Explanation, Unification, and What Chemistry Gets from Causation

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I consider a way the concept of causation could be excised from chemical practice, suggested by Kitcher's view that causes are just a subset of unifying patterns which play a particular psychological role for us. Kitcherian chemistry is at first blush well equipped to handle explanatory tasks. However, it would force chemists to accept certain unifying patterns as explanatory, which they do not think are at all explanatory. This might head off some descriptive lines of enquiry and damage prospects for the identification of potentially larger-scale explanations. More important than this, to chemists, it could put them off from finding the explanatory patterns that are true—true because they get at the real structure of the chemical phenomena in the world.

1. Introduction. Chemists use a great deal of causal talk in their professional practice. They deploy causal verbs peculiar to chemistry, like "hydrolyze," "oxidize," and "chelate," as well as commonsense causal verbs like "push," "pull," "bend," and "block." In this paper, I examine the role a concept of causation plays in the practice of chemistry. The mere presence of causal discourse in a field, it might be argued, is no indication that a concept of causation is necessary to the endeavors of that field. Perhaps causal talk in chemistry is gratuitous, in which case it could be excised and chemistry could perfectly well proceed in its researches.

Would a chemistry working in the absence of a concept of causation be able to find out the same things about the world? In the absence of a concept of causation, would there still be a motivation for chemistry to find out what it does find out about the world? In a nutshell, what we are asking is this: If, in a flash, the concept of causation were removed from chemical practice as we know it today, would there be any significant

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‡I am grateful to Peter Godfrey-Smith, Michael Strevens, and Michael Weisberg for helpful discussions and valuable comments on earlier versions of this paper.

Philosophy of Science, 71 (December 2004) pp. 1060–1070. 0031-8248/2004/7105-0036$10.00
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https://doi.org/10.1086/428010 Published online by Cambridge University Press

damaging change in how that practice as a whole went on? Would chemists carry out the same sorts of experiments, study the same sorts of phenomena, and produce the same sorts of information about the world? In other words, would there be any detectable differences in the findings of chemistry or in the practices that generate them to let us know that the concept of causation had been removed other than an absence of causal talk in chemical discourses? And would chemistry be worse off?

To explore what chemistry might look like in the absence of a concept of causation, we will take as our starting point a picture of science without causes suggested by Philip Kitcher in "Explanatory Unification and the Causal Structure of the World."

2. A Kitcherian Picture of Science without Causes. In "Explanatory Unification and the Causal Structure of the World," Philip Kitcher claims that explanation is best understood as a process of unifying the phenomena in the world—basically, a matter of describing the most phenomena using the least patterns. Kitcher further claims that causal claims are grounded in claims about explanatory dependence rather than the other way around. The claim "A caused B" requires first that A explains B.

What makes some, but not all, of our explanations count as causes? Kitcher writes,

> The scientific tradition has articulated some general patterns of derivation—sometimes explicitly considering how the phenomena within a domain could be unified, sometimes only under the tacit guidance of the methodological directive to use the minimum of patterns in generating the maximum of conclusions. Derivations that accord with these patterns become explanatory, and the phenomena described in their conclusions are viewed as objectively dependent on the phenomena described in their premises. So there passes into our common ways of thinking, and our common ways of talking, a view of the ordering of phenomena, and this picture of how phenomena are ordered is expressed, often though not invariably, in our recognition of causal dependencies. (Kitcher 1989, 436)

Explanation (i.e., unification) is a cognitive task of great importance for us. And, Kitcher argues, the project of achieving unification is a big part of what motivates scientific investigations: "The growth of science is driven in part by the desire for explanation, and to explain is to fit the phenomena into a unified picture insofar as we can" (Kitcher 1989, 500). As we engage in this task, we fill our explanatory store with patterns that let us fit more and more phenomena within them. Given the success of these patterns, we come to view it as an objective matter of fact that the explanandum phenomena depend on the explanans phenomena. To the extent that we

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are successful in our attempts to achieve a unification of phenomena, we are inclined to assume nature has a certain structure independent of our explanatory projects which makes the phenomena happen as they do. We believe that our explanations, when they work, get the structure of nature right. As Kitcher claims elsewhere, "The causal structure of the world, the divisions of things into kinds, the objective dependencies among phenomena are all *generated from our efforts at organization*" (Kitcher 1993, 172). The "joints of nature" are only reflections of the stable elements in the organization of our beliefs.

