补充材料：

生成式人工智能解决大学化学教学问题的能力与局限

——基于学生小组实践的研究报告

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I. 研究小组调查任务描述

评估主流 AI 聊天机器人在回答 29 道大学化学题目时的准确性，分析不同题目类别下的表现差异，确定表现最佳的模型及其擅长的题目类型，并评估这些模型作为教学辅助工具的潜力。

1 问题设计

本项研究于 2024 年 11 月 24 日启动，至 11 月 30 日结束，历时 7 天。在此期间，研究人员从山东大学基础医学院 2023 年秋季学期和 2024 年春季学期所用大学化学教材中选取问题，精心设计了 29 道开放式化学题目，用于评估 5 款 AI 聊天机器人的表现。这些题目曾在学生学习过程中使用，覆盖了一学年大学化学课程的核心内容，并分为五类：概念型、解释型、机理型、计算型和综合型题目。同时，为避免文章发表时与平台发展现状脱节，研究者在 2025 年 12 月中旬再次运用这些题目对 5 款 AI 聊天机器人进行了评估。

研究人员将 1-19 题划定为有机化学部分，20-29 题划定为无机化学部分。各类题型的顺序采用随机分布方式，以尽可能模拟真实的学习与测试场景，从而为评估 AI 聊天机器人的问题处理与应对能力提供更客观、准确的数据。随后，研究人员向这 5 款 AI 聊天机器人分别提出同一套题目，并记录其回答以进行详细分析。

2 分析统计

研究人员与授课教师合作，对 AI 聊天机器人回答的正确性和完整性进行了全面评估。评估标准包括以下几个方面：答案的准确性、解释的清晰度、回答的详尽程度以及对概念理解的帮助性。为便于后续数据分析，研究人员在每道题目下方列出了对人工智能聊天机器人回答的评估结果，错误之处用黄色标记，重新评估的内容与结果用 2025.12 标注。

针对每种题型，研究人员统计了正确回答的数量及准确率，确定了在各类题型中准确率最高的 AI 聊天机器人，并对各聊天机器人的整体表现进行了比较。通过这些数据，明确了 AI 聊天机器人擅长回答的化学题型，为其在化学教育中的应用提供了有价值的参考。

II . 29 个开放式问题（错误用黄色标出）

1. Given an IUPAC name for CH_2ClF

ChatGPT: chlorofluoromethane
Kimi Assistant（Kimi 智能助手）: chloro(fluoro)methane
Doubao（豆包）: chlorofluoromethane
ERNIE Bot（文心一言）: chlorofluoromethane
iFLYTEK Spark（讯飞星火）: fluoromethyl chloride

Student's Judgement:

ChatGPT: √
Kimi Assistant: √
Doubao: √
ERNIE Bot: √
iFLYTEK Spark: √

2. Explain why boat conformation is less stable than the chair conformation for cyclohexane.

ChatGPT:

The boat conformation of cyclohexane is much less stable than the chair conformation due to several factors:

Torsional Strain: In the boat conformation, there is significant eclipsing of bonds. Specifically, the hydrogen atoms on adjacent carbon atoms in the boat are positioned in an eclipsed conformation, which increases torsional strain. In contrast, the chair conformation allows for staggered bonds, minimizing torsional strain.

Steric Strain (Flagpole Interactions): The boat conformation has steric clashes between the hydrogen atoms at the "flagpole" positions (the two hydrogen atoms on the carbons that are adjacent to the "bow" and "stern" of the boat). These hydrogens are too close to each other, causing van der Waals repulsion, which increases the strain in the boat form. In the chair conformation, these interactions are minimized, as the substituents are positioned farther apart.

Lack of Ring Strain Relief: The chair conformation allows for the most stable distribution of bond angles (around 109.5°, the ideal tetrahedral angle), and minimizes ring strain. In contrast, the boat conformation is forced into a shape that cannot achieve this ideal bond angle, leading to angle strain (or Baeyer strain), making it less stable.

As a result, the chair conformation is much more stable due to the absence of eclipsing interactions, fewer steric clashes, and better bond angle alignment. The boat conformation, while still a valid conformation, is energetically less favorable due to these increased strains.

Kimi Assistant:

The stability of cyclohexane conformations, such as the boat and chair forms, is largely determined by the amount of strain present in the molecule. Here's why the boat conformation is less stable than the chair

conformation:

1. Axial-Equatorial Strain: In the boat conformation, some of the substituents (like hydrogen atoms or methyl groups) are in axial positions, which means they point directly upwards or downwards from the ring. This results in significant steric hindrance and crowding, leading to increased energy and instability.
2. Baeyer Strain: The boat conformation has a structural feature called Baeyer strain, which arises from the fact that the two ends of the boat are not coplanar, causing the carbon atoms at the ends to have significant angle strain. This is because the carbon atoms in the boat conformation are forced out of the ideal sp3 tetrahedral angle of 109.5°.
3. Van der Waals Strain: The boat conformation has more van der Waals interactions between the axial hydrogens on adjacent carbons, which increases the energy of the molecule. In contrast, the chair conformation minimizes these interactions by allowing all substituents to be either equatorial (in the plane of the ring and experiencing less crowding) or axial (but with less severe steric interactions than in the boat form).
4. Dihedral Angle Strain: The boat conformation has dihedral angles that deviate significantly from the ideal 60° angles found in an idealized planar hexagon. This deviation leads to additional strain and energy.
5. Energy Difference: The energy difference between the chair and boat conformations is significant, with the chair conformation being more stable by several kilocalories per mole. This energy difference makes the chair conformation the predominant form at equilibrium.
6. Transition State: The transition state between the chair and boat conformations involves a half-chair conformation, which has even more strain than the boat conformation, making the interconversion unfavorable.

Due to these factors, the chair conformation is significantly more stable and is the preferred conformation for cyclohexane at room temperature. The boat conformation is a high-energy, minor conformation that is not typically observed under normal conditions.

Doubao:

1. Torsional Strain

In the chair conformation of cyclohexane, the carbon - hydrogen bonds are in a staggered conformation. Staggered conformations have the least torsional strain because the electron clouds of the C - H bonds are as far apart as possible in the Newman projection.

In the boat conformation, there are several eclipsed C - H bonds. Eclipsed bonds lead to a significant torsional strain because the electron clouds of the adjacent bonds are in close proximity and interact unfavorably. This torsional strain in the boat conformation makes it less stable than the chair conformation.

2. Steric Strain

The boat conformation has a flagpole interaction. In the boat shape, the two hydrogen atoms at the “bow” and “stern” of the boat (the 1,4 - diaxial hydrogens) are in close proximity to each other. These are called flagpole hydrogens.

The close approach of these flagpole hydrogens results in steric strain. Steric strain is due to the repulsion between atoms or groups of atoms that are too close together. In contrast, the chair conformation does not have such a close - proximity interaction of hydrogens that would lead to steric strain.

3. Overall Energy Consideration

The combination of torsional strain from the eclipsed bonds and steric strain from the flagpole interactions makes the boat conformation have a higher energy than the chair conformation. Molecules

tend to exist in the lowest energy conformation, so cyclohexane prefers the chair conformation over the boat conformation due to its greater stability.

ERNIE Bot:

The boat conformation of cyclohexane is less stable than the chair conformation due to several key factors related to molecular geometry and steric hindrance. Here's a detailed explanation:

Molecular Geometry:

Chair Conformation: In the chair conformation, cyclohexane adopts a shape resembling a chair, with four carbon atoms forming the base (or "seat") of the chair and two carbon atoms forming the "legs" that extend upward. This conformation minimizes the steric hindrance between the hydrogen atoms attached to the carbon atoms.

Boat Conformation: In the boat conformation, cyclohexane adopts a shape resembling a boat, with all six carbon atoms lying in the same plane. This planar arrangement leads to greater steric hindrance between the hydrogen atoms, particularly those attached to the carbon atoms that are adjacent to each other in the plane.

Steric Hindrance:

In the chair conformation, the hydrogen atoms are positioned in such a way that they avoid close contact with each other, minimizing repulsive forces. This results in a lower energy state and greater stability.

In the boat conformation, the hydrogen atoms are closer together, leading to increased repulsive forces (steric hindrance). This higher energy state makes the boat conformation less stable.

