

# Epistemic Dependence & Understanding: Reformulating through Symmetry

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## ABSTRACT

Science frequently gives us multiple, compatible ways of solving the same problem or formulating the same theory. These compatible formulations change our understanding of the world, despite providing the same explanations. According to what I call ‘conceptualism’, reformulations change our understanding by clarifying the epistemic structure of theories. I illustrate conceptualism by analyzing a typical example of symmetry-based reformulation in chemical physics. This case study poses a problem for ‘explanationism’, the rival thesis that differences in understanding require ontic explanatory differences. To defend conceptualism, I consider how prominent accounts of explanation might accommodate this case study. I argue that either they do not succeed, or they generate a skeptical challenge.

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## 1 Introduction

Throughout science and engineering, we often have multiple, compatible methods for answering explanatory why-questions. Paradigmatic examples include various formulations of classical mechanics and quantum mechanics, along with common variable

changes such as Laplace and Fourier transforms. In physics and chemistry, ‘dispensable symmetry arguments’ provide another class of examples. In such cases, we can use a symmetry argument, but we do not have to: alternative elementary methods suffice. Both these elementary and symmetry-based methods answer many of the same explanatory why-questions, while agreeing on the way the world is. In all of these cases, compatible formulations provide—in some sense—the same explanation, despite formulating these explanations very differently. These differences in formulation lead to objective and non-pragmatic differences in understanding. For short, I will call these kinds of differences in understanding ‘intellectual differences’. This essay aims to provide a positive account of how compatible formulations generate intellectual differences, focusing on dispensable symmetry arguments in particular.

Compatible formulations pose a problem for ‘explanationism’, a position commonly defended or assumed by accounts of scientific explanation.<sup>1</sup> Explanationism claims that intellectual differences require differences in ontic explanatory information, such as nomological or causal structure. According to explanationism, a theory or problem-solving procedure provides an objective difference in understanding if and only if it represents a corresponding ontic difference. Against explanationism, I will argue that compatible formulations provide intellectual differences without any concomitant ontic differences. They thereby pose a counterexample to explanationism.

If not through explanatory differences, how can we account for the intellectual differences that compatible formulations provide? To answer this question, I will introduce and defend ‘conceptualism’, an account of scientific understanding that addresses the deficiencies of explanationism.<sup>2</sup> Conceptualism accommodates intellectual differences between reformulations by appealing to differences in their epistemic or organizational structure. Concretely, this structure is constituted by what I will call ‘epistemic dependence relations’ (EDRs). These characterize what we need to know or what suffices to know to solve a problem, including answering why-questions. I will argue that differences in epistemic dependence relations generate the striking intellectual differences we see between compatible formulations of the same theory.

I begin in Section 2 by clarifying my target: explanationism. Remaining neutral on whether explanations are best understood ‘ontically’ or ‘epistemically’, the thrust of my challenge will be that ontic differences alone cannot account for all the myriad intellectual differences we see in science. Section 3 articulates conceptualism as a framework for analyzing scientific understanding. I illustrate conceptualism with some brief examples. Section 4 proceeds to develop my account through one of the simplest yet sufficiently rich examples of dispensable symmetry arguments, taken from crystal field theory—an idealized model in chemical physics and inorganic chemistry. I introduce three compatible formulations of crystal field theory: the elementary, non-group-theoretic, and group-theoretic approaches. Each approach references the same ontic explanatory features, while nonetheless leading to different understandings of the

<sup>1</sup> 20th century proponents include Hempel ([1965], pp. 337, 488), Railton ([1981], pp. 247–8), and Salmon ([1989], pp. 120, 161). 21st-century proponents include Woodward ([2003], pp. 86, 223) and Strevens ([2008], pp. 117, 154). Khalifa ([2012], [2017]) has defended a particularly thorough characterization of explanationism.

<sup>2</sup> I call this view ‘conceptualism’ to emphasize the role that concepts play in theory reformulation and understanding. By ‘concepts’, I intend what Kenneth Manders ([2008], [unpublished]) calls ‘expressive means’. These include the mathematical, linguistic, diagrammatic, and notational resources we use to express theories. Despite some interesting analogies, I do not intend to endorse scholastic or early modern ‘conceptualism’ about universals.

phenomena. These formulations thereby provide a counterexample to explanationism. In Sections 5 and 6, I consider and rebut two objections against conceptualism. The first argues that existing accounts of explanation can easily accommodate the intellectual differences I identify. Considering two leading accounts of causal explanation, I show that this is not the case. The second objection argues that what I am calling cases of the same explanation are in fact different explanations and can be accommodated as such. I argue that this response faces a skeptical challenge that conceptualism avoids.

## 2 Explanationism

Recent accounts of understanding sometimes allege that traditional theories of explanation neglected scientific understanding (de Regt [2017], p. 16). Regardless of the fairness of this charge, both proponents and opponents of traditional accounts of explanation agree on a central schema connecting understanding with explanation. According to this ‘received view of understanding’, understanding why a phenomenon occurs consists in grasping an explanation of that phenomenon.<sup>3</sup> By tightly connecting understanding-why with explanation, the received view transforms even traditional accounts of scientific explanation into a minimal account of scientific understanding.

The received view suggests that there are only two possible sources for differences in understanding why a phenomenon occurs. These correspond to pragmatic vs. non-pragmatic differences in understanding-why, respectively. First, on the pragmatic side, these differences can spring from variation in how agents grasp explanations. Most recent accounts of scientific understanding have focused their attention here, arguing that understanding involves special skills or abilities for grasping explanations.<sup>4</sup> This feature of understanding-why is inherently pragmatic because it depends on features of agents. It is ideally intersubjective but often idiosyncratic.<sup>5</sup> Secondly, on the non-pragmatic side, differences in understanding can arise from grasping different explanatory information, such as different states of affairs or other ontic features of reality. Differences in ontic explanatory features straightforwardly provide objective and non-pragmatic differences in understanding. Insofar as traditional accounts of explanation have been interested in scientific understanding, it has been in this second sense.

This traditional focus leads to ‘explanationism’, which claims that all objective and non-pragmatic differences in understanding arise from differences in the ontological content represented or picked out by explanations.<sup>6</sup> Phrased as a biconditional, ex-

<sup>3</sup> For statements of this position see Strevens ([2013]), Khalifa ([2017], pp. 16–8), de Regt ([2017], p. 23), and Potochnik ([2017], pp. 123–4).

<sup>4</sup> See, for instance, de Regt and Dieks ([2005]), de Regt, Leonelli et al. ([2009]), Grimm ([2010]) and Hills ([2016]). Along with scientists’ cognitive abilities, Potochnik’s account of understanding relies on scientists’ research interests, background information, space-time location, and psychological characteristics ([2017], p. 100).

<sup>5</sup> de Regt ([2017], p. 44) argues that the pragmatic nature of skills does not entail that the resulting understanding is problematically subjective. Potochnik makes a similar claim regarding her account of understanding, where ‘features of scientists themselves, including their interests and intentions, influence what generates understanding’ ([2015b], p. 74). However, these pragmatic features are certainly less objective than explanatory differences in understanding and the epistemic differences I consider in Section 3.

<sup>6</sup> What I am calling ‘explanationism’ might more precisely be called ‘ontic explanationism’. It is distinct from weaker positions seeking to reduce intellectual differences to both ontic and non-ontic features of explanation.

planationism contends that an intellectually significant difference occurs if and only if there is a corresponding ontic explanatory difference. Such ontic differences comprise differences in the worldly features responsible for the phenomenon of interest, such as laws of nature, causes, mechanisms, grounds, and difference-makers. As already noted, explanations that appeal to different ontic features straightforwardly lead to intellectual differences; this establishes one direction of the explanationist biconditional. Many accounts of explanation also treat such ontic differences as necessary for an intellectual difference, establishing the second direction. For instance, according to Hempel, ‘all scientific explanation [...] seeks to provide a systematic understanding of empirical phenomena by showing that they fit into a nomic nexus’ ([1965], p. 488). Similarly, Trout argues that the only kind of understanding that we should focus on is an objective kind coming from explanations, namely ‘the state produced, and only produced, by grasping a true explanation’ ([2007], pp. 584–5). Strevens defends this same claim ([2008], p. 3), arguing further that ‘science understands a phenomenon just in case it can provide a standalone explanation of the phenomenon’, namely ‘an explanation that is complete, that is not missing any of its parts’ ([2008], p. 117). Woodward also frequently makes remarks that are congenial to explanationism, such as his claim that ‘once we have been given information about the complete patterns of counterfactual dependence [...] it appears that nothing has been left out that is relevant to understanding why matters transpired as they did’ ([2003], p. 86). On this traditional conception, non-ontic differences—such as differences in the mode of presentation of an explanation—are seen as merely pragmatic.

As a thesis about the relationship between understanding and explanation, explanationism is not itself an account of explanation. As such, there are a great variety of explanationists, distinguished by their preferred accounts of scientific explanation. This includes defenders of both ‘ontic’ and ‘epistemic’ conceptions of explanation. As characterized by Salmon, the ‘ontic conception’ views explanations as objective and non-pragmatic features of the world that exist independently of explanatory arguments or discoveries ([1989], p. 133). In this ontic sense, an explanation is ‘a relation among features of the world’, namely the features ‘that cause, produce, or are otherwise responsible for the phenomena we seek to explain’ (Craver [2014], pp. 30, 36). In contrast, the ‘epistemic conception’ of explanation focuses on the representation of these ontic features. The epistemic conception privileges ‘explanation-texts’ or ‘explanatory arguments’ as being explanations proper. Nevertheless, as Craver ([2014]) has argued, these explanation-texts must still refer to ontic explanatory information to discharge their central normative duty of distinguishing explanations from non-explanations. Thus, at least for my purposes, the debate between epistemic and ontic accounts is merely terminological.<sup>7</sup> For instance, the three approaches to crystal field theory discussed in Section 4 provide the same explanation in an ontic sense, but of course they each provide a different explanation-text (and hence a different epistemic explanation). What matters is that they agree on the ontic explanatory information, and it is immaterial if we characterize this information within an ontic vs. an epistemic conception of explanation. Hence, I intend to argue against any account of explanation that takes grasping ontic explanatory information as necessary and sufficient for objective and non-pragmatic differences in understanding.

