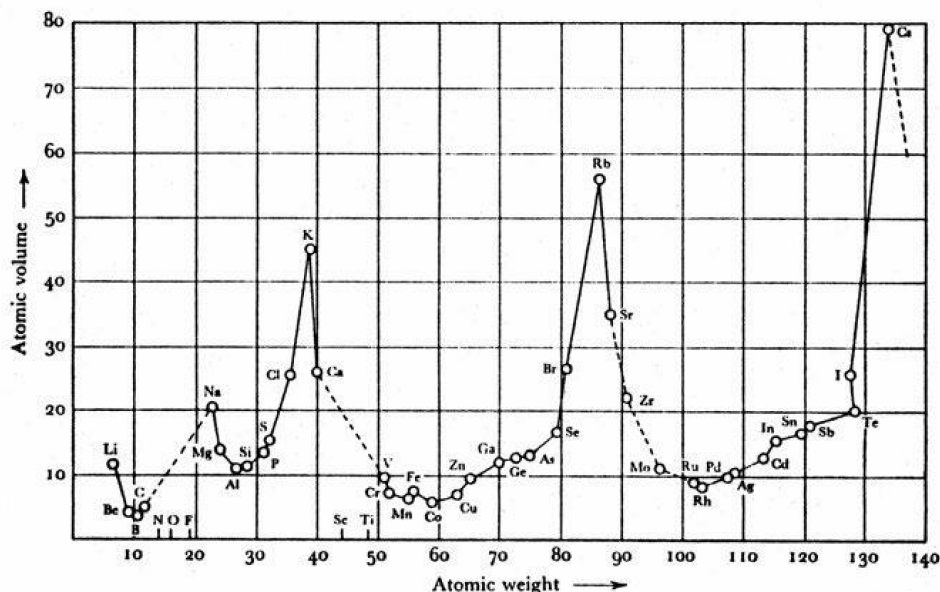
Figure 1: Meyer (1870): periodicity in graphical format

in the future many of these imperfections were largely resolved after the implementation of a new ordering principle in the early 20th century–viz. atomic number. The discovery of x-rays and developments in research on radioactivity led to the identification of positive charge in the nucleus, which would be associated with the number of protons in an element, reflected by atomic number. Ordering elements on the basis of atomic (or proton) number produced a more consistent periodic pattern than ordering on the basis of atomic weight. While the exact reason for this would be pursued in further work, it was at least clear that proton number reliably increased by a single unit through element ordering, while atomic weight was much more variable. Atomic weight didn't increase by a standard amount through serially ordered elements and it could vary across different samples of the same element. These features would later be explained by variations in neutron number, which are uncharged particles located in the nucleus of an atom. While both protons and neutrons contribute to atomic weight, neutrons don't reliably track increases in proton number and they can vary across different samples of the same element (as in the case of isotopes). This clarified how an ordering on the basis of atomic weight and atomic number could differ and why imperfections found in the former were resolved with the later. If an element with fewer protons than another had far more neutrons it could have a lower atomic number but a higher atomic weight. This made sense of the Tellurium and Iodine case: although Tellurium had a lower number of protons (52) (and thus, a lower atomic number) than Iodine (53), naturally occurring samples of Tellurium had far more neurons than Iodine and, thus, weighted more (Scerri, ASI p. 82). Ordering on the basis of atomic number placed Tellurium before Iodine, which captured a more consistent periodic pattern.

Throughout this early work the main phenomena of interest were various chemical and physical properties and the periodic nature of these properties across elements. Of course, identifying this periodicity required the right kind of ordering principle. While both atomic weight and atomic number worked well enough to reveal much of this pattern, they were quite limited in explaining

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                              Ti=50      Zr=90      ?=180.
                              V=51       Nb=94      Ta=182.
                              Cr=52      Mo=96      W=186.
                              Mn=55      Rh=104,4   Pt=197,1.
                              Fe=56      Ru=104,4   Ir=198.
                           Ni=Co=59      Pd=106,6   Os=199.
    H=1                       Cu=63,4    Ag=108     Hg=200.
               Be= 9,4 Mg=24  Zn=65,2    Cd=112
               B=11    Al=27,3   ?=68    Ur=116     Au=197?
               C=12    Si=28     ?=70    Sn=118
               N=14    P=31    As=75     Sb=122     Bi=210?
               O=16    S=32    Se=79,4   Te=128?
               F=19    Cl=35,5 Br=80     I=127
    Li=7  Na=23        K=39    Rb=85,4   Cs=133        Tl=204.
                       Ca=40   Sr=87,6   Ba=137        Pb=207.
                        ?=45   Ce=92
                      ?Er=56   La=94
                      ?Yt=60   Di=95
                      ?In=75,6 Th=118?
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Figure 2: Mendeleev (1869): periodicity in tabular format

aspects of this pattern that interested scientists, such as why it was present at all and why it had particular features. For example, nothing about these ordering principles explained why elements in a particular row all shared the same set of properties or why other properties varied periodically across serially ordered elements. In some sense, many early periodic tables represented *that* elements have these chemical characteristics, without involving any underlying explanation for *why* they do.