So, Kitcher thinks our causal talk plays a psychological role. However, the purpose of such talk is not just to make us feel good. Rather, it helps us to perform epistemic tasks, to gain and organize knowledge of the world. Our causal talk identifies patterns with demonstrated success in unificatory projects—success so striking that we project these patterns onto the world. The success of these patterns seems like a reason to believe that there is stuff in the world that can be counted on to make the phenomena fit these patterns. And, even if such success cannot logically warrant our belief in causes, it is a psychological fact about us that we do believe in them. Indeed, perhaps beings like us cannot help but project the structure of our explanatory store onto the ordering of phenomena.

But, we need not make this extra step of holding that our patterns have delivered to us the "joints of nature" in order to achieve successful unifications or to find patterns which let us generate many useful conclusions. Kitcher holds up mathematics as an example of a field in which explanation is clearly a matter of unification, but where explanations are not projected onto the world as causes. It seems plausible that other scientists (like chemists) could be tough-minded enough, in the laboratory if not in everyday life, to recognize that successful projects of unification are no proof that the predicates they use in their explanations will continue to be projectable, that the entities they discuss are natural kinds, or that the dependencies they identify are objective. And, like mathematicians, they could still perfectly well develop explanatory schemata that unify the phenomena of interest in the absence of causal talk.

What would a Kitcherian science without causes look like? Given Kitcher's view of causation, losing causation requires a small alteration in our psychology. We would no longer project any of our explanatory patterns onto the world, or believe that their success results from actually capturing natural kinds, projectable predicates, or objective dependencies. Instead, all our explanations would be judged only on how well they unify. A Kitcherian science without causes, then, would just look to develop the smallest set of (most stringent) patterns which allows for the derivation of the most (true) consequences. Patterns that unify in this way explain.

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3. Kitcherian Chemistry. The test of Kitcher's view is whether chemistry would change significantly if it was guided *solely* by the unification approach to explanation, and if these explanations didn't carry with them the assumption of a certain causal structure in the world. Clearly, many explanations in chemistry do unify. But it is possible that some chemical explanations, viewed as perfectly good in a chemistry with causes, will need to be thrown out because they do not unify. Another possibility is that a Kitcherian chemistry will have to accept as explanatory certain unifying patterns which are not taken to be explanatory by the current cause-laden chemistry. It is the second of these possibilities that will end up creating the biggest problem for Kitcher's view.

There is no question that some progress in chemistry is a matter of unification of phenomena. Kitcher himself offers a persuasive chemical example of this sort. He points to the issue of fixed weight ratios in multi-element compounds, identifying the following pattern as a first attempt to answer the question of why a given compound of elements X and Y always has a fixed weight ratio $m : n$ of X and Y:

1. There is a compound Z between X and Y that has the atomic formula $XpYq$.
2. The atomic weight of X is x; the atomic weight of Y is y.
3. The weight ratio of X to Y in Z is $px : qy$ $(= m : n)$. (Kitcher 1989, 446)

This pattern counts as unifying because it explains the weight ratios in terms of the combining ratios of X and Y and their atomic weights. The pattern was subsequently modified to account for why X and Y combined in certain ratios in terms of valence numbers associated with different elements, numbers which allowed prediction of combining ratios. Valence was later fit into the pattern of electronic shell structure within the atoms, a pattern which itself, Kitcher claims, can be fit within quantum mechanical descriptions of atoms and their electron configurations. Kitcher observes:

> These derivations provide a deeper understanding of the conclusions than was given by the simple invocation of the concept of valence because they show us *in a unified way* how the apparently arbitrary valence rules are generated. Moreover, the appeal to the model of the atom enables us to derive instances of (2) from premises that characterize the composition of atoms in terms of protons, neutrons, and electrons. (Kitcher 1989, 446)

Indeed, the task of removing seemingly arbitrary rules, of finding patterns of explanation which could properly be applied to *any* element, rather

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than having to regard each element as a unique sort of entity, seems to have been the bread and butter of much chemical investigation.