Pragmatic accounts of understanding also aim to challenge explanationism, but they

<sup>7</sup> Even defenders of the epistemic conception, such as Bokulich, agree that ‘ontic constraints still play a central role’ in explanation ([2018], p. 794).

are dialectically less effective for this purpose. Following Elgin ([2004]), Potochnik ([2017], p. 95) rejects the traditional factivity assumption that understanding requires truth, requiring instead that the relevant claims be ‘true enough’. According to Potochnik, whether a scientific claim is true enough to provide understanding depends partly on pragmatic considerations, including ‘the purpose of the research to which it contributes’ ([2017], p. 96). Ultimately, Potochnik extends these pragmatic considerations to explanation, arguing that the audience ‘helps determine the nature of the explanatory facts, that is, the ontic explanation’ ([2017], p. 128).<sup>8</sup> However, it is unlikely that explanationists would willingly grant the assumptions of a framework where ontic explanation depends on features of agents. In general, explanationists are simply less interested in more subjective, pragmatic conceptions of explanation or understanding.<sup>9</sup> Additionally, Khalifa ([2012]) has noted that accounts of explanation already implicitly involve another pragmatic dimension of understanding, namely the use of skills. Obviously, agents require some cognitive abilities to construct and grasp explanations. For instance, Woodward’s manipulationist account of causal explanation implicitly references the relevant skills for constructing and analyzing what-if-things-had-been-different questions. Thus, explanationism already seems compatible with skills-based accounts of understanding. In contrast, I intend to rebut explanationism on its own terms by privileging its preferred sense of understanding. I will argue in Section 3 that explanationism is incomplete even with regards to these objective and non-pragmatic differences in understanding. Whereas pragmatic accounts of understanding criticize explanationism for reasons it might not find compelling, conceptualism points out a shortcoming that even explanationists should regard as important.

### 3 Conceptualism

The chief shortcoming of explanationism is its failure to accommodate a common occurrence in science and engineering. In these disciplines, we often have at hand multiple compatible formulations of the same underlying explanatory features. Explanationism does not account for how compatible formulations sometimes provide different understandings, despite referencing the same explanatory information. To address this oversight, I will propose an alternative account of understanding: conceptualism. Conceptualism agrees with explanationism that ontic explanatory differences suffice for intellectual differences. It is clearly intellectually significant to find out that some ontic feature plays an explanatory role. However, against explanationism, conceptualism holds that these explanatory differences are not necessary for intellectual differences. Instead, certain kinds of differences in the organization of explanatory information are intellectually significant.<sup>10</sup> This kind of understanding has been neglected by both accounts of

<sup>8</sup> Morrison ([2000], pp. 28–9) makes a similar claim that the explanatory power or acceptability of an explanation depends partly on the scientific community or even individual scientists.

<sup>9</sup> Hempel ([1965], pp. 425–32) discusses pragmatic features of explanation at length, noting that although they are important, they can be separated from his non-pragmatic account of explanation and understanding. He remarks that ‘to propound those [non-pragmatic] models is therefore neither to deny the pragmatic “dimension” of explanation nor to belittle its importance’ ([1965], p. 426).

<sup>10</sup> In a footnote, Railton ([1981], p. 256) notes that not only the content of an explanation but also ‘the *organization* of its components’ can be important. Salmon ([1989], p. 131) makes a similar point. However, whereas Railton and Salmon both view this organizational information as ‘explanatory information’, conceptualism denies that it necessarily matters for explanation, a claim I defend in Section 5.

scientific explanation and recent accounts of understanding, the former owing to their focus on ontological features, the latter owing to their focus on pragmatic features of agents.

The intellectual differences that motivate conceptualism arise whenever we have two or more compatible ways of formulating a theory or solving a problem. By ‘compatible’, I mean that the formulations do not disagree about the way the world is: they are logically and physically consistent. Believing one does not preclude us from believing the others; we can consistently believe them all.<sup>11</sup> Examples include both various formulations of classical mechanics (Lagrangian, Hamiltonian, and Hamilton-Jacobi) and quantum mechanics (wave mechanics, matrix mechanics, path integrals, and density matrices). Within a shared domain of problems, compatible formulations do not present ontic explanatory differences. Nevertheless, each formulation provides a distinctive way of understanding the world and in particular of understanding why phenomena occur. Dispensable symmetry arguments in physics and chemistry provide another kind of compatible formulation. In these cases, we have an elementary formulation that eschews symmetries along with at least one formulation that takes advantage of symmetry (possibly through the mathematical language of group representation theory). Both the elementary and the symmetry-based approaches provide different understandings of the same phenomena, despite describing the same ontic explanatory information. Section 4 illustrates this moral in detail. Other examples of dispensable symmetry arguments include the Wigner–Eckart matrix element theorem, symmetry-based explanations of hydrogen’s energy spectrum, and selection rules in spectroscopy.

What constitutes the non-explanatory intellectual differences that compatible formulations provide? Conceptualism locates these differences in how formulations organize explanatory information, rather than in that information itself. Different formulations package the same ontic explanation within dramatically different epistemic structures. Conceptualism formalizes these organizational differences through the notion of ‘epistemic dependence relations’ (EDRs). Epistemic dependence relations characterize what we need to know or what suffices to know in order to solve particular problems, such as answering explanatory why-questions. The *relata* related by an EDR are the inputs needed (or sufficient) for obtaining knowledge of a given output. In the context of explanations, the inputs are typically *explanans*, with the output being a given *explanandum*.

EDRs are useful because they succinctly characterize organizational differences between formulations. To illustrate this, consider a toy example from arithmetic: calculating the absolute value of the product of two integers,  $|xy|$ .<sup>12</sup> One formulation of this problem involves first calculating  $x$  times  $y$  and then taking the absolute value. This involves knowing the signs of both integers. Alternatively, one could reformulate this problem by recognizing that the absolute value of a product equals the product of the absolute values:  $|xy| = |x||y|$ . In this formulation, we don’t need to know the sign of each integer. It suffices to know their absolute values. Hence, this reformulation uses different epistemic dependence relations to solve the problem. Conceptualism claims that in cases like this, we not only solve the problem differently, we also gain a different

<sup>11</sup> Bokulich ([2013]) considers how different models of geomorphology can produce different understanding of the same phenomena, but these models are competing, rather than compatible. Similarly, Potochnik ([2015b], p. 77) discusses competing approaches to both human sexuality and population biology.

<sup>12</sup> I thank Dave Baker for suggesting this example.

understanding of the solution.

Section 4 will show how dispensable symmetry arguments affect understanding through two general kinds of epistemic dependence relations: modularization and unification. ‘Modularization’ occurs when a formulation breaks a problem or a why-question into separately treatable sub-problems. Modularizing a problem shows that some parts of it can be treated independently of other parts. ‘Unification’ occurs when a single derivation and its solution applies to a family of different systems that all display shared behaviour. For instance, organizing systems into symmetry-based families unifies them. Noticing such epistemic dependence relations changes our understanding of a given phenomenon by clarifying what suffices or is necessary to understand it. Furthermore, this kind of intellectual difference does not rely on any particular details about agents, skills, or capacities. We can thereby abstract away agents, analyzing EDRs as objective, agent-independent features of a theory formulation.<sup>13</sup>

Compatible formulations pose a problem for explanationism only if these intellectual differences concern understanding-why, rather than some other kind of understanding. Hence, it is incumbent upon conceptualism to argue that different EDRs lead to differences in understanding-why. To see this, note first that reformulating a theory changes our understanding of that theory. Moreover, it is through theories or problem-solving procedures that we answer explanatory why-questions and thereby acquire understanding-why. Hence, by changing our understanding of the theory used to provide an explanation, EDRs affect the resulting understanding-why. Indeed, some epistemologists have argued that understanding-why deals directly with grasping the relations that hold between various propositions in a subject matter. In particular, this involves situating a proposition within a broader theory or methodology. For instance, Zagzebski has argued that understanding ‘involves seeing the relation of parts to other parts and perhaps even the relation of part to a whole’ ([2001], p. 241). Similarly, Elgin has argued that understanding a proposition is a matter of integrating it within a coherent and comprehensive body of knowledge ([2007]). She notes in particular that having ‘more non-trivial inferential connections between propositions’ constitutes greater understanding ([2007], p. 36). Articulating EDRs certainly clarifies these inferential connections. For at least these reasons, epistemic dependence relations matter for understanding-why.<sup>14</sup>

Of course, not all differences in the organization of explanatory information are intellectually significant. Many differences are merely convenient, conventional, or otherwise pragmatic. In such cases, the alternative formulations constitute ‘trivial notational variants’. For instance, many scientists and engineers prefer working in right-handed rather than left-handed Cartesian coordinates systems. This difference in handedness is merely convenient rather than intellectually significant. We do not acquire an objectively different understanding of a problem by reformulating it in a mirror-image coordinate system. Similarly, many physicists prefer using Einstein summation convention for expressing equations, but laboriously writing out the suppressed summation symbols would not lead to objective differences in understanding. Conceptualism distinguishes these trivial notational variants from ‘nontrivial reformulations’, where

<sup>13</sup> This non-agentive approach to understanding captures one facet of understanding that does not depend on agents, allowing agent-dependent features to be subsequently added. Ultimately, psychological ‘grasping’ should be treated naturalistically, sensitive to the concerns of Trout ([2007]).

<sup>14</sup> Hunt ([forthcoming]) further defends this claim, along with providing an independent argument against explanationism by appealing to theoretically equivalent formulations.

only the latter provide intellectually significant differences. This distinction calls for a criterion: on what basis can we separate cases of reformulations into intellectually trivial vs. nontrivial formulations? Conceptualism proposes that differences in EDRs are sufficient for generating nontrivial reformulations.<sup>15</sup> For as we have seen, different epistemic dependence relations lead to differences in understanding-why. In contrast, since trivial notational variants provide the same EDRs, they do not provide objective and non-pragmatic differences in understanding.

Having motivated the need for a positive account of compatible formulations, the rest of this essay defends conceptualism by applying it to a paradigmatic instance of reformulation. The use of symmetry arguments in crystal field theory shows how reformulating a problem-solving procedure can lead to differences in understanding phenomena without requiring explanatory differences. My account of how symmetry arguments contribute to understanding involves disentangling three compatible formulations. First, there are ‘elementary approaches’, which proceed on a case-by-case basis without appealing to symmetry. Often in physics and chemistry, elementary approaches involve a brute-force application of perturbation theory to each system of interest. Secondly, in ‘non-group-theoretic approaches’, we make the system’s symmetries explicit but without using an abstract language for symmetry. Finally, ‘group-theoretic approaches’ take advantage of symmetry by using the more sophisticated mathematics of group representation theory. In Section 4.3, I show how at each stage in this process of reformulation, we acquire different EDRs, leading to different understandings of the phenomena. Since these intellectual differences do not arise from explanatory differences, they pose a counterexample to explanationism.