Bond Angles and Bond Lengths:

The chair conformation allows for bond angles and bond lengths that are closer to the ideal values for carbon-carbon single bonds and carbon-hydrogen bonds. This contributes to the overall stability of the conformation.

The boat conformation, on the other hand, results in bond angles and bond lengths that deviate more from the ideal values, leading to increased strain and decreased stability.

Energetics:

The chair conformation is the most stable conformation of cyclohexane because it minimizes the strain caused by steric hindrance and deviations from ideal bond angles and bond lengths.

The boat conformation, with its higher energy state due to increased steric hindrance and strain, is less stable and is therefore less likely to be adopted by cyclohexane molecules in their ground state.

In summary, the boat conformation of cyclohexane is less stable than the chair conformation due to increased steric hindrance, deviations from ideal bond angles and bond lengths, and a higher energy state. The chair conformation, with its lower energy and reduced strain, is the preferred conformation for cyclohexane molecules in their ground state.

iFLYTEK Spark:

The boat conformation of cyclohexane is significantly less stable than the chair conformation due to several key factors related to molecular geometry, bond angles, and torsional strain. Here's a detailed explanation:

1. Bond Angle Deviation:

Chair Conformation: In the chair form, each carbon atom in the ring adopts an approximate tetrahedral arrangement with bond angles close to 109.5°, which is the ideal angle for sp^3 hybridized carbon atoms. This minimizes angle strain.

Boat Conformation: In the boat form, the carbon atoms at positions 2 and 5 (the "bow" or "stern" of the boat) have internal bond angles that deviate significantly from the ideal tetrahedral angle. Specifically,

these angles are compressed to around 90°, leading to increased angle strain.

2. Torsional Strain:

Chair Conformation: The chair form has all substituents in equatorial positions, which minimizes torsional strain. Equatorial bonds are staggered, reducing the repulsive interactions between them.

Boat Conformation: In the boat form, some substituents must occupy axial positions, where they experience significant 1,3-diaxial repulsions. These repulsions occur because the axial hydrogens or substituents on carbons 2 and 5 are directly across from each other, leading to unfavorable eclipsing interactions.

3. Conformation Energy:

Chair Conformation: The chair form represents the global energy minimum for cyclohexane. It is the most stable conformation due to its ability to place all substituents in equatorial positions, minimizing both angle and torsional strains.

Boat Conformation: The boat form is a higher energy conformation because it cannot avoid the severe angle strain at the bow and stern positions and the unfavorable 1,3-diaxial interactions. This makes it a local energy maximum rather than a minimum.

4. Flexibility:

Chair Conformation: The chair form can easily flip into its mirror image (chair-to-chair interconversion), allowing it to adapt to different substituent patterns without incurring significant strain.

Boat Conformation: While the boat form can also undergo pseudorotation to convert into the twist-boat or other conformers, it is inherently less flexible and more prone to strain compared to the chair form.

Summary:

The chair conformation of cyclohexane is much more stable than the boat conformation primarily because it minimizes angle strain by maintaining near-ideal tetrahedral bond angles and reduces torsional strain by avoiding 1,3-diaxial interactions. These factors contribute to the overall lower energy of the chair conformation, making it the preferred structure for cyclohexane under normal conditions.

Student's judgement:

ChatGPT: √

Kimi Assistant: √

Doubao: √

ERNIE Bot: √

iFLYTEK Spark: √

3. Write equations for all of the steps (initiation, propagation, and termination) in the free-radical chlorination of methane to form methyl chloride.

ChatGPT:

The free-radical chlorination of methane to form methyl chloride proceeds through three main stages: initiation, propagation, and termination. Here's a breakdown of the process with the relevant equations for each step:

1. Initiation

The process begins with the homolytic cleavage of chlorine molecules (Cl_2) to form two chlorine radicals ($Cl•$). This step requires energy, usually in the form of heat or UV light.

Cl2→2Cl·(UV light *or heat)*

2. Propagation

During propagation, the chlorine radical reacts with methane (CH_4) to generate a methyl radical ($CH_3•$) and hydrogen chloride (HCl). The methyl radical then reacts with another chlorine molecule (Cl_2) to form methyl chloride (CH_3Cl) and another chlorine radical, which can continue the chain reaction.

Step 1 (Chlorine reacts with methane):

Cl•+CH4→CH3•+HCl

Step 2 (Methyl radical reacts with chlorine):

CH3•+Cl2→CH3Cl+Cl•

These two propagation steps continue cyclically, with the chlorine radical generated in step 2 being used in step 1.

3. Termination

The chain reaction can be terminated when two radicals combine. There are several possible termination steps:

Two chlorine radicals combine to form chlorine gas:

Cl•+Cl•→Cl2

A chlorine radical combines with a methyl radical to form chloromethane (methyl chloride):

CH3•+Cl•→CH3Cl

Two methyl radicals combine to form ethane:

CH3•+CH3•→CH3CH3

In practice, termination steps result in the termination of the free-radical chain and the cessation of the chlorination process.

Summary of Overall Reaction:

The overall reaction for the free-radical chlorination of methane to form methyl chloride is:

CH4+Cl2→CH3Cl+HCl

Kimi Assistant:

The free-radical chlorination of methane to form methyl chloride involves three main steps: initiation, propagation, and termination. Here are the equations for each step:

Initiation:

1. Homolytic cleavage of the Cl2 molecule to form two chlorine radicals:

Cl2→2Cl·

Propagation:

2. The chlorine radical reacts with methane (CH4) to form methyl radical (CH3•) and hydrogen chloride (HCl):

Cl•+CH4→CH3•+HCl

3. The methyl radical then reacts with another Cl2 molecule to form methyl chloride (CH3Cl) and another chlorine radical:

CH3•+Cl2→CH3Cl+Cl•

Termination:

4. Two radicals react with each other to form a stable molecule, ending the chain reaction. This can happen in several ways, but two common ones are:

Two methyl radicals combining to form ethane (C2H6):

CH3•+CH3•→CH3CH3

A methyl radical and a chlorine radical combining to form methyl chloride and a chlorine molecule:

$CH_3\bullet + Cl\bullet \rightarrow CH_3Cl$

The propagation steps are repeated many times, leading to the formation of a significant amount of methyl chloride. The termination steps are less frequent but are necessary to stop the reaction from continuing indefinitely.

Doubao:

1. Initiation:

Chlorine molecules (Cl_2) absorb energy (usually in the form of ultraviolet light or heat) to break the Cl - Cl bond homolytically. This forms two chlorine radicals ($Cl\bullet$).

The equation for the initiation step is: $Cl_2 \rightarrow 2Cl\cdot (h\nu \text{ or } \Delta)$

2. Propagation:

The first propagation step: A chlorine radical ($Cl\cdot$) attacks a methane molecule (CH_4). The chlorine radical abstracts a hydrogen atom from methane, forming a methyl radical ($CH_3\bullet$) and a molecule of hydrogen chloride (HCl).

The equation is: $Cl\bullet + CH_4 \rightarrow CH_3\bullet + HCl$

The second propagation step: The methyl radical ($CH_3\bullet$) then reacts with a chlorine molecule (Cl_2) to form methyl chloride (CH_3Cl) and a new chlorine radical ($Cl\bullet$).

The equation is:$CH_3\bullet + Cl_2 \rightarrow CH_3Cl + Cl\bullet$

3. Termination:

There are several possible termination steps. One is the combination of two chlorine radicals to form a chlorine molecule.

The equation is: $Cl\bullet + Cl\bullet \rightarrow Cl_2$

Another is the combination of a chlorine radical and a methyl radical to form methyl chloride.

The equation is: $CH_3\bullet + Cl\bullet \rightarrow CH_3Cl$

The third is the combination of two methyl radicals to form ethane (C_2H_6).

The equation is: $CH_3\bullet + CH_3\bullet \rightarrow C_2H_6$

ERNIE Bot:

Sure, here are the equations for the steps involved in the free-radical chlorination of methane to form methyl chloride:

Initiation Step:

$Cl_2 \rightarrow 2Cl\cdot (h\nu)$

Propagation Steps:

$CH_4 + Cl\cdot \rightarrow CH_3\cdot + HCl$

$CH_3\cdot + Cl_2 \rightarrow CH_3Cl + Cl\cdot$

These two propagation steps repeat multiple times.

