

## QTAIM and the Interactive Conception of Chemical Bonding

Quantum physics is the foundation for chemistry, but the concept of chemical bonding is not easily reconciled with quantum mechanical models of molecular systems. The quantum theory of atoms in molecules (QTAIM), developed by Richard F.W. Bader and colleagues, seeks to define bonding using a topological analysis of the electron density distribution. The “bond paths” identified by the analysis are posited as indicators of a special pairwise physical relationship between atoms. While elements of the theory remain subject to debate, I argue that QTAIM embodies a distinctive interactive conception of bonding that is an attractive alternative to others previously discussed.

## 1. Introduction

The notion of the chemical bond played a key role in the development of modern chemistry and remains central to our understanding of molecular structure and chemical transformations. However, with the advent of quantum mechanics (QM) and its successful application to molecules, it has become difficult to reconcile the traditional idea of bonds with the underlying physical theory. Some philosophers of science have grappled with this problem, discussing ways to conceive of bonds or bonding in light of QM models of molecular systems. At the same time, the quantum theory of atoms in molecules (QTAIM), a program in theoretical chemistry, provides a intriguing method for linking QM to traditional chemical concepts including bonding.

This paper is organized as follows. Section two briefly reviews the challenges facing the notion of the bond in light of modern modelling techniques, and highlights the structural and energetic conceptions discussed by Hendry (2008) and Weisberg (2008) as possible responses. An overview of QTAIM is presented in section three. While various philosophical implications of this theory have been discussed by proponents and others, I focus on the contrast it provides with these two other conceptions. In section four I argue that QTAIM provides a distinctive and appealing notion of bonding—appropriately described as an *interactive* conception. Section five briefly summarizes and suggests that the interactive conception has potential to illuminate how the idea of mechanistic explanation applies to chemistry.

## 2. Conceptions of the Chemical Bond in the Wake of Quantum Theory

Beginning in the 19<sup>th</sup> century, several scientists developed models of molecular structure, particularly as an avenue to explain phenomena in organic chemistry. A key figure in developing the theory of chemical bonds in the early 20<sup>th</sup> century was G.N. Lewis. Lewis (1916) distinguished two types of compounds, polar and non-polar. The former came to be described in terms of so-called ionic bonds: here electrostatic forces (which act in all directions) are responsible for the combination of oppositely charged ions. The non-polar type, Lewis reasoned, required the sharing of electrons. Specifically, the sharing of a pair of electrons between two atoms creates a covalent bond. In the theory, each element has a characteristic configuration of unpaired outer shell electrons: this is the raw material for creating covalent bonds and resulting molecules.

QM offers a very different picture of electrons, atoms and molecules. For instance, for a free particle moving in space, one cannot ascertain its position at a given time, but instead must determine its wave function  $\Psi$ , which is a function from the possible positions to a (complex) number. To interpret what this means for possible measurements of the particle's position, one calculates the probability of finding the particle in a given volume of

space at a given time from the product of  $\Psi$  and its complex conjugate  $\Psi^*$ . Absent a measurement interaction, the particle has no defined spatial location.<sup>1</sup>

For an atom, the behavior of the system is described by the time-independent Schrödinger equation,<sup>2</sup>  $\hat{H}\psi = E\psi$ , where  $\psi$  is the wave function,  $E$  is the energy, and  $\hat{H}$  is the Hamiltonian operator appropriate for the system. For an atom, the Hamiltonian will contain a kinetic energy term and a potential energy term that is based on the electrostatic attraction between the electrons and the nucleus (along with repulsion between electrons). By solving the equation, one finds the wave function and the energy: in fact there are many solutions corresponding to many energy states (the lowest energy state is the ground state). In the case of the hydrogen atom (where the nucleus is assumed to be stationary at the origin of the coordinate system), the calculated wave functions (called orbitals) indicate the position state of the electron: again this is in terms of complex-valued amplitudes over the possible position configurations. For multi-electron atoms an approximate description of possible electronic states is built up from successive hydrogen-like orbitals of increasing energy. In the context of multiple electrons, one can use the wave function as the basis for calculating the *electron*

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<sup>1</sup> The domain of the wave function for an  $N$ -particle system is a configuration space with  $3N$  dimensions.

