AI in basic chemistry

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Abstract

Chemists are more and more using artificial intelligence (AI) to do a variety of tasks, including expediting drug discovery and lowering its enormous costs and the time to market for new treatments (1). However, the use of artificial intelligence in chemistry is not just for the formation of new drugs. The fundamental building blocks of science, molecules and chemical bonds, are just the beginning of it. AI can assist with everything from molecular property identification to molecule synthesis when it comes to chemistry and related fields(2) (3).

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Introduction:-

Basic chemistry provides a wide range of possible applications for AI. Here are some applications of AI in this area:

Based on a compound's structure, AI can be used to predict its chemical properties, such as its boiling point, melting temperature, solubility, and reactivity. This can aid in the discovery of new compounds and their attributes (4; 5).

Chemical synthesis: By anticipating reaction conditions, identifying suitable catalysts, and recommending changes to reaction routes to maximise yield and reduce waste, AI can be used to optimise chemical synthesis processes (6; 7).

Analyzing spectroscopic data: To identify substances and their functional groups, AI can be used to analyse and interpret spectroscopic data, such as infrared or mass spectra (8).

Predicting molecular interactions: AI can be used to predict molecular interactions, such as the binding of proteins to ligands, which may assist in the design and discovery of new drugs (9).

Chemical education: AI may be used to create and improve educational tools and platforms for educating students about chemistry. (10).

on the whole, AI can speed up and improve many parts of basic chemistry, ranging from predicting compound characteristics to optimising chemical reactions and analysing spectroscopic data.

Basic chemistry:-

The study of the constitution, characteristics, and behaviour of matter is known as basic chemistry. It serves as the foundation for many other branches of study, including biology, physics, and geology. Here are some basic chemistry principles and topics to get you started (11; 12):

Matter and its properties: The properties and states of matter, including solids, liquids, and gases, as well as their behaviour under various conditions.

Atoms and molecules: The fundamental constituents of matter, including their structure, properties, and behaviour.

Chemical reactions: Matter transformation, encompassing reaction types, balance equations, and reaction rates.
Stoichiometry: The quantitative relationship among reactants and products in a chemical reaction, particularly mole-to-mole conversions and limiting reactants.
Solutions: Solute and solvent behaviour, including concentration units, colligative qualities, and acid-base reactions.
Acids and bases: pH, acid-base interactions, and buffer solutions, in addition to the properties and behaviours of acids and bases.
Thermochemistry: Enthalpy, entropy and Gibbs free energy are all studied concerning how much heat and energy are altered during chemical processes.
Fundamental knowledge of the physical and chemical properties of matter is provided by basic chemistry, which is crucial for many fields of research and technology, including drug development, environmental science, and materials engineering.

1. Chemical reactions:

AI has many potential applications in the field of chemical reactions. Here are some ways AI can be used in this field:

1.1 Reaction prediction:

By using AI to anticipate chemical reaction outcomes based on the reactants and reaction circumstances, new reactions can be discovered and old ones can be optimised. By utilising machine learning algorithms to analyse enormous volumes of chemical data and forecast reactions, AI has the potential to significantly speed up and advance this process. Here are a few applications of AI in reaction prediction:

1.1.a. Predicting reaction products: Based on the reactants and reaction circumstances, AI can be trained on a vast library of chemical reactions to predict the products of a specific reaction.

1.1.b. Reaction route identification: Based on the energy of the reaction and the accessibility of reaction intermediates, AI can be used to determine the most likely reaction pathway for a given collection of reactants.

1.1.c. Predicting reaction kinetics: Based on the composition and characteristics of the reactants as well as the reaction conditions, AI can be used to forecast the rate and mechanism of a reaction.

1.1.d. Virtual screening: Large databases of chemicals can be screened using AI to find those most likely to undergo a desired reaction (13).
in general, AI has the potential to greatly accelerate and enhance the prediction of chemical reactions, which can have broad implications in many fields, from drug discovery to materials science and beyond.