Termination Steps:

Combination:

$2Cl\cdot \rightarrow Cl_2$

$CH_3\cdot + CH_3\cdot \rightarrow C_2H_6$

Disproportionation:

$CH_3\cdot + Cl\cdot \rightarrow CH_3Cl$

Note that termination steps can occur in various ways, and the above are examples of common pathways.

iFLYTEK Spark:

The free-radical chlorination of methane (CH4) to form methyl chloride (CH3Cl) involves a series of steps, including initiation, propagation, and termination. Below are the equations for each step:

Initiation

1. Formation of Chlorine Radicals: The initiation step typically involves the homolytic cleavage of chlorine molecules (Cl2) into two chlorine radicals (Cl•). This can be induced by heat, light, or a catalyst.

$Cl2 \rightarrow 2Cl•$

Propagation

2. Chlorine Radical Addition: A chlorine radical adds to a methane molecule, forming a chloromethyl radical (CH3•) and a hydrogen chloride (HCl) molecule.

$Cl• + CH4 \rightarrow CH3• + HCl$

3. Radical Halogenation: The chloromethyl radical then reacts with another chlorine molecule, producing methyl chloride (CH3Cl) and regenerating a chlorine radical (Cl•).

$CH3• + Cl2 \rightarrow CH3Cl + Cl•$

Termination

4. Radical Combination: Two radical species combine to form stable molecules, terminating the chain reaction. This can occur in several ways:

Two chlorine radicals combine to form a chlorine molecule.

$Cl• + Cl• \rightarrow Cl2$

A chloromethyl radical and a chlorine radical combine to form methyl chloride.

$CH3• + Cl• \rightarrow CH3Cl$

Two chloromethyl radicals combine to form ethane (not observed under typical conditions but shown here for completeness).

$CH3• + CH3• \rightarrow CH3CH3$

These steps illustrate the mechanism by which methane is converted into methyl chloride through a free-radical process.

Student's Judgement:

ChatGPT: √
Kimi Assistant: √
Doubao: √
ERNIE Bot: √
iFLYTEK Spark: √

4. Explain with the aid of conformational structures why cis-1,3-dimethylcyclohexane is more stable than trans-1,3-dimethylcyclohexane, whereas the reverse order of stability is observed for the 1,2 and 1,4 isomers.(Within 100 words)

ChatGPT:

In cyclohexane derivatives, stability is influenced by steric hindrance and 1,3-diaxial interactions. For cis-1,3-dimethylcyclohexane, both methyl groups are positioned in equatorial positions, minimizing steric

strain, which enhances stability. In contrast, trans-1,3-dimethylcyclohexane has one methyl in the axial position, leading to significant 1,3-diaxial interactions and higher strain. For the 1,2 and 1,4 isomers, the relative stability reverses because, in these cases, axial positions cause more steric strain in the cis isomer, while the trans isomer places substituents in more favorable positions (either both equatorial or alternating between axial and equatorial).

Kimi Assistant:

The stability of cis-1,3-dimethylcyclohexane compared to trans-1,3-dimethylcyclohexane is due to the absence of 1,3-diaxial interactions in the cis isomer. In the trans isomer, the two methyl groups on opposite sides of the ring are in an axial position, leading to significant steric hindrance and increased energy.

For 1,2-dimethylcyclohexane, the trans isomer is more stable because the methyl groups are equatorial, minimizing steric hindrance. In the cis isomer, one methyl group is axial, leading to higher energy due to 1,2-axial interactions.

In 1,4-dimethylcyclohexane, both isomers have minimal steric hindrance, but the trans isomer is slightly more stable due to the greater distance between the methyl groups, reducing van der Waals repulsion.

Doubao:

In cis - 1,3 - dimethylcyclohexane, both methyls can be in equatorial positions in the more stable chair conformation. In trans - 1,3 - dimethylcyclohexane, one methyl is axial. For 1,2 and 1,4 isomers, the trans isomers have less steric hindrance as the groups can be equatorial.

ERNIE Bot:

In cis-1,3-dimethylcyclohexane, the two methyl groups are on the same side of the ring, allowing for better steric packing with less crowding. This leads to lower energy and greater stability.

Conversely, in trans-1,3-dimethylcyclohexane, the methyl groups are on opposite sides, causing greater steric hindrance and higher energy.

For 1,2- and 1,4-dimethylcyclohexane, the trans isomers are more stable due to less steric hindrance between the methyl groups, which are farther apart compared to the cis isomers where they are closer and cause more crowding.

iFLYTEK Spark:

The stability of cyclohexane derivatives can be explained by conformational structures and the principles of equatorial versus axial bonds.

cis-1,3-Dimethylcyclohexane: The cis isomer predominantly adopts a diequatorial conformation where both methyl groups are in equatorial positions, minimizing steric strain and leading to greater stability.

trans-1,3-Dimethylcyclohexane: The trans isomer has one methyl group in an axial position, which introduces significant 1,3-diaxial interactions with adjacent hydrogens, increasing steric strain and reducing stability.

For 1,2- and 1,4-dimethylcyclohexane:

trans-1,2-Dimethylcyclohexane: Both methyl groups can be equatorial, making it more stable than the cis isomer.

cis-1,4-Dimethylcyclohexane: One methyl group must be axial, causing destabilizing interactions.

These differences in steric strain and bond orientation explain the observed stability trends.

Student's Judgement:

ChatGPT: √

Kimi Assistant: √

Doubao: √

ERNIE Bot: √

iFLYTEK Spark: √

5. The acid-catalyzed hydration of 1-methylcyclohexene gives 1-methylcyclohexanol. Write each step in the mechanism of this reaction. (Within 150 words)

ChatGPT:

The acid-catalyzed hydration of 1-methylcyclohexene proceeds via a three-step mechanism:

1. Protonation of the Alkene:

The double bond of 1-methylcyclohexene reacts with a proton (H+) from the acid catalyst ($H3O^+$ or H_2SO_4). The proton adds to the carbon of the double bond that has the greater number of hydrogen atoms, forming a secondary carbocation at the more stable position (adjacent to the methyl group).

$CH2=C(CH3)\rightarrow CH_2=C^+(H)CH_2 \quad (H^+)$

2. Nucleophilic Attack by Water:

Water (H_2O) attacks the carbocation, forming a protonated alcohol (oxonium ion).

$CH_2=C^+(H)CH_2+H_2O\rightarrow CH_3C(OH_2^+)(H)CH_2$

3. Deprotonation:

The protonated alcohol undergoes deprotonation, typically by water, to form the neutral alcohol.

$CH_3C(OH_2^+)(H)CH_2\rightarrow CH_3C(OH)(H)CH_2 \quad (H_2O)$

The result is 1-methylcyclohexanol.

2025.12：The mechanism involves electrophilic aromatic substitution. Initially, benzene reacts with excess D_2SO_4 to form a cyclohexadienyl cation intermediate after protonation of the ring by H^+ from sulfuric acid. The deuterium from D_2SO_4 then acts as a nucleophile, substituting for hydrogen on the aromatic ring. This process can occur multiple times, leading to a gradual replacement of hydrogens with deuteriums. As more deuterium is incorporated, the reaction continues until the hydrogens are predominantly replaced by deuteriums, demonstrating the effectiveness of D_2SO_4 in facilitating this isotope exchange at room temperature.

Kimi Assistant:

The acid-catalyzed hydration of 1-methylcyclohexene to form 1-methylcyclohexanol involves the following steps:

1. Protonation of the double bond: The pi electrons of the double bond attack the proton (H+) from the acid catalyst, forming a carbocation intermediate. Since 1-methylcyclohexene can form a more stable carbocation with the positive charge on the more substituted carbon, it will protonate at the carbon adjacent to the methyl group.

2. Formation of the carbocation: The double bond breaks, and the electrons from the broken bond pair up with the proton, leaving a carbocation with a positive charge on the carbon.

3. Nucleophilic attack by water: A water molecule acts as a nucleophile and attacks the carbocation, with the oxygen atom donating a pair of electrons to form a new bond.