<sup>2</sup> The assumption required here is that the potential energy of the system does not change with time.

*density distribution* ( $\rho$ ): this gives the expected number of electrons one would find at a particular location upon measurement.<sup>3</sup>

Given that electrons are not localized in quantum theory in the absence of measurement, Lewis' idea that a molecule is formed by sharing particular electrons is problematic. Linus Pauling (1960) prominently sought to reconcile the two pictures. His approach was to interpret quantum theory as describing "resonance" structures, which were hybrid combinations of multiple possible classical configurations. Some critics, however, viewed this perspective as unhelpful in the search for a purely quantum foundation for chemistry. While precise solutions to the Schrödinger equation for molecules are generally intractable, techniques to estimate a molecular wave function and thus calculate molecular energies and other properties were quickly developed.<sup>4</sup> One approach to calculation (which retains a conceptual link to the Lewis model and resonance theory) uses what are called valence bond (VB) models. This approach starts with the wave functions associated with

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<sup>3</sup> For multi-electron systems, the possible position configurations will reflect that electrons are fermions and their composite wave functions are anti-symmetric. This underlies the Pauli exclusion principle, whereby only two electrons may occupy the same orbital, and they must have opposite spins.

<sup>4</sup> One feature which figures in all of these approaches is the Born-Oppenheimer approximation: calculations start with the assumption that the nuclei are in a fixed configuration (which can be altered iteratively to find the best solution).

individual atoms (two at a time) and creates hybrid orbitals from their overlap. As a result, VB-based calculations preserve a degree of localization in the resulting orbital structure, and the idea of overlapping orbitals provides an intuitive notion of a bond. Over time an alternative to the VB approach has become dominant: this features the use of molecular orbital (MO) models.<sup>5</sup> Here, one constructs orbitals for all of the electrons in the molecule together (given fixed nuclear coordinates). These orbitals are not localized: they “cover” the entire molecule. The success of MO methods for calculating molecular wave functions leads to a puzzle about how the notion of a chemical bond should be viewed given the state of the science.

In assessing this question, Hendry (2008) describes two conceptions of the chemical bond. The first, the structural conception, seeks to “retain the explanatory insights afforded by classical structural formulas (Hendry 2008, 917).” To maintain these insights in the context of quantum theory, Hendry suggests a functional approach that would identify “physical realizers” of the role traditionally played by bonds. The requirements are that the realizers would be “material parts of the molecule that are responsible for spatially localized submolecular relationships between individual atomic centers (Hendry 2008, 917).”

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<sup>5</sup> For discussion of VB and MO models, see Weisberg (2008). Another family of models utilizing Density Functional Theory (DFT) is also frequently employed. These estimate functions on the electron density distribution to extract information about molecular properties.

Weisberg (2008) offers a slightly different definition whereby the conception says “a covalent bond is a directional, submolecular relationship between individual atomic centers that is responsible for holding the atoms together (Weisberg 2008, 934).” The main challenges facing this conception are the indistinguishability and non-localized nature of electrons in a molecule. A possible solution Hendry discusses is the identification of bonds with “nonarbitrary” components of the electronic wave function and/or electron density distribution of the molecule (Hendry 2008, 918).

The alternative Hendry outlines is called the energetic conception. Here, no part of the molecule responsible for bonding is identified. Instead facts about chemical bonding are facts about “energy changes between molecular or super-molecular states (Hendry 2008, 919).” If a molecule in a bonded state has lower energy compared to its separated atoms, this represents the formation of bonds. For two atoms forming a diatomic molecule, one can plot total potential energy as a function of inter-nuclear separation and identify the minimum value associated with bonding. For a polyatomic molecule, a potential energy surface in higher dimensions can likewise be calculated from trial wave functions. The energetic conception is, as Hendry puts it, “more a theory of chemical *bonding* than a theory of *bonds* (Hendry 2008, 919, emphasis added).” Weisberg (2008) argues that the idea that bonding involves energetic stabilization is a consistent, or robust, feature of various molecular models. This favors the energetic conception. He also argues that across the models he surveys, greater delocalization of electrons correlates with an increased match between calculated values for molecular properties and empirical estimates. This puts pressure on the

structural conception, which depends on identifying the realizers of the bond role in localized regions between atomic centers.