Conceptions of the proper ordering principle would undergo one more change before influencing our modern periodic table. This change involved the incorporation of electronic structure into an ordering based on atomic number. We now know that atomic (or proton) number also reflects the number of electrons in an element–in neutrally charged atoms changes in proton number track changes in electron number. In modern chemistry, scientists frequently appeal to atomic structure in explaining the chemical and physical properties of the elements and their periodic character. As Moeller states, "Mendeleev's ordering of the elements is completely explained by modern atomic theory" p. 159. While these explanations typically cite subatomic particles including protons and electrons, they typically place significant emphasis on electronic structure. As Scerri states, "it is still generally believed that the electron holds the key to explaining the existence of the periodic table and the form it takes" (Scerri p. 183). Furthermore, these explanations often appear causal in nature–chemists claim that electronic structure "determines" "dictates" and "is responsible for" the behavior of the elements and, relatedly, that these behaviors "depend on" and are a "consequence of" this structure (Housecroft p. 20). This interpretation is consistent with other statements in the literature. For example, it is claimed that "the concept of electronic configuration as a *causally explanatory* feature has become very much the domain of chemistry or to be more precise it is the dominant paradigm in modern chemistry" (Scerri p. 236, emphasis added).

If electronic and atomic structure play a role in explaining the periodic behavior of the elements, how should these explanations be understood? What role does the periodic table play in these explanations and it is correct to view them as causal in nature? I address these questions in the next section, by turning to an examination of the modern periodic table.

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3   The modern periodic table.   Before considering the role of electronic and atomic structure in modern explanations in chemistry it will help to briefly clarify the basic account of causal explanation I rely on, the relevant explanatory targets or explananda in this example, and how information about these targets is represented in the modern periodic table. Once these are specified, I will provide an account of what it means to say that these factors explain various properties of the elements and I will show that the periodic table contains causal information that figures in these explanations.

My analysis relies on an interventionist account of causation, which maintains that causes are factors that "make a difference" to their effects (Woodward 2003). On this account, causal relationships take place between variables, which represent properties capable of taking on differing values. Consider the following minimal interventionist criterion (I): to say that X is a cause of Y means that, in some background circumstances B, changes in X produce changes in Y. In other words, if one were to intervene on X and change its values, this would lead to changes in the values of Y.[5] For example, suppose we have a light switch X and a light bulb Y, which can each take on the values (0, 1) representing the 'off' and 'on' states of the switch and bulb, respectively. When we say that the switch causes the light to turn 'on' or 'off,' we mean that manipulating the switch provides control over these states of the bulb. This "change relating" conception of causation relates changes in a cause variable to changes in an effect variable where these changes have to do with the hypothetical control a cause exerts over an effect and, relatedly, the way in which an effect depends on its causes.[6]

Two features of this account should be highlighted. First, in order to capture changes in causes and effects the variables representing them need to take on at least two different values (and sometimes they will take on a larger range of values). Second, it needs to be clear how values of the cause variable systematically relate to values of the effect variable in a way that meets the minimal interventionist criterion (I) mentioned above. In other words, in identifying causal relationships it isn't enough to simply specify two properties that have a purported causal connection or even two properties that can each take on some range of different values. It needs to be clear how particular values of the cause variable produce (control) particular values in the effect variable or, similarly, how values of the effect depend on values of the cause. These considerations suggest three criteria that a scientific figure should meet if it contains causal structure or causal information. At the very least, such figures should specify (i) some cause variable C that can take on different values, (ii) an effect variable E that can take on different values, and (iii) how values of C systematically relate to values of E in the interventionist sense (I) captured above.[7]

What does this account of causation have to do with explanation? Causal explanations are often characterized as the explanation of some effect by appealing to its causes. On the interventionist account an explanandum is represented by some range of values in an effect variable. The corresponding explanans involves some cause variable (or variables) and how its different values systematically relate–in an interventionist sense–to the range of values in the effect. Intervening on

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[5]The notion of an intervention is an ideal intervention, which precisely intervenes on X without also intervening on factors that cause or are associated with Y. For more on this see (Woodward 2003).

[6]The control is "hypothetical" because we often talk about factors causing particular outcomes, even though we lack the ability to actually intervene on them. What we mean is that if such factors were manipulated, they would produces changes in their purported effect (Woodward 2003).

[7]A further requirement that is assumed in this analysis is that these variables and relationships represent true claims about actual properties in the world (Woodward 2015) (Woodward 2014).

and changing values of the cause, produces systematic changes in the value of the effect or, alternatively, varying states of the effect depend on the varying states of the cause. In the philosophical literature there is a long tradition of distinguishing explanation from the scientific activities of classification, description, and prediction. The interventionist account follows this tradition and distinguishes causal explanation from these activities on the basis of their identification of relationships with interventionist causal control, in the sense captured in (I). Of course, scientists are interested in all sorts phenomena and relationships, which fail to meet this interventionist standard (I). For example, they may be interested in classifying or describing organisms on the basis of "surface level" phenotypic features, without concerning themselves with the causes such features. Moreover, these features might help in predicting the presence of some future phenotypic outcome, without it being the case that they cause of the outcome itself (perhaps there is a mere correlation). This is all to say that legitimate classificatory, descriptive, and predictive projects in science can be guided by considerations that don't involve causal relationships. However, where the hallmark of causal explanation involves supplying "difference making" information–i.e. information relevant to manipulation and control–these projects will not be viewed as explanatory and instead "merely" classificatory, descriptive, or predictive.

3.1 Explananda. Consider the modern periodic table, shown in figure 3, which represents various chemical and physical properties of the elements and their periodic nature. Each box in this table represents an element where the letters and numbers indicate the element's abbreviated symbol and atomic number, respectively. Elements are organized in horizontal rows called "periods" and vertical columns called "groups."[8] Ordering on the basis of atomic number starts at the top left of the table with Hydrogen (which has an atomic number of 1) and continues from left-to-right and top-to-bottom throughout the table. Elements are "defined" by their atomic number–no two elements have the same atomic number and substances with the same atomic number are the same element (Nath, p. 94).

