# Decoding Atomic behavior: Exploring the logic of interactions Through game theory in chemistry

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## Abstract

The comprehension of atomic structures and the interactions between atoms is crucial for a thorough understanding of chemistry. This paper explores the application of game theory concepts to elucidate the reactions occurring between elements in the periodic table. The study's results indicate that coordination, anti-coordination, cooperation, and non-cooperation among atoms and molecules play a significant role in the formation of chemical bonds, as predicted by game theory. Moreover, the predictability of chemical reactions and their resulting chemical behavior and physical properties can be inferred. Several illustrative examples of various chemical reactions are provided to validate the practicality of these assertions.

**Keywords:** *game theory*, *cooperative game*, *chemical bond*

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## 1. Introduction

Von Neumann and Morgenstern (1953) were the first to acknowledge game theory in relation to human economic behavior. Since then, game theory has found extensive application in social and behavioral sciences, spanning domains such as politics, market economics, ecosystems, and biological phenomena. In game theory, a player is considered rational when they aim to maximize their own payoff through their strategic choices. The term "game theory" was first explicitly used in the context of evolution by Hamilton (1967) when studying the optimal sex ratio in the presence of local mate competition. Hamilton's concept of an "unbeatable strategy" aligns with the notion of an Evolutionarily Stable Strategy (ESS) as later defined by Maynard Smith and Price (1973). Evolutionary game theory provides a framework for understanding evolution at the phenotypic level, where the fitness of specific phenotypes is contingent upon their frequencies within the population [1]. Chemistry, as a scientific discipline, focuses on the understanding of matter in terms of its characterization, composition, and transformations [2]. In 1869, Dmitri Mendeleev, a Russian chemist, created the initial systematic arrangement of all 63 known elements at that time, known as the periodic table. It was later discovered by Moseley that the appropriate structure of the periodic table could be correlated to the atomic number of elements. The periodic table serves as a valuable tool for establishing relationships and connections between the properties of different elements. Within chemistry, molecules and ions are two significant types of particles that arise from atoms. Chemical bonds are responsible for holding atoms together within molecules [2]. In classical game theory, a fundamental assumption is that players will act rationally, guided by self-interest. However, applying this assumption directly to a chemical context would be inappropriate. Instead, in the chemical domain, the notion of rationality is replaced by considerations of population dynamics and stability. The criterion for evaluating interactions shifts from self-interest to the formation of stable bonds. The paper aims to address fundamental questions related to the bonding of atoms, the prevalence of materials in nature, and the atomic nature of noble gases. By exploring these questions, we can elucidate the relationship between stability and game theory. The answers lie in the properties of atoms themselves. Noble gases exhibit stability because they have eight electrons in their valence shell, except for helium. To answer the first and second questions, it is important to note that atoms bond together in order to attain stability. Thus, elements achieve stability through the formation of chemical bonds. The behavior of atoms in reactions is influenced by various factors, with the nuclear charge, electron configuration, and effective size of the atom being particularly significant. The distribution of electrons around the nucleus determines the behavior of elements. Specifically, the arrangement of electrons in the valence shell and energy levels shapes the characteristic behavior patterns, often referred to as "types" or "behavior kinds," associated with specific electron configurations. This diversity in behavior gives rise to the heterogeneous nature of the periodic table, where different properties are observed within periods and groups. The behavior of individual atoms within a population is not a result of conscious choice but rather arises naturally from specific combinations of electrons, protons, and neutrons. Atoms consist of two electrically charged components: the negatively charged electrons and the positively charged nucleus. Each element's atoms or molecules involved in a reaction can be considered as players in a game. However, these players do not make deliberate choices.

Interactions between these atomic players lead to the formation of chemical bonds. These interactions involve attractive and repulsive forces, which cause atoms to approach each other and form bonds. The ultimate objective of these interactions is to achieve a stable state for each player involved.

In summary, the behavior of atoms in reactions is influenced by factors such as electron configuration, nuclear charge, and atom size. This behavior gives rise to diverse properties within the periodic table. Interaction between atoms, driven by attractive and repulsive forces, leads to bonding formation and the attainment of stable states. Noble gases, with their limited inclination for bonding, are generally more stable. However, we exclude the study of Noble gases in this paper.