#### 4 A Case Study from Crystal Field Theory

Crystal field theory provides an idealized model for describing properties of coordination complexes. These consist of a positively charged metal ion surrounded by negatively charged or polarized species known as ‘ligands’. Figure 1 shows two examples: nickel(II) hexahydrate and nickel(II) hexammine. Both complexes comprise a  $Ni^{2+}$  ion bound to six ligands occupying the vertices of an octahedron (see Figure A.1). Often, the colour of coordination complexes changes according to the ligands bound to the metal ion. Whereas nickel(II) hexahydrate is green, nickel(II) hexammine is purple. Chemists use crystal field theory to understand these differences in colour, along with differences in thermodynamic and magnetic properties (Figgis and Hitchman [2000]).

To explain these properties, chemists focus on how the valence electrons of the metal ion change when surrounded by ligands. For instance, an isolated  $Ni^{2+}$  ion has eight valence electrons that occupy five energetically ‘degenerate’ orbitals, meaning that they have the same energy (depicted by the left side of Figure 2).<sup>16</sup> Surrounding  $Ni^{2+}$  with ligands breaks this degeneracy, causing previously degenerate orbitals to ‘split’ into new energy levels with new degeneracies. Crystal field theory describes this splitting phenomenon by treating ligands as point dipoles that create an electrostatic ‘crystal’ field, perturbing the energy levels of the metal ion.<sup>17</sup> In the case of nickel(II)

<sup>15</sup> Indeed, it is plausible that a difference in epistemic dependence relations is necessary for an intellectually significant difference. It is difficult to imagine that two formulations could be significantly different without providing at least one different epistemic dependence relation.

<sup>16</sup> Atomic orbitals are one-electron wavefunctions used to approximate the overall state of an atom or molecule.



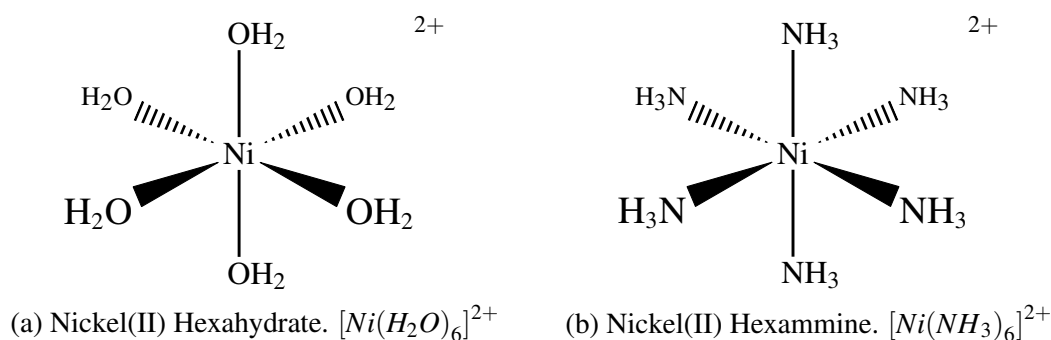


Figure 1: Octahedral coordination complexes

hexahydrate, the fivefold degenerate valence orbitals split into two new levels that are two-fold and three-fold degenerate, shown in Figure 2. The difference between these energy levels is denoted ' $\Delta_O$ '. Electronic transitions between these levels help explain the characteristic colours of many metal complexes.

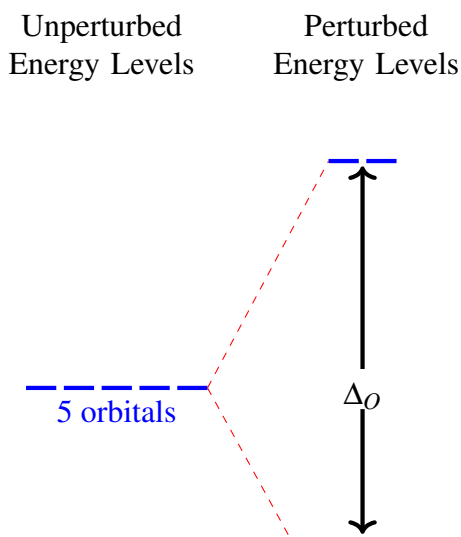


Figure 2: Splitting of valence orbitals in an octahedral crystal field

Crystal field theory solves three connected problems about electronic structure, each posing its own why-question. The 'splitting problem' is to determine how many new energy levels form from a previously degenerate energy level. The 'degeneracy problem' is to determine how many orbitals constitute each new level, i.e. its degeneracy. Finally, chemists estimate the energy difference  $\Delta_O$  by finding the eigenvalues of each new energy level, giving rise to the 'eigenvalue problem'. For brevity, I will refer to these three problems collectively as 'the crystal field theory problem'. Section 4.1 begins by sketching three different compatible approaches to explaining this phenomenon. Armed with these approaches, Section 4.2 develops them as a counter-example to explanationism. They provide different ways of understanding crystal field theory without concomitant explanatory differences. Finally, in Section 4.3, I show

<sup>17</sup> Crystal field theory idealizes interactions as purely ionic, neglecting chemical bonds between the metal ion and ligands. It underlies more sophisticated models such as ligand field theory (Cotton [1990], p. 254). For simplicity, I suppress additional philosophical issues pertaining to idealization, since the same questions about reformulations arise outside this context.

how conceptualism easily accommodates the intellectually significant features of this case study. The group-theoretic approach modularizes and unifies crystal field theory by providing distinctive epistemic dependence relations. Throughout, I will focus on nickel(II) hexahydrate as a concrete example, although my discussion applies more generally.

### 4.1 Three approaches to crystal field theory

The first approach to crystal field theory is ‘elementary’ in the sense that it makes no explicit appeal to symmetry properties of the molecule. Instead, it relies entirely on perturbation theory, approximating the eigenvalues of the coordination complex relative to those of the unperturbed, free metal ion. We begin by measuring the electrostatic potential, representing it as a perturbation operator  $H'$ . The eigenvalues of this perturbation operator provide a first-order correction to the known energy states of the free metal ion. We calculate these eigenvalues by solving a ‘secular equation’ (Equation A.1), which functions as the relevant law-like statement for this explanation. With the eigenvalues in hand, the splitting and degeneracy follow immediately. The number of distinct eigenvalues and their degeneracies corresponds to the number of new energy levels and their degeneracies. For nickel(II) hexahydrate, we obtain two distinct eigenvalues that are three-fold and two-fold degenerate. Figure 3a represents the schematic structure of this approach.<sup>18</sup>

The second approach relies on the same schematic structure: it uses perturbation theory to calculate the eigenvalues, from which the energy-level structure follows. However, we now take explicit advantage of symmetry, although without using the formal apparatus of group representation theory. Hence, I will refer to this first symmetry-based formulation as the ‘non-group-theoretic approach’.<sup>19</sup> Unlike the elementary approach, we begin by characterizing the electrostatic potential in terms of the symmetry of the coordination complex. For nickel(II) hexahydrate, the resulting potential (Equation A.2) applies to any coordination complex with six ligands at the vertices of an octahedron. We then follow the same procedure as the elementary approach but now using this symmetry-based potential. Solving the secular equation leads to two distinct eigenvalues:  $\lambda_1 = -\frac{2}{5}\Delta_O$  (three-fold degenerate) and  $\lambda_2 = \frac{3}{5}\Delta_O$  (two-fold degenerate), expressed in terms of their energy difference  $\Delta_O$ . As in the elementary approach, the splitting and degeneracy follow immediately from these eigenvalues. The two distinct eigenvalues and their degeneracies entail that two new energy levels form that are three-fold and two-fold degenerate.

In the third approach, we take advantage of not only symmetry but also the formal apparatus of group (representation) theory. This ‘group-theoretic approach’ extensively reformulates the crystal field theory problem, leading to a dramatically different organizational structure, shown in Figure 3b.<sup>20</sup> Rather than deduce the splitting and degeneracy from the eigenvalues (as in the other two approaches), we now determine them without solving a secular equation. To begin, we identify the symmetry groups of both the free metal ion and the coordination complex. An unperturbed metal ion,

<sup>18</sup> See Appendix A for a more detailed account of each formulation.

<sup>19</sup> See Dunn et al. ([1965], pp. 9–16) and Figgis and Hitchman ([2000], pp. 30–8) for detailed applications of this approach.

<sup>20</sup> Adopting an abbreviation common throughout physics and chemistry, ‘group theory’ will typically refer more precisely to ‘group representation theory’. See Appendix A.3 for details.

such as  $Ni^{2+}$ , is invariant under arbitrary rotations, so its symmetry group is the rotation group. In the case of nickel(II) hexahydrate, since its ligands sit at the vertices of an octahedron, its symmetry group is accordingly the octahedral group.

The next step is to extract information about the energy levels from these symmetry groups, using the mathematics of group representations. Recall from Figure 2 that our task is to determine how the initially five-fold degenerate valence orbitals of  $Ni^{2+}$  rearrange into the new energy-level structure of the coordination complex. For both the initial and final systems, each distinct energy level corresponds to a ‘representation’  $\Gamma$  of the corresponding symmetry group. Hence, to determine the new splitting and degeneracy, it suffices to determine how many representations of the octahedral group occur (corresponding to the number of new energy levels) and their dimensions (corresponding to the degeneracy of each energy level). First, we determine the representation of the rotation group associated with the nickel ion’s valence orbitals. We then exploit a precise mathematical relationship characterizing how this initial representation from the rotation group ‘decomposes’ into a sum of new representations from the octahedral group. Executing a simple algorithm (demonstrated in Appendix A.3), we find that the initial representation decomposes into two new representations of dimensions two and three. This solves the splitting and degeneracy problems: two new energy levels form that are, respectively, two-fold and three-fold degenerate.

Finally—as in the other two approaches—the group-theoretic approach uses perturbation theory to solve the eigenvalue problem. The key difference is that group theory reorganizes the secular equation using properties of the representations. By knowing the group representations of the new energy levels, we can diagonalize the perturbation operator,  $H'$ . Diagonalization provides a separate secular equation for each distinct energy level. This modularizes the eigenvalue problem into a separate sub-problem for each distinct eigenspace. We learn that we can calculate each distinct eigenvalue separately, rather than solving a larger secular equation for all of them.