Elements in the table are organized in a way that captures various patterns in their properties. Two types of these patterns are group trends and periodic trends. Group trends refer to clusters of chemical behaviors that are shared among elements in the same group or column of the table. These columns of elements are referred to as "chemical families" due to the fact that they contain "chemical homologues" or elements that exhibit similar chemical behaviors (Seaborg 1959, 472). For example, group 17 is the halogen family, which contains highly reactive, non-metals (poor conductors or heat and electricity) that frequently combine with other elements to form compounds. Another example is the noble gas family, or group 18, which is comprised of odorless, colorless, nonflammable gases with low reactivity in standard conditions. Where many of Mendeleev's earlier tables (e.g., figure 2) captured these chemical similarities or "family resemblance" relations along the horizontal dimension, the modern table captures these similarities vertically.[9] Group trends exhibit

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[8]This 18-column layout is sometimes expanded into a 32-column "long form" of the table where the Lanthanide and Actinide series (shown in the two disconnected rows at the bottom) are inserted between the second and third periods (following Barium (Ba) and Radium (Ra)). When they are spliced into the table in this location they continue the serial ordering of elements by atomic number.

[9]In order to see the similarities between Mendeleev's table in figure 2 and the modern periodic table, Mendeleev's table should be rotated by 90 degrees and reflected across the vertical axis (Gordin 2004, 28). Some of Mendeleev's later tables captured group trends in a vertical manner, similar to the modern table.

Group →	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
↓ Period																		
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

Lanthanides	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Actinides	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Figure 3: The modern periodic table

periodicity in the sense that they identify clusters of chemical properties that periodically reoccur throughout serially ordered elements. The modern table is organized so that these reoccurrences line up in a vertical manner. While these "family resemblance" relations are not strictly found for all columns in the periodic table they are typically discussed for groups 1, 2, 13-18 and the lanthanide and actinide series. Standard inorganic chemistry textbooks usually dedicate individual chapters or large sections to groups 1, 2, 13-18 and their characteristic features.

A second set of patterns found in the table are periodic trends. Where group trends capture changes in clusters of properties, periodic trends capture changes in single properties. Examples of standard periodic trends include atomic radius, electron affinity, ionization energy, and metallic character. The modern table is organized in a way that captures trends in these single properties throughout all elements in the table. These trends are explicitly shown in figure 4. In order to see this clearly, consider atomic radius–the arrows in figure 4 indicate directions of increasing atomic radius throughout all elements in the table. This property increases from top-to-bottom and right-to-left throughout the table. In other words, atomic radius increases as one moves down groups and leftward in periods. Other periodic trends can be read off this figure in a similar fashion.

Group and periodic trends represent one layer of information in the modern periodic table. Inorganic chemists refer to this information as "descriptive chemistry" because it describes the brute, observable "hard facts" about properties of the elements (Williams 1979, viii) (Weller, Overton, Rourke, and Armstrong 2014, 271). The table organizes these facts in a way that captures trends in these properties and renders them more comprehensible than a rote study of individual elements. Instead of memorizing the unique features of over 100 individual elements, a qualitative understanding of these features is provided by spatial trends in the table and the relative location of any element (Scerri 2011, 28). This involves "discussing the chemistry of an element in terms of
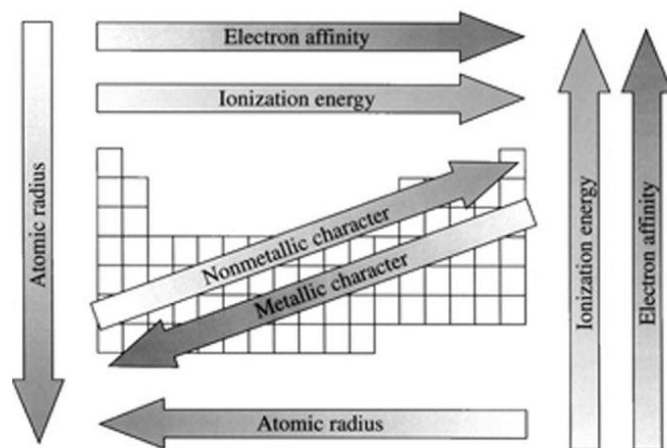
Figure 4: Periodic trends

its position in the periodic table" (Williams 1979, 277). Impressively, the table serves this role for all known or naturally occurring elements, which leads chemists to speak of its "unifying" nature and the fact that it is a "single chart" that "embodies the whole of the discipline" (Scerri 2012, 329). This descriptive information serves other purposes as well: the "close neighbor" relations of nearby elements in the table facilitates comparisons and suggests elements that could replace others in chemical reactions (Woody 2014, 139) (Scerri 2011, 10-11). These features of the modern periodic table have led to its use as a key pedagogical tool in teaching descriptive chemistry (Moeller, Bailar, Kleinberg, Guss, Castellion, and Metz 1980, xxv). In fact, Mendeleev's earliest periodic tables were motivated by an interest in pedagogical utility and making the periodic patterns easily accessible (Gordin 2004, 28-9). As the study and organization of these "facts" about the properties of elements led to the earliest periodic tables it is claimed that "descriptive chemistry forms the historical basis of the periodic table" (Houten 2009, 11).

However, chemists aren't just interested in describing and organizing these facts about the properties of elements–they also want to explain them. Inorganic chemists distinguish "descriptive chemistry," which *describes* facts about the properties of elements, from "theoretical chemistry," which employs theories and principles to *explain* these facts. The theories and principles that they view as providing these explanations have to do with the atomic and electronic structure of the elements. Consider the following quotes:

> This part of the book describes the physical and chemical properties of the elements as they are set out in the periodic table. This 'descriptive chemistry' of the elements reveals a rich tapestry of patterns and trends, many of which can be rationalized and explained by application of the [atomic] concepts developed in Part 1" (Weller, Overton, Rourke, and Armstrong 2014, 271).

