

## Structure in Chemistry: A Case Study of Cumulativity and Retention

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In this paper I tentatively explore the historical evidence for a bold claim: that theories of molecular structure have, since the 1860s, developed through a series of conservative extensions, despite some apparently radical theoretical and conceptual change during this time. A conservative extension of a theory is one where its inferential content before the extension (i.e. that which determines its explanatory and predictive power) is a proper subset of its inferential content afterwards. This will happen when a theory is extended or reinterpreted so that inferences can be made concerning phenomena about which no inferences were previously made.

As a body of theory, molecular structure presents a number of apparent difficulties for historians and philosophers of science. Firstly, it was presented via a diverse range of visual representations. The visual nature of these interpretations makes it difficult to specify the predictive and explanatory content of the theory. Secondly, it was presented amid considerable controversy concerning the reality of atoms, and whether hypotheses about structure at the atomic scale could have any legitimate role in chemical explanation. This has meant that the interpretative caution of contemporary chemists has sometimes been misunderstood by historians and philosophers as a blanket form of instrumentalism. These difficulties can be addressed by paying careful attention to the inferential uses to which the various visual representations are put, which reflect sophisticated interpretative stances that the chemists took towards their representation schemes. I examine three key developments in structural theory.

### 1. Structure in organic chemistry (1860s)

Although presented via a diverse range of representational media (e.g. Kekul's sausage formulae, Hofmann's glyptic formulae' and the chemical graphs of Crum Brown and Frankland), structure in organic chemistry has long been interpreted by historians as a relatively unified body of theory (see Alan Rocke 1984, 2010). Like many contemporary chemists, Edward Frankland was careful to point out that structural formulae were intended to represent neither the shape of the molecules, nor the relative position of the constituent atoms'. This caution is sometimes mistaken for instrumentalism, but I argue that it reflects instead an awareness that the use of structural formulae in chemical explanations required inferences to be made concerning only the order of the connections between the atoms. The shapes of the molecules and the relative positions of the atoms played no more part in the representation than the particular colours chosen to represent the different kinds of atoms in Hofmann's glyptic formulae.

### 2. Stereochemistry (1870s)

The explanatory scope of the structures in (1) were soon extended so that inferences could be made about the relative positions of their constituent atoms. In 1874, Jacobus van't Hoff explained why there are two isomers of compounds in which four different groups are attached to a single carbon atom by supposing that the valences are arranged tetrahedrally (the two isomers are conceived of as mirror images of each other). Adolf von Baeyer explained the instability and reactivity of some organic compounds by reference to strain in their molecules, which meant their distortion away from some preferred structure (see Ramberg 2003, Chapters 3 and 4). These stereochemical theories were intrinsically spatial, because their explanatory power depended precisely on their describing the

arrangement of atoms in space. The extension of the theory did not require a wholesale revision of the structures that had previously been assigned to organic substances. Hence I argue that stereochemistry constituted a conservative extension of the earlier structural theory of the 1860s.

### 3. Structure in motion (1920s onwards)

The structural formulae of the nineteenth century are sometimes described as static. This could be misleading. Nineteenth-century chemists clearly entertained the thought that matter must be dynamic at the atomic scale, but they had no means to make reliable inferences about any such atomic motions. Hence they made no such inferences. The structural formulae may have been static, but they were not interpreted as representing molecules to be static. This caution began to change in the twentieth century. In 1911, Nils Bjerrum applied the 'old' quantum theory to the motions of molecules and their interaction with radiation, potentially explaining their spectroscopic behaviour (see Assmus 1992). From the 1920s onwards, Christopher Ingold applied G.N. Lewis' understanding of the covalent bond as deriving from the sharing of electrons to give detailed insight into reaction mechanisms: how, when chemical reactions occur, the structure of the reagents transforms into the structure of the products (see Goodwin 2007). I argue that these developments were conservative extensions of the structures in (2), allowing inferences to be made about their motions, and various spectroscopic and kinetic phenomena explained.

I conclude the paper by considering the prospects for extending my argument into the era of quantum mechanics. This might seem like a hopeless task: surely the quantum-mechanical molecule is radically different from the classical one! But this is too quick: firstly, 'classical' chemical structures are not classical in any way that has any connection with physics. They involve no application of (for instance) classical mechanics or Boltzmann statistics. Secondly, when quantum mechanics did come to be applied to molecules, the resultant theory was a synthesis of classical' structure and quantum mechanics. At first the classical structures were preserved by simple inclusion. Only later did quantum-mechanical facsimiles of them become available.