To summarize central intellectual differences between the three approaches, we can represent the structure of their solution procedures as flowcharts. I represent the elementary and non-group-theoretic approaches together, since they differ only in the first step, namely whether or not we first construct a symmetry-based form for the electrostatic potential. Figure 3 shows how the additional epistemic dependence relations provided by group theory restructure the solution procedure. The dashed ovals indicate modularization, where we have broken a problem into separately treatable sub-problems. Group theory shows us how to separate the splitting and degeneracy problems from the eigenvalue problem, indicated by the first dashed oval in Figure 3. Furthermore, group theory separates the eigenvalue problem into a separate problem for each distinct eigenvalue, indicated by the second dashed oval. Finally, the flowchart illustrates how group theory unifies the crystal field theory problem by indicating that symmetry properties are sufficient for determining the splitting and degeneracy. I expand on these points in Section 4.3, but first I will clarify how the three approaches pose a problem for explanationism.

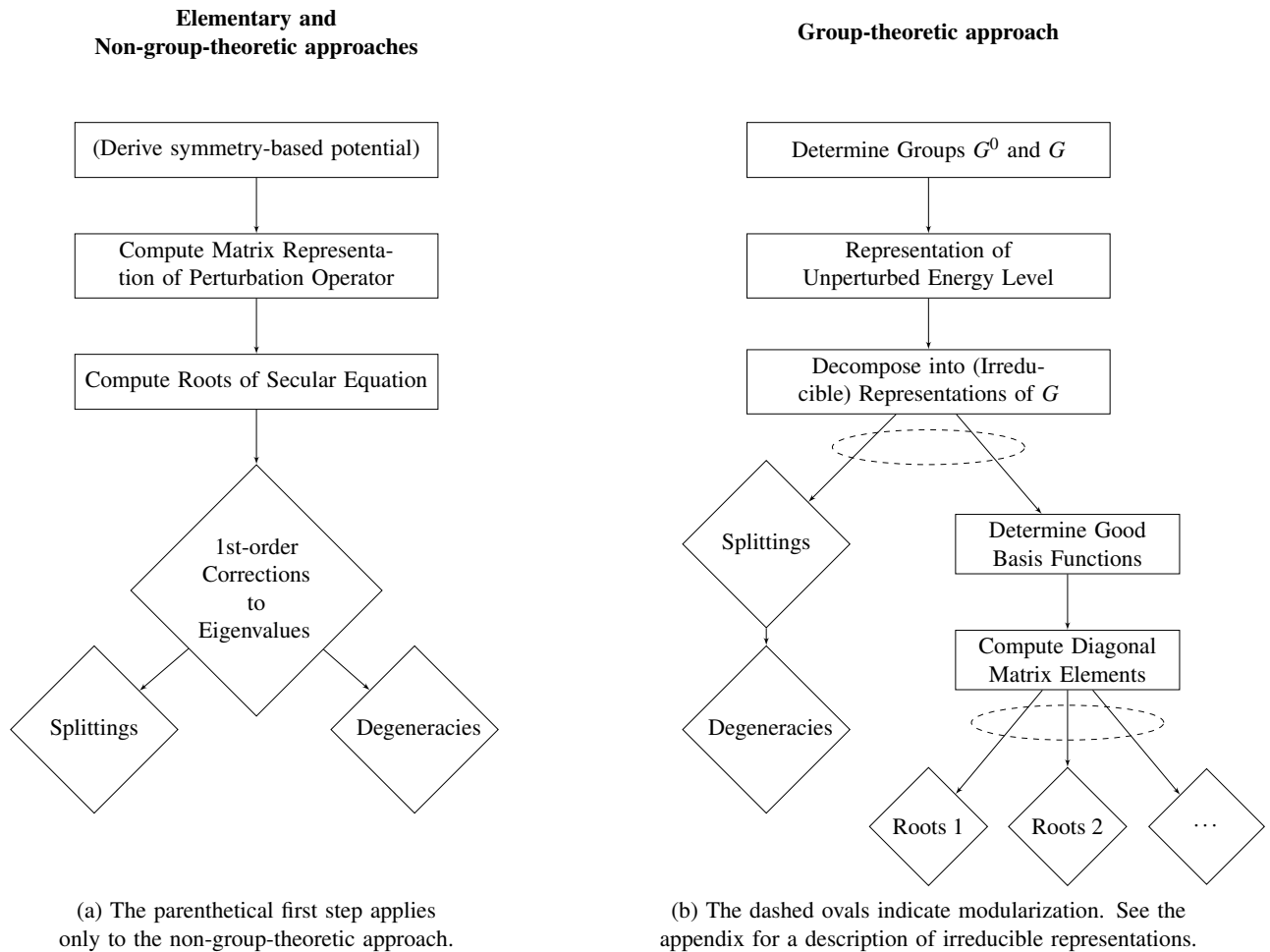


Figure 3: Schematic step-by-step flowcharts for the three approaches

## 4.2 A problem for explanationism

With the approaches to crystal field theory before us, I will now show how they pose a serious challenge to explanationism. To simplify the exposition, I will focus on how the two symmetry-based approaches explain the splitting and degeneracy (i.e. the energy-level structure). Similar points arise when comparing these two approaches to the elementary approach, along with considering how each approach explains the eigenvalues. My argument involves establishing three premises, which together entail that explanationism provides an incomplete account of the non-pragmatic and objective dimensions of understanding. First, I will show that—on many accounts of explanation—both symmetry-based approaches provide not only derivations but also explanations of the relevant phenomena.<sup>21</sup> Secondly, I will argue that both approaches reference the same ontic explanatory information; hence, they do not involve explanatory differences. Finally, I will argue that the approaches nevertheless provide different understandings of the crystal field theory phenomena. Hence, explanationism is incorrect: not all intellectual differences stem from corresponding explanatory differences.

Since explanationism is concerned only with explanatory understanding (i.e. understanding-why), my case study poses a problem only if the compatible formula-

<sup>21</sup> Section 6 extends my argument to explanationists who might refuse to grant this premise.

tions are genuine explanations, rather than mere derivations. However, due to persistent disagreements about the nature of explanation, it is impossible to conclusively demonstrate that these approaches are explanatory. The best one can do is motivate interpreting them as such. To this end, it suffices to note that many established accounts of explanation would treat these three approaches as explanatory.<sup>22</sup> To make just one representative analysis, I will consider Woodward and Hitchcock's ([2003a]) 'manipulationist' (or 'interventionist') account of causal explanation, since it avoids many well-known problems facing 20th-century accounts of explanation. Manipulationism recasts explanation as the pursuit of answering 'what-if-things-had-been-different questions': how would the explanandum have differed if one of the explanans had been changed? For instance, we might wonder how a coordination complex's energy levels would have differed if we had changed its symmetry. Answering these what-if questions requires an 'explanatory generalization': a law-like statement characterizing how the explanandum depends on the explanans, in function–variable form. This lets us derive the explanandum from input variables characterizing the explanans (such as initial or boundary conditions). To qualify as an explanatory generalization, a law-like statement must be invariant under 'testing interventions' (Woodward and Hitchcock [2003b], p. 182). This means that the generalization must continue to hold even as we intervene on the system of interest, changing its explanans variables within some nontrivial range.<sup>23</sup> Coulomb's law provides a paradigmatic example, characterizing how the electrostatic force between two charged bodies depends on their charges and the distance between them.

Manipulationism straightforwardly renders both symmetry-based approaches—and also the elementary approach—as genuinely explanatory. In each formulation, the secular equation (A.1) functions as a suitable explanatory generalization for solving the eigenvalue problem. The secular equation remains invariant under a wide range of interventions, including modifying the charges and configuration of the surrounding ligands. It thereby answers many kinds of what-if-things-had-been-different questions. In the non-group-theoretic approach, we explain the splitting and degeneracy as a consequence of these eigenvalues. Thus, by causally explaining the eigenvalues, we also causally explain the energy-level structure. In the group-theoretic approach, a different explanatory generalization—the character decomposition formula—characterizes how the splitting and degeneracy depend on the symmetry.<sup>24</sup> Since the character decomposition formula is also invariant under a variety of interventions, manipulationism would interpret this as a genuine explanation too. Hence, both approaches provide not merely derivations but also causal explanations of the splitting and degeneracy.

Next, we must show that both symmetry-based approaches reference the same ontic explanatory information. Otherwise, an explanationist could seek to reduce any intellectual differences between the approaches to concomitant explanatory differences. In both cases, we appeal to the geometric arrangement of the coordination complex, i.e.

<sup>22</sup> Although space precludes a fuller discussion, these derivations count as explanatory on Hempel and Oppenheim's ([1965 [1948]]) deductive-nomological model, Railton's ([1981]) ideal explanatory text account, Lewis's ([1986], pp. 217–21) similar account of causal explanation, and Kitcher's ([1989]) unificationist account. I briefly discuss the latter in Section 5.2.

<sup>23</sup> These testing interventions need not be experimentally feasible or even physically possible (although they often are); an intervention simply needs to be 'logically or conceptually possible' (Woodward [2003], p. 132).

<sup>24</sup> Appendix A.3 describes this formula (Equation A.5) in detail.

its symmetry, to determine its energy-level structure. The non-group-theoretic approach uses this structural information to determine the symmetry-based form of the potential (Equation A.2). This potential is then fed into the secular equation to determine the quantitative form of the eigenvalues. Although the symmetry-based potential technically references the charge of the central metal ion, this information could be suppressed without changing the derivation of the energy-level structure. Likewise, in the group-theoretic approach, we appeal to the geometric structure of the coordination complex to determine its abstract symmetry group. Then, using mathematical properties of this abstract symmetry group—namely, properties of its representations—we determine the energy-level structure. Hence, in both cases, we appeal to the same ontic explanation, namely the same state of affairs in the world.<sup>25</sup>

Finally, it remains to show that the two approaches provide different ways of understanding the crystal field theory phenomena, despite relying on the same ontic explanatory information. In the non-group-theoretic approach, we understand the splitting and degeneracy as a consequence (or feature) of the eigenvalues. In contrast, the group-theoretic approach provides a way of understanding the splitting and degeneracy as a consequence of symmetry independently of the quantitative form of the eigenvalues. Below, I will describe how conceptualism accommodates this intellectual difference in terms of ‘modularization’, a general kind of epistemic dependence relation. Moreover, the two approaches differ in how they unify coordination complexes into symmetry-based families. In the non-group-theoretic approach, we understand the system’s features as an instance of a particular instantiation of octahedral symmetry. Whereas in the group-theoretic approach, our understanding does not depend on the particular instantiation of octahedral symmetry; it applies to any possible instantiation of this symmetry. These differences in unification amount to differences in understanding.<sup>26</sup>

To summarize, the two symmetry-based approaches to crystal field theory provide a counterexample to explanationism. They each explain the splitting and degeneracy while referencing the same ontic explanatory information. Nevertheless, they provide objective and non-pragmatic differences in understanding why the phenomenon occurs. Hence, they show that explanationism is incomplete: it fails to account for all relevant intellectual differences. In the next section, I will demonstrate how conceptualism easily accommodates the intellectual differences between these two approaches, interpreting them in terms of different epistemic dependence relations.