> The principles of chemistry are the explanations of the chemical facts; this is where you meet the hypothesis, the laws, and the theories. Descriptive chemistry, as you might expect, is the description of the elements and compounds, their physical states, and how they behave. No matter how chemistry is used, a good balance between principles and descriptive chemistry is a necessity. We will attempt to maintain such a

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balance throughout this textbook" (Moeller, Bailar, Kleinberg, Guss, Castellion, and Metz 1980, 7).

[I]norganic chemistry is not just the study of properties and reactions; it includes explanations. To explain "why" it is necessary to look at the principles of chemistry, such as atomic structure, bonding, intermolecular forces, thermodynamics, and acid-base behavior" (Rayner-Canham 1996, xii).

"So far in this book we have explored ways in which the chemical reactions and physical properties of the elements and their compounds are related to some more fundamental properties of the atoms of the elements: their radii, electronegativities, charges, covalent-bond types and energies, and periodic table positions. But in chemistry we also seek to explain periodic variations in atomic radii, electronegativities, charges, and covalent bond types in terms of our theory of the electronic structure of the atom itself. This is the job of the field of *theoretical chemistry*" (Wulfsberg 1991, 371).

These quotes and the previous analysis help reveal a number of things. First, chemists are interested in explaining properties of the elements and they distinguish this project from merely describing these properties (I'll say more about this later). Second, some of the properties they seek to explain are group and periodic trends, which are explanatory targets captured by the modern periodic table. I am going to suggest that these patterns represent an *explananda* or *effect* overlay in the table–they represent changes in the chemical and physical properties of the elements that scientists are interested in explaining. The interventionist framework provides a natural way to understand such explananda. For a particular group or periodic trend the property in question can be represented by a variable P, which is capable of taking on a range of values. These values are the varying state of the property depicted in the table (in what I am called the explananda overlay). For example if P_p is atomic radius the different values of this property are qualitatively depicted by the arrows in figure 4, which captures the consistent, step-wise changes in this property across all elements in the table. The table captures how P_p changes when one starts at any element in the table and moves to another. This basic point is true for group behaviors as well. Group behaviors are best thought of as variables P_g that take on discrete, binary values (as opposed to the continuous values taken on by P_p), which are present in some groups (1) and absent (0) in others. Changes in these values are represented by the spatial location of elements within the vertical columns in the table. The values of P_g change when moving horizontally in the table, because elements in the same column have the same value.[10] The values of both P_p and P_g vary periodically when one follows elements ordered by atomic number. A third point, which relates to the second, is that this explanandum overlay clarifies how the periodic table meets one of the three criteria for causal structure. It meets the second criteria because it contains information about an effect variable and the different values that it takes. This doesn't deny that chemists are often interested in this layer solely for its descriptive information about the properties of the elements. The point is that, when they want to explain these properties they serve as an explanatory target. The effect variable is a given property specified by the group and period trends. The different values that it takes are specified by changes in the value as one moves throughout the table. Fourth, these quotes

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[10]For example, if P_g represents the cluster of chemical behaviors displayed by group 17, elements in this column have value of 1 for this variable (representing the presence of these behaviors), while elements in other others have a value of 0 for this variable (as they lack these behaviors).

don't just reveal what chemists want to explain, but also what provides these explanations. They clearly view something about electronic and atomic structure as explanatorily relevant to various properties of the elements. These structures do some kind of explanatory work in these cases. I am going to argue that some of these explanations have a causal interpretation and that information about these causal relationships is captured in the modern periodic table. In order to see this I turn to an examination of electronic and atomic properties of the elements, their representation in the periodic table, and how they figure in these explanations.

3.2 Explanantia. As mentioned earlier electronic structure is importantly related to atomic number. In particular, atomic number doesn't just reflect the number of protons in an atom of an element, but also the number of electrons.[11] For elements of increasing atomic number the additional protons are located in the nucleus (or center) of the atom, while electrons are added to shells–and orbitals within these shells–that surround the nucleus. Different shells contain different orbital types as shown in figure 5. In this figure, shells (n) are represented horizontally and orbital types (l) vertically: the first shell contains one s orbital, the second contains one s and one p orbital, the third contains one s, p, and d orbital, and so on. Distinct orbitals within these shells hold different maximum amounts of elections. Orbital types s, p, d, and f can hold a maximum of 2, 6, 10, and 14 electrons, respectively. The order in which these shells and orbitals are filled with electrons is specified by the Madelung rule, which is represented by the winding arrow in figure 5 (Allen and Knight 2002) (Housecroft and Sharpe 2010).[12] This arrow shows that in following elements of increasing atomic number electrons are first added to the s orbital of the first shell (1s), then the s orbital of the second shell (2s), the p orbital of the second shell (2p) and so on.[13] While this holds generally, it should not be viewed as a "strict rule" as there are exceptions (Myers 2003, 67) (Scerri 1997b, 552). Following this principle, the atomic number of an element can be used to determine its electronic configuration or the relative location of its electrons in particular orbitals and shells.

When scientists explain group and periodic trends they place significant emphasis on electron configuration and, in particular, on an atom's "valence electrons," which are those electrons in its outermost orbitals. The outermost position of these electrons influences: chemical reactivity because they are more available for bonding, the stability of an atom due to how full the respective orbitals are, and properties like atomic radius because their orbital location alters how close protons can pull them centrally (Rayner-Canham and Overton 2010, 30-31) (Myers 2003, 66). Consider how chemists appeal to these electrons in their discussions of the periodic table and chemical explanations:

> "the electron configurations of the elements provide the basis for explaining many aspects of chemistry. Particularly important are the electrons in the outermost orbital of an element. These electrons, known as the valence electrons, are responsible for the

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[11]This is the case with neutrally charged atoms, which are assumed in characterization of the periodic table (Myers 2003, 41), (Hofmann 2002, 6).