### 3. Overview of QTAIM

The quantum theory of atoms in molecules developed by Bader (1990) and colleagues offers an alternative approach to thinking about bonding.<sup>6</sup> The approach involves analyzing the topological features of the electron density distribution ( $\rho$ ) and linking these to chemical concepts. In examining  $\rho$  for a given molecule, the most obvious characteristic is its concentration near atomic centers and low concentration elsewhere. However, a detailed examination reveals more features. Since one can treat  $\rho$  as a scalar field in three-dimensional space, one can proceed to examine the associated gradient vector field (by applying the vector differential operator  $\nabla$ ): this shows the direction in which the density is increasing the most at a given point (and the magnitude of the increase). In this way, one identifies features such as critical points associated with extrema (minima, maxima and

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<sup>6</sup> Concise expositions of QTAIM include Gillespie and Popelier (2001, chaps. 6-7), and Popelier (2000, 2016).

saddle points), as well as gradient paths—trajectories that follow the line of steepest “ascent” at successive points.<sup>7</sup>

In examining  $\rho$  for a given molecule, a set of gradient paths originating at infinity will converge on maxima associated with each nucleus.<sup>8</sup> According to QTAIM, the space traversed by all of these paths (called the atomic basin), along with the nuclear “attractor” itself, defines an individual atom: “An atom, free or bound, is defined as the union of an attractor and its associated basin (Bader 1990, 28, emphasis original).” There is also a critical point (a saddle point) between nuclei: the set of gradient paths originating at infinity and converging on these points define a boundary, called the interatomic surface.<sup>9</sup> The atom is bounded inside the molecule by this surface and extends to infinity in the open directions away from the rest of the molecule: in practice the boundary in these directions may be defined using a pragmatic cut-off level of electron density (e.g. 0.001 a.u.). Next, one can

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<sup>7</sup> Further details can also be found by examining the second differential operator or Laplacian  $\nabla^2(\rho)$ , which is interpreted as indicating local concentration and depletion of density. This can be used to identify (imperfect) analogues of localized electron pairs (see Bader 1990, chap. 7).

<sup>8</sup> Technically, these maxima are not true critical points due to discontinuities, but are treated as such as a practical matter (see Bader 1990, 19).

<sup>9</sup> This surface is also referred to as a zero-flux surface, in that no gradient vectors cross it at any point (see Bader 1990, 28-9).

observe gradient paths that mark out lines of concentrated density linking two atomic centers to these same inter-nuclear critical points. These are called “bond critical points” and the paths that run from it to the paired nuclei are used to define what QTAIM calls “bond paths:” the full set of bond paths comprises what is called the molecular graph (Bader 1990, 32-3).

What is the relationship between QTAIM’s bond path and other notions of the chemical bond? Gillespie and Popelier (2001) caution that “a bond path is not identical to a bond in the sense used by Lewis (Gillespie and Popelier 2001, 152).” A molecular graph will not be identical to a Lewis structure, for instance, because “double and triple bonds are represented by only one bond path (Gillespie and Popelier 2001, 152).”<sup>10</sup> Still, they assert that “the existence of a bond path between two atoms tells us that these atoms are bonded together (Gillespie and Popelier 2001, 153).” Given this claim, one might ask if QTAIM is a way to “hold on to the structural conception of the bond understood functionally (Weisberg, Needham, and Hendry 2016, section 4.3).”

On this point, it is important to note that the QTAIM definition of a bond path also includes a stipulation that draws on the *energetic* conception of bonding. The identification of a bond path depends not only the presence of the signature pattern of electron density, but also requires that “the forces on the nuclei are balanced and the system possesses a minimum energy equilibrium internuclear separation (Bader 1990, 33).” Otherwise the feature is

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<sup>10</sup> Part of the QTAIM approach is to look closely at the characteristics of the BCP’s and neighboring topology to show how they correspond with various types of bonds.

referred to as an “atomic interaction line” (see Bader 1990, 32). But there is no reason a structural understanding of bonding cannot include this energetic component, and the QTAIM approach does at first appear to include important elements of the structural conception (as defined in Weisberg 2008): bond paths map a directional, submolecular relationship between atomic centers. With regard to Weisberg’s last criterion, Bader at times seems to endorse the notion that this feature “is responsible for holding the atoms together” (Weisberg 2008, 934). He says “nuclei...are linked by a line through space along which electronic charge density, the glue of chemistry, is maximally accumulated (Bader 1990, 33).”<sup>11</sup> But is this line of concentrated electronic charge density literally the “glue”? While the issues here are subtle, the answer is no.