4. Deprotonation: The hydroxyl group (OH) formed in the previous step can donate a proton to the acid catalyst, regenerating the protonated acid and forming the alcohol.

5. Catalyst regeneration: The acid catalyst is regenerated and available to protonate another molecule of 1-methylcyclohexene.

The overall reaction is:

1-methylcyclohexene+H_2O→1-methylcyclohexanol(acid)

This mechanism is an example of an electrophilic addition reaction, where water acts as the nucleophile.

Doubao:

1.Protonation: The double bond of 1 - methylcyclohexene attacks a proton (H+) from the acid catalyst, forming a carbocation. The more stable tertiary carbocation is formed.

2. Nucleophilic Attack: Water acts as a nucleophile and attacks the carbocation, forming a protonated alcohol.

3. Deprotonation: Another water molecule (or a base in the reaction mixture) removes a proton from the protonated alcohol, yielding 1 - methylcyclohexanol.

ERNIE Bot:

The acid-catalyzed hydration of 1-methylcyclohexene to produce 1-methylcyclohexanol involves several key steps. Here's a concise outline of the mechanism:

Protonation: The double bond in 1-methylcyclohexene is protonated by the acid catalyst, forming a carbocation intermediate. This step polarizes the double bond, making it more susceptible to attack by water.

Addition of Water: Water then attacks the positively charged carbon of the carbocation, adding a hydroxyl (-OH) group and forming an alcohol intermediate with a positive charge on the oxygen.

Proton Transfer: A proton from the acid catalyst is then transferred to the oxygen atom of the alcohol intermediate, neutralizing the charge and producing the final product, 1-methylcyclohexanol.

Regeneration of Catalyst: The acid catalyst is regenerated in this process and is available to catalyze further reactions.

This mechanism is characteristic of acid-catalyzed hydration reactions, where the acid acts as a catalyst to facilitate the addition of water to an olefin.

iFLYTEK Spark:

The acid-catalyzed hydration of 1-methylcyclohexene to form 1-methylcyclohexanol involves several steps, primarily driven by the electrophilic nature of protons. Here is a step-by-step mechanism:

Step 1: Protonation

1. Protonation of the Double Bond: The double bond in 1-methylcyclohexene is protonated by a hydronium ion (H_3O^+), resulting in a carbocation intermediate.

$CH3\text{-}C5H8 + H3O^+ \rightarrow CH3\text{-}C5H9^+ + H2O$

Step 2: Nucleophilic Attack

2. Nucleophilic Addition of Water: A water molecule acts as a nucleophile and attacks the carbocation at the positively charged carbon, forming a new C-OH bond and regenerating a proton.

$CH3\text{-}C5H9^+ + H2O \rightarrow CH3\text{-}C5H9(OH) + H^+$

Step 3: Deprotonation

3. Deprotonation to Form Alcohol: The protonated alcohol intermediate loses a proton to a base (often another water molecule or an anion) to form the final product, 1-methylcyclohexanol.

$CH3\text{-}C5H9(OH) + H2O \rightarrow CH3\text{-}C5H10(OH) + H_3O^+$

These steps illustrate the overall mechanism for the conversion of 1-methylcyclohexene into 1-methylcyclohexanol through acid-catalyzed hydration.

2025.12：The mechanism proceeds via acid-catalyzed electrophilic addition:

Protonation: H^+ (from H_3O^+) adds to the less substituted carbon of 1-methylcyclohexene, forming a stable tertiary carbocation at C1 (adjacent to the methyl group).
Nucleophilic attack: Water attacks the tertiary carbocation, yielding an oxonium ion (protonated alcohol).
Deprotonation: A water molecule deprotonates the oxonium ion, regenerating H_3O^+ and producing 1-methylcyclohexanol.
Regioselectivity follows Markovnikov's rule due to the greater stability of the tertiary carbocation intermediate. The acid catalyst (H^+) is regenerated, enabling catalytic turnover.

Student's Judgement:

ChatGPT: × 化学反应式中的反应错误。 ×（2025.12）反应物叙述错误
Kimi Assistant: √
Doubao: √
ERNIE Bot: √
iFLYTEK Spark: × 化学反应式中的反应物错误。 √（2025.12）

6. Describe two simple chemical tests that could be used to distinguish methylcyclohexane from methylcyclohexene. (Within 100 words)

ChatGPT:

1.Bromine water test: Methylcyclohexene, being an alkene, will undergo electrophilic addition with bromine water, decolorizing it. Methylcyclohexane, an alkane, will not react, and the bromine water will remain reddish-brown.

2. Baeyer's test (Potassium permanganate): Methylcyclohexene reacts with potassium permanganate ($KMnO_4$) in the presence of a dilute acid or neutral medium, causing the purple color to fade and forming a diol (vicinal alcohols). Methylcyclohexane does not react and the purple color persists.

Kimi Assistant:

1. Bromine Water Test: Methylcyclohexene will decolorize bromine water due to its double bond, which reacts with bromine in an addition reaction. Methylcyclohexane, lacking a double bond, will not react and thus the bromine water will remain colored.

2. Acid-Catalyzed Hydration Test: Methylcyclohexene can be hydrated in the presence of an acid catalyst to form methylcyclohexanol. Methylcyclohexane, being already saturated, will not undergo this reaction. The formation of a new compound (alcohol) in the case of methylcyclohexene can be confirmed by further tests such as the Lucas test, which would show a cloudy precipitate with zinc chloride in the presence of the alcohol.

2025.12：

1. Bromine water test: Add bromine water (reddish-brown) to each compound. Methylcyclohexene will decolorize it via addition across the double bond; methylcyclohexane will not.

2. Baeyer's test: Add dilute, cold $KMnO_4$(purple). Methylcyclohexene will decolorize it and form a brown precipitate (MnO_2); methylcyclohexane will not react.

Doubao:

1. Bromine water test: Methylcyclohexene decolorizes bromine water due to the addition reaction of the double bond, while methylcyclohexane doesn't react and the solution stays brown.

2. Acidified potassium permanganate test: Methylcyclohexene turns it from purple to colorless, but

methylcyclohexane doesn't.

ERNIE Bot:

Two simple chemical tests to distinguish methylcyclohexane from methylcyclohexene are:

Bromine Water Test: Add bromine water (Br_2 in H_2O). Methylcyclohexene reacts, causing the solution to turn colorless due to double bond saturation, while methylcyclohexane does not.

KMnO4 Test: Using potassium permanganate (KMnO4), which is reduced by unsaturated compounds. Methylcyclohexene causes KMnO4 to decolorize, indicating its unsaturation, whereas methylcyclohexane doesn't.

iFLYTEK Spark:

Two simple chemical tests can be used to distinguish methylcyclohexane from methylcyclohexene:

1. Bromination Test: Add a small amount of bromine (Br_2) to the compound. Methylcyclohexane, being an alkane, will not react with bromine and remain unchanged. In contrast, methylcyclohexene, an alkene, will react with bromine by undergoing electrophilic addition, resulting in the formation of a dibromide derivative and a visible color change (brown).

2. KMnO4 Test: Add a solution of potassium permanganate (KMnO4) to the compound. Methylcyclohexane will not react and the purple color of KMnO4 will remain unchanged. Methylcyclohexene, however, will react with KMnO4, causing it to be reduced and decolorized as the double bond in the alkene is oxidized.

Student's Judgement:

ChatGPT: √

Kimi Assistant: × Lucas 试剂主要用于鉴别一级、二级和三级醇，但不能简单直接地判断是否在此处生成了醇类物质，通常用 Lucas 试剂来区分不同种类的醇。 √ （2025.12）

Doubao: √

ERNIE Bot: √

iFLYTEK Spark: √

7. Explain the mechanism of electrophilic aromatic substitution of benzene with chlorine under the catalysis of ferric chloride. (Within 100 words)

ChatGPT:

The electrophilic aromatic substitution of benzene with chlorine (Cl_2) in the presence of ferric chloride ($FeCl_3$) proceeds as follows:

1. Activation of Cl2: $FeCl_3$ acts as a Lewis acid and coordinates with Cl2, generating a more reactive electrophilic species, Cl+.