[12]The Madelung rule is also sometimes referred to as the $(n + l)$ rule, the Janet rule, and the Klechkowsky rule. This rule is related Bohr's Aufbau (or "building up") principle which states that atoms are built up by adding protons and electrons, where electrons occupy orbitals of lowest energy.

[13]Notice that electrons are not added in a manner that tracks increasing shell number. For example, electrons are added to the s orbital of the fourth shell (4s) before the d orbital of the third shell (3d).
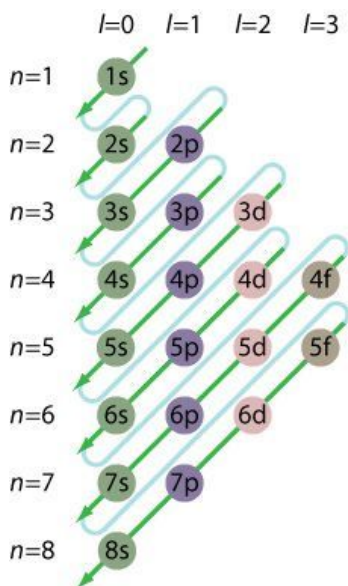
Figure 5: Madelung rule and filling of orbitals

chemical properties elements display, bonding, the periodic table, and many chemical principles" (Myers 2003, 43-44).

I am going to suggest that the way to understand these claims–and the main feature of these explanations–is that electronic structure and to a significant extent atomic structure, are causally responsible for various chemical and physical properties of the elements in an interventionist manner. These atomic features "make a difference" to these properties in the sense that changes in these features produce changes in these properties. Before I explore this in more detail, it will help to connect this discussion of electronic structure up to the periodic table and the explicitly *periodic* nature of elemental properties displayed in the table. Even if electronic structure were causally relevant to chemical behavior how could this explain the distinctively periodic nature of this behavior? One might wonder "how a simple arrangement could provide such regularities" (Niaz 2009, 69) or how a simple ordering would produce such an elaborate and consistent periodic pattern.

The answer chemists provide has to do with the fact that as elements are ordered by increasing atomic number there is a periodic pattern in their valence electron configuration. This results from a pattern in the Madelung rule or in the types of orbitals that electrons successively fill. As seen in figure 5 this filling cycles through s, p, d, and f orbitals such that serially ordered elements have a repeating pattern in the types of orbitals occupied by their outermost electrons. This is represented by different "blocks" of the periodic table, shown in figure 6, which reflect the different orbital types occupied by an element's outermost electrons (Allen and Knight 2002). In following elements of increasing atomic number in the table, the sequence of blocks one moves through mirrors the sequence of orbitals specified by the Madelung rule. Elements in the s block have valence electrons in s orbitals, elements in the p block have their valence electrons in p orbitals, and so on. Each orbital is "progressively filled across a period" where each position (or vertical column) in the block indicates how many electrons occupy the respective orbital (Myers 2003, 66). For example, elements in the first position of the p block (group 13) have a single valence electron in a p orbital,

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while elements in the second position (group 14) have two valence electrons in this orbital. This creates an alignment in the table where groups (or vertical columns in the table) contain elements with similar valence electron configurations and where periods capture repeating sequences of these configurations. The fact that groups in the table contain elements with the same valence electron configuration is cited as the reason for their shared behavior (Myers 2003, 66) (Scerri 2011, 27-28). Relatedly, periodic changes in these configurations are cited as the reason for periodic changes in other properties of the elements (Myers 2003, 66). As chemists state, "periodicity is a consequence of the variation in ground state electronic configurations" and "[e]lectron configurations of elements help to explain the recurrence of physical and chemical properties" (Housecroft and Sharpe 2012, 20) (Chang 2007, 326). Thus, serially ordered elements exhibit periodic changes in their properties, because these properties are caused by atomic features which themselves vary periodically with this ordering. This involves explaining repeating changes in an effect by appealing to repeating changes in its causal factors.
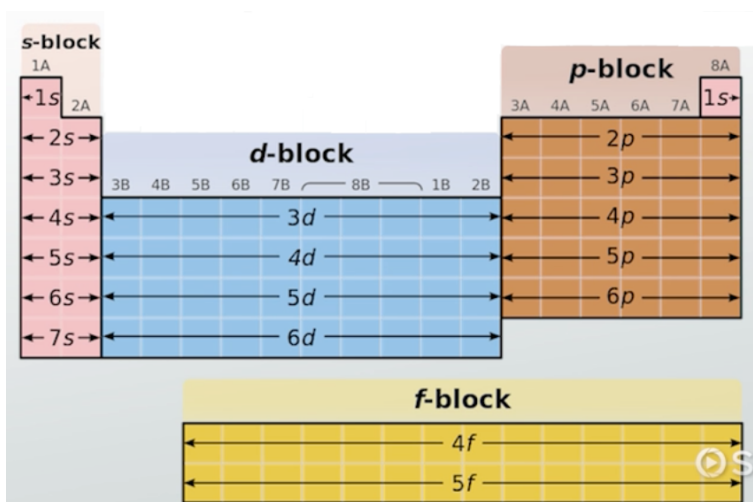

Figure 6: Blocks of the periodic table

This reveals another layer of information in the table–information about the electronic configuration and the proton number of the elements. I am going to suggest that this information represents an *explanantia* or *cause* overlay in the table–it contains information that chemists appeal to in explaining what causes the chemical and physical properties of the elements. The table captures how these atomic features change across the elements and how these changes follow a periodic pattern. We now have two layers of information in the table, which both reveal periodic changes in the elements–one at the level of chemical and physical properties and another at the level of atomic structure. These layers are superimposed in the table in a way that reveals how they are systematically related. In particular, these connections reveal how particular changes in atomic features correspond to particular changes in elemental properties.