The collision theory and transition state theory are widely used in evaluating chemical reactions. Both theories rely on the occurrence of collisions between particles as a necessary condition. In this work, the collision theory is employed, and the collisions between particles are conceptualized as a game between the elements.

The subsequent sections of this paper delve into the description of the collision game. Chemical bonds are formed when atoms combine through alterations in electron distribution. There exist three fundamental types of bonding: ionic bonding, covalent bonding, and metallic bonding. In this paper, we however discuss only ionic and covalent bonding between elements. It is important to note that all reactions involving two reactants necessitate collisions between particles for the reaction to proceed [2]. Through the formation of bonds, elements can achieve stability. Our framework allows for the implementation of different games for these types of reactions.

## 2. Ionic bonding:

An ion refers to a particle composed of either an atom or a group of atoms that carries an electric charge. There are two types of ions:

- **Cation:** A cation bears a positive charge, which occurs when one or more electrons are lost by the atom or group of atoms.
- **Anion:** An anion carries a negative charge, which happens when one or more electrons are gained by the atom or group of atoms.

Ionic bonding occurs when there is a transfer of electrons from one type of atom to another. In this process, the atoms of one reactant lose electrons and become positively charged ions (cations), while the atoms of the other reactant gain electrons and become negatively charged ions (anions).

The resulting electrostatic attraction between the oppositely charged ions holds them together in a crystal structure. This net attraction can be considered as an ionic bond. The strength of this bond holds the crystal together and is responsible for the stability of the ionic compound [2].

In the reaction between a potassium ion and a chloride ion, potassium ion loses one electron, and the chloride ion gains an electron.

Now let's consider a population of two atoms, where there are two types: one type can gain electrons

(G) and the other type can lose electrons (L). In this population, the atoms cannot share electrons. The desirable condition for achieving stability is either losing electrons or gaining electrons, depending on the type of atom.

The key aspect of this particle game is to achieve stability through bonding formation, which benefits and gains both particles. Each atom is considered a player in this game, assuming different roles within the population. Two players with the same role (either both losing electrons or both gaining electrons) earn a reward denoted as S, while for a non-matching pair, they receive a payment represented by P.

To represent this game, we can use a matrix, as shown in Table 1. Each row of the matrix represents a possible type within the population, and each column represents another possible type within the population. It's important to note that the players cannot choose between "losing electrons" or "gaining electrons" directly, but rather between the type that loses electrons and the type that gains electrons.

| | G | L |
|---|---|---|
| G | (S,S) | (P,P) |
| L | (P,P) | (S,S) |

Table 1: *A symmetric game between sodium and chlorine atoms with no symmetric Nash equilibrium*

Please note that the specific values for the rewards (S) and payments (P) would depend on the specific context and can be determined based on the desired outcomes of the game.

In the described game, there are two Nash equilibria: (G, L) and (L, G). A Nash equilibrium is a situation in which no player has an incentive to unilaterally change their strategy, given the strategies chosen by the other players. In this case, both equilibria involve one player losing electrons (L) while the other gains electrons (G). Additionally, both equilibria are polymorphic and homogeneous in stable strategy.

This game resembles an anti-coordination game, where the players' objectives are to choose different strategies to avoid duplication. In the context of the potassium and chloride ions, this means that the number of potassium ions produced is equal to the number of chloride ions produced. Consequently, the formula KCl represents the compound with the simplest ratio of ions present, which is a 1:1 ratio [2].

$$K^+ + Cl^- \rightarrow KCl.$$

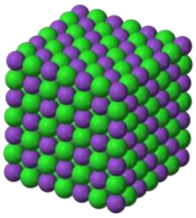

Fig. Potassium Chloride

In the updated example, the population now consists of two types of ions: cations (C) and anions (A), which are referred to as mutated ions. During collisions, members of the new population, referred to as congeners, repel each other, while non-kind ions attract each other.

To analyze this collision scenario within the framework of game theory and map it to Nash equilibria, we consider cations and anions as the players in the game.

Let's denote the rewards and payments as follows:

Congeners of the same type (C-C or A-A) earn a reward S. Non-kind ions (C-A) receive a payment P, which is shared by both players.