It should be noted, however, that some doubt whether this example really exemplifies unification to the extent that Kitcher claims it does. The electronic shells, or orbitals, which are used to unify valency rules are an extremely important pattern in many chemical explanations. Chemists use orbitals (very roughly, places in atoms or molecules where electrons can be) to account for chemical structure and reactivity. Each electron in an orbital in a multi-electron atom has ascribed to it four distinct quantum numbers. Scerri has argued that, although it is widely assumed by chemists that quantum mechanics explains orbitals and the behavior of atoms with particular orbital arrangements, it turns out that quantum mechanics is at odds with the orbital concept and that "[d]efinite quantum numbers for individual electrons do not have any meaning in the framework of quantum mechanics" (Scerri 1991, 122). If this is the case, the last unifying step that Kicher identifies in his chemical example does not, in fact, unify; the electronic shells do not fit within the quantum mechanical descriptions of atoms and their electrons.[1]

Would this serve as an indictment of Kitcherian chemistry? It might, if arguably chemists were preferring a pattern that unifies fewer phenomena over one that unifies more. Indeed, in practice many chemists who deal with issues of structure and reactivity actually use the orbital pattern and merely gesture toward the quantum mechanical pattern without actually using it. But perhaps the real reason for this is that the quantum mechanical pattern (at least in its present form) *fails* to unify the phenomena chemists are most concerned to explain. If this is the case, Kitcherian chemists could easily justify the choice of the orbital pattern.

Kitcher can respond, in almost any case we could find where chemists prefer a pattern that appears to unify less over one that appears to unify more, that there must be some reason behind this choice. Intuitively, chemists would argue that the main reason they might prefer a pattern that does not seem to achieve the best unification is if the pattern which does seem to best unify the phenomena gets the causal structure of the system wrong. But Kitcher has a clear response to this sort of argument. What sort of grounds could chemists have for thinking a pattern gets the structure wrong? This judgment will be based on some sort of experimental or observational result or on some kind of theoretical consideration. If measurements indicate problems with the pattern that seems to unify more, these new measurements, of course, can be counted among the phenomena that chemists desire to unify. And theoretical considerations

1. I do not think, however, the conflict between strict quantum mechanical theory and chemical explanatory patterns is as big as Scerri thinks it is.

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can easily be seen as considerations that seek a global unification of the different specific unifying patterns chemists employ. In any case, once the particulars of the situation are understood, the choice will be seen to be a truly unifying choice.

In the absence of a clear example of chemists preferring a pattern which unifies less to a pattern which unifies more, we can still criticize Kitcherian chemistry if we can find a pattern which unifies well but is not regarded by chemists as explanatory. Just such a pattern can be found in a little-used principle of minimal action in studies of reaction mechanisms.

> Perhaps, the first step in this direction had been taken . . . when A. Muller, in 1886, i.e., at a time when molecular theory was still young, introduced *the rule of least molecular deformation* in the course of chemical transformation. The idea was appealing, and found its place in a number of textbooks as *the principle of minimal structural change*. In its most general terms it was formulated by F. Rice and E. Teller, who in 1938 proposed the principle of least motion (PLM) according to which "Those elementary reactions will be favored that involve the least change in atomic position and electronic configuration." (Hoffmann et al. 1996, 120)

The pattern identified by PLM has a number of virtues. It rests on a clear underlying idea, the minimization of nuclear motions in a reaction. It is simple to make the computations required in applying this principle. Moreover, PLM makes very good predictions of the reaction pathways real chemical systems actually take.

However, given the question of why a reaction proceeds along pathway A rather than pathway B, chemists would not judge "Because pathway A involves the least change in atomic position and electronic configuration" to be an explanatory answer. A proper answer to this question will invoke the stability of the different sets of products along the two competing pathways (which is itself a matter of the energy required to break old bonds and the energy released when new bonds are formed), the type of reactive collision required in each pathway, etc. Nuclear motions in a reaction are *related* to these other structural features, but not in a straightforward way.

Given the simplicity of PLM—one needn't know anything about bond energies for specific types of bonds, about the likelihood of particular sorts of collision, etc.—as long as its predictions are as good as those generated by other means, this would seem to be a pattern that unifies the phenomena well. On this basis, chemists should recognize PLM as explaining the reaction pathways along which chemical reactions occur.

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But good predictions not withstanding, chemists reject PLM as truly explanatory because it does not identify the right causal structure.[2]

This example challenges Kitcher because it identifies phenomena which are symmetrical, but where there is no such explanatory symmetry. The least nuclear motions allow us to predict a reactive pathway just as a particular pathway allows us to predict the nuclear motions involved in going from reactants to products along that pathway. However, where the pathway can explain the nuclear motions, it is denied that the minimization of nuclear motions really explains the pathway taken. But if unification proceeds equally well in either direction, it would seem that Kitcher is committed to saying both count as good explanations.