In order to explore this further, recall that chemists cite atomic and electronic features to explain the chemical and physical properties of the elements. What exactly does it mean to say that these atomic features explain these properties? Some of these explanations have a causal interpretation and are well understood within an interventionist framework. In these cases, chemists are stating that these atomic features are causally responsible for these chemical and physical properties in the

sense that if one were to intervene on and manipulate these features this would produce changes in these properties and, relatedly, variations in these properties depend on variations in these features. This is suggested by Krebs in the following passage:

> "What makes chemistry so interesting is that each specific chemical element is related to its own kind of atom. Elements with specific characteristics have unique atoms. Each type of atom is unique to that element. *If you change the basic structure of an atom, you change the structure and properties of the element related to that atom*" (Krebs 2006, xxiv; emphasis added).

This change-relating relationship is captured by the two overlays of information in the modern periodic table. These overlays contain information about properties that stand in a causal relationship. Variations in atomic structure are represented by different locations in the explanantia or *cause* overlay, while variations in elemental properties are represented by different locations in the explananda or *effect* overlay. The systematic connection between these two properties is captured by the superimposition of each overlay over the other–manipulating atomic structure involves spatial movement along the cause overlay, which produces subsequent movement in the effect overlay. Movement in the effect overlay reveals how elemental properties change as a result of this manipulation. This involves reading the causal information in the table "forward" from cause to effect. In other words, reading out what elemental changes are produced from atomic alterations. Alternatively, the table can be read "backward" from changes in elemental properties to atomic structure. The forward reading captures causal control of atomic features over elemental properties, while the backward reading captures the dependency of these properties on such features. These features of the table help clarify how it meets the criteria for causal structure. Where the explananda or effect overlay meets the second criteria of causal structure, the explanantia or cause overlay meets the first criteria of causal structure, because it captures changes in a cause variable of interest. Furthermore, the superimposition of these overlays indicates how the table meets the third criteria for causal structure, which has to do with specifying the systematic relation between values of a cause and effect variable. The particular layering of these overlays on top of each other is no accident–it serves to show how particular values of atomic features relate to particular values of elemental properties.

What further reasons do we have to accept such an interventionist interpretation? This interpretation is supported by current theories about Big Bang and interstellar nucleosynthesis, experiments used in the discovery and synthesis of "man-made" elements, and our general understanding of nuclear transmutation (and related concepts like radio active decay, nuclear fission, and fusion, etc.). Each of these relies on the interventionist causal control that atomic features have over elemental properties. Nuclear transmutation involves the conversion of one element into another. Interest in transmutation dates back to the alchemists of ancient Greece who sought to turn base metals into gold and silver and who postulated that a special material called "the philosopher's stone" was a required catalyst for such a process (Hofmann 2002, 1) (Krebs 2006, 4). Such efforts were viewed as heretical by 18th and 19th century chemists until Soddy and Rutherford witnessed transmutation during a radioactive decay process and Rutherford conducted transmutation experiments, converting nitrogen into oxygen though alpha particle bombardment (Rutherford and Soddy 1903) (Rutherford 1919). This work revealed that atomic alternations could in fact cause changes in the chemical and physical properties of a substance and result in the conversion of one element into another. These conversions became the focus of 19th and 20th century experiments designed to

synthesize previously unidentified elements, which capture a second set of phenomena in chemistry that supports the interventionist interpretation.[14] These experiments changed one element into another by intervening on atomic structure. These atomic interventions involve bombarding target atoms with high speed particles or small atoms that alter the proton and electron constitution of the resulting atoms. The original target could combine with these particles forming an element of a larger atomic number or it could break into many elements of smaller atomic number. The periodic table is often consulted in these experiments–it helps identify suitable target elements, suitable projectiles, what products their interaction would form, and what chemical and physical properties such products were likely have. In fact, the (reoccurring) periodic nature of elemental properties in the lanthanide and actinide series (rows) played an invaluable role in identifying successful synthetic products in these experiments (Seaborg 1959, 472). This use of the table exploits its two overlays and treats it as a sort of "ladder" that one can move up and down (Hofmann 2002, 24). Starting with any target element in the table, atomic changes can move one up or down a period, where the final ending point reveals the resulting element and associated properties. Finally, the relationship between atomic features and elemental properties underlies current theories of naturally occurring nucleosynthesis. It is theorized that the first synthesis of elements in our universe took place during the early part of the Big Bang and then later within the high heat and pressure of stars. Both of these environments supplied sufficient energy (in the form of high pressure and heat) that allowed for atomic alternations, which in turn produced the variety of elements that make up our universe (Clayton 1983). Each of these three cases involves chemical concepts and theories, which characterize atomic features as having interventionist causal control over elemental properties, i.e. where changes at the atomic level produces changes in elemental properties.