Bader says that the appearance of an atomic interaction line (AIL) between a pair of nuclei is a “necessary condition” for bonding, but its presence is a sufficient condition only when “the system possesses a minimum energy equilibrium internuclear separation” (Bader 1990, 33). It is then that the AIL is designated a bond path. In order to better understand this definition, the role of the accumulation of charge between two nuclei *in the process of*

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<sup>11</sup> The notion that a region of electron density provides the “glue” or “cement” holding atoms together in a molecule is widespread in chemical texts, presumably for its heuristic value in some contexts (see, e.g., Loudon 1995). This provides the backdrop for Bader’s comment.

*achieving bonding* and the meaning of the presence of a bond path *in equilibrium* must be distinguished.<sup>12</sup>

If one pictures separated atoms being brought closer, then bonding is “the situation obtained when the initially attractive Hellmann-Feynman forces acting on the approaching nuclei, and resulting from the accumulation of electron density associated with the formation of the atomic interaction line, vanish (Bader 1998, 7314).” Bader is referring here to the role of electrostatic forces, the reliance on which is justified by reference to the Hellmann-Feynman theorem. This theorem implies that, given a wave function and associated  $\rho$ , all the forces on a nucleus in a molecule can be calculated based on classical electrostatics (see Gillespie and Popelier 2001, 134-36). As shown by Berlin (1951), this result can also be used to identify so-called binding and anti-binding regions of electron density in molecules. In the case of a diatomic system, charge density in the binding region between nuclei is seen as drawing the nuclei together, while density in anti-binding regions on the far side of the nuclei works to draw them apart (along with nuclear repulsion).<sup>13</sup>

*Outside* the equilibrium inter-nuclear separation, we can ascribe to the binding region the responsibility for a (net) attractive force. *At* equilibrium distances, all forces on the nuclei

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<sup>12</sup> See discussion in Popelier (2000), 60-1.

<sup>13</sup> This electrostatic picture of how bonding is achieved has been challenged by a competing theory of the bonding process (discussed recently by Needham 2014). See Bader (2011) for a response.

are balanced. Now, one can still divide the electronic density distribution into binding and anti-binding regions (it should be noted here that the binding region encompasses much more than the line of density marked out by the bond path). But if there is no net force at work, it would be oversimplifying to say the binding region is “holding the atoms together.” This would only tell part of the story, since one could say the anti-binding region also holds the atoms in place by keeping the inter-nuclear distance from compressing beyond the equilibrium separation. This point is perhaps clearer in comparison to Hendry’s formulation of bonds as “material parts of the molecule that are responsible for spatially localized sub-molecular relationships between individual atomic centers (Hendry 2008, 917).” Binding and anti-binding regions both clearly play a role in defining the equilibrium inter-nuclear distance. And since these regions together encompass the entire molecule, there is no basis for concluding that the bond paths of QTAIM, despite highlighting a concentrated area of  $\rho$ , pick out a region that plays the functional role envisioned by the structural conception. Instead, the presence of the bond path at equilibrium appears to represent “forces [which] act on the nuclei for *any* displacement from their final equilibrium position (Bader 1998, 7314-315, emphasis added).”<sup>14</sup> As such, the bond path is a “universal *indicator* of bonding (Bader 1998, 7315, emphasis added).” According to QTAIM, then, the bond path is a *sign* that the bonding relationship exists, but it does not represent a region responsible for holding the atoms in place.

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<sup>14</sup> See also Popelier (2000), 55-56.

