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Overview of the complex but fruitful relationship between molecular chemistry and quantum mechanics, in celebration of the Year of Quantum Sciences and Technologies.

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Abstract

The United Nations General Assembly has officially designated 2025 as the International Year of Quantum Science and Technology (IYQ). This global initiative, supported by UNESCO and co-sponsored by several countries, marks the centenary of quantum sciences, which encompass quantum mechanics, quantum chemistry, and related fields. These disciplines serve as the foundation for fundamental research across the natural sciences. Quantum mechanics provides the theoretical framework for understanding matter and energy at the microscopic scale. While public celebrations of the International Year of Quantum Science and Technology often showcase quantum technologies to engage a broader audience, it is crucial to remember that the emergence of quantum theory primarily represented a ground-breaking shift in the basic sciences.

This article explores the complex relationship between quantum mechanics and concepts of traditional chemistry, particularly concerning the microscopic world of atoms and molecules. It highlights how quantum mechanics, a holistic and nonlocal theory, features concepts such as entanglement and the indistinguishability of components that challenge classical chemical notions of distinct interatomic interactions and well-defined molecular structures. While quantum mechanics excels at determining the overall stability and dynamics of the system, the article explains that quantum chemistry relies on the classical Born-Oppenheimer approximation to maintain the view of local interactions and identifiable atoms within a molecule. Then, the article discusses the historical development and limitations of transition state theory in explaining chemical reactions, highlighting chemistry's specific focus on bond breaking and bond making as a fundamental explanatory principle.

Introduction

It has now been a century since Werner Heisenberg published his seminal work on the quantum-theoretical reinterpretation of kinematic and mechanical relationships [1]. Quantum mechanics has since demonstrated its profound capacity to elucidate the sub-microscopic realm of matter, a domain fundamental to our chemical understanding of the natural world. From its very origins, quantum mechanics has not only provided a description of the atom as a system composed of multiple constituents but has also enabled the investigation of how assemblies of atoms combine to form molecules. Indeed, within the context of nineteenth-century science, the molecule posed a far greater conceptual challenge than the atom itself.

In that era, an atom, in the literal sense—a piece of matter endowed with mass, with or without a specific shape—struggled to explain its interactions with other atoms, and even more so, the selective interactions associated with the chemical affinities of substances. Since the seventeenth century, physicists had rationalised atomic interactions by assimilating them to gravitational and/or electrical forces, often "dematerialising" atoms into points of force endowed with mass [2]. Chemists, from Dalton onwards, conceptualised atoms as particles of matter, differentiated by mass (the so-called "atomic weight"), but observed regularities and periodicities among different atoms—evident in Mendeleev's periodic table—that were difficult to understand without probing the atom's interior.

After the discovery of atomic components—first the electron, then the nucleus, and finally its differentiation into protons and neutrons—the problem of atomic structure could no longer be ignored. The solution found in the early twentieth century fused the immateriality (points of force) of physicists and the materiality (particle of matter) of chemists into a dual atomic world, a wave/particle for both atomic constituents and the atom as a whole. Ultimately, the molecule found its “nature” in the energetic stability of an ensemble of atoms distributed in space.

Nevertheless, whether and how certain theoretical features of quantum mechanics could be related to concepts developed within chemical tradition, chiefly those of interatomic bonding and molecular structure, remains to be understood. Here, we will analyse three essential quantum features: the non-locality of interactions, the indistinguishability of atomic/molecular components, and the relationship between the characteristics of sub-microscopic entities and macroscopic properties—features that have a complex relationship with the chemical perspective on the sub-microscopic world.

Non-locality in Quantum Mechanics and Its Relationship with Chemistry

The non-locality of interactions between microscopic entities is an essential aspect of Quantum Mechanics and implies that even entities separated by great distances can influence one another. This property has no analogy in classical physics and contradicts the principle of locality, which states that an object is only influenced by its immediate environment, not by distant objects. In ancient and classical physics, interactions were always considered local, either involving contact (as in collisions) or decreasing in intensity with distance (as in Newton’s and Coulomb’s laws).