This analysis suggests that the periodic table meets the three criteria for causal structure specified in the beginning of section 3. However, in order for a scientific figure to have causal structure it doesn't need to represent causal structure in exactly the same way that the periodic table does. To see this consider the third criteria, which the periodic table meets by means of superimposing information about cause and effect variables. A scientific figure can have causal structure without representing the systematic relationships between cause and effect variables by means of superimposition or in the layered manner found in the periodic table. In fact, it seems that this representation format is fairly uncommon in scientific contexts and relatively unique to the periodic table. These systematic relationships are more often represented by partitioning cause and effect variables in one-dimensional figures such that they don't overlap. This is seen in many tables, graphs, and equations which locate cause and effect variables in different areas of one a single figure as opposed to superimposing them. Thus, this third criteria can be met by figures that differ in representational style. The same point holds for the other two criteria for causal structure. Distinct diagrams can meet these criteria in different ways in the sense of employing varying forms of representing cause and effect variables. Different representational formats may serve different purposes, highlight important features of a causal relationship, or be more perspicuous in some contexts than others. The important point is that a diagram represents the causal properties referenced in the three criteria for causal structure, while acknowledging that there will be a variety of ways or representational formats in which it can successfully do so.

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[14]These experiments included elements in the lanthanide and actinide series which are too heavy to occur naturally in large quantities.

4 Explanation, classification, and causal structure. I have suggested that the modern periodic table has causal structure in the sense of containing causal information that figures in explanations in chemistry. This isn't to say that the table explains everything about elemental properties that one might be interested in or that it contains maximal atomic detail about such explanations. Surely there are explananda that the table doesn't address and it clearly omits details that may provide "deeper" or more "complete" understandings of those phenomena it does. A main goal of this paper is to show how this table contains at least some causal structure and, thus, that figures in at least some explanations without suggesting that these are the only explanations of periodicity in this domain or even that they are as detailed as (other) explanations that invoke more atomic theory. These features of the table are sometimes cited to argue that it isn't explanatory because the information it contains fails to fully explain elemental properties and their periodicity. One example of this involves the common claim that electronic configurations don't fully account for the "closure of the periods" or the number of elements that span each period (viz. 2, 10, 18, 36, 54, and 84, respectively) (Scerri 1997b, 551-2) (Scerri 2007, 234). This criticism appears to be guided by an expectation that proper explanations should be "complete" in some sense and should involve derivation from lower-level theories, similar to a deductive nomological (DN) approach. Thus, the purported problem in this case is that the order of shell filling represented in figure 5 is merely supported by empirical and experimental considerations, but it has not been explained itself in the sense of being derived from any underlying theory (viz. quantum mechanics) (Scerri 1997b, 551-2) (Scerri 2007, 234) (Woody 2014, 142). As these claims suggest that derivation from first principles is a necessary feature of explanation, the lack of such a derivation–and the reliance on "mere" empirical data–is said to poses a serious "objection" to viewing this case as genuinely explanatory (Scerri 1997b, 551).

A first point to make is that such criticisms place an unrealistically high bar on what counts as explanatory, in the sense of assuming that explanations should be "rigorous" or "complete" with respect to the number of phenomena that are addressed. Where chemists appeal to the order of electron filling to explain patterns in elemental properties, these criticisms suggest that a genuine explanation goes deeper–it should also explain *why* electrons fill in this order. One clear worry with this approach is that it can lead to an infinite regress in the phenomena to be explained. It seems to expect that for something to be explanatory it should explain everything (or many things) about a topic or in a domain–it either explains everything in full detail or nothing at all. This is an inappropriate standard to expect explanations to meet–it means that nothing will ever qualify as explanatory because their will always be some why-questions that a given body of information doesn't answer. In some sense this makes explanation impossible. This is problematic because it conflicts with common views that successful explanations are provided in scientific and ordinary life contexts. Furthermore, it doesn't make sense of the fact that chemists claim that periodicity has some kind of explanation.

Second, these criticisms assume that if chemists' explanations don't fit a DN-type framework, then they don't qualify as genuinely explanatory. One problem with this assumption is that it isn't clear that this framework well-accommodates explanation in this domain. In fact, chemists' insistence that they are providing explanations despite their unintelligibility within the DN model should raise worries about how well this model reflects the explanations they have in mind. One advantage of the interventionist account is that it captures some of these explanations without being impeded by the aforementioned criticisms related to lack of derivation from underlying theory. Even if period length can't be deduced from theory this doesn't change the fact that alterations in proton

and electron number produce changes in elemental properties and that this relationship is useful for purposes related to explanation and control. The lack of a deductive explanation of electron filling doesn't prevent experiments on transmutation, efforts to synthesize elements, or modern accounts of cosmic nucleosynthesis. These change-relating relationships exist between atomic features and elemental properties even if some of these features can't be derived from the first principles of quantum mechanics. Furthermore, chemists don't appear to downgrade empirical evidence or view this evidence as inferior to theoretical derivations as suggested by these criticisms. The fact that such information is "merely" empirical or experimental is no issue–it's simply how information about these relationships is discovered and it's not inferior to information derived from theoretical principles.

Another criticism of the explanatory role of the table has to do with classification. This criticism is associated with the worry that the table merely classifies elements on the basis of their properties without explaining them. For example, as Scerri states:

> The periodic systems, both naive and sophisticated, are systems of classification which are devoid of theoretical status in much the same way as the Linnean [sic] system of biological classification or the Dewey decimal system of library classification. None of these systems can be regarded as theories since they do not seek to explain the facts but merely to classify them (Scerri 1997a, 239).