2. Aromatic substitution: The electron-rich benzene ring donates electrons to the Cl+ ion, forming a sigma complex (arenium ion).

3. Restoration of aromaticity: The sigma complex loses a proton (H+) to regenerate the aromatic ring, yielding chlorobenzene (C6H5Cl) as the product.

This mechanism involves the generation of an electrophile and the formation of a transient carbocation intermediate.

Kimi Assistant:

Electrophilic aromatic substitution of benzene with Cl2 under ferric chloride (FeCl3) as a catalyst involves

a two-step mechanism:

1. Electrophile Generation: FeCl3 acts as a Lewis acid, accepting a pair of electrons from Cl2 to form a ferric chloride complex and a chlorine radical (Cl•).

2. Aromatic Substitution: The chlorine radical, an electrophile, attacks the benzene ring, forming a sigma complex. This is followed by the migration of a hydrogen atom to the chlorine, forming HCl and leaving a chlorobenzene with a positive charge on the carbon.

3. Regeneration of Catalyst: The positively charged carbon is then attacked by another Cl•, forming dichlorobenzene and regenerating the ferric chloride catalyst.

This process is highly regioselective, typically occurring at the ortho and para positions relative to existing substituents due to the stabilizing effect of the positive charge on the transition state by resonance.

2025.12: $FeCl_3$ chlorinates benzene via electrophilic aromatic substitution (EAS):

$FeCl_3 + Cl_2 \rightarrow Cl^+ \cdots FeCl_4^-$ (π-complex)

Cl^+ attacks π cloud $\rightarrow$ σ-complex (arenium ion)

Aromaticity restored as $FeCl_4^-$ removes ring H^+

Regenerate $FeCl_3$; product = chlorobenzene + HCl

Doubao:

In this reaction, $FeCl_3$ reacts with Cl2 to form Cl+ (electrophile). The electrophile attacks the benzene ring, breaking its aromaticity. Then, through deprotonation, the aromaticity is restored, and HCl and FeCl3 are regenerated.

ERNIE Bot:

The mechanism of electrophilic aromatic substitution of benzene with Cl2 under $FeCl_3$ involves two main steps:

Electrophile Formation: $FeCl_3$ catalyzes the formation of Cl+ as the electrophile by accepting an electron from Cl2.

Substitution Reaction: The aromatic π-bond of benzene attacks Cl+, forming a carbocation intermediate. This intermediate then loses a proton to reform the aromatic π-bond, resulting in the substitution of a chlorine atom on the benzene ring.

This process leads to the formation of chlorobenzene.

iFLYTEK Spark:

Electrophilic aromatic substitution (EAS) of benzene with Cl_2 in the presence of ferric chloride ($FeCl_3$) as a catalyst proceeds through the following mechanism:

1. Formation of Electrophile: Ferric chloride abstracts a chloride ion from Cl_2, forming a positive chlorine electrophile (Cl^+).

2. Electrophilic Attack: The Cl^+ electrophile attacks one of the carbon atoms in the benzene ring, leading to the formation of a carbocation intermediate.

3. Rearrangement and Delocalization: The carbocation intermediate undergoes rapid delocalization of the positive charge around the ring, stabilizing it.

4. Nucleophilic Attack: A chloride ion acts as a nucleophile, attacking the carbocation at the position where the positive charge is most stabilized, resulting in the formation of chlorobenzene and regenerating the ferric chloride catalyst.

The overall reaction results in the substitution of one hydrogen atom on the benzene ring with a chlorine atom.

2025.12: $FeCl_3$ acts as a Lewis acid catalyst, coordinating with Cl_2 to generate the electrophile Cl^+ (as $[Cl–FeCl_3]^+$ or via heterolytic cleavage). This electrophile attacks the electron-rich benzene ring, forming a

resonance-stabilized arenium ion (sigma complex) where the positive charge is delocalized over three carbon atoms. Deprotonation by the weak base $[FeCl_4]^-$ then restores aromaticity, yielding chlorobenzene and regenerating $HFeCl_3$ (which dissociates to HCl and $FeCl_3$). The catalyst enables milder conditions by facilitating Cl^+ formation.

Student's Judgement:

ChatGPT: √

Kimi Assistant: × 该解释是错误的，因为它错误地声称亲电体是氯自由基（Cl·）而不是氯离子（Cl^+），错误地描述了取代和催化剂再生步骤，并不恰当地提到了取代苯的区域选择性。 √（2025.12）

Doubao: √

ERNIE Bot: √

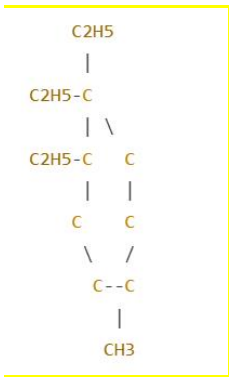
iFLYTEK Spark: × 不存在亲核攻击。 ×（2025.12）反应过程仍存在错误

8. Write structural formula for 2,4,6-triethyltoluene

ChatGPT:

```
      CH2CH3
        |
  CH3-C6H4
        |
      CH2CH3
```

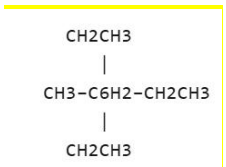
2025.12:



Kimi Assistant:

```
      CH3       CH3
        |       |
  CH2-C-CH2-C6H4-CH3
        |       |
      CH3       CH3
```

2025.12:



Doubao:

```
  CH3
```

|

CH3 - C - CH2 - CH3

| |

H - C - C - H

| |

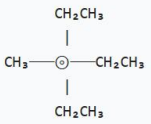
H - C - C - H

|

CH2 - CH3

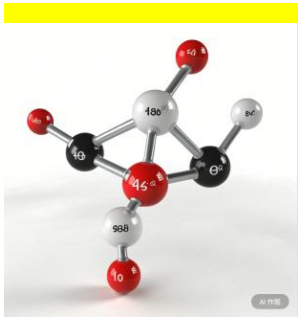
2025.12：

plaintext



(where "⊙" represents the benzene ring; the methyl group is at C1, and ethyl groups are at C2, C4, C6).

ERNIE Bot:



2025.12：

```
CH₃
        |
   CH₂CH₃–C₆H₃–CH₂CH₃
        |     |
   CH₂CH₃   (positions 2,4,6)
```

iFLYTEK Spark:

H2C

|

CH2--CH=CH2

|

CH2--CH=CH2

|

CH2--CH=CH2

|

CH2--CH=CH2

|

CH2--CH=CH2

|

CH2--CH=CH2

2025.12：

- If you draw benzene, label one carbon as **C1–CH_3**.
- Count clockwise:
  - C2: –CH_2CH_3
  - C3: H
  - C4: –CH_2CH_3
  - C5: H
  - C6: –CH_2CH_3

Student's Judgement:

ChatGPT: × × (2025.12)

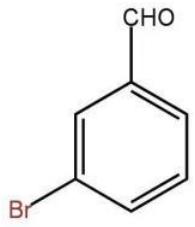
Kimi Assistant: × × (2025.12)

Doubao: × √ (2025.12)

ERNIE Bot: × × (2025.12)

iFLYTEK Spark: × √ (2025.12)

9. Name this compound:



ChatGPT: 3-bromobenzaldehyde

Kimi Assistant: 2-bromo-benzaldehyde

2025.12:bromomethane

Doubao: 2 - bromobenzaldehyde

2025.12:3-bromobenzaldehyde

ERNIE Bot: 1-Bromo-2-phenylethanone

2025.12: 3-Bromobenzaldehyde

iFLYTEK Spark: 4-Bromobenzaldehyde

2025.12:4-Bromopheno

Student's Judgement:

ChatGPT: √

Kimi Assistant: ×

× **(2025.12)**

Doubao: ×

√ **(2025.12)**

ERNIE Bot: ×

√ **(2025.12)**

iFLYTEK Spark: ×

× **(2025.12)**

10. When benzene is treated with excess D_2SO_4 at room temperature, the hydrogens on the benzene ring gradually replaced by deuterium. Write a mechanism that explains this observation.(Within 100 words)

ChatGPT:

When benzene is treated with excess D_2SO_4 at room temperature, the hydrogens on the benzene ring are gradually replaced by deuterium through a proton-deuterium exchange mechanism. The D_2SO_4 dissociates into D^+ and HSO_4^- . The benzene ring is protonated to form a sigma complex, and the proton on the ring is exchanged with a deuteron (D^+) from D_2SO_4. This process occurs repeatedly, with the hydrogens on the ring gradually being replaced by deuterium. The final product is deuterated benzene (C_6H_5D), with varying degrees of deuterium incorporation depending on the reaction conditions.