### 4.3 Illustrating conceptualism

Unlike explanationism, conceptualism accounts for the intellectual differences between compatible formulations. As an illustration, I will show how conceptualism interprets the differences between the two symmetry-based approaches. These amount to organizational differences of the same ontic explanatory information, leading to objective and non-pragmatic differences in understanding. First, I will explain how the notion of modularization accommodates two key intellectual differences between the approaches.

<sup>25</sup> Similarly, when it comes to explaining the eigenvalues, each of the three approaches references the same explanatory information, including the charge of the central metal ion, the charges of the ligands, the arrangement of the ligands and metal ion, and the secular equation. This provides a further counterexample to explanationism.

<sup>26</sup> Many philosophers nevertheless view unification as having no bearing on explanation (see Section 5).

Secondly, I will explain how unification accommodates a remaining intellectual difference.

When it comes to understanding the splitting and degeneracy, the two symmetry-based approaches provide different understandings because they appeal to different EDRs. In the non-group-theoretic approach, we rely on the EDR that knowledge of the quantitative form of the eigenvalues is sufficient for knowledge of the splitting and degeneracy. In contrast, the group-theoretic approach modularizes the crystal field theory problem into distinct sub-problems, solving for the splitting and degeneracy without solving for the eigenvalues. This modularization constitutes the following EDR: knowledge of the eigenvalues is not necessary for knowledge of the splitting and degeneracy. Instead, it is possible to derive the splitting and degeneracy without knowing even the quantitative form of the eigenvalues. These different EDRs thereby provide different ways of understanding the splitting and degeneracy, in virtue of how they structure the derivation. A similar moral about modularization applies to the eigenvalue problem. In the non-group-theoretic approach, we understand the eigenvalues from a single secular equation, whereas in the group-theoretic approach, we modularize the larger secular equation into a set of smaller secular equations, one for each distinct eigenspace. Thus, we learn that we can understand each distinct eigenspace separately.

A third key intellectual difference between the approaches stems from differences in how they unify phenomena. Unlike the elementary approach, both symmetry-based approaches unify the crystal field theory problem into symmetry-based families.<sup>27</sup> The symmetry-based derivations apply not only to a given coordination complex but also to coordination complexes in the same geometric family. Specifically, they provide the following kind of epistemic dependence relation: knowledge of the energy-level structure for one coordination complex in this family suffices for knowledge of the energy structure for other complexes in this family. Unifying coordination complexes into symmetry-based families enables us to understand each one as an instance of a larger class with the same behaviour. Moreover, due to the differences in their respective EDRs, the group-theoretic approach unifies more than the non-group-theoretic approach. In the latter, a given symmetry-based potential applies only to coordination complexes that have the same geometric arrangement of ligands around the central metal ion. For nickel(II) hexahydrate, this is a particular instantiation of octahedral symmetry, with each ligand at the vertex of an octahedron. In contrast, the relevant group-theoretic argument applies to any coordination complex with octahedral symmetry, independently of how it is instantiated. For instance, the derivation sketched in Section 4.1 applies just as well to a coordination complex with eight ligands at the vertices of a cube, rather than an octahedron.<sup>28</sup> The group-theoretic approach unifies more because it tells us that knowledge of the abstract symmetry group suffices for knowledge of the energy-level structure.

Despite my focus on non-pragmatic differences in understanding, some EDRs are pragmatically beneficial as well. For agents interested in knowing only the splitting and degeneracy, modularization provides a beneficial way of obtaining this knowledge

<sup>27</sup> The elementary approach cannot unify the energy-level structure because it treats each coordination complex on a case-by-case basis. This piecemeal approach results from its central EDR, namely that knowledge of the eigenvalues is sufficient for knowledge of the splitting and degeneracy. To calculate these eigenvalues, it—like the other two approaches—appeals to the particular strength of the interaction, a feature specific to each coordination complex.

<sup>28</sup> Since cubes are dual to octahedra, they have the same symmetry group.

without needing to determine further properties of the eigenvalues. Similarly, for agents who wish to determine the energy-level structure of a class of coordination complexes, the additional unification provided by group theory hastens this task. In this way, different EDRs can lead to pragmatic benefits, based on agents' goals. But, unlike many recent pragmatic accounts of scientific understanding, conceptualism keeps these two aspects of theory reformulation separate, i.e. the pragmatic benefits vs. the objective and non-pragmatic differences in understanding. The former depend on the preferences and goals of agents, whereas the latter are formal properties of a theory's formulation.<sup>29</sup>

## 5 Is Conceptualism Redundant?

Section 4.2 developed a counterexample to explanationism. This counterexample targets explanationists who view each approach to crystal field theory as explanatory—an interpretation sanctioned by many accounts of explanation. To rebut my argument, these explanationists might argue that other non-pragmatic features of scientific explanation—such as differences in explanatory depth—account for all intellectual differences between the approaches. This would render conceptualism's account of scientific understanding redundant, relative to existing accounts of explanatory differences.

In response, I will argue that conceptualism is not redundant when compared with leading accounts of explanation that treat the approaches to crystal field theory as explanatory. Because I view them as the most promising theories in their respective traditions, I will focus on Skow's ([2016]) account of reasons-why and Woodward and Hitchcock's manipulationist account.<sup>30</sup> I will argue that both accounts fail to accommodate modularization and unification. Additionally, even Kitcher's ([1989]) unificationist account of explanation does not accommodate the relevant kind of unification illustrated by crystal field theory.

### 5.1 Skow's account of reasons-why

Skow's account of reasons-why continues the causal explanation tradition of Railton and Lewis, while treating grounding as an additional explanatory feature. For a given concrete event *Q*, Skow's theory characterizes a hierarchy of reasons why *Q* occurred. At bottom, there are the 'first-level reasons why *Q*'. These are always either causes or grounds. For each reason-why, there might be further reasons why that reason is a reason, and so on ([2016], p. 124). Nevertheless, when it comes to answering the initial, bottom-level why-question regarding *Q*, answering these higher-level why-questions is optional on Skow's account. Hence, explanatory arguments that agree on the first-level reasons-why provide the same explanation. Since the three approaches to crystal field

<sup>29</sup> Against my approach, Potochnik ([2015a], p. 1172) argues that it is a mistake to seek a clean-divide between the pragmatic and the non-pragmatic in the context of explanation and understanding. Defending the utility and coherence of this traditional distinction—which explanationists necessarily grant—lies outside the scope of this paper.

<sup>30</sup> Potochnik's causal pattern account of explanation provides an interesting approach that amalgamates and develops aspects of Woodward's, Achinstein's, Strevens', and van Fraassen's accounts of explanation ([2015a], [2017], pp. 127, 134). However, since it relies on pragmatic features of agents ([2015a], pp. 1172–5, [2017], p. 127), it is not amenable to a defender of explanationism. Bokulich's ([2011]) rich account of model explanations modifies Woodward's account to accommodate idealization, a complication that I suppress here.



theory agree on the underlying ontic reasons for the crystal field theory phenomena, Skow's account would treat each of them as explanatory.<sup>31</sup> Thus, his account falls within the scope of Section 4.2's argument against explanationism.

Although Skow's account has its attractions, it is too circumscribed to capture many of the intellectually significant differences brought out by symmetry arguments. The chief utility of Skow's theory derives from characterizing a hierarchy of reasons-why. This enables us to see how multiple arguments can agree on a set of lower-level reasons-why while differing in the higher-level reasons that they articulate. However, Skow's theory focuses exclusively on answers to why-questions, and modularization is not an answer to a why-question. Instead, modularization is a feature of how some explanatory arguments are organized, based on the epistemic dependence relations they deploy. As a property of EDRs, modularization characterizes what it 'suffices to know' to answer a certain why-question. Characterizing what-it-takes-to-know something is different in kind from answering a why-question about a physical phenomenon.

For a different reason, Skow's account cannot accommodate the symmetry-based unification discussed in Section 4.3. Skow restricts his account to reasons why for 'concrete events', excluding law-like generalizations such as Galileo's law of freefall ([2016], pp. 27–8, 37). This restriction faces difficulties explaining generalizations, such as the claim that all coordination complexes with octahedral symmetry display a particular energy-level structure. To accommodate such generalizations, Skow's account must treat them as a conjunction of concrete events, explained by a concatenation of reasons-why for each system ([2016], p. 134). This sort of aggregative explanation leaves open that these different systems only coincidentally display the same pattern of behaviour. Aware of this worry, Skow claims that 'to show that it is no coincidence that all the facts in some collection obtain it is enough to find a *common reason* why they all obtain' ([2016], p. 134). In this case, the common reason would presumably be that all these different coordination complexes have octahedral symmetry. Nevertheless, as Lange ([2010], pp. 307, 319–22, [2014], pp. 508–9) notes, there is an important difference between conjoining explanations (even those sharing a common explainer) vs. providing a single, unified explanation. Skow's account cannot afford any special significance to the single, unified derivation that group representation theory provides. For indeed, the non-group theoretic symmetry argument provides the same common reason—octahedral symmetry—but without providing a single unified derivation that covers all instantiations of this symmetry group. Hence, Skow's account would have to view these two approaches as being on a par with respect to unification, although they are not.

