

Swiss Scientific Society for Developing Countries SWISSSDC Open Repository & Archive Zürichstrasse 70 8600 Dübendorf Switzerland info@swisssdc.ch www.swisssdc.ch

Year: 2024

Beyond Disorder: A New Perspective on Entropy in Chemistry

Alzeer, Jawad

ABSTRACT

The concept of entropy, a fundamental principle in the field of chemistry, has traditionally been oversimplified as a mere measure of disorder. However, this simplistic perspective fails to capture the intricate and multifaceted nature of entropy, along with its profound influence on various phenomena. This paper seeks to delve deeper into the understanding of entropy by moving beyond the conventional disorder- centric viewpoint and adopting a more nuanced approach that integrates both disorder and energy considerations. Through the redefinition of potential energy and microstates as integral components of entropy, the study explores the intricate interplay between disorder, energy, and molecular transformations within chemical systems. The implications of this refined conceptualization extend beyond the boundaries of chemistry, impacting fields such as physics, biology, and medicine. The potential transformative effects of this enhanced understanding hold promise for advancing scientific knowledge and applications across diverse disciplines.

Originally published at:

Alzeer, Jawad (2023). Beyond Disorder: A New Perspective on Entropy in Chemistry. Am. J. Med. Chem, 2024;5(1):1-5.

https://www.sciencerepository.org/beyond-disorder-a-new-perspective_AJMC-2024-1-101 DOI: https://10.31487/j.AJMC.2024.01.01



Available online at www.sciencerepository.org

Science Repository



Review Article

Beyond Disorder: A New Perspective on Entropy in Chemistry

Jawad Alzeer^{1,2*}

¹College of Medicine, PPU, Wadi Al-haria, Hebron, Palestine

²Swiss Scientific Society for Developing Countries, Zurich, Switzerland

ARTICLEINFO

Article history:

Received: 23 January, 2024 Accepted: 12 February, 2024 Published: 14 March, 2024

Keywords:
Entropy
disorder
energy
potential energy
microstates
chemical reactions
molecular transformations
thermodynamics

ABSTRACT

The concept of entropy, a fundamental principle in the field of chemistry, has traditionally been oversimplified as a mere measure of disorder. However, this simplistic perspective fails to capture the intricate and multifaceted nature of entropy, along with its profound influence on various phenomena. This paper seeks to delve deeper into the understanding of entropy by moving beyond the conventional disorder-centric viewpoint and adopting a more nuanced approach that integrates both disorder and energy considerations. Through the redefinition of potential energy and microstates as integral components of entropy, the study explores the intricate interplay between disorder, energy, and molecular transformations within chemical systems. The implications of this refined conceptualization extend beyond the boundaries of chemistry, impacting fields such as physics, biology, and medicine. The potential transformative effects of this enhanced understanding hold promise for advancing scientific knowledge and applications across diverse disciplines.

© 2024 Jawad Alzeer. Hosting by Science Repository.

Introduction

In the field of chemistry, the concept of entropy presents a particular challenge as it leads to a confusing misunderstanding that makes it difficult to understand. This challenge arises from the inherent dual nature of entropy, where one perspective focuses on the order and disorder within a system, while another is concerned with energy associated with the breaking and formation of bonds during chemical reactions [1]. The coexistence of these perspectives creates a cognitive conflict for chemists, forcing them to reconcile between different perspectives for better understanding of this fundamental thermodynamic concept. The initial perspective on entropy often draws parallels with the order and disorder observed in a system, akin to the analogy of a tidy room. In this analogy, the organized state of toys represents low entropy, while the subsequent scattered and disorganized state signifies high entropy. The intuitive understanding that disorder tends to increase over time, in the absence of external influences, aligns with the common perception of entropy association with the second law of thermodynamics, stating that the entropy of an isolated system always increases [2]. Entering the domain of chemical reactions opens up

another dimension of entropy, which is closely associated with energetic shifts in bond transformations [3]. In this context, entropy is more than just a measure of disorder; it influences the overall energy status of a system. As chemical bonds break and new ones form, particles undergo a rearrangement, akin to the analogy of scattered toys in a tidy room [4]. This rearrangement results in the creation of structures that can be either more ordered or less ordered, accompanied by the release or absorption of energy.