Kimi Assistant:

The deuteration of benzene with D_2SO_4 involves a sigmatropic rearrangement known as the deuterium shift:

1. Protonation: D_2SO_4 protonates benzene, forming a protonated benzene intermediate.
2. Deuterium Shift: A deuterium from D_2SO_4 migrates to an adjacent carbon on the ring, forming a deuterated carbocation.
3. Reprotonation: The carbocation is reprotonated by D_2SO_4, and the process repeats, leading to further deuteration.
4. Catalyst Regeneration: D_2SO_4 is regenerated, allowing the reaction to continue.

This mechanism results in the gradual replacement of hydrogens by deuterium on the benzene ring.

Doubao:

Benzene is protonated by H^+ from D_2SO_4 to form a carbocation. D^+ from D_2SO_4 then attacks the carbocation. The released H^+ can protonate another benzene molecule, repeating the process and replacing H with D.

ERNIE Bot:

Benzene reacts with excess D_2SO_4 at room temperature via a substitution mechanism. The D2SO4, analogous to H2SO4, acts as an electrophile. It forms a complex with benzene, polarizing the π-bond. A deuterium atom (D^+) from D_2SO_4 attacks the benzene ring, substituting a hydrogen. This results in the formation of a deuterated intermediate, which releases D2SO4−. The aromaticity of the ring is restored, and the process repeats, gradually replacing all hydrogens with deuterium. Note that D_2SO_4 is hypothetical; typically, benzene undergoes sulfonation with H2SO4.

2025.12：The mechanism involves electrophilic aromatic substitution. D_2SO_4 dissociates into D^+ and DSO_4^-. Benzene's π-electrons attack D^+, forming a resonance-stabilized sigma complex (arenium ion). This intermediate loses a proton (H^+) to restore aromaticity, but in excess D_2SO_4, H^+ is replaced by D^+ from the solvent, substituting H with D. The process repeats for all ring hydrogens. Room temperature facilitates slow, controlled substitution without disrupting aromaticity. Key steps: electrophilic attack → sigma complex formation → deprotonation/deuteration → aromaticity restoration.

iFLYTEK Spark:

The mechanism involves electrophilic aromatic substitution. Deuterated sulfuric acid (D_2SO_4) dissociates to produce deuterium ions (D^+), which act as electrophiles and attack the benzene ring, forming a

carbocation intermediate. This intermediate quickly rearranges through 1,2-hydride shifts to form a more stable carbocation. The stabilized carbocation loses a proton (H^+), regenerating the aromatic benzene ring with one deuterium atom incorporated. The released proton can react with another DSO_4^- to regenerate D_2SO_4, allowing the cycle to continue, leading to gradual replacement of hydrogen atoms by deuterium on the benzene ring.

2025.12： The reaction proceeds via electrophilic aromatic substitution with deuterium exchange. D_2SO_4 generates D^+ as the electrophile. Benzene undergoes reversible protonation (deuteration) to form a non-aromatic arenium ion (sigma complex). Due to the kinetic isotope effect, C–H bonds cleave faster than C–D bonds. Thus, the arenium ion preferentially loses H^+ (rather than D^+) to restore aromaticity, yielding monodeuterated benzene (C_6H_5D). Excess D_2SO_4 drives repeated cycles: subsequent electrophilic attacks incorporate additional deuterium atoms, replacing all ring hydrogens with deuterium over time.

Student's Judgement:

ChatGPT: √

Kimi Assistant: √

Doubao: √

ERNIE Bot: × "释放 D2SO4"不够准确 √ （2025.12）

iFLYTEK Spark: × D2SO4 未再生 √ （2025.12）

11. Show how pure 3,5-dinitrochlorobenzene can be prepared, starting from a disubstituted benzene.

ChatGPT:

Start with chlorobenzene.

Perform nitration to produce 3-nitrochlorobenzene.

Perform a second nitration to introduce the second nitro group at position 5, yielding 3,5-dinitrochlorobenzene.

2025.12： To prepare pure 3,5-dinitrochlorobenzene from a disubstituted benzene, we can follow a multi-step synthetic route. Here's a step-by-step synthesis pathway:

Starting Material:

Let's consider starting with 1,4-dichlorobenzene (p-dichlorobenzene) as the disubstituted benzene.

Step 1: Nitration of 1,4-Dichlorobenzene

Reagents: Nitric acid (HNO_3) and sulfuric acid (H_2SO_4)

Reaction: Perform nitration to introduce a nitro group onto the benzene ring.

Products: The reaction will predominantly yield 3-nitro-1,4-dichlorobenzene, as the nitro group is a meta-directing group due to the presence of chlorine atoms.

Step 2: Further Nitration

Reagents: Again use nitric acid and sulfuric acid.

Reaction: Subject 3-nitro-1,4-dichlorobenzene to further nitration.

Products: This will lead to the formation of 3,5-dinitro-1,4-dichlorobenzene, where another nitro group is introduced at the 5-position relative to the first nitro group.

Step 3: Separation and Purification

To obtain pure 3,5-dinitrochlorobenzene from the mixture, we would need to carry out a purification process such as recrystallization or column chromatography, depending on the solubility properties of the products.

Summary of Reaction Steps:

Nitration of 1,4-dichlorobenzene → 3-nitro-1,4-dichlorobenzene

Further nitration of 3-nitro-1,4-dichlorobenzene → 3,5-dinitro-1,4-dichlorobenzene

Purification to isolate pure 3,5-dinitrochlorobenzene.

Kimi Assistant:

To prepare pure 3,5-dinitrochlorobenzene from a disubstituted benzene, you would typically follow a multi-step synthesis process. Here's a general outline of the steps involved:

1. Starting Material: Begin with a disubstituted benzene that has at least one hydrogen atom at the 3 and 5 positions. For example, you might start with chlorobenzene or methylchlorobenzene.

2. Nitration: The first step is to nitrate the benzene ring. This is typically done using a mixture of concentrated nitric acid (HNO_3) and concentrated sulfuric acid (H_2SO_4) as a catalyst. The nitration process will introduce nitro groups (-NO2) into the benzene ring. To obtain 3,5-dinitro substitution, the nitration must be carefully controlled to avoid over-nitration or the formation of other isomers.

3. Selective Nitration: If the starting material is not already chlorinated at the desired position, a chlorination step may be necessary. This can be achieved using chlorine (Cl_2) in the presence of a catalyst like iron(III) chloride ($FeCl_3$) or ultraviolet (UV) light.

4. Purification: After nitration and chlorination, the product will need to be purified to remove any unreacted starting material, byproducts, or other isomers. This can be done through methods such as fractional crystallization, distillation, or chromatography.

5. Confirmation: Finally, the structure of the synthesized compound should be confirmed using analytical techniques such as nuclear magnetic resonance (NMR), infrared (IR) spectroscopy, or mass spectrometry.

It's important to note that the synthesis of 3,5-dinitrochlorobenzene can be a hazardous process due to the use of strong acids and the potential formation of explosive dinitro compounds. Therefore, it should be carried out with proper safety precautions and in a controlled laboratory environment.

The search results provided do not contain specific procedures for the synthesis of 3,5-dinitrochlorobenzene, but they do highlight the importance of controlling the nitration process to avoid the formation of undesired isomers, such as 2,4-dinitrochlorobenzene. The nitration of chlorobenzene with nitric acid in a continuous installation has been developed, which could be relevant to the nitration step in the synthesis. However, the specific details of the synthesis would require a more detailed chemical protocol or a consultation with chemical literature and databases.

2025.12：🩹 Reaction Steps

Step 1: Nitration of 1,3-dichlorobenzene

Reagents: Conc. HNO_3 / Conc. H_2SO_4

Conditions: Heat

Product: 3,5-dinitro-1-chlorobenzene

Reaction:

1,3-dichlorobenzene + 2 HNO_3/H_2SO_4 → 3,5-dinitrochlorobenzene

✓ Purification

Recrystallization from ethanol or benzene to obtain pure 3,5-dinitrochlorobenzene.