Kitcher examines a famous everyday case of this sort, the case of the flagpole and its shadow (Kitcher 1989, 484–487). While, given the sun elevation, it is just as easy to calculate the height of the flagpole from the height of its shadow as it is to calculate the height of the shadow from the flagpole, common sense judges that the height of the flagpole explains the height of the shadow in a way the height of the shadow does not explain the height of the flagpole. Despite the apparent symmetry, however, Kitcher argues that there is a real asymmetry in how good a unification each sort of explanation provides.

The most obvious problem with a pattern that seeks to explain the heights of objects in terms of the heights of their shadows is that there are conditions in which such objects do not cast shadows—e.g., because they are not illuminated, or are not opaque to light, or are microscopic, or have internal light sources—yet still have heights. Unless this problem is addressed, the shadow pattern can only account for the height of illuminated objects (which are also medium-sized, not transparent, and without light sources of their own), and thus cannot unify as many phenomena as can origin-and-development patterns[3]. Recasting the pattern in terms of the height of the shadow an object has a *disposition* to cast in particular circumstances results in a disjunctive list which lumps together a heterogeneous collection of dispositions:

> *x* has the disposition to cast a shadow if illuminated by a light source or *x* has the disposition to produce an absorption pattern if suitably coated and irradiated or *x* has the disposition to cast a shadow if *x* is covered with opaque material or *x* has the disposition to cast a shadow if *x* is sectioned and unrolled or *x* has the disposition to cast

2. Note that chemists do not need to have a fully worked out description of the right causal structure in order to identify the nuclear motions as the wrong causal structure.

3. These are patterns that make reference to the intentions of a designer, or, in the case of natural objects, to facts about how their careers affect their sizes.

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> a shadow after x has been treated to block its own light sources or . . . (Kitcher 1989, 486–487)

This disposition is not homogeneous. The dispositional-shadow patterns will be gerrymandered relative to what Kitcher identifies as origin-and-development patterns they stand in for—they are an illegitimate fusing of many distinct patterns into one. Such a fusion is especially suspect if a simpler, nondisjunctive, homogeneous pattern is available for the explanatory task at hand. The dispositional-shadow patterns will result in a worse unification of the full set of phenomena, since they actually require more patterns to account for the same phenomena.

As Kitcher sees it, the height of objects should really be explained in terms of how they were designed and constructed, or how they developed and persisted by way of natural processes—i.e., they are best explained with origin-and-development patterns. Such patterns *could* be included in the set which seeks to explain object heights in terms of shadow heights, but this set would also need a pattern "that derives conclusions about dimensions from premises about the characteristics of shadows" (Kitcher 1989, 485). In other words, explaining the object height from the shadow height requires more patterns than the explanation in the other direction. So this approach to an explanation which starts with the shadow height unifies less well that the explanation which starts with the object height.

In general, Kitcher thinks such problems of apparent symmetries will be dissolved by identifying the more fundamental features.

> Explanation proceeds by tracing the less fundamental properties of things to more fundamental features, and the criterion for distinguishing the less from the more fundamental is that appeal to the latter can be made on a broader scale. Thus an attempt to subvert the order of explanation shows up in the provision of an impoverished set of derivations . . . or in the attempt to disguise an artificial congeries of properties as a single characteristic. (Kitcher 1989, 487)

Chemists would agree that PLM fails as an explanation for why a reaction occurs along one pathway rather than another because it fails to invoke the more fundamental features. What chemists think makes a feature more fundamental, however, is not precisely the criterion Kitcher identifies. As a matter of fact, they would expect that appeal to more fundamental features generally can be made on a broader scale, but this is because they are the features that make the phenomena happen the way they do. And, on Kitcherian grounds it is not as easy to defeat the PLM pattern as the shadow height pattern. For one thing, although an unilluminated flagpole still has height—even in the absence of a shadow—we cannot have a chemical reaction without there being motion of the nuclei in the

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molecules reacting. Thus, PLM does not force an impoverished set of derivations. For another thing, the pattern the chemists identify as the wrong one here looks much less gerrymandered than the right one. Tracking the motions of nuclei is simple compared to determining stabilities of different molecules, energies of different bonds, what is required of reactive collisions, etc. Nuclear motion lends itself to a very clean pattern. In contrast, the considerations chemists identify as important here would seem hard to capture in a single homogeneous characteristic. Why, then, shouldn't nuclear motions be identified as the more fundamental property? As far as the unification approach is concerned, it should be. Since chemists deny that it is, their explanations must not be explanations in virtue of their unifying power.