Understanding entropy in the context of chemical reaction is particularly important when considered together with enthalpy and Gibbs free energy. The breaking and forming of chemical bonds not only rearranges atoms, but also causes significant changes in the energy state of the system [5]. Enthalpy, serving as the measure of the total energy content within chemical bonds, undergoes changes during chemical processes. When chemical bonds break, energy is consumed, and, conversely, when bonds form, energy is released. The rearrangement of atoms and the associated changes in enthalpy and entropy contribute to shifts in the Gibbs free energy of the system. The interplay of entropy, enthalpy and Gibbs free energy illustrates the intricate thermodynamics of chemical

^{*}Correspondence to: Jawad Alzeer, College of Medicine, PPU, Wadi Al-haria, Hebron, Palestine; Swiss Scientific Society for Developing Countries, Zurich, Switzerland; E-mail: jawad.alzeer@uzh.ch

reactions, where disorder, energy changes and the overall feasibility of the process are closely intertwined [6, 7].

Essentially, for chemists, understanding entropy is incomplete without considering its relationship with enthalpy and free Gibbs energy [8-10]. Explaining entropy outside this context risks either non-acceptance or misunderstanding, as these three factors collectively add layers of complexity to deciphering the thermodynamics governing chemical reactions. To comprehend the intricate nature of entropy, one must delicately balance their understanding between disorder and energy. This duality introduces inherent complexities in interpreting this fundamental thermodynamic concept, giving rise to a sophisticated framework within the field of chemistry. In our pursuit of understanding, we delve into the intricacies of entropy, exploring both the disorder and energy perspectives. Our aim is to establish a cohesive connection between these seemingly disparate dimensions, unraveling the complexity within the field of chemistry.

Moving Beyond Disorder in Chemistry

Entropy, a cornerstone of chemistry, often represents a confusing duality between disorder and energy. This inherent ambiguity stems from the multifaceted nature of entropy and challenges chemists to move beyond a simplistic, disorder-centered perspective [11]. Instead, a comprehensive understanding requires an integrated approach that reconciles disorder and energy and establishes a meaningful connection between these seemingly disparate dimensions. The prevalent analogy of a tidy room, often employed to illustrate entropy's increase as disorder takes hold, serves as a simplified representation. While disorder undoubtedly plays a crucial role in entropy, it alone cannot dictate the direction of a chemical reaction. In the field of chemical transformations, enthalpy (ΔH) and entropy change (ΔS) emerge as pivotal determinants of the reaction's course. Entropy, viewed not merely as a measure of disorder but as a form of energy, extends beyond its simplistic portrayal, intertwining with the energetic dynamics of molecular transformations [12].

Chemical reactions involve the breaking and forming of chemical bonds, resulting in a rearrangement of atoms accompanied by an exchange of energy [13]. This process goes beyond a mere spatial rearrangement and involves a significant exchange of constitution, configuration and conformation associated with these molecular transformations [14, 15]. Chemists commonly start by interpreting entropy through the lens of disorder and then connecting the concept to energy. The misconception of the entropy concept begins to unfold at this point, prompting chemists to gently broaden their perspective and gradually narrow down the misconception [16].

Gibbs free energy ($\Delta G=\Delta H$ - $T\Delta S$) serves as a comprehensive summary that considers both the influences of enthalpy change (ΔH) and entropy change (ΔS) to predict the spontaneity of a reaction [1]. This means that not only the energetic aspect represented by enthalpy (bond forming and bond breaking) is taken into account, but also the degree of changes in constitution, configuration and conformation determine the overall spontaneity of the reaction. To further clarify the complicated relationship between entropy and energy, it is useful to look at the interaction of these terms in the context of a chemical reaction. In

spontaneous reactions, the system might smoothly transitions from a state of higher order (lower entropy) to one of lower order (higher entropy) [17]. This shift in order is accompanied by the release of energy, typically in the form of heat. The energy released corresponds to a decrease in potential energy as the system moves to a more disordered state. Essentially, the spontaneity of the reaction is connected to the system's inherent tendency to move towards increased disorder, leading to the release of energy. Conversely, in non-spontaneous reactions, the system might undergoes a transition from a lower order state to a higher order state [18, 19]. To build order in the system or drive the reaction forward, energy must be supplied. Therefore, energy is provided, in form of catalyst or co-factors, to facilitate the occurrence of the reaction, counteracting the natural tendency towards disorder by promoting a state of increased order.