Quantum non-locality represents one of the most profound and counterintuitive aspects of Quantum Mechanics [3]. At its theoretical core, quantum non-locality is intimately connected to quantum entanglement, which describes correlations between particles regardless of their spatial separation. When two particles are prepared in an entangled state, for example, with correlated spin parameters, they become a single quantum system in a certain sense. If these particles are separated and the spin of one is measured, the spin of the other is determined instantaneously, regardless of distance.

Historically, the famous Einstein-Podolsky-Rosen (EPR) [4] paper of 1935 marked the beginning of the problem of quantum non-locality. In this work, Einstein and his colleagues first recognised this “spooky” feature of quantum mechanics, suggesting non-local behaviour in multi-particle systems. Einstein believed this indicated that quantum mechanics was incomplete and proposed the search for a realistic, local theory with hidden variables as an alternative. The theoretical debate between these alternative views was empirically resolved when Aspect and colleagues [5], in pioneering experiments in the early 1980s, measured correlations between entangled particles, providing compelling evidence for the non-local behaviour of sub-microscopic entities.

Since then, many theoretical proposals have sought to understand non-locality. Recently, some researchers [6] have suggested that the Heisenberg uncertainty principle—one of the cornerstones of quantum mechanics—determines the non-locality of the theory, suggesting that these two fundamental aspects are deeply interconnected.

Quantum non-locality can be interpreted differently across various interpretations of quantum mechanics, offering distinct perspectives on this phenomenon. In the standard Copenhagen interpretation, non-locality emerges during the measurement process, when the wave function collapses. By contrast, Bohmian mechanics explicitly incorporates non-locality as a fundamental feature, postulating that particles always have well-defined positions and follow deterministic trajectories, but are guided by a quantum potential [7]. Other interpretations go further, emphasising non-locality: some models of quantum reality [8,9] postulate that the entire universe forms an "indivisible whole" that is "extremely non-local," where particles retain memory of their space-time history through phase entanglement. In this view, quantum non-locality may not be a "problem to solve," but rather a feature leading to a deeper understanding of space-time itself.

It is worth noting, however, that some physicists have argued that non-locality is not necessary in quantum theory and that it depends solely on the interpretative frameworks employed. For example, if the quantum wave function is not given a realistic interpretation and its "collapse" is not considered a physical change, locality could be recovered even within the standard quantum framework.

The discovery of quantum non-locality and subsequent experimental confirmations have led to profound philosophical implications that continue to reshape our understanding of the universe. The revelation that the universe may exhibit non-local behaviour represents one of the most subtle yet profound insights into the physical world. Philosophically, quantum non-locality forces us to abandon at least one of our assumptions about reality. Experimental findings on non-locality tell us that we cannot simultaneously maintain both the principle of locality (that objects are influenced only by their immediate surroundings) and realism (the idea that physical properties exist independently of observation). This conclusion confronts us with several uncomfortable philosophical options: must we accept that reality is fundamentally non-local, or abandon the idea that unobserved properties have definite values? Ultimately, non-locality compels us to reflect on our very understanding of causality in the quantum world.

How does all this relate to the chemical perspective on the atomic/molecular world? This is the question we now address.

Already Schrödinger [10], examining these quantum issues, identified the conceptual basis of what we now recognise as entanglement in the existence of global states of composite systems that could not be written as products of the states of their individual subsystems. From the quantum perspective, as noted, entangled particles constitute a single quantum system, so it is not necessary to transfer information between its spatially separated parts. Thus, in this view, quantum mechanics is necessarily a non-local theory, but it respects ordinary causality.

For chemists studying the atomic/molecular world, both the particles and their interactions are local. The locality of particles will be addressed later; here, we focus on the locality of interactions between atoms—what chemists call chemical or interatomic bonds. Within a molecule, chemists identify which pairs of atoms are bonded and which are not. This is the conceptual basis of molecular structure. The concept of molecular structure, developed in the second half of the nineteenth century [11,12], has since played a fundamental role in chemistry. As Hendry notes [13], "molecular structure is so central to chemical explanation that to explain molecular structure is pretty much to explain the whole of chemistry."

Molecular structure is certainly closely related to the spatial distribution of atoms, but for chemists, it is not exhausted by this relationship. Given the spatial positions of an aggregate of atoms, to arrive at the concept of a molecule and its structure, further logical steps are required [14]. For example, if we specify the spatial arrangement of an aggregate consisting of 25 hydrogen atoms and one oxygen atom (system $H_{25}O$), it would not constitute a molecule, and we could not speak of its "molecular structure." Such a system would not be stable and thus would not be a molecule that could be found in nature or synthesized in the laboratory; its structure would not correspond to a minimum on any potential energy hypersurface. This highlights an important general principle of the sub-microscopic world: not every aggregate of atoms is a molecule.