🩹 Alternative Route (if starting from other disubstituted benzenes)

If you start from other disubstituted benzenes, you may get mixtures due to competing directing effects.

For example:

Chlorobenzene + nitration → mixture of ortho, meta, para (not selective).

Nitrobenzene + chlorination → meta-chloronitrobenzene, but further nitration is difficult due to deactivation.

✓ Conclusion

The best and most selective way to prepare pure 3,5-dinitrochlorobenzene is:

Start from 1,3-dichlorobenzene and perform double nitration with HNO_3/H_2SO_4 under heat, followed by recrystallization.

This gives 3,5-dinitrochlorobenzene as the major product.

Doubao:

Starting Material Selection:

We start with chlorobenzene as the disubstituted benzene. Chlorobenzene has a chlorine atom attached to the benzene ring.

Nitration Reactions:

The first nitration step:

Chlorobenzene undergoes nitration. The nitration reaction is carried out using a mixture of concentrated nitric acid and concentrated sulfuric acid. The electrophile in this reaction is the nitronium ion.

Chlorobenzene reacts with to form a mixture of ortho - and para - nitrochlorobenzene. The reaction mechanism involves the electrophilic aromatic substitution. The major product is para - nitrochlorobenzene due to steric and electronic effects.

The second nitration step:

Para - nitrochlorobenzene is further nitrated. Using the same nitrating mixture (and), another nitronium ion attacks the benzene ring.

The second nitration occurs at the position meta to the chlorine atom and ortho to the first nitro group, resulting in the formation of 3,5 - dinitrochlorobenzene. This is because the nitro group is a meta - directing deactivator, and the chlorine atom is an ortho/para - directing activator. The combined directing effects lead to the formation of 3,5 - dinitrochlorobenzene.

2025.12：

1. Starting Material

1,3-dinitrobenzene (m-dinitrobenzene, disubstituted benzene):

$O_2N-C_6H_4-NO_2$ (two $-NO_2$ at positions 1 and 3).

2. Reaction: Regioselective Chlorination (Electrophilic Aromatic Substitution)

Reagents & Conditions:

- Halogenating agent: Cl_2 (chlorine gas)
- Catalyst: $FeCl_3$ or $AlCl_3$ (Lewis acid, activates Cl_2 to form electrophilic Cl^+)
- Temperature: Moderate heating ($60–80^\circ C$; required because 1,3-dinitrobenzene is highly deactivated, so higher reactivity is needed for substitution).

Reaction Equation (Structural Formula):

plaintext

```
      O2N                 O2N
       |                   |
H3C6H3-NO2 + Cl2 → H3C6H2(NO2)2-Cl
       |                   |
      NO2                 NO2
(1,3-dinitrobenzene)   (1-chloro-3,5-dinitrobenzene)
```

(Note: The product is 3,5-dinitrochlorobenzene, with Cl at position 5 relative to the two $-NO_2$ groups.)

三、Rationale for Purity & Regioselectivity

1. **Directing Effect Synergy**:

   In 1,3-dinitrobenzene, the two $-NO_2$ groups are meta to each other. Each $-NO_2$ directs electrophiles (Cl^+) to its meta position:

   - The $-NO_2$ at position 1 directs Cl^+ to positions 3 and 5.
   - The $-NO_2$ at position 3 directs Cl^+ to positions 1 and 5.

   The **only common meta position** is position 5, so Cl^+ exclusively attacks position 5. No ortho/para substitution occurs (since $-NO_2$ deactivates ortho/para positions).

2. **Minimal Byproducts**:

   Due to the strong deactivating effect of $-NO_2$, o[illegible]nochlorination occurs (no further chlorination of the benzene ring). Thus, the product is nearly pure and requires no complex separation.

ERNIE Bot:

To prepare pure 3,5-dinitrochlorobenzene starting from a disubstituted benzene, a strategic synthesis pathway needs to be employed, given that direct substitution at the specific 3 and 5 positions from an arbitrary disubstituted benzene may not be feasible. Here's a plausible synthetic route:

Synthesis Pathway

Selection of Starting Material:

Although not explicitly stated, a common precursor for synthesizing 3,5-dinitrochlorobenzene is 1,3-dichlorobenzene. This compound can serve as a practical starting point due to its availability and reactivity.

First Nitration Reaction:

Subject 1,3-dichlorobenzene to a nitration reaction to introduce the first nitro group (-NO_2). This typically involves using a mixture of concentrated nitric acid and sulfuric acid as the nitrating agent, under controlled temperature conditions. The reaction will yield a mixture of isomers, primarily 1,3-dichloro-5-nitrobenzene, along with minor amounts of other nitro isomers.

Isolation and Purification:

Employ suitable isolation techniques, such as distillation or crystallization, to separate 1,3-dichloro-5-nitrobenzene from the reaction mixture. This step is crucial to minimize the presence of

unwanted isomers.

Second Nitration Reaction:

Subject the isolated 1,3-dichloro-5-nitrobenzene to a second nitration reaction to introduce the second nitro group on the remaining chlorine atom. Precise control of reaction conditions is essential to minimize the formation of byproducts.

Further Isolation and Purification:

Utilize advanced separation techniques, such as column chromatography or recrystallization, to purify 3,5-dinitrochlorobenzene from the second nitration reaction mixture. These techniques are necessary to achieve the desired purity.

Considerations

Reaction Conditions: Nitration reactions are exothermic and can produce harmful byproducts. Therefore, reaction temperatures and concentrations must be carefully controlled.

Separation Techniques: Due to the similar physical properties of nitrobenzene isomers, isolation and purification can be challenging. Advanced separation methods may be required to achieve high purity.

Safety: The chemicals used, such as concentrated nitric acid and sulfuric acid, are corrosive, oxidizing, and/or flammable. Synthesis should be conducted in a properly ventilated hood and under the supervision of a professional.

Conclusion

While direct synthesis of 3,5-dinitrochlorobenzene from a specific disubstituted benzene may not be straightforward, a practical synthesis pathway involves using 1,3-dichlorobenzene as the starting material and proceeding through a series of controlled nitration reactions, followed by rigorous isolation and purification steps. This process requires precise control of reaction conditions, advanced separation techniques, and stringent safety measures.

2025.12： To prepare pure 3,5-dinitrochlorobenzene starting from a disubstituted benzene, follow these steps based on electrophilic aromatic substitution (EAS) principles:

Step 1: Synthesis of the Disubstituted Starting Material

Start with nitrobenzene (monosubstituted). Chlorinate nitrobenzene using $Cl_2/AlCl_3$ or $FeCl_3$. The nitro group ($-NO_2$) is a meta-director and deactivating group, so chlorination occurs at the meta position relative to the nitro group:

$$\text{Nitrobenzene} \xrightarrow{Cl_2/AlCl_3} \text{3-Chloronitrobenzene (1-chloro-3-nitrobenzene).}$$

This yields meta-nitrochlorobenzene, a disubstituted benzene with Cl and NO_2 at positions 1 and 3.

Step 2: Introduction of the Second Nitro Group

Nitrate 3-chloronitrobenzene using HNO_3/H_2SO_4. The existing nitro group ($-NO_2$) directs the incoming nitro group to the meta position relative to itself. Since the ring already has Cl at position 1 and NO_2 at position 3, the second nitro group enters position 5 (meta to the first nitro group, avoiding the occupied position 1):

$$\text{3-Chloronitrobenzene} \xrightarrow{HNO_3/H_2SO_4} \text{3,5-Dinitrochlorobenzene.}$$

Key Reaction Mechanisms & Directing Effects

Chlorination of Nitrobenzene:

The nitro group ($-NO_2$) is a strong electron-withdrawing, meta-directing group. Chlorination occurs at the meta position (position 3) to avoid steric/electronic repulsion with the nitro group.

Nitration of 3-Chloronitrobenzene:

The nitro group at position 3 directs the second nitro group to position 5 (meta to itself). The chlorine at position 1 (ortho /para-director) has minimal influence here due to the stronger deactivating /meta-directing effect of the nitro group.