## 5.2 Woodward and Hitchcock's manipulationism

Manipulationism also fails to accommodate both modularization and unification. As described in Section 4.2, manipulationism focuses on answering what-if-things-had-been-different questions, using possible interventions on the system of interest. However, just as modularization is not a reason-why, it is also not subsumed under answers to what-if questions—again because modularization is an organizational feature of ex-

<sup>31</sup> Technically, Skow recommends abandoning the explanation-idiom in favor of answers to why-questions that describe the reasons why an event occurs ([2016], pp. 7–10). Nonetheless, 'explanation' remains a convenient catchall for the particular kinds of reasons-why and why-questions pertinent to science.

planatory arguments. Thus, it *prima facie* lies outside the scope of manipulationism. In particular, manipulationism neglects a crucial instance of modularization, namely the epistemic dependence relation that we do not need to know the charges and distances in order to determine the splitting and degeneracy. The group-theoretic approach provides us with this EDR by demonstrating that knowledge of symmetry suffices for knowledge of the energy structure. However, manipulationism cannot accommodate this EDR using interventions and what-if-things-had-been-different questions. The problem stems from Woodward and Hitchcock's stricture that explanations depend solely on 'invariance under some range of changes in the variables figuring in the [explanatory generalization] itself' ([2003a], p. 7). Changes to other variables left out of the explanatory generalization—such as background conditions—do not figure in the explanation. Crucially, the group-theoretic approach gives us the above EDR by setting aside explicit dependence on the charges and distances, treating them as background conditions. Hence, when it comes to explaining the splitting and degeneracy, the group-theoretic approach is silent on interventions that affect these variables.<sup>32</sup>

Nevertheless, an explanationist might point to manipulationism's additional account of explanatory depth as a source of intellectual differences. According to Woodward and Hitchcock ([2003a], [2003b]), one generalization is—*ceteris paribus*—deeper than another if the former incorporates an explanans that the latter treats as a background condition. Explicitly incorporating background conditions shows how the phenomenon depends on additional explanans, thereby providing a deeper explanation. For instance, the group-theoretic character decomposition formula (Equation A.5) explicitly incorporates symmetry as an explanans variable. This makes the group-theoretic approach deeper than the non-group-theoretic approach because the latter fixes symmetry as a background condition. While this might be a welcome result, Woodward and Hitchcock's account of depth also has counterintuitive consequences. In particular, it seems to classify the elementary approach as deeper than the group-theoretic approach: the elementary approach allows for interventions on not only the symmetry but also the charges and ligand distances, whereas the group-theoretic approach treats these latter features as background conditions. Yet, the group-theoretic EDRs tell us something important about crystal field theory that the elementary approach neglects. Independently of whether either approach is deeper, we need an account of this intellectual difference. This is what conceptualism provides.

Moreover, Woodward and Hitchcock explicitly disavow that unification matters for causal explanation. Recall that symmetry arguments unify by focusing on families of systems that share a set of features or properties, such as the set of all coordination complexes with octahedral symmetry. Woodward and Hitchcock argue that this kind of generalization is not crucial for accounts of explanation at all. Instead, they focus exclusively on a second kind of generalization, based on varying the properties of a particular system. They characterize this as 'generality with respect to *other possible prop-*

<sup>32</sup> Woodward does discuss a completely different notion of 'modularity' in the context of representing causal structure by systems of equations ([2003], pp. 48, 327–9). This notion of modularity requires that each equation represents a distinct causal mechanism, so that we can intervene on one equation without affecting others. The crystal field theory equations are not modular in this sense because they are not causally independent of each other.

erties of the very object or system that is the focus of explanation' ([2003b], p. 182).<sup>33</sup> Having specified a particular system of interest, one considers varying features that are properties of that system only. They thus deny any need to interpret unification *qua* explanation. As Woodward argues, many kinds of unification involve classificatory schemes or general mathematical formalisms that are not intrinsically connected with causal explanations ([2003], pp. 362–4). This illustrates how accounts of explanation can neglect intellectually significant features such as unification. Not everything that matters for understanding necessarily has to do with explanation.<sup>34</sup>

Still, an explanationist might wonder whether Kitcher's ([1989]) account of unification already accommodates the intellectual differences wrought by unification. Perhaps surprisingly, it does not. According to Kitcher, an argument pattern counts as explanatory provided that it best unifies the phenomena. This is quantified in terms of deriving the largest number of phenomena relative to the smallest number of assumptions. Only these unificatory argument patterns earn a place in the 'explanatory store' of arguments that are genuinely explanatory. But, problematically for Kitcher, the explanatory store is deductively closed, and this prevents it from distinguishing the three approaches to crystal field theory on unificatory grounds. Recall that the group-theoretic approach relies on the same perturbation-theoretic argument schema as the other two approaches. Hence, including the group-theoretic approach within Kitcher's explanatory store *ipso facto* includes the other two approaches. Thus, even though only the group-theoretic approach maximally unifies crystal field theory, Kitcher's account does not distinguish it from the other approaches. This shows that Kitcher's notion of unification is actually too weak to adequately characterize the relevant EDRs that I have identified.<sup>35</sup>

## 6 Explanatory Exclusion

Short of denying that there are intellectual differences between compatible formulations, only one plausible strategy for defending explanationism remains: an explanationist could deny that the three formulations of crystal field theory are each explanatory. If only the group-theoretic approach provides a genuine explanation, then its intellectual differences would arise from explanatory differences after all. Mounting this strategy requires adopting an 'exclusionary account' of explanation. Compared to the accounts considered in Section 5, exclusionary accounts posit more restrictive criteria for explanatory relevance. By making the criteria for explanation more demanding, exclusionary accounts generate an explanatory difference between compatible formulations. These putative explanatory differences can ground corresponding differences in understanding, thereby precluding counterexamples to explanationism.

To illustrate this strategy, I will consider two exclusionary accounts: Strevens' ([2008]) kairetic account and Lange's ([2017]) account of distinctively mathematical

<sup>33</sup> Likewise, Woodward claims that 'the explanatory depth of a generalization is connected to its range of invariance rather than its scope; hence, the unificationist approach focuses on the wrong sort of generality in explanations' ([2003], p. 366).

<sup>34</sup> See Gijsbers ([2013]) for a similar conclusion. Gijsbers ([2007]) provides a detailed argument for why unification is not inherently connected with explanation. Similarly, Morrison ([2000]) argues through numerous case studies that unification is often either in tension with or has nothing to do with explanation.

<sup>35</sup> For additional criticisms of Kitcher's account of unification, see Barnes ([1992]) and Woodward ([2003], pp. 366–73).

explanations. Both accounts focus on abstraction of allegedly irrelevant causal details, thereby excluding many causal influences from counting as explanatorily relevant. We will see that only the group-theoretic approach satisfies their restrictions, making it the only genuine explanation for crystal field theory. However, this exclusionary strategy runs afoul of an important desideratum: we should be able to accommodate the apparent differences in understanding without appealing to epistemically inaccessible ontic features. Positing more restrictive explanatory relevance relations generates a skeptical problem because we cannot easily know whether these additional relevance relations exist or are satisfied.<sup>36</sup> My goal here is not to reject these accounts of explanation *per se*, but rather to point out that no one should adopt them merely for the sake of upholding explanationism. Conceptualism provides a more epistemically secure and parsimonious account of the relevant differences in understanding.

### 6.1 Strevens' kairetic account

Strevens' account focuses on identifying causal 'difference-makers', the only causal influences that are explanatorily relevant. According to his 'kairetic condition', a causal influence counts as a difference-maker provided it remains in at least one maximally abstract model explaining the phenomenon. To apply this test, we begin with a model that causally entails the explanandum.<sup>37</sup> We then make this causal model as abstract as possible, replacing specific descriptions of causal influences with increasingly abstract characterizations, i.e. less exact or specific claims (Strevens [2008], p. 97). Causal influences that survive this abstraction procedure qualify as difference-makers. On Strevens' account, only these maximally abstract causal models genuinely explain.<sup>38</sup>

Applying the kairetic account to the three formulations of crystal field theory, we see this abstraction procedure in action. Regarding the splitting and degeneracy, the non-group-theoretic approach abstracts from the particular charges and field strength used by the elementary approach.<sup>39</sup> In their stead, it offers the symmetry-based potential as a putative causal difference-maker. The group-theoretic approach abstracts further, eliminating the particular way that symmetry is instantiated. Assuming that we can always re-express knowledge of symmetries using group theory, the symmetry-based potential would be explanatorily irrelevant. What remains are the symmetries themselves—the initial metal ion and the resulting coordination complex—as the putative causal difference-makers for the splitting and degeneracy. Since only the group-theoretic approach successfully represents these difference-makers, it is the only approach we have considered that would provide a genuine explanation. It shows that symmetry is a difference-maker, but not the particular way that symmetry is instantiated. In this way, Strevens' kairetic account could ground the intellectual differences between the two

<sup>36</sup> Woodward defends a similar epistemic accessibility criterion for explanation ([2003], pp. 23, 179–81, 308).

<sup>37</sup> Causal entailment goes beyond logical entailment by representing an actual causal process that produces the explanandum (Strevens [2008], pp. 71–2, 93). Potochnik weakens this entailment relation to better accommodate idealizations ([2017], pp. 155–6).

<sup>38</sup> Note that a single application of this kairetic procedure only identifies all of the difference-makers that appear in a given causal model, rather than all of the difference-makers for a given event.

<sup>39</sup> We cannot, however, conclude from this single application of the kairetic procedure that the charges and field strength are explanatorily irrelevant for the splitting and degeneracy. To do that, we would have to show that we can abstract them away from any model that causally entails the splitting and degeneracy.

symmetry-based approaches in corresponding ontic explanatory differences, thereby preserving explanationism.

However, the kairetic abstraction procedure for identifying causal difference-makers faces a skeptical challenge. In general, it is impossible to conclusively prove that any causal factor is or is not a difference-maker. On the one hand, to show that a factor is a difference-maker, we must show that it survives under maximal abstraction within a causal model. Yet, how can we know that no further abstractions in our model are possible? A scientist taught the non-group-theoretic approach—and with no knowledge of group theory—might reasonably think that this is a maximally abstract causal model. On the other hand, to show that a causal factor is not a difference-maker, we must show that the kairetic procedure eliminates or abstracts away that causal factor from any and all causal models for the given explanandum (Strevens [2008], pp. 69–70, 87). For instance, to show that the specific eigenvalues are genuinely irrelevant for explaining the splitting and degeneracy, it is not enough to see how group theory eliminates them to provide a more abstract causal model. Instead, we would have to show that any causal model for the splitting and degeneracy lets us abstract away the specific eigenvalues.

Conceptualism avoids these skeptical worries by analyzing the relevant intellectual differences in terms of epistemic dependence relations, rather than putative causal difference-makers. It shows that we do not have to consider other possible but currently unconceived causal models to account for the change in understanding provided by group theory. Although considering such models would no doubt be illuminating—since it would amount to considering further reformulations—conceptualism lets us analyse the intellectual differences between the symmetry-based approaches by considering those two approaches alone. The hard task of identifying causal difference-makers may reasonably be hostage to the existence of even more abstract models, but the task of identifying intellectually significant differences surely is not.