To determine the Nash equilibria in this game, we need to analyze the possible strategies and payoffs for both cations and anions. The equilibria will be situations where neither player has an incentive to unilaterally deviate from their chosen strategy, given the strategies of the other players.

The specific Nash equilibria for this game would depend on the values of the rewards S and payments P, as well as the strategic choices of the players (cations and anions). Analyzing the strategies and payoffs can help identify the equilibria and understand the outcomes of the collisions in terms of ion

population dynamics.
In the given payoff matrix game between cations (C) and anions (A), let's consider the repulsive energy of congeners to be equal. The payoff matrix is as follows:

| | C | A |
|---|---|---|
| C | (S,S) | (P,P) |
| A | (P,P) | (S,S) |

Table 2: *Payoff matrix game between cations and anions.*

If $S < P$ the game has asymmetric Nash equilibrium. If $S > P$ the game has symmetric Nash equilibrium.

If the reward S (for congeners of the same type) is less than the payment P (for non-kind ions), the game has an asymmetric Nash equilibrium. In this case, the equilibrium occurs when cations (C) and anions (A) are paired, resulting in two Nash equilibria: (C, A) and (A, C). These equilibria are polymorphic and homogeneous in stable strategy.

On the other hand, if the reward S is greater than the payment P, the game has a symmetric Nash equilibrium. In this scenario, both cations and anions prefer to pair with the same type. Therefore, the equilibria are (C, C) and (A, A), and these equilibria are polymorphic and heterogeneous in stable strategy.

The difference in the magnitudes of the rewards and payments determines the nature of the equilibrium. When the attractive force between non-kind players (S) is greater than the repulsion force between congeners (P), the crystal structure forms and remains intact. However, if the attractive force is weaker than the repulsion force ($S < P$), the crystal body is likely to rupture.

## 3. Covalent bonding:

In covalent bonding, electrons are shared between atoms rather than being transferred. A single covalent bond consists of a pair of electrons shared by two atoms. Molecules are formed when atoms are covalently bonded to each other, creating a tightly bound particle.

The collision theory, which describes reactions in terms of collisions between reacting molecules, can be applied to understand the dynamics of covalent bonding. Let's consider the hypothetical gas-phase reaction:

$$A_2(g) + B_2(g) \rightarrow 2AB(g)$$

In this reaction, the $A_2$ and $B_2$molecules serve as the players in the collision game. When an A2 molecule and a $B_2$molecule collide, the old A-A and B-B bonds break. Simultaneously, two new A-B bonds are formed, resulting in the creation of two AB molecules. These newly formed AB molecules then separate from the collision site.

During the collision, when two slow-moving molecules approach each other closely, they experience a repulsive force due to the charges of their electron clouds. This repulsion prevents the molecules from merging or bonding directly. Instead, the collision results in the rearrangement of bonds, breaking the old bonds and forming new ones, leading to the formation of the AB molecules [2].

The game involves the bonding of two oxygen atoms ($O_2$). In this population of two atoms, each atom alone cannot achieve a stable state. They need to share electrons to reach a stable configuration. The bonding pair of electrons is absorbed from the nuclei of the two atoms and is shared between them. Consequently, the atoms compete to attract this bonding pair of electrons.

In this game, each player (atom) has two strategies: attract (A) or repulse (R) the bonding pair of electrons. The outcome of the game depends on the combination of strategies chosen by the players. The payoffs for each combination of strategies are as follows:

If both atoms attract (A, A), they both earn a reward S.

If one atom repulses (R) and the other atom attracts (A), the repulsing atom gains a payoff P, while the attracting atom receives the reward S (where $S > P$).

If both atoms repulse (R, R), they both have a payment P.

The game can be represented in the following table:

| | A | R |
|---|---|---|
| A | (S,S) | (P,P) |
| R | (P,P) | (S,S) |

Table 3. *A purely covalent bond in molecule formed form two identical atoms, such as* $O_2$

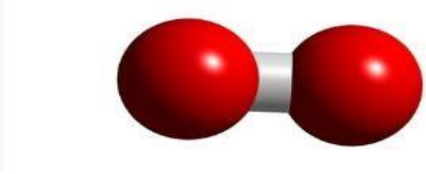

Fig. Oxygen molecule

A purely covalent bond in molecule formed form two identical atoms, such as $O_2$.