The temperature (T) dependence of entropy further adds to the complexity of understanding its role in chemical reactions. At low temperatures, the system's thermal energy is insufficient to overcome the energy barrier associated with the reaction. As a result, enthalpy (ΔH) dominates the spontaneity of the reaction, with entropy (ΔS) playing a lesser role. However, as temperature increases, the system gains more thermal energy, allowing entropy to exert a greater influence on the reaction's spontaneity. This interplay between temperature, enthalpy, and entropy is crucial for predicting the direction and feasibility of chemical reactions under varying conditions [17]. While increasing temperature generally favours product formation according to Gibbs free energy, this is not always the case, particularly when the product possesses a higher potential energy (higher order) compared to the reactant [20]. In such instances, the entropy change (ΔS) becomes negative, and a temperature rise further increases the overall negative entropy, rendering the Gibbs free energy change (ΔG) positive, indicating an endothermic reaction [21, 22].

Discussion

Entropy, a fundamental concept pervading chemistry, physics, and biology, has often been misconstrued as a simplistic measure of disorder. This narrow view fails to capture the multifaceted nature of entropy and its profound impact on various phenomena. To dispel these misconceptions and establish a comprehensive understanding of entropy, we must transcend this limited perspective and embrace a more nuanced approach. In chemistry, entropy is frequently equated with disorder, leading to difficulties in explaining the direction and spontaneity of chemical reactions [23]. Similarly, in physics, entropy is often associated with energy dissipation, making it challenging to reconcile this notion with the concept of entropy as a measure of disorder in statistical mechanics [24]. Moreover, in medicine, entropy is often misinterpreted as a mere indicator of disease progression, overlooking its crucial role in maintaining cellular homeostasis [25-28].

To overcome these misconceptions and establish a unified perspective, we need a representation of anti-entropy, the force that counteracts disorder and promotes order. Potential energy, the energy stored within a system due to its arrangement, emerges as a promising candidate for this role [29]. Potential energy can be used to quantify the order or disorder of a system, and changes in potential energy can be directly linked to changes in entropy. However, the traditional definition of

chemical potential energy, limited to the energy stored in chemical bonds, is insufficient to capture the full complexity of entropy. A more comprehensive definition of potential energy should encompass the energy stored in the constitution, configuration, and conformation of an object, particle, or molecule. This expanded definition encompasses the energy associated with the three-dimensional arrangement of atoms or molecules, their flexibility and rigidity, and the overall structure of the system. The flexibility or freedom of a molecule expands its range of possible arrangements, known as microstates, fostering a more adaptable conformation and enhancing entropy [30]. Conversely, rigidity restricts

the number of microstates, promoting a rigid conformation and augmenting potential energy. Microstates represent distinct arrangements of atoms or molecules within a system. The number of microstates associated with a system directly correlates with its entropy. A system with a vast array of microstates is considered more disordered and has higher entropy, whereas a system with a limited number of microstates is considered more ordered and exhibits lower entropy. Table 1 illustrates the factors that can influence both potential energy and entropy.

Table 1: Factors that can influence both potential energy and entropy.

| Factor | Effect on Potential Energy | Effect on Entropy |
|-----------------------------------|----------------------------|-------------------|
| Bond Formation | Increases | Decreases |
| Bond Breaking | Decreases | Increases |
| Bond Stretching | Increases | Decreases |
| Bond Bending | Increases | Decreases |
| Increase in Microstates | Decreases | Increases |
| Breakdown of Ordered Structure | Decreases | Increases |
| Build Ordered Structure | Increases | Decreases |
| Increase in Flexibility | Decreases | Increases |
| Increase in Rigidity | Increases | Decreases |
| Increase in Temperature | Decreases | Increases |
| Increase in Carbon Atoms | Increases | Decreases |
| Increase in Structural Complexity | Increases | Decreases |
| Increase in Conformers | Decreases | Increases |
| Increase in Molecular Movement | Decreases | Increases |