## 6.2 Lange’s distinctively mathematical explanations

Faced with the limitations of causal accounts of explanation, an explanationist might try to locate ontic differences between reformulations within the realm of non-causal explanations. Perhaps what is needed to save explanationism is an account of how mathematical facts explain physical phenomena. Lange’s theory of distinctively mathematical explanations provides one such account. According to Lange, sometimes causal structure alone cannot account for the inevitability of certain physical phenomena ([2017], pp. 5–6). In these cases, we require a ‘distinctively mathematical explanation’, wherein a mathematical fact ‘constrains’ the causal structure of reality. Such constraints possess a higher degree of necessity than the laws or contingent facts that they constrain (Lange [2013], [2017], p. 10). Recognizing the relevant constraints shows not only why the explanandum occurred, but also why the explanandum was inevitable—in a modal sense stronger than nomic inevitability. In such cases, arguments that appeal to causal structure alone are merely derivations of the relevant phenomenon, rather than explanations.

When it comes to explaining splitting and degeneracy, Lange’s account classifies only the group-theoretic approach as explanatory. On this interpretation, the character decomposition formula (Equation A.5) constrains the possible form of all resulting energy levels, given initial and final symmetry groups. In other words, it constrains

all possible causal relations governing the energy-level structure of coordination complexes. For instance, if the force law governing coordination complexes weren't Coulomb's law—e.g. if it were an inverse cubic force law instead—the splitting and degeneracy would remain the same. Although naturally necessary, such force laws would be interpreted as less necessary than the mathematically necessary facts governing the representations of symmetry groups. Hence, the group-theoretic approach shows that the splitting and degeneracy are more necessary than both the relevant force laws and the resulting eigenvalues. Since the other two approaches cannot explain this difference in modality, Lange would argue that they are non-explanatory: the causal mechanisms they reference are explanatorily irrelevant.

However, just like Strevens' account, Lange's account faces a skeptical challenge. His account successfully distinguishes the group-theoretic approach from the other two approaches only if the world possesses this rich modal structure of mathematical facts constraining physical facts. Commitment to this kind of graded natural modality is decidedly controversial, in part because it is epistemically inaccessible. We do not have empirical access to this hierarchy of modal facts. Nevertheless, Lange's account applies only if the world possesses this structure. If the world turned out to lack sufficient modal structure, then distinctively mathematical explanations would devolve into ordinary causal explanations.

A further problem arises from this skeptical worry. Worlds that lack Lange's requisite modal structure are empirically indistinguishable from worlds that possess it. Hence, the intellectual differences described in Section 4 would be equally apparent in either kind of world. Regardless of whether or not the world possesses this modal structure, the three formulations would still provide different understandings of crystal field theory. Since these differences do not depend on corresponding facts about modality, we should be able to accommodate them without further metaphysical theorizing. For instance, to appreciate the central insight that modularization provides, we don't need there to be graded modality in the world. Specifically, we don't need group-theoretic facts to constrain the causal structure of the world. By supplying epistemic dependence information, the group-theoretic approach makes a distinctive contribution to our understanding of crystal field theory, independently of further ontic commitments. Hence, conceptualism provides a superior strategy for accommodating these intellectual differences.

Plausibly, any exclusionary account of explanation will face similar problems. For the basic idea behind this explanationist strategy is to posit additional ontic features that might ground the intellectual differences between compatible formulations. Since compatible formulations superficially posit the same states of affairs, any such additional ontic features will be epistemically less accessible. In contrast, conceptualism provides an account of these intellectual differences using features that we have easy epistemic access to—namely, epistemic dependence relations. Determining epistemic dependence relations is simply a matter of analyzing the epistemic structure of a theory formulation. Since these differences in EDRs persist independently of whether they are grounded in further ontic differences, our account of understanding should likewise be independent of these further differences. Whereas conceptualism satisfies this desideratum, the exclusionary strategy canvassed here seemingly does not.

## 7 Conclusion

We began with two questions: what accounts for the intellectual differences that compatible formulations provide, if not explanatory differences? And in particular, what makes a symmetry argument intellectually significant in cases where it is not needed to explain the phenomenon? To answer these questions, I have developed conceptualism as a framework for analyzing objective and non-pragmatic differences in understanding. By reformulating theories, we gain epistemic dependence relations that clarify what we need to know to solve problems. The three formulations of crystal field theory considered in Section 4 illustrate the dramatic differences that can arise. Group representation theory radically restructures how we understand the energy levels of coordination complexes. It does this by modularizing the crystal field theory problem into separately treatable sub-problems while unifying systems into symmetry-based families.

Sections 5 and 6 considered what seem to be the only two strategies available for defending explanationism—short of denying that compatible formulations lead to differences in understanding. By rebutting these strategies, I have shown that existing accounts of explanation face the burden of accommodating non-explanatory intellectual differences. One easy way to meet this burden is simply to renounce explanationism and adopt conceptualism. Conceptualism provides a general approach to interpreting the intellectual and methodological significance of reformulations.<sup>40</sup> This includes mathematical reformulations in particular, which have recently sparked debates over the existence of non-causal explanations. Promisingly, conceptualism lets us interpret mathematized explanations while skirting seemingly insoluble metaphysical disputes. It focuses attention away from epistemically inaccessible features of scientific ontology and toward the manifestly accessible epistemic structure of scientific theories (and problem-solving procedures more generally). Overall, conceptualism provides an attractive account of the intellectual differences that undergird a central and ubiquitous component of scientific progress, namely, compatible formulations.

## A Appendix

### A.1 The elementary approach

The elementary approach solves the crystal field theory problem exclusively through perturbation theory. We begin with an initial Hamiltonian  $H^0$  (with known eigenvalues and eigenfunctions) that characterizes the energy and dynamics of the unperturbed system, such as  $Ni^{2+}$ . We characterize the perturbation from the six water molecules by an operator  $H'$ . The sum of these two operators equals an approximate Hamiltonian,  $H$ , for nickel(II) hexahydrate:  $H = H^0 + H'$ . To approximate the eigenvalues of  $H$ , we first calculate the matrix elements of the perturbation operator  $H'$  by measuring the electrostatic potential. Calculating these matrix elements requires choosing a basis for the five unperturbed d-orbitals of  $Ni^{2+}$ , such as the five spherical harmonics,  $Y^{2,m}$  ( $m \in \{-2, -1, 0, 1, 2\}$ ).<sup>41</sup> In this basis, we compute all twenty-five elements of the  $5 \times 5$

<sup>40</sup> Moreover, despite its focus on objective and non-pragmatic differences in understanding, conceptualism can be combined with recent pragmatic accounts of understanding for a more complete picture.

<sup>41</sup> These functions belong to the separable Hilbert space  $L^2(\mathbb{R}^3)$  of square-integrable complex-valued functions defined over Euclidean three-space  $\mathbb{R}^3$ . For details, see Cornwell ([1984], Appendix B).

matrix  $H'$  and use them to solve the secular equation of the perturbation operator:

$$\text{determinant}[H' - \lambda I] = 0 \quad (\text{A.1})$$

where  $\lambda I$  is a constant multiple of the identity matrix. The roots (i.e. zeros) of the secular equation equal the eigenvalues of  $H'$ , which provide a first-order correction to the eigenvalues of  $H^0$ . The number and degeneracy of the distinct eigenvalues corresponds to the number of new energy levels and their degeneracies.

## A.2 The non-group-theoretic approach

The non-group-theoretic approach begins by determining a general form for the electrostatic potential in terms of the symmetry of the coordination complex. Using Coulomb's law, we express the potential at an arbitrary point  $P$  as a sum of six contributing potentials, one from each of the ligands. After manipulating this expression using Legendre polynomials, we arrive at a tractable formula in Cartesian coordinates  $x$ ,  $y$ , and  $z$ . This constitutes a 'symmetry-based form of the potential' (Figgis and Hitchman [2000], p. 38):

$$V = \sum_{i=1}^6 V_i = 6 \frac{Ze^2}{a} + \frac{35Ze^2}{4a^5} (x^4 + y^4 + z^4 - \frac{3}{5}r^4) \quad (\text{A.2})$$

Here,  $Z$  is the charge of the central metal ion,  $r$  is the distance from the point  $P$  to the central metal ion, and  $a$  is the distance between each ligand and the central metal ion.

Using equation (A.2) for the crystal field potential  $V$ , we then proceed as in the elementary approach. We calculate the matrix elements of the perturbation operator  $H'$  and solve the resulting secular equation for its roots. Since this derivation uses a symmetry-based expression for the potential, it applies not just to nickel(II) hexahydrate but to any coordination complex with octahedral symmetry instantiated in the same way. We find two distinct roots:  $\lambda_1 = -\frac{2}{5}\Delta_O$  (three-fold degenerate) and  $\lambda_2 = \frac{3}{5}\Delta_O$  (two-fold degenerate), expressed in terms of their energy difference  $\Delta_O$ . The existence of two distinct roots entails that two new energy levels form. Since these roots are three-fold and two-fold degenerate, so are the resulting energy levels (Dunn et al. [1965], p. 16).

## A.3 The group-theoretic approach

To apply group theory, we first identify the symmetry group  $G^0$  of the unperturbed  $Ni^{2+}$  metal ion.<sup>42</sup> This is the set of transformations that leave the initial Hamiltonian,  $H^0$ , invariant. An unperturbed metal ion possesses spherical symmetry, so  $H^0$  is invariant under any rotation around any axis passing through the centre of  $Ni^{2+}$ . This uncountably infinite set of rotations constitutes the 'pure rotation group'  $SO(3)$ , (i.e. the 'special orthogonal group in three dimensions').<sup>43</sup>

Next, we identify the symmetry group  $G$  of the final, perturbed state—in this case nickel(II) hexahydrate. In Figure A.1,  $Ni^{2+}$  sits at the centre of an octahedron, surrounded by a water ligand at each vertex. The symmetry operations that leave this coordination complex's Hamiltonian,  $H$ , invariant are the twenty-four operations of the

<sup>42</sup> A 'group' is a set equipped with a closed, invertible, and associative binary operation, containing an identity element.

<sup>43</sup> To simplify the exposition, I neglect inversion transformations in both the initial and final symmetry groups.



octahedral group,  $O$ . These comprise a variety of  $90^\circ$ ,  $120^\circ$ , and  $180^\circ$  rotations through various axes passing through the octahedron's centre.