This issue leads us to note that in ancient Greek atomism, although it was implicit that atoms would aggregate to form everyday objects, the concept of a molecule was absent. There could be no conceptual difference between different "aggregates of atoms." Nothing would distinguish the atomic aggregates H_2O and $H_{25}O$—both would be possible and compatible with such atomism. In modern terms, for Greek atomism, "every aggregate would be a molecule."

Elsewhere, one of us has shown the evolution of the concept of the molecule and its conceptual and philosophical relevance in modern science [11]. Summarising the aggregate/molecule problem, valence and chemical bonding concepts clarified in the nineteenth century why the H_2O molecule could exist and $H_{25}O$ could not. After extensive theoretical and experimental work, nineteenth-century chemists "determined" that the oxygen atom was bivalent (with two valences to be saturated in molecule formation, thus forming two chemical bonds), while hydrogen was monovalent (saturating only one valence to form a single bond). This made it possible for oxygen to bond with two hydrogen atoms (as in H_2O), but not with twenty-five hydrogen atoms (as in $H_{25}O$). From this chemical perspective, hydrogen atoms are "bonded" to the oxygen atom (and vice versa), but the two hydrogen atoms are not bonded to each other.

The modern concept of molecular structure, therefore, not only provides the spatial arrangement of atoms but also information on the organization of interactions within a molecule. Chemists identify, for each atom in a molecule, to which other atoms it is bonded, and the structural formula highlights this difference atom by atom. In practice, the concept of molecular structure "summarises" the set of intramolecular atomic bonds.

The concept of molecular structure has allowed the rationalisation of the properties of chemical compounds, enabling their classification into homogeneous groups, such as those in organic chemistry: alcohols, ethers, etc. The same concept has also made it possible to understand the transformation properties of such groups of substances—their reactivity. Chemistry without chemical bonds and the corresponding molecular structure would, in fact, be radically different from what it is today. The question, therefore, of whether the chemical bond emerges directly from the study of these systems using quantum mechanics has a negative answer, and the relationship between the chemical bond and molecular structure with quantum mechanics is complex and must be analysed in detail [15].

The Indistinguishability of Atoms in a Molecule in Quantum Mechanics and Chemical Perspective

Quantum mechanics is a holistic theory in the sense that, once a system is defined, its stationary states are global states distributed over the entire system and lack a "specific" connection to the constituents. This does not mean, of course, that these global states are uniformly distributed among all the constituents, but rather that the states of the system's components no longer have their own reality within the system. Even when the theory uses the states of the components to obtain these global states—as in the LCAO-MO approach to molecular electronic states, where the global stationary states of the molecule (molecular orbitals, MO) are linear combinations of the atomic orbitals of the components (linear combination of atomic orbitals, LCAO)—the states of the constituents are merely one of the possible (in the mathematical sense) bases for constructing the stationary states of the global molecular system. The atomic states (and, with them, the related atomic systems) lose any "real" significance within the molecule, and their combination (the coefficients of the linear composition in the LCAO approach) serves only as a possible description and determination of the global state. Any other basis, distributed in molecular space, could serve the same purpose (perhaps less efficiently, requiring more functions, i.e., a larger basis set).

This aspect of quantum mechanics has been scarcely emphasised in the literature and entails a complex relationship with the sub-microscopic world of chemistry. The latter, in fact, presupposes that the global system (the molecule) "in some way" contains the constituents (the atoms), that the properties of the new system (the molecule) are "in some way" connected to the properties of the constituents (the atoms), and that it is appropriate to project the system's properties onto its constituents. There is much to be said to clarify the expression "in some way," but this is a general issue that cannot be exhaustively addressed here. In what sense, the constituents "persist" in a system that "is more than its constituents" by definition is, in fact, a problem relevant to all systems, not just molecular ones [16]. Many of the specific issues and difficulties related to projecting molecular properties onto atoms are connected to these general problems. For example, the calculation of "atomic charges" in a molecule is carried out via many different approaches [17] precisely because there is no simple and unique way to assign the molecular characteristic of electron density to atoms, even though this is rarely specified in the literature.