Changes in constitution, configuration, and conformation play a crucial role in altering entropy in chemical reactions. The constitution of a molecule refers to the types and number of atoms in the molecule, while the configuration refers to the spatial arrangement of its atoms within a specific molecular framework. Additionally, it's essential to note that configuration is often accompanied by constitutional changes. Conformation, on the other hand, describes the detailed three-dimensional shape of atoms in space, including rotations and bond angles (Figure 1). Expanding the tidy room analogy to the macromolecular level provides a nuanced understanding of entropy. Just as the organized arrangement of objects contributes to low entropy in a tidy room, a protein's rigid and ordered structure in its native state reflects a state of low entropy and high potential. The proper functioning

of proteins relies on the preservation of structural information. However, when exposed to heat, inducing denaturation, the protein undergoes a transformative conformational shift. This alteration leads to enhanced flexibility, an increase in microstates, and consequently, heightened disorder within the protein's structure. Consequently, the entropy of the system rises significantly, driven by the proliferation of possible orientations for the atoms constituting the protein. Despite the transformative shifts in conformation that contribute to the protein's increased entropy, the essential constitution and configuration remain intact [31, 32]. As this structural change persists, a growing sense of disorder becomes more apparent, accompanied by the gradual fading of function and information.

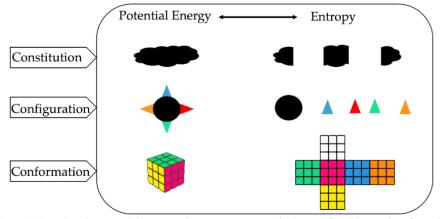


Figure 1: Interchanging potential energy and entropy across constitution, configuration, and conformation.

At the molecular level, the oxidation of glucose, analogous to other chemical transformations, exemplifies the loss of constitution, configuration, and conformation as complex molecules disassemble into simpler ones. Glucose's intricate six-carbon structure unravels into simpler forms, namely water and carbon dioxide, marking a simplification of its constitution. Both the constitution and configuration of glucose fade away, and its characteristic chair conformation disappears (Figure 2). Compared to glucose, the resulting molecules exhibit a lower degree of organization, increased mobility, distinct

intermolecular forces, and an overall decrease in potential energy accompanied by a rise in entropy. This chemical reaction progresses from a highly ordered state (high potential) to a state of reduced order (low potential). During cellular respiration, as glucose undergoes oxidation, the potential energy difference serves a dual purpose: a portion is utilized to store ATP for anabolic processes, while the remaining energy is employed to generate heat, contributing to the maintenance of body temperature [32].

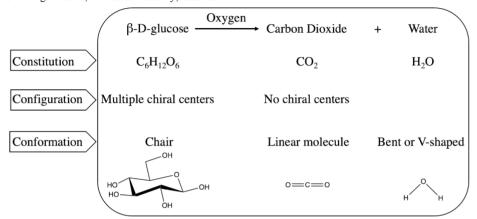


Figure 2: Conversion of potential energy to ATP and heat: reduction in potential energy and increase in entropy.

The redefined understanding of entropy, which essentially moves beyond the oversimplified notion that entropy is limited to disorder, has profound implications for various scientific fields. In chemistry, it provides a deeper explanation for reaction spontaneity, linking entropy changes to energy exchanges. This multifaceted concept, deeply intertwined with molecular structure and rearrangement, transcends the simplistic notion of disorder [33]. In physics, the revised understanding resolves the apparent contradiction between entropy's role in ordering and its connection to energy dissipation. By incorporating the interplay of potential energy and microstates, order and disorder are harmoniously connected. This expanded perspective fosters a unified comprehension of entropy's role in physical phenomena, paving the way for transformative advancements in thermodynamics and related fields [34]. In medicine, macromolecules possess well-defined constitution, configuration, and conformation, endowing them with substantial potential, information, and the ability to function as essential components within biological systems. This refined understanding paves the way for a comprehensive understanding of cellular processes and their intricate relationship to entropy. By appreciating the role of proteins in counteracting entropy-driven disorder, we can develop novel strategies to combat disease and promote human health [35, 36]. Harnessing the anti-entropic potential of proteins opens doors to a deeper understanding of biological complexity and the development of innovative medical treatments [37, 38].