In the case of the bond formed by hydrogen and oxygen molecules to create a water molecule ($H_2O$), we again consider a population of two molecules that share electrons to achieve a stable state. Each molecule alone cannot attain stability and thus competes for the bonding pair of electrons.

In this game, each player (atom) has two strategies: attract (A) or repulse (R) the bonding pair of electrons. However, in a water ($H_2O$) molecule, the electrons of the covalent bond are more strongly attracted by the oxygen (O) atom. In a covalent bond, atoms share electrons to achieve a stable electron configuration. Oxygen has a higher electronegativity compared to hydrogen, which means it has a greater ability to attract electrons towards itself in a chemical bond. In the case of water ($H_2O$), the oxygen atom has a stronger pull on the shared electrons in the covalent bonds. As a result, the oxygen atom partially carries a negative charge (δ-) due to the higher electron density, while the hydrogen atoms carry partial positive charges (δ+). This gives rise to a polar covalent bond, with the oxygen atom being slightly negative and the hydrogen atoms being slightly positive in the $H_2O$ molecule.

The payoffs for different strategy combinations are as follows:

If both players attract (A, A), player 1 (hydrogen) earns a reward S, while player 2 (chlorine) earns a reward P.

If both players repulse (R, R), player 1 earns a reward K, and player 2 earns a reward T.

Other combinations are not explicitly mentioned in the given information.

The given payoffs are ranked as follows: $K < T < S < P$.

The specific values of the rewards K, T, S, and P are not provided in the given information, so the payoff matrix cannot be determined.

| | A | R |
|---|---|---|
| A | (S,P) | (S,T) |
| R | (K,P) | (K,T) |

Table 4. *The outcomes of play between hydrogen and oxygen molecules*.

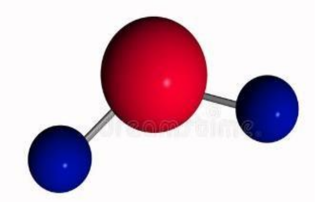

Fig. $H_2O$ molecule

In the given game, pairs of members of a population engage in interactions where atoms in a molecule can share electrons with either a congener (atom of the same kind) or a non-kind atom in another molecule. The objective is to reach a stable state by sharing electrons.

Each player has two strategies: cooperate (C) by sharing electrons with a non-kind atom, or defect (D) by not sharing electrons with the non-kind atom and keeping them within their own molecule. The payoffs for different strategy combinations are as follows:

If both players cooperate (C, C), they both earn a reward S. If one player defects (D) and the other cooperates (C), the defector gains a payoff P, while the cooperator receives zero payoff.

If both players defect (D, D), they both have a payment P.

The given information states that the payoffs satisfy the inequality $0 < P < S$, indicating that the reward for cooperation is greater than zero, and the reward for defection is less than the reward for cooperation.

Based on this information, it can be observed that the strategy of defecting (D) strictly dominates cooperation (C) for each player. Therefore, the strategy pair (D, D) is a Nash equilibrium in this game. Players have an incentive to defect rather than cooperate, regardless of the other player's choice.

However, it's important to note that the specific values of the rewards S and P are not provided, so the exact payoff matrix and the magnitudes of the rewards cannot be determined from the given information.

| | C | D |
|---|---|---|
| C | (S,S) | (0,P) |
| D | (P,0) | (P,P) |

Table 5. *A symmetric game between atoms of two different molecule*

## 4. Conclusion:

Indeed, game theory can be a valuable tool for analyzing and predicting the behavior of various phenomena, including chemical reactions and the formation of materials. By applying game theory to the interactions between atoms and molecules, we can gain insights into the dynamics and stability of chemical systems.

In the context of equilibrium in chemical reactions, game theory can help us understand the interplay between different species and their strategies (such as cooperation or defection) in achieving stability. The concept of Nash equilibrium allows us to identify stable strategies where no player has an incentive to unilaterally change their strategy.

Furthermore, game theory can be utilized in the design and optimization of experiments for producing new materials. By considering the interactions between the constituent elements of a material as a game, researchers can assess the feasibility and success of the experimental process based on the predicted outcomes of the game.

Overall, applying game theory to chemical systems can provide valuable insights into the behavior of elements and molecules, leading to a better understanding of equilibrium states, stability, and the formation of materials.

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