To the holistic issue in the study of molecular systems with quantum mechanics, we must add a peculiarity of the quantum world: the indistinguishability of a system's components. For example, the current quantum treatment of a molecular system is carried out using atomic nuclei and electrons. Due to the mass difference between these two atomic components, the former is considered using the classical mechanics approach (Born-Oppenheimer approximation), with fixed positions and velocities, while electrons are treated as fully quantum and indistinguishable from one another. The Slater determinant in the study of the electronic states of a molecule serves to emphasise that we are unable to distinguish which electron belongs to which atomic nucleus, since all electrons are identical; thus, for each electron, all possible permutations over the atomic nuclei must be considered. This poses problems for chemists who, following Lewis's reasoning, place electrons around atomic nuclei and "move" them—visually, with curved arrows—during the formation of new molecular systems.

The Born-Oppenheimer approximation can be avoided in the treatment of some simple molecular systems, but in this case, the issues with the chemical perspective become more pronounced [18]. For the chemist, for example, it is essential to distinguish between the two types of hydrogen present in ethyl alcohol (C_2H_5OH): those bonded to carbon atoms and the one bonded to the oxygen atom. In a fully quantum treatment, however, for this molecule, the distinguishability of the two types of hydrogen atoms would be lost. It would no longer be possible to associate this substance with the class of alcohols based on the presence of an O-H functional group. The existence of a hydrogen atom “bonded” to the oxygen atom (or even simply “close” to the oxygen nucleus) and thus different from the other hydrogens “bonded” to carbon atoms (or “close” to the carbon nuclei) would no longer be determinable.

Atomic/Molecular Properties and Macroscopic Properties: The Quantum and Chemical Perspectives

Having touched upon the “locality and distinguishability” of the components of a quantum system, let us now consider the significance, for quantum mechanics and chemistry, of connecting atomic properties with molecular properties and the latter with those of the macroscopic substance.

To answer the first part of the question—namely, the connection between atomic and molecular properties—we must recall the different meanings that the parts of a system have in these two scientific domains. As mentioned, quantum mechanics is a holistic theory that aims to calculate the stationary states of the isolated molecular system and thus recognizes the states of the constituent parts (in this case, the atoms) only as “mathematical support” to start from a description sufficiently similar to the final one, which is obtained by optimizing the molecular potential energy. Chemistry, on the other hand—including quantum chemistry—holds that it is useful to “connect” molecular states and their properties to atomic states and their properties. This does not mean that the quantum chemist believes that atomic states continue to exist within the molecule. However, since the aim is not only to calculate molecular properties but also to “project” them onto the constituent atoms in order to compare and group molecules, it is considered essential that the constituents (both the states and the entities) remain essential. To simplify and clarify this point: for quantum mechanics, the basis used to construct molecular states can be generic, and the atomic states basis is only useful; for quantum chemistry, the atomic states basis is the one to use in order to decompose molecular properties onto the atoms. It is clear to the quantum chemist that the decomposition of a molecular property onto atoms can be performed in several ways, but this issue can be addressed by noting that each type of decomposition identifies a particular model of the atoms within the molecule. The classic example is that of atomic charges in a molecule: Mulliken populations, atomic natural orbital (ANO) charges, or other methods [17].

A specific discussion should be reserved for the study of chemical reactions with quantum mechanics and theoretical chemistry. Between 1915 and 1940, two groups of problems regarding the theoretical treatment of chemical reactions underwent intense reworking: the mechanism of reactions, i.e., identifying all the steps in the course of a chemical reaction, and the nature of the elementary act of the reaction [1].

In this context, we wish to highlight a general aspect of the philosophy of science that has received little attention. The concept of reaction mechanism has acquired, at the beginning of the twenty-first century, an increasingly general and important role in the scientific explanation of reality [20,21]. This has been achieved, however, with little attention to the mechanism of chemical processes, which have employed this concept for a century [22].

In our view, it is important for those engaged in the philosophy of chemistry to reclaim the primary role that chemistry has played in developing the concept of the mechanism of a process. In current theoretical chemistry, the main approach to studying chemical reactions is transition state theory (TST), also known as the theory of absolute reaction rates (ART) and the theory of the activated complex, with roots dating back to the early twentieth century.