1.2 Stoichiometry

The quantitative study of chemical reactions known as stoichiometry includes calculating the quantities of the reactants and products using stoichiometric ratios. Stoichiometry research can be accelerated and improved with the help of AI (14) in several ways:

1.2.a. Reaction stoichiometry calculations: Stoichiometric ratios and reaction yields for chemical reactions can be computed automatically using artificial intelligence (AI). The Reaction Stoichiometry

Calculator, an AI tool that can automatically calculate the remaining values of a chemical reaction given any known value, can be used to make stoichiometry calculations (15). To analyse chemical reactions and comprehend the connection between reactants and products, stoichiometric calculations are utilised. The number of components on both sides of the equation must be equal for balanced reactions to occur. Chemical formulas serve as the basis for the calculations (16).

1.2.b. Limiting reagent identification: AI can assist predict the maximum yield of a product by identifying the limiting reagent in a chemical reaction. By comparing the molar ratios of the reactants with the actual stoichiometric ratio, it is possible to limit reagent identification. The reactant with fewer moles than required is the limiting agent. The amount of the reaction's product and the amount of excess reagent still present should next be calculated (17). By analysing the balanced chemical equation and determining how much reactant B is needed to react with reactant A, artificial intelligence (AI) can be used to find limiting reagents. Given any known value, the AI tool can automatically determine the remaining values of a chemical reaction (18).

1.2.c Mole-to-mole conversions: Stoichiometric calculations sometimes involve mole-to-mole conversions, which AI can help with. Stoichiometry can be used to perform conversions from one mole to another. Chemistry's field of stoichiometry examines the quantitative interactions between reactants and products in chemical reactions. It entails figuring out how many reactants are necessary to generate a specific volume of product. By analysing the balanced chemical equation and determining how much reactant B is needed to react with reactant A, AI can do mole-to-mole conversions. Given any known value, the AI tool can automatically determine the remaining values of a chemical reaction (19).

1.2.d. Multi-step stoichiometry problems: More difficult stoichiometry issues, including those involving numerous stages and reactions, can benefit from AI assistance. Stoichiometry can be used to address problems involving multiple steps in stoichiometry. Chemistry's field of stoichiometry examines the quantitative interactions between reactants and products in chemical reactions. It entails figuring out how many reactants are needed to make a certain amount of product (20).

AI can be used to solve multi-step stoichiometry problems by comparing the balanced chemical equation and checking the amount of reactant B required to react with reactant A. The AI tool can automatically calculate the remaining values of a chemical reaction given any known value (21).

1.3. Error analysis:

Accuracy and reliability can be increased by using AI to detect and analyse flaws in stoichiometric calculations.

There are several ways artificial intelligence (AI) can help with mistake analysis in chemistry. Using machine learning methods to spot and fix flaws in experimental data is one example. To find patterns in the data and spot flaws, machine learning algorithms can be taught on enormous datasets of experimental outcomes. The expected values of the experimental results can then be predicted, and compared to the actual experimental results, and any differences or errors can be found. AI can also be used to improve experimentation processes and lessen error-proneness. The analysis of data from prior studies, for instance, can be used to pinpoint locations where errors are most likely to occur. Then, with the use of this knowledge, experimental protocols can be improved to reduce the possibility of mistakes.

The creation of prediction models for chemical reactions is another potential application of AI in error analysis. These models can be used to forecast the consequences of chemical reactions after being trained on vast databases of experimental results. These models can be used to find mistakes and enhance the models' accuracy by comparing the anticipated results to the actual experimental results.In general,

using AI for error analysis has the potential to greatly enhance the precision and dependability of experimental results in chemistry, ultimately leading to more precise scientific conclusions and better-informed decision-making.

Overall, AI has the potential to advance and quicken the study of stoichiometry by automating repetitive computations, assisting with more challenging issues, and enhancing accuracy and reliability. This can have wide-ranging effects on a variety of sectors, including materials science, drug discovery, and more.

1.4. Reaction optimization:

By determining the ideal reaction conditions, catalysts, and reagents to maximise yield and reduce waste, AI can be used to optimise chemical reactions.