To be fair, Kitcher has another move available here. He could argue that PLM failed to unify chemical phenomena, not by virtue of any flaw with the PLM pattern itself, but because it did not fit well with the other explanatory patterns that were part of chemistry when it was introduced. However, the chemist's objection to PLM is more basic: regardless of how well or badly PLM might have fit with other patterns, PLM doesn't identify causal structure. That pathway A involves the least change in atomic position and electronic configuration simply does not bear the right structural relation to a chemical reaction's proceeding along pathway A rather than pathway B. In view of this shortcoming, PLM was never a serious candidate for an explanatory pattern, even before its fit with other explanatory patterns was considered.

Would chemistry be better off if it adopted a Kitcherian approach? This translates to the question of whether the goal of chemistry is, or ought to be, just to find patterns that best unify the phenomena of interest, or to get a grip on structure of the world that is more than a reflection of the organization of chemists' beliefs. There certainly exist appealingly simple patterns, like PLM, which chemists could adopt. Accepting such patterns as explanatory would provide "answers" to questions of interest and wrap up certain lines of enquiry. But, lurking in the chemists' practice is an awareness that the world could turn out to be messier and less unified than some of the models our minds could construct of it. And, this awareness appears to drive a great deal of chemical investigation.

If PLM were regarded as a good explanation in chemistry, the need for chemists to pursue information about the stabilities of molecules, bond energies, reactive collisions, and the like, would be less pressing. Tracking such features is the sort of project that arises when the features are invoked by explanatory patterns, or if one thought they might be helpful in identifying *truly* explanatory patterns (perhaps because an existing pattern that unifies doesn't seem to invoke causally relevant features). So, ruling on whether patterns are explanatory based solely on Kitcher's unification

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standard, which would judge a pattern like PLM as explanatory, might put chemists off the search for the actual patterns of structural connections that are really at work here—the patterns that unify *because* they get at the true causes. Identifying these seems more likely to be the starting point for further meaningful investigations. PLM may do a good enough job at unifying reaction pathway phenomena, but at this point its unifying power reaches a dead end. Ultimately, more complicated features than nuclear motions may let us unify more. But, rather than seeking these more complicated features and the unifying patterns into which they fit, chemists may be lulled into a pattern which achieve a local—but not global—unificatory optimum. If any good unification is a stopping point, more complicated competing patterns may be discarded too soon.

It is certainly the case that good chemical theories are expected to unify phenomena, but this is because they aim to get the causal structure right—and this structure is thought to underlie a great many diverse chemical phenomena. Moreover, looking for ways to capture the most known phenomena under the least number of stringent patterns might entrench mistaken ways of understanding the world. In turn, this could rule out more complex patterns that suggest other potentially fruitful ways of organizing phenomena, different experiments that could generate new phenomena. And in the end, chemists want chemistry to yield true stories about the connections between chemical substances in the world, not just about connections between chemical phenomena in our *understanding* of the world. They are seeking information about the connections between physical structure, not about the structures created by our cognitive efforts at organization.

4. Conclusion. This paper has considered a way the concept of causation could be excised from chemical practice and argued that this excision would create significant changes in chemistry. Kitcherian chemistry is at first blush well equipped to handle explanatory tasks. However, it would force chemists to accept certain unifying patterns, like PLM, as explanatory. This might head off some descriptive lines of enquiry and damage prospects for the identification of potentially larger-scale explanations. More important than this, to chemists, it could put them off from finding the explanatory patterns that are *true*—true because they get at the real structure of the chemical phenomena in the world. Chemistry is a bundle of projects of description, prediction, control, and explanation, projects which are seen as interacting in important ways. To move all of these projects forward, chemists rely on a concept of causation which looks for structural connections in the world. These connections, no matter how simple or complicated, are what explain phenomena. Capturing them precisely in models improves predictive power and allows chemists to plot

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particular interventions which will produce the desired results. And the desire to see these connections—to characterize the relevant structural features of cause and effect as well as possible—is what motivates novel measurements on chemical systems.

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