The statistical theory of chemical reactions begins with Marcelin's work in 1915 [23]. It was then developed primarily by Eyring in 1935 as the calculation of absolute reaction rates [24] for bimolecular reactions and by Evans and Polanyi as transition state theory" [25,26]. The basic idea of this theory is that during the reaction, the system must overcome a critical region (the transition state) in configuration space to move from the initial state (reactants region) to the final state (products region). Assuming thermal equilibrium in both the initial and transition states, the formula for the reaction rate was derived based on the probabilities of finding the system in the initial and final states, the average velocity with which the system passes through the narrow intermediate region of configuration space, and the probability that the system, having passed the transition state, reaches the final product state [27,28]. Subsequently, Pelzer and Wigner [29] introduced the use of potential energy surfaces in this statistical treatment of chemical reactions, identifying the transition state with the saddle point (a minimum in all coordinates except one, in which there is a maximum) of a potential surface. In this way, it is possible to define a "reaction path" as the line of minimum potential energy connecting the two potential wells of reactants and products, passing through the saddle of the transition state. Wigner [30] replaced probabilities with the corresponding quantum partition functions, and Eyring developed the theory in the form of the "activated complex," where the transition state, called the activated complex, was considered sufficiently stable to be in thermal equilibrium with the reactants in all degrees of freedom except for movement along the reaction coordinate. Hirshfelder and Wigner [31] were the first to discuss the validity of the activated complex theory from the perspective of quantum mechanics.

They demonstrated that the concept of an activated complex aligns with Heisenberg's uncertainty principle only when the potential energy along the reaction path in the saddle region is sufficiently flat. This condition is met when the energy $h\nu^{\#}$ (h being the Planck's constant and $\nu^{\#}$ the vibration frequency of the activated complex at the saddle point) is significantly less than the thermal energy KT (K being the Boltzmann constant and T the absolute temperature)

This condition was necessary both for the definition of the activated complex and for motion along the reaction coordinate. If this condition was not satisfied, quantum mechanical tunnelling through the barrier had to be considered [32]. If the condition was met instead, motion along the reaction coordinate could be described classically. However, this condition alone was not sufficient for defining the activated complex as a stable configuration for which it made sense to speak of vibrations and rotations. It was also necessary to assume that the lifetime of the activated complex was sufficiently long that, while the system passed through the intermediate region of configuration space, many vibrations and rotations could occur. In practice, the theory of the activated complex was justified when movement along the reaction coordinate was slow enough to allow adiabatic variation of vibrations and rotations, thus preserving the quantum state of the system. This ensured both the possibility of treating vibrations and rotations quantum mechanically and thermal equilibrium in the transition state.

A critical point of the activated complex theory was the assumption that this complex was in equilibrium with the reactants. Recently, different approaches have been proposed to overcome the equilibrium assumption. Here, we will only make explicit the general problems that have led to them. There are many reasons to introduce non-equilibrium theories. First, the validity of the assumption of thermal equilibrium between the initial state and the transition state can be questioned, and it is desirable to have an alternative formulation. Moreover, there are situations where one wishes to know the detailed molecular dynamics of a chemical process, requiring a more detailed treatment than a statistical approach. These non-equilibrium theories are necessarily more complicated than the original equilibrium theory, and it is difficult to obtain numerical values from them to compare with experimental results.

Let us now analyse the fundamental concepts underlying TST. In the kinetic theory of collisions, it is assumed that molecules do not interact except during an infinitesimally brief period when they collide. These collisions allow for the thermal equilibrium of molecular velocities and, when the exchanged energy randomly exceeds a pre-set threshold, trigger the reaction. This theory is based on a classical mechanical view of molecules as groups of balls that break apart upon collision. The problem is that this simplistic view is suitable only for a few types of reactions, particularly unimolecular reactions, in which two molecules of the same species collide and one acquires enough energy to fragment. In general, a chemical reaction leads to a global restructuring of the molecules involved in the collision, so extensive as to give rise to new molecules. A theory of reactions must therefore explain the complex mechanisms that allow for the substitution of atoms and the formation of selective bonds, as well as the breaking of certain bonds. It is, so to speak, the "reorganization" aspect of molecules, rather than just the breaking, that is missing. In our view, this theory is still substantially tied to the concept of the molecule as a "set of rigid spheres," that is, a system in which "molecular structure" coincides with the "arrangement" of atoms. We have already shown, however, that, beyond the variation in atomic positions, a chemical reaction can be seen as "a disorganisation followed by a reorganisation." Furthermore, this theory seeks to interpret all phenomena in purely mechanistic terms and does not consider specific chemical interactions. This issue becomes increasingly evident as molecular size increases, particularly with macromolecules. The active and allosteric sites of proteins are an excellent example [33].

