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&HPS2 Submission Abstract

Crystals and Natural Kinds

In the twentieth century, developments in crystallography resulted in great advances in the scientific understanding of material substances. Though crystallography has been crucial to disciplines as important and diverse as solid-state physics and molecular biology, it has received relatively sparse treatment by historians and philosophers of science. In this essay, I provide a historical and philosophical study of crystallography and crystal classification. On the basis of this historical sketch, I argue against the claim that natural kinds cannot overlap in extension. Call this 'the hierarchy requirement.' One and the same crystal is classified as a member of a chemical kind, a structural kind, and a symmetry class. Thus, either the hierarchy requirement is incorrect in the domain of x-ray crystallography or these various kinds into which crystals are classified are not distinct. I argue that the second disjunct is false. Therefore, the hierarchy requirement is incorrect in the domain of x-ray crystallography.

I divide the essay into three sections. In the first section, I provide a historical sketch of crystallography. I focus on the changes in crystallography that accompanied the integration of x-ray analysis into the discipline by William Henry Bragg and William Lawrence Bragg from 1913—1929. This historical sketch demonstrates that the diverse kinds into which a crystal is classified cannot be reduced to a single kind or unified into a hierarchy. Prior to the advent of x-ray analysis, crystallography included two relatively independent research programs: geometric and chemical. Geometric crystallographers employed mathematical methods to classify crystals on the basis of symmetry. Crystals may be symmetric relative to planes, axes, or points. These combine to form thirty-two symmetry classes into which a particular crystal may be classified. These thirty-two classes were first identified by J. F. C. Hessel in 1830 and have since become a standard basis for the classification of crystals. Chemical crystallographers employed analytical methods to classify crystals on the basis of properties such as molecular weight and chemical composition. The early methods of chemical crystallography were sufficiently powerful to determine the chemical properties of few crystals. However, after the initial application of x-ray analysis to crystals by William Henry and William Lawrence Bragg, information about the internal structure and composition of a wide range of crystals was made available. Subsequent taxonomies of crystals included symmetry classes, chemical properties and internal structure as independent categories for classification. This resulted in a complex array of crystal kinds that overlap in extension: chemical kinds, structural kinds, and symmetry classes. For example, the crystals Calcite and Vaterite are of the same chemical kind ($CaCO_3$) but of distinct structural kinds. This complex array was not unified into a single set or hierarchy of kinds. Attempts were made at unification but the properties that distinguish kinds of crystals could not be either eliminated or explained away. Instead, each independent kind was retained because each is important for explaining other properties of crystals.

In the second section, I argue that the classification of crystals in incompatible with the hierarchy requirement for natural kinds. I take Brian Ellis as a model advocate of the claim that kinds cannot overlap in extension. More precisely, he claims that two natural kinds can overlap in extension only if there is some broader genus of which both natural kinds are species. The classification of crystals presents a challenge to this view since crystal kinds overlap and these kinds do not share a common genus. There are two responses available to the advocate of the hierarchy requirement. First, he could claim that one set of non-overlapping kinds is primary. Some philosophers of science, including Ellis, distinguish between causal explanations which have ontological import and theoretical explanations which do not. Chemical kinds are most important for causal explanation and thus are the true kinds; structural kinds and symmetry classes have pragmatic value only. I argue that this response fails. Chemical kinds, structural kinds, and symmetry classes are all important for causal explanations. For example, the structure of a crystal is crucial to the causal explanation of the diffraction pattern produced during x-ray analysis. The second response available to the advocate of the hierarchy requirement is to claim that chemical kinds, structural kinds, and symmetry classes in fact form a unified hierarchy. Structural kinds are species of symmetry classes which are species of chemical kinds. This response also fails. For, there are crystals which share their chemical kind and lattice structure but fall into different symmetry classes. This is possible because the orientation of the Sulfur atoms within the lattice varies between the two crystals. Though the arrangement of atoms in the lattice is identical, the difference in orientation results in a difference in symmetry. Thus, structural kinds could not be a non-overlapping species of symmetry classes. No other arrangement of these kinds into a hierarchy of non-overlapping kinds is possible. Thus, the second possible response fails. I see no other plausible response available to the advocate of the hierarchy requirement and, therefore, conclude that the hierarchy requirement is incorrect in the domain of crystallography.

In the third section of the paper, I situate my discussion of the hierarchy requirement as it applies to crystal kinds in the context of the broader philosophical discussion of natural kinds. Chemistry is frequently cited as a stronghold for advocates of the hierarchy requirement. The periodic table of elements provides a foundation for the categorization of material substances into non-overlapping kinds. The argument presented in section two shows that, relative to the periodic table, as the material substances get more complex, so do the taxonomies. This result is continuous with much work on natural kinds within the biological sciences. It is common to recognize that organisms cannot be classified into a hierarchy of non-overlapping species. The same is true of crystals.