Chemical reaction optimisation has made use of artificial intelligence (AI) to increase reaction yields, shorten reaction durations, and reduce waste (22). AI can be used to predict reaction outcomes, optimize reaction conditions, and design new reactions. AI can also be used to identify reaction pathways and mechanisms (23). AI can assist chemists in exploring wider chemical space and discovering novel reactions that would be challenging to identify with conventional techniques4. By foreseeing the ideal reaction conditions, AI can also assist chemists in optimising already-existing reactions.

1.5. Mechanism analysis:

AI can be used to examine the workings of reactions and identify their essential phases and intermediates. This can cut down experimental times and costs while also accelerating the discovery of new reactions and improving already-existing ones(24).

1.6. Reaction design:

AI can be used to design new chemical reactions by suggesting modifications to existing reaction pathways or by creating entirely new pathways based on specific chemical goals (25).

1.7. Predicting reaction outcomes:

Large databases of chemical reactions can be used to train AI algorithms to forecast new reactions' results depending on their input conditions. This can assist chemists in finding the ideal reaction conditions rapidly to produce the desired product with a high yield and selectivity (26).

AI can be used to predict reaction outcomes, which is a crucial role in reaction design. AI algorithms can anticipate the results of new reactions based on the input conditions by studying massive databases of chemical reactions in order to identify patterns and correlations between reactants and products.

1.8. Designing new reactions:

By examining huge datasets of chemical structures and attributes to pinpoint prospective reactants and reaction pathways, AI systems can also be used to create new chemical reactions. This can be very helpful in the drug development process because it calls for novel interactions to create new molecules with certain biological properties (27).

1.9. Optimizing reaction conditions:

By examining the data from several tests, AI may also be used to determine the ideal reaction parameters, such as temperature, pressure, and catalysts, to achieve high yield and selectivity (28).

1.10. Predicting properties of reaction products:

Based on their chemical structure, AI systems can be trained to anticipate the characteristics of possible reaction products, such as their solubility, stability, and toxicity. Before performing experiments, this can assist chemists in identifying potential problems with a new reaction (29).

1.11. Synthesis planning:

By recommending the most successful and economical synthetic routes depending on the availability of starting materials and reaction conditions, AI can be used to plan the synthesis of complicated compounds. (30).

Overall, AI can significantly speed up and improve the discovery and optimisation of chemical reactions, which might have wide-ranging effects on a variety of industries, including drug development, materials research, and other areas.

Conclusion

By enhancing research effectiveness, precision, and predictive capacity, artificial intelligence (AI) has the potential to have a significant impact on the subject of basic chemistry. The study of vast volumes of chemical data, such as molecule structures and characteristics, which can be utilised to create new medications or materials, is one area where AI can be especially helpful. To speed up and lower the cost of the drug development process, machine learning algorithms can also be trained to predict the qualities of molecules, such as their toxicity or reactivity, based on their structural traits.

Additionally, AI can be used to reproduce complex chemical reactions and processes, providing insights into the underlying mechanisms and allowing scientists to optimize reaction conditions and design new catalysts. AI tools can also assist in the design of experiments, helping to identify the most promising conditions to test and reducing the amount of time and resources required for experimentation. on the whole, AI has the potential to revolutionize the field of basic chemistry, and we can expect to see continued growth and development in this area in the coming years.

Ethical Approval

Not applicable

Informed Consent

Not applicable

Statement Regarding Research Involving Human Participants and/or Animals

Not applicable

Consent to Participate

Not applicable

Consent to Publish

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Author's Contribution

Dongapure Avinash Chandrakant and Choudhari Prafulla Prabhakarrao both contributed equally to this study. They were involved in the conception and design of the study, acquisition and analysis of the data, and interpretation of the results. Both authors drafted the manuscript and revised it critically for important intellectual content. They have both read and approved the final version of the manuscript

Competing Interests

No any conflict of interest

Availability of data and materials

All data and materials used in this study are described in the manuscript and are available to readers upon request from the corresponding author.

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