Other general problems are implicit in quantum potential energy surfaces. In the transition state theory, in fact, the concept of molecule is altered, at least in the usual sense used in chemistry. For chemistry, it is a spatially well-defined structure, except for small oscillations around the equilibrium positions. Instead, the potential energy surface of a reactive system, and in general we must speak of a system and not of a molecule, is obtained by calculating the potential energy for all possible spatial positions of the atoms, even for those that, from a chemical point of view, could hardly give rise to a molecule. The value of the potential energy of the system has no physical meaning except at some specific points of the surface: minimums, inflexion points, and maximums. It is only these points, and the areas around them, the parts of the surface that can be related to specific situations of the molecule. Furthermore, as the number of atoms in the system increases, this hypersurface becomes impossible to explore. In this system, chemical bonds, i.e., directional and privileged interactions, disappear, and the position of the atoms in the molecule is recovered only a posteriori by placing the atoms in the potential energy wells to minimize the energies. Furthermore, for large molecules and for macromolecules on a potential energy hypersurface, many positions of relative minima are possible, i.e., many systems with spatial arrangements of the atoms that are very different from those of the molecule under examination. Finally, once the transition state has been determined, the system evolves along the line that leads to the minimization of the energy of the products and it is this curve that gives us the reaction path. This approach also clashes with the chemical approach in which the chemical reaction is centred on the breaking and formation of interatomic bonds.

In conclusion, chemical transformations are a fundamental part of the chemical approach to the study of the material world. For this science, in fact, the millions of entities that characterize it, the molecules in the microscopic plane and the chemical substances in the macroscopic one, are the qualitative plural of the world, but they are also the basis with which to explain its transformation. The ability to hold together both the static aspects, properties of the entities, and the dynamic ones, their transformation, is the historical result of a science that has always given considerable importance to the aspect of variety and transformability of matter. Furthermore, nowadays, quantum mechanics is only in the early stages of explaining the dynamic reactive transformation of the molecular structure.

Conclusion

In conclusion, we can summarize the essential aspects analysed of the relationship of quantum mechanics with the chemical tradition.

The general approach of chemistry and quantum mechanics are different. Chemistry aims to master a complex world of millions of different substances (mainly compounds) on the macroscopic level and an equally complex world at the microscopic level (mainly molecules). The strategy used is to group substances/molecules into categories that, although they identify common essential characteristics, linking them to macroscopic reactivity and microscopic molecular structure. In particular, from a microscopic chemical perspective it is essential to determine the organization of interatomic interactions and in particular "who is linked to whom". The concept of chemical bond becomes, therefore, the cornerstone of the structuring of the molecular building and its transformation in chemical reactions.

Quantum mechanics applied to the molecular world can play an important role in determining whether a particular structure is stable and in which particular states, in determining the constrained movements of the molecular structure (roto-vibrations), with the possibility of starting from these to analyse the reactive path that modifies the global state of the system. In this global view of the molecule, its components are not essential and their *in situ* characteristics and their modifications in the reactive process can be found a posteriori by projection from the global characteristics. The non-locality of quantum interactions and the indistinguishability of atomic components within the molecule do not represent a problem if the quantum approach is supported by a classical approach with the Born-Oppenheimer approximation. In the few and recent cases of a completely quantum treatment of a molecule, only global properties can be obtained, such as the stability of the system. In any case, these studies are too recent to be able to make a significant comparison of the information that Quantum Mechanics can provide to chemistry.

Note*:* The opinions expressed in this contribution are personal and do not in any way commit the Ministry of Foreign Affairs and International Cooperation.

Declarations

Conflict of Interest

The authors declare no conflict of interest.

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