Consider the Linnaean and Dewey Decimal systems–both involve classifying entities on the basis of some property or set of properties. In the former, organisms are classified and distinguished from one another on the basis of whether they exhibit particular properties (Ereshefsky 2004). For example, within this taxonomy different species of plants are differentiated on the basis of distinct characteristics of their fructification systems (sex organs) (Ereshefsky 2004). Similarly, the Dewey Decimal system classifies books on the basis of differences in their subject matter. In this system library books are categorized into main classes such as literature, religion, history and geography, and pure science, and then more specific sub-groups within these classes (Seyler 1987, 186-7). Both of these systems involve classifying, sorting, or distinguishing items on the basis of various properties. However, notice that these classifications don't rely on or provide causal information–they don't contain difference-making information in the sense of specifying how changes in one property produce changes in another. They tell one how to sort and identify entities on the basis of identifying various properties, but not what factors can be manipulated to change these properties or what manipulating these properties will produce. In these cases classification requires the successful identification of relevant properties, but it doesn't require knowing what the causes or effects of these properties are. For example, you can know that a plant has various features without knowing what causal relationships these features figure in. This information can be used to classify the plant (and distinguish it from other plants), without explaining why the plant has these features. Of course, these classifications may generate interest in understanding and discovering these causal relationships, but the classifications themselves aren't contingent on this information.[15]

This is all to say that classification is possible without causal information and that the Linnaean

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[15]Of course, some classifications do involve causal information. This makes the "merely" classificatory claim somewhat puzzling, because classification and explanation are not mutually exclusive. I take it that worries about cases of "mere" classification are situations where a system can can classify, but not explain.

and Dewey Decimal systems classify in this manner.[16] Thus, in the context of causal explanation, it makes sense to view these systems as "mere" classifications that don't explain. However, it is incorrect to equate them with the modern periodic table in this sense. The modern periodic table differs from these systems in that it involves classifying elements on the basis of various properties, while also containing information about what causes–and, thus, what explains–these properties. Unlike these classification systems, the modern periodic table contains difference-making information as it specifies how changes in atomic features cause changes in elemental properties. Because of the this, the modern periodic table provides information about how to control and change things in the world, which is not the case with the Linnaean and Dewey Decimal systems. These systems clarify how to identify and sort things in the world, but not what properties can be manipulated to change other properties in the world. This is central to what it means to say that the modern periodic table has causal structure.

This suggests that the modern periodic table is not "merely" classificatory in the way that the Linnaean and Dewey Decimal systems are. However, these concerns about the table being "merely" classificatory are not entirely misguided. In order to motivate this, recall how chemists divide up information in the modern table on the basis of whether it is representative of "descriptive" or "theoretical" chemistry. Descriptive information captures the observable "facts" about chemical and physical properties of elements, while theoretical information involves the relationship between these properties and the atomic-level features that they depend on. It is this atomic level information, which gives the periodic table is explanatory character–these atomic level features explain why the elements have the properties that they have. However, notice that information about atomic structure was completely absent in the earliest periodic tables, as little to nothing was known about this structure at the time. Instead, these tables relied solely on chemical and physical properties of the elements–properties that are still found in the modern periodic table and that are associated with descriptive chemistry. This descriptive information is viewed as the starting point or the "original basis" of the earliest periodic tables and identifying elemental features that chemists ultimately sought to explain (Houten 2009, 13). As Hofman states, "All that looking at natural substances and experimenting with the ways in which they interacted with one another did, in the course of time, throw up a vast amount of empirical information which eventually demanded explanation" (Hofmann 2002, 1). This descriptive information is similar to the information used in classifications such as Linnaean taxonomy and the Dewey Decimal system, because it involves properties of entities of interest, without an understanding of the causal relationships they figure in.

While this descriptive information helped to classify and organize the elements, it didn't explain their properties or why they exhibited periodicity. The absence of such an explanation is reflected by the lack of causal structure in the earliest periodic tables. In these tables, elemental properties were indexed to atomic weight, which was one of the earliest ordering principles. Why isn't atomic weight viewed as an explanation of elemental properties and their periodicity? If atomic weight were causally or explanatorily relevant to elemental properties, it should be possible, hypothetically, to change the properties of an element by altering its atomic weight, but we know this relationship not to be true. Atomic weight doesn't "make a difference" to elements properties in this sense– the atomic weight of an element can be altered by changing its neutron number, but this doesn't change its elemental properties (unless proton and electron number are also changed). When atomic weight was replaced with atomic number, the table began to include atomic level features

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[16]For further support of this first point, see (Ereshefsky and Reydon 2014).

and causal information. The reason for this is that atomic number contains information about proton and electron structure, which does "make a difference" to elemental properties. What this shows is that the periodic table originated as more of a classification system, which only became explanatory as information about what explains elemental properties–viz. atomic level features–was discovered and incorporated into its later versions. It makes sense to hesitate in attributing the table anything more than "mere" classificatory status, because it originated with such a constraint and only figured in explanation once it was modified to include information about atomic structure.

5   Conclusion.   This analysis raises an interesting puzzle. If it is true that the earliest periodic tables lacked causal structure and thus lacked an explanatory role, how were they able to predict the properties of undiscovered elements? The reason for this is that while atomic weight doesn't cause the physical and chemical properties of elements, it is reliably correlated with factors that do–it is reliably correlated with the proton number and electron configuration of the elements. In this manner, it can be used as a fairly accurate tool for ordering elements by incremental changes in their atomic structure, without being a direct measure of this structure itself. A similar rationale guides the identification and search for biomarkers in medicine–goal is to identify factors that are reliably indicators of disease even if they are not disease causes themselves. These factors can be useful for prediction, without figuring in causal explanation of the outcome of interest. Such predictive factors can also be exploited in the discovery of causal structure as seen in the case of the periodic table–in this case the identification of a pattern ultimately took on a causal interpretation. The periodic table is an example of how a system that is originally restricted to classification, description, and prediction, can develop into one that explains. This is likely to be a common developmental trajectory for causal discovery in science. While particular patterns and regularities can point to causal structure actually finding this structure often requires significant work.

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