By recognizing potential energy as a reservoir of anti-entropy, we effectively bridge the gap between order and disorder. Embracing this multifaceted perspective dispels long-held misconceptions, providing a cohesive framework for comprehending entropy's far-reaching implications across scientific domains. This refined understanding holds immense transformative potential, propelling advancements in chemistry, physics, biology, and beyond.

Conclusion

In essence, entropy, a central concept in chemistry, physics, and biology, is often oversimplified as a mere measure of disorder. This hinders our understanding of its complexity and impact on chemical reactions, physics contradictions, and cellular processes. To address this, a nuanced approach redefines entropy to include potential energy as anti-entropy, offering a broader perspective that encompasses a system's constitution, configuration, and conformation. At the molecular level, changes in these aspects influence entropy, seen in protein denaturation and glucose oxidation. This refined entropy has broad implications, explaining reaction spontaneity, reconciling physics contradictions, and enhancing our understanding of cellular processes in medicine. Recognizing potential energy as anti-entropy bridges the gap between order and disorder, dispelling misconceptions and providing a cohesive framework. Embracing this perspective propels advancements in chemistry, physics, biology, and beyond, driving innovative discoveries and applications in various scientific fields.

Acknowledgments

We would like to thank Prof. Quamrul Hasan, Prof. Khaled Abou Hadeed for their useful discussion and support.

Ethical Statement

The authors are accountable for all aspects of the work in ensuring that questions related to the accuracy or integrity of any part of the work are appropriately investigated and resolved.

Conflicts of Interest

None.

REFERENCES

- Smith JM (1950) Introduction to chemical engineering thermodynamics. *Journal of Chemical Education* 27: 584.
- Janbozorgi M, Sheikhi MRH, Metghalchi H (2013) Principle of detailed balance and the second law of thermodynamics in chemical kinetics. *Journal of Energy Resources Technology* 135: 041901.
- Usacheva T, Terekhova I, Alister D, Agafonov M, Kuranova NN et al. (2021) Entropy effects in intermolecular associations of crown-ethers and cyclodextrins with amino acids in aqueous and in non-aqueous media. Entropy 24: 24. [Crossref]
- Lambert F (2007) Configurational entropy revisited. *Journal of Chemical Education* 84: 1548.
- Schmitt C, Kaiser L, Schween M (2019) Learning to Think in Mechanistic Alternatives: SN1 vs. E1 and the Gibbs-Helmholtz Equation. World Journal of Chemical Education 7: 102-108.
- Huang J, Sheehan RJ, Langer SH (2005) Entropy—enthalpy compensations in solutions of dual character molecules with polymeric chromatographic liquid phases. J Phys Chem B 109: 1736-1743.
 [Crossref]
- Nakamura K, Mizuta R, Suganuma S, Tsuji E, Katada N (2017) Compensation between activation entropy and enthalpy in reactions of aromatic hydrocarbons catalyzed by solid acids. *Catalysis Communications* 102: 103-107.
- Calderone CT, Williams DH (2001) An enthalpic component in cooperativity: the relationship between enthalpy, entropy, and noncovalent structure in weak associations. J Am Chem Soc 123: 6262-6267. [Crossref]
- Wang LS (2021) Progress in entropy principle, as disclosed by nine schools of thermodynamics, and its ecological implication. International Journal of Design & Nature and Ecodynamics 16: 359-372.
- Haglund J, Andersson S, Elmgren M (2015) Chemical engineering students' ideas of entropy. Chemistry Education Research and Practice 16: 537-551.
- Lambert F (2012) The misinterpretation of entropy as "disorder". *Journal of Chemical Education* 89: 310-310.
- Leff HS (2007) Entropy, its language, and interpretation. Foundations of Physics 37: 1744-1766.
- Prigogine I (2003) Chemical kinetics and dynamics. Ann N Y Acad Sci 988: 128-132. [Crossref]
- López Rosa S, Esquivel RO, Angulo JC, Antolín J, Dehesa JS et al. (2009) Fisher information study in position and momentum spaces for elementary chemical reactions. *J Chem Theory Comput* 6: 145-154. [Crossref]
- Nielsen SN, Müller F, Marques JC, Bastianoni S, Jørgensen SE (2020)
 Thermodynamics in ecology-an introductory review. *Entropy (Basel)*
 22: 820. [Crossref]
- Martyushev LM (2013) Entropy and entropy production: old misconceptions and new breakthroughs. *Entropy* 15: 1152-1170.