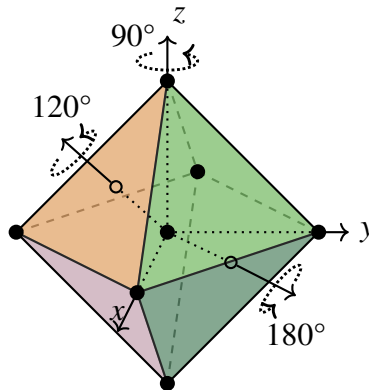


Figure A.1: Some symmetry operations of an octahedron

These symmetry transformations form five distinct ‘conjugacy classes’: (1)  $360^\circ$ , (8)  $120^\circ$ , (6)  $180^\circ$ , (3)  $180^\circ$ , and (6)  $90^\circ$ , corresponding to distinct kinds of rotations. Here, ‘(1)  $360^\circ$ ’ indicates a conjugacy class consisting of one 360 degree rotation, namely the identity element of the group.<sup>44</sup>

To extract information about the energy levels from these symmetry groups, we move from group theory to group representation theory. This involves constructing ‘matrix representations’ for the symmetry groups of interest.<sup>45</sup> To form a matrix representation, we map each geometrical symmetry transformation  $B$  to an invertible matrix  $\rho(B)$ . For finite groups, such as the octahedral group, each representation can be decomposed into a finite number of ‘irreducible representations’.<sup>46</sup> Since these irreducible representations cannot be decomposed further, they function as the basic building blocks of all other representations. For instance, the octahedral group has five irreducible representations, labeled  $A_1, A_2, E, T_1$ , and  $T_2$ .<sup>47</sup>

Irreducible representations express important symmetry properties of physical systems. In particular, the irreducible representations of a system’s symmetry group label the Hamiltonian’s eigenvalues, i.e. the energy of each orbital. This means that each distinct energy level (each distinct eigenspace) corresponds to an irreducible representation.<sup>48</sup> For example, an irreducible representation ‘ $\Gamma_{rot}^{(2)}$ ’ of  $SO(3)$  labels the five-fold

<sup>44</sup> A ‘conjugacy class’ is a collection of operations that is invariant under conjugation: letting  $A$  be a member of the conjugacy class and  $X$  any member of the group, the combination  $XAX^{-1}$  is also a member of the conjugacy class.

<sup>45</sup> A matrix representation is a group homomorphism  $\rho$  from the group of interest to the group of invertible linear transformations over a vector space  $V$  (i.e. the general linear group  $GL(V)$ ). Requiring this map to be a ‘group homomorphism’ means that the matrix representatives must compose under matrix multiplication in the same way as the symmetry transformations do:  $\rho(AB) = \rho(A)\rho(B)$ .

<sup>46</sup> A representation is ‘irreducible’ if there is no proper subspace of basis vectors left invariant by the transformations of the symmetry group, i.e. the vector space for the representation contains no smaller, nontrivial invariant subspaces. Otherwise, a representation is ‘reducible’.

<sup>47</sup> The capital letters correspond to the dimensionality of the irreducible representation, with ‘A’, ‘E’, and ‘T’ corresponding to one, two, and three dimensional representations, respectively.

<sup>48</sup> In general, each  $d$ -dimensional eigenspace provides a basis for a  $d$ -dimensional representation of the Hamiltonian’s symmetry group. In cases of accidental degeneracy, this representation is reducible, rather than irreducible.

degenerate d-orbitals of  $Ni^{2+}$ . This correspondence between eigenspaces and irreducible representations allows us to derive facts about energy levels by considering relationships between representations.

For many applications, it is unnecessary to determine explicit matrix representations for each irreducible representation (illustrating another epistemic dependence relation). Instead, we can often rely on group characters. For a given irreducible representation, a ‘character’ is the trace of a matrix from that representation (the ‘trace’ is the sum of the elements along the principal diagonal). Since matrix traces are invariant under changes in basis, characters are invariants of an irreducible representation, meaning that they do not depend on the basis chosen for the representation. Thus, each irreducible representation has a well-defined set of characters. Furthermore, since the trace of a matrix is invariant under conjugation, members of the same conjugacy class have the same trace, and thus the same characters. As a result, we can organize the characters in a table, where the rows label the irreducible representations and the columns label the conjugacy classes. The character table for the octahedral group is shown in Table A.1.

Table A.1: Character table for the octahedral group

<b>O</b>	(1) <b>360°</b>	(8) <b>120°</b>	(3) <b>180°</b>	(6) <b>180°'</b>	(6) <b>90°</b>	Good basis functions
<b>A<sub>1</sub></b>	1	1	1	1	1	$x^2 + y^2 + z^2$
<b>A<sub>2</sub></b>	1	1	1	-1	-1	
<b>E</b>	2	-1	2	0	0	$(2z^2 - x^2 - y^2, x^2 - y^2)$
<b>T<sub>1</sub></b>	3	0	-1	-1	1	
<b>T<sub>2</sub></b>	3	0	-1	1	-1	$(xz, yz, xy)$
$\Gamma_{rot}^{(2)}$	5	-1	1	1	-1	

Affixed to the bottom of Table A.1 are the characters of the representation  $\Gamma_{rot}^{(2)}$  for each conjugacy class of the octahedral group. These characters follow from a general equation for the character of a rotation through  $\alpha$  radians for an irreducible representation characterized by angular momentum  $\ell$  (Cotton [1990], p. 261):

$$\chi^\ell(\alpha) = \frac{\sin[(\ell + \frac{1}{2})\alpha]}{\sin[\alpha/2]} \quad (\text{A.3})$$

For instance, the character of the  $\Gamma_{rot}^{(2)}$  matrix representatives for 120° rotations is  $-1$ , obtained by substituting ‘ $\frac{2\pi}{3}$  radians’ for  $\alpha$  and ‘2’ for  $\ell$  (since we are dealing with d-orbitals, which have an orbital angular momentum of two).

When we perturb the spherical symmetry by surrounding the metal ion with ligands, we break its spherical symmetry into octahedral symmetry. Consequently, irreducible representations from the octahedral group now label the energy levels of the system. Therefore, the irreducible representation  $\Gamma_{rot}^{(2)}$  that labels the initially degenerate energy levels decomposes into a direct sum of irreducible representations  $\Gamma^r$  from the octahedral group:

$$\Gamma_{rot}^{(2)} \approx \sum_r \oplus n_r \Gamma^r \quad (\text{A.4})$$

where the multiplicity,  $n_r \in \mathbb{N}$ , indicates the number of times that the irreducible representation  $\Gamma^r$  occurs in this decomposition.

Each distinct  $\Gamma^r$  in the decomposition (A.4) labels an eigenspace of nickel(II) hexahydrate. Thus, the number of distinct  $\Gamma^r$  in the decomposition provides the splitting, i.e. the number of distinct eigenspaces, and the dimension of  $\Gamma^r$  equals the degeneracy of the corresponding eigenspace. Hence, the decomposition of  $\Gamma_{rot}^{(2)}$  determines the splitting and degeneracy.

To determine this decomposition, we do not need to know explicit matrix representations for the irreducible representations. Instead, it suffices to use a ‘character decomposition formula’:

$$n_r = (1/g) \sum_k N_k \chi^r(T)^* \chi_{rot}(T) \quad (\text{A.5})$$

This equation provides a general relation for decomposing a reducible representation into a sum of irreducible representations of a finite group (Cornwell [1984], p. 85). As before,  $n_r$  denotes the multiplicity of the  $r$ -th irreducible representation in the decomposition of  $\Gamma_{rot}^{(2)}$ .  $g$  denotes the cardinality of the symmetry group of the coordination complex, in this case the octahedral group (which has 24 elements). The sum is taken over each conjugacy class (i.e. column) of the character table, indexed by  $k$ .  $N_k$  denotes the number of symmetry operations in the  $k$ -th conjugacy class. In Table A.1,  $N_k$  corresponds to the number preceding the type of symmetry operation at the top of the table.  $\chi^r(T)^*$  denotes the complex conjugate of the character of a symmetry operation  $T$  in the  $k$ -th class for the  $r$ -th irreducible representation. Since the characters for the octahedral group are real, these are simply the characters in Table A.1. Likewise,  $\chi_{rot}(T)$  denotes the character of the same symmetry operation for the representation  $\Gamma_{rot}^{(2)}$ .

To illustrate the use of Equation A.5, we can compute the multiplicities  $n_r$  in the decomposition of the representation  $\Gamma_{rot}^{(2)}$ . In each equation below, the three factors in the  $k$ -th summand all come from the  $k$ -th column of Table A.1. The first number in each summand is the class size  $N_k$  from the top row. The second number is  $\chi^r(T)$  from the row of the given irreducible representation. The third number is  $\chi_{rot}(T)$  from the bottom row of the table.

$$\begin{aligned} n_{A_1} &= \frac{1}{24} [(1)(1)(5) + (8)(1)(-1) + (3)(1)(1) + (6)(1)(1) + (6)(1)(-1)] = 0 \\ n_{A_2} &= \frac{1}{24} [(1)(1)(5) + (8)(1)(-1) + (3)(1)(1) + (6)(-1)(1) + (6)(-1)(-1)] = 0 \\ n_E &= \frac{1}{24} [(1)(2)(5) + (8)(-1)(-1) + (3)(2)(1) + (6)(0)(1) + (6)(0)(-1)] = 1 \\ n_{T_1} &= \frac{1}{24} [(1)(3)(5) + (8)(0)(-1) + (3)(-1)(1) + (6)(-1)(1) + (6)(1)(-1)] = 0 \\ n_{T_2} &= \frac{1}{24} [(1)(3)(5) + (8)(0)(-1) + (3)(-1)(1) + (6)(1)(1) + (6)(-1)(-1)] = 1 \end{aligned} \quad (\text{A.6})$$

This calculation shows that the only irreducible representations that occur in the decomposition of  $\Gamma_{rot}^{(2)}$  are  $E$  and  $T_2$ . Thus, the fivefold degenerate d-orbitals split into two new energy levels, with symmetry type  $E$  and  $T_2$ , respectively. This solves the splitting problem. It also solves the degeneracy problem. In Table A.1, the character of the identity transformation (found in the column under  $360^\circ$ ) equals the dimension of the corresponding irreducible representation. Thus, we see that the  $E$  irreducible representation is two-dimensional, while the  $T_2$  irreducible representation is three-dimensional. Recalling that the dimension of an irreducible representation equals the dimension of

the corresponding eigenspace, we see that the resulting energy levels are two-fold and three-fold degenerate, respectively. Finally, through the method of projection operators, representation theory allows us to determine good basis functions that diagonalize the perturbation operator,  $H'$  (Cornwell [1984], pp. 92–8). These are listed in the final column of the character table. They help modularize the eigenvalue problem into separate calculations for each eigenvalue.

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