Consistent with this conclusion is another departure QTAIM takes from a traditional view of bonds. Bonds are often pictured as localized *between* atoms in a molecule. However, bond paths (with the exception of the bond critical point) fall *inside* atomic boundaries. Atoms lie adjacent to one another along the interatomic surface. QTAIM offers a different picture that “requires the replacement of the model of structure that imparts an existence to a *bond* separate from the atoms it links – the ball and stick model or its orbital equivalents of atomic and overlap contributions – with the concept of *bonding* between atoms (Bader 1998, 7322, emphasis original).”

#### 4. Interpreting QTAIM’s Conception of Atoms and Bonding

Bader’s distinction between “bonds” and “bonding” is in keeping with a difference Hendry identifies between the structural and energetic conceptions.<sup>15</sup> Given this, and given its reliance on energy equilibrium in its definition of bonding, one might ask how closely the QTAIM picture should be identified with the energetic conception. The key difference is that while the energetic conception emphasizes achieving a stabilizing minimum molecular energy, QTAIM goes further to provide an indicator that particular atoms are indeed bonded.

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<sup>15</sup> Bader says that “a bond path is not to be understood as representing a ‘bond,’” rather “the presence of a bond path linking a pair of nuclei implies that the corresponding atoms are bonded to one another (Bader 1990, 35).”

Only some pairs of atoms in a polyatomic molecule at an energy minimum are bonded, and bond paths pick these out. As a first pass, one might view the QTAIM conception as a hybrid of the conceptions considered above: while it relies on energetic considerations, its bond paths define directional relationships between atomic centers in keeping with the structural conception.

But seeing the QTAIM idea as a hybrid arguably misses what makes it distinctive. The goal of QTAIM is to provide not only a conception of bonding, but also of the bonded *atoms*: it seeks to show that atoms in molecules should be seen as bona fide physical systems in their own right. Bader notes that “quantum mechanics has been shown to account for the properties of isolated atoms and for the total properties of a molecular system” but there is a “lack of a quantum definition of an atom in a molecule (Bader 1990, 131).” The approximated solutions to the molecular wave function feature delocalized electron orbitals around a configuration of stationary nuclei. As discussed, QTAIM uses a topological examination of  $\rho$  to define atoms. In doing so, QTAIM also provides a way to calculate various atomic properties. To calculate atomic charge, for example, one integrates  $\rho$  over the topologically defined volume of an atom and then subtracts it from the associated nuclear charge: Bader argues that the consistency of these calculated values across molecules that incorporate the same atom demonstrates the success of the approach.<sup>16</sup> QTAIM extends this approach to other properties, including atomic energies, although this involves more complex

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<sup>16</sup> Bader uses Li in LiF, LiO, and LiH as an example (Bader 1990, 135).

derivations.<sup>17</sup> Bader's ultimate claim is that QTAIM provides a full account of atoms in molecules as quantum physical subsystems: the topologically defined atom is also a quantum atom.<sup>18</sup> This claim continues to be the subject of debate in the theoretical chemistry literature, and no definitive judgments on its technical merits can be made here. Rather, with this sense of the goals of the program, we can return to the question of what QTAIM's approach implies for the conceptions of atoms and bonding.

Instead of describing a molecule as a system featuring interactions between electrons and nuclei, QTAIM posits atoms as interacting systems within the molecule. An atom in a molecule is an "open quantum subsystem, free to exchange charge and momentum with its environment (Bader 1990, 169)." Of course the relationship of interest is between two bonded atoms along an interatomic surface: "it is through the exchange of electrons and the fluxes in properties across the surface described by the physics of a proper open system that atoms adjust to the presence of their bonded neighbors (Bader 1998, 7322)." Bonding is a special physical relationship between pairs of atoms in a molecule where displacement

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<sup>17</sup> Popelier (2016) gives a concise account of QTAIM's derivation of atomic energies. In response to some criticisms of the approach he concedes that it is not ruled out that some molecular fragments, which are not QTAIM's topological atoms, may also have a well-defined energy (see Popelier 2016, 37).

<sup>18</sup> Bader's arguments that quantum mechanical principles apply to QTAIM's atoms are given in Bader (1990), chaps. 5-6, 8.