- Ott JB, Boerio-Goates J (2000) Chemical thermodynamics: principles and applications. Elsevier Ltd.
- Bu S, Yang X, Li W, Wang X, Liu X (2022) Thermodynamic performance judgment of organic rankine cycle based on gibbs free energy change.
- Song Z, Yi J, Qi J, Zheng Q, Zhu Z, et al. (2021) Line defects in monolayer TiSe2 with adsorption of Pt atoms potentially enable excellent catalytic activity. *Nano Research* 15: 4687-4692.
- Wolfenden R, Snider MJ, Ridgway C, Miller BG (1999) The temperature dependence of enzyme rate enhancements. *Journal of the American Chemical Society* 121: 7419-7420.
- Xu J, Li Z, Bao W, Liu F, Liu Y et al. (2019) Recyclable biobased materials based on diels-alder cycloaddition. *Journal of Applied Polymer Science* 136: 47362.
- Yin P, Qu R, Chen H, Tian Y, Yin G et al. (2008) Thermodynamic and kinetic properties of scandium (i) ion reacting with sco in gas phase. Open Chemistry 6: 438-442.
- Abell TN, Bretz SL (2019) Macroscopic observations of dissolving, insolubility, and precipitation: general chemistry and physical chemistry students' ideas about entropy changes and spontaneity. *Journal of Chemical Education* 96: 469-478.
- Christensen WM, Meltzer DE, Ogilvie CA (2009) Student ideas regarding entropy and the second law of thermodynamics in an introductory physics course. *American Journal of Physics* 77: 907-917.
- Huang DM, Chandler D (2000) Temperature and length scale dependence of hydrophobic effects and their possible implications for protein folding. *Proc Natl Acad Sci U S A* 97: 8324-8327. [Crossref]
- Alzeer J (2022) Halalopathy: role of entropy in the aging process. Am J Biomed Sci & Res 16: 147-154.
- Alzeer J (2022) Halalopathy: Anxiety and depression from logic and energetic perspectives. Am J Biomed Sci & Res 16: 378-384.
- Alzeer J (2023) The role of buffers in establishing a balance of homeostasis and maintaining health. Am J Med Chem 4: 1-6.
- Moore MA (1974) Statistical mechanics: a set of lectures. Physics Bulletin 25: 191
- Karshikoff A, Nilsson L, Ladenstein R (2015) Rigidity versus flexibility: the dilemma of understanding protein thermal stability. FEBS J 282: 3899-3917. [Crossref]
- Saffran M (1992) Introduction to protein structure. Trends in Endocrinology & Metabolism 3: 380.
- Alzeer J (2022) Directionality of chemical reaction and spontaneity of biological process in the context of entropy. *International Journal of Regenerative Medicine* 5: 1-7.
- Atkins P, Paula Jde, Keeler J (2022) Atkins' physical chemistry. Oxford University Press.
- 34. Ben-Naim A (2007) Entropy demystified the second law reduced to plain common sense. Word Scientific.
- Alzeer J (2020) Entropy and potential energy as a key role of Halalopathy in disease prevention and cure. Longhua Chin Me 3: 20.
- Alzeer J. (2022) Halalopathy: Improving potential energy and minimising entropy offer an integrative approach for more effective treatment. *Medicon Med Sci* 2: 21-24.
- 37. Gruebel M (2002) Protein folding: the free energy surface. *Curr Opin Struct Biol* 12: 161-168. [Crossref]
- 38. Alzeer J (2023) Recognizing limitations: overcoming challenges in enhancing health and preventing disease. *Eur J Gen Med* 3: 1-7.