(within limits) leads to particular restorative responses within the molecular framework.<sup>19</sup> In equilibrium, the nature of this relationship can be examined via the topological properties of density at the points where the atoms meet and where charge or other properties would be exchanged – the bond critical points on the interatomic surfaces. But even though bond paths are defined at equilibrium, the distinctive feature of the conception is that it embodies the idea of a particular pairwise interaction between atoms (not just between the electrons and nuclei). Rather than a combination of the energetic and structural conceptions discussed above, the QTAIM conception is better labeled an *interactive* conception of bonding.

It should be noted that QTAIM's claim of a close extensional match between its definition of bonding and traditional chemical definitions has been challenged. Bader had put the claim this way: "the network of bond paths...is found to coincide with the network generated by linking together those pairs of atoms that are assumed to be bonded to one another on the basis of chemical considerations (Bader 1990, 33)." However, Weisberg, Needham, and Hendry note that Bader's approach appears to be "too permissive (Weisberg, Needham, and Hendry 2016, section 4.3):" citing Cerpa, Krapp, Vela, and Merino (2008), they say the problem is that bond paths appear between non-bonded atoms (one example given was that of an Argon atom trapped within a C<sub>60</sub> molecule which features a bond path

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<sup>19</sup> For a challenge to QTAIM's association of bond paths/BCP's with stabilizing interactions see Poater, Solà, and Bickelhaupt (2006). The present discussion is limited to arguing that this notion is conceptually central to the theory.

connecting it with all sixty carbon atoms).<sup>20</sup> In recent papers, Bader clearly acknowledges that bond paths are present in contexts not traditionally associated with chemical bonds. However, he attempts to turn this into a virtue, saying QTAIM offers a more theoretically precise approach to bonding that extends beyond traditional notions but also offers analytic tools to more precisely characterize different cases (see Bader 2011, 20). On balance, while the criticism has some merit given claims made in Bader's earlier work, it must be considered in the larger context of debates about chemical bonding: neither Lewis's theory nor any successor account is free of challenges.<sup>21</sup>

## 5. Summary and Implications

The interactive conception embodied in QTAIM has advantages over the others discussed: it offers more detail about how atoms relate to one another inside a molecule compared to the energetic conception, and unlike traditional structural approaches it relies

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<sup>20</sup> See Bader (2009) for a response. For another critique see Foroutan-Nejad, Shahbazian, and Marek (2014), who emphasize that bond paths may disappear/re-appear due solely to nuclear vibrations in some cases. They also note that atoms in molecules that are not linked by bond paths may be seen as interacting.

<sup>21</sup> This is true even of a minimalist energetic account. For example, Berson (2008) argues there are cases where covalent bonding leads to energetic destabilization.

only on information drawn from quantum mechanically derived calculations. It also invites one to consider that bonding is not best understood in static terms. While analyses of physical systems often center on idealized equilibrium conditions, molecules should perhaps be understood as constituted from patterns of repeated characteristic interactions between atoms in an environment of ongoing change.

This idea suggests that the interactive conception has implications for the philosophy of explanation as it pertains to chemistry. In particular, despite the successes of quantum models, approaches to mechanistic explanation typically used elsewhere in the context of complex (often biological) systems would still be applicable to molecules. First, I note that in the constitutive dimension of mechanistic explanation, systems are typically conceived of as composite entities whose properties and behaviors are due to both the properties of and the organized pattern of interaction among its constituent parts.<sup>22</sup> This comports well with the interactive conception of bonding. Further, the interactive view may help to elucidate the notion of mechanism in the context of chemical transformations. Goodwin (2012) describes chemists as using both a thick and thin conception of mechanism. In the thick sense of a reaction mechanism, for instance, a reaction is conceived of as a continuous evolution from reactants to products and might be represented as a path along a potential energy surface. The thin conception, on the other hand, breaks the reaction into a sequence of steps, and may feature a description of links between discrete classical structures. If atoms can be given an

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<sup>22</sup> An example is Wimsatt's discussion of reductive explanation (see Wimsatt, 2007, 275).

energetic analysis while also being treated as interacting entities both inside and outside of molecules, this offers a potential path toward bridging these two conceptions of mechanism.

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