Purification

The final product, 3,5-dinitrochlorobenzene, is purified via recrystallization from ethanol or acetone to remove unreacted starting material and byproducts (e.g., ortho- or para-isomers).

iFLYTEK Spark:

Step 1: Preparation of Starting Material

Ensure that you have a sufficient quantity of 1,3-dichlorobenzene, which is commercially available or can be synthesized by known methods if not readily accessible.

Step 2: Nitration Reaction

Setup: Place the 1,3-dichlorobenzene in a flask equipped with a stirrer and a dropping funnel.

Reagents: Slowly add a mixture of concentrated nitric acid and sulfuric acid (often in a ratio of 1:1) to the flask while maintaining a low temperature (usually around 0°C to 5°C) to control the exothermic reaction.

Reaction Time: Stir the mixture for several hours at this controlled temperature to ensure complete nitration.

Step 3: Isolation and Purification

Quench the Reaction: Carefully pour the reaction mixture into ice water to quench any remaining acid and precipitate the organic product.

Filtration: Filter the precipitate to collect the crude product.

Purification: Purify the crude product using recrystallization from an appropriate solvent (such as ethanol or hexane), or use column chromatography if necessary. Ensure that the final product is free of impurities by checking its melting point and purity through techniques like NMR or IR spectroscopy.

Step 4: Final Product

The purified 3,5-dinitro-1-chlorobenzene should be a yellow crystalline compound. Confirm its identity and purity through spectral analysis if required.

By following these steps, you can prepare pure 3,5-dinitrochlorobenzene starting from a disubstituted benzene.

2025.12 : To prepare pure 3,5-dinitrochlorobenzene (1-chloro-3,5-dinitrobenzene) starting from a disubstituted benzene, follow this synthetic route beginning with 1,3-dinitrobenzene (m-dinitrobenzene), which is a suitable disubstituted benzene precursor. The key is to leverage the meta-directing nature of the nitro group and selective transformations to achieve the desired substitution pattern.

Step-by-Step Synthesis:

1.Selective Reduction of One Nitro Group to Amino Group:

Treat 1,3-dinitrobenzene with sodium sulfide (Na_2S) or ammonium sulfide ($(NH_4)_2S$) in aqueous ethanol or water. This selectively reduces one nitro group to an amino group, yielding 3-nitroaniline (m-nitroaniline).

Reason: Sulfide reagents reduce one nitro group in meta-dinitrobenzenes due to the electron-withdrawing effect of the adjacent nitro group, which makes one nitro group more susceptible to reduction.

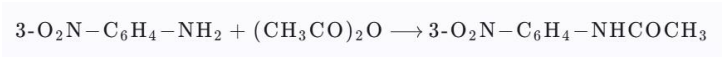
$$1,3\text{-}(O_2N)_2C_6H_4 + Na_2S \longrightarrow 3\text{-}O_2N-C_6H_4-NH_2$$

2.Protection of the Amino Group by Acetylation:

Acetylate 3-nitroaniline using acetic anhydride (Ac_2O) or glacial acetic acid to form 3-nitroacetanilide.

Reason: The amino group is a strong activator and ortho/para director, which would interfere with

subsequent nitration. Acetylation converts it to a moderately activating acetamido group (–$NHCOCH_3$), which is still ortho/para directing but less nucleophilic, allowing controlled nitration.



$$3\text{-}O_2N-C_6H_4-NH_2 + (CH_3CO)_2O \longrightarrow 3\text{-}O_2N-C_6H_4-NHCOCH_3$$

3.Nitration to Introduce the Second Nitro Group:

Nitrate 3-nitroacetanilide using a mixture of concentrated nitric acid (HNO_3) and sulfuric acid (H_2SO_4) at 0 – 10 ° C. This yields 3,5-dinitroacetanilide.

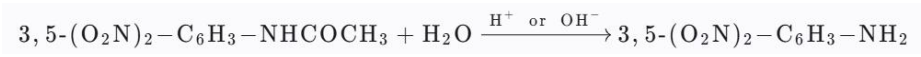
Reason: The nitro group at position 3 is meta-directing, while the acetamido group at position 1 is ortho/para directing. Position 5 (meta to the nitro group and meta to the acetamido group) is favored for electrophilic attack due to the strong meta-directing influence of the nitro group. Low temperature prevents over-oxidation or undesired byproducts.

$$3\text{-}O_2N-C_6H_4-NHCOCH_3 + HNO_3/H_2SO_4 \xrightarrow{0\text{-}10\ ^\circ C} 3,5\text{-}(O_2N)_2-C_6H_3-NHCOCH_3$$

4.Hydrolysis of the Acetamido Group:

Hydrolyze 3,5-dinitroacetanilide under acidic conditions (e.g., HCl, H_2O, reflux) or basic conditions (e.g., NaOH, H_2O, reflux) to remove the acetyl group, yielding 3,5-dinitroaniline.

Reason: The acetamide protecting group is cleaved to regenerate the free amino group for the next step.



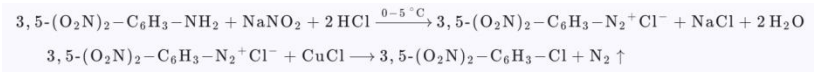
$$3,5\text{-}(O_2N)_2-C_6H_3-NHCOCH_3 + H_2O \xrightarrow{H^+ \text{ or } OH^-} 3,5\text{-}(O_2N)_2-C_6H_3-NH_2$$

5.Conversion of Amino Group to Chloro Group via Sandmeyer Reaction:

Diazotization: Treat 3,5-dinitroaniline with sodium nitrite ($NaNO_2$) in aqueous hydrochloric acid (HCl) at 0 – 5 ° C to form the diazonium salt.

Sandmeyer Reaction: Add copper(I) chloride (CuCl) to the diazonium salt solution, which replaces the diazonium group with chlorine, yielding 1-chloro-3,5-dinitrobenzene (3,5-dinitrochlorobenzene).

Reason: The strongly electron-withdrawing nitro groups stabilize the diazonium intermediate, making the Sandmeyer reaction feasible. Direct halogenation is not possible due to the deactivating nature of the nitro groups.



$$3,5\text{-}(O_2N)_2-C_6H_3-NH_2 + NaNO_2 + 2\,HCl \xrightarrow{0-5\ ^\circ C} 3,5\text{-}(O_2N)_2-C_6H_3-N_2^+Cl^- + NaCl + 2\,H_2O$$

$$3,5\text{-}(O_2N)_2-C_6H_3-N_2^+Cl^- + CuCl \longrightarrow 3,5\text{-}(O_2N)_2-C_6H_3-Cl + N_2\uparrow$$

Why This Route Ensures Purity:

Regioselectivity: The meta-directing nitro group in 1,3-dinitrobenzene ensures the second nitro group installs at position 5 (via the protected aniline intermediate), avoiding ortho/para mixtures.

No Isomeric Contamination: Starting from 1,3-dinitrobenzene (symmetrical meta-disubstituted) avoids regiochemical ambiguities. Subsequent steps are high-yielding and selective:

Selective reduction targets only one nitro group.

Acetylation controls nitration to position 5.

Sandmeyer reaction cleanly replaces – N_2^+ with – Cl without rearrangement.

Purification Points: Intermediates (3-nitroaniline, 3-nitroacetanilide, 3,5-dinitroacetanilide, 3,5-dinitroaniline) can be purified by recrystallization before the final step, ensuring the product is pure.

Student's Judgement:

ChatGPT: × × (2025.12)
Kimi Assistant: × × (2025.12)
Doubao: × √ (2025.12)
ERNIE Bot: × × (2025.12)
iFLYTEK Spark: × × (2025.12)

12. Write an equation for each of the following reactions:

A. 2-methyl-2-butanol + HCl

B. cyclohexanol + PBr_3

ChatGPT:
$CH_3CH_2C(OH)(CH_3)+HCl \rightarrow CH_3CH_2C(Cl)(CH_3)+H_2O$
$C_6H_{11}OH+PBr_3 \rightarrow C_6H_{11}Br+HPO_3$
2025.12：$(CH_3)_2C(OH)C_2H_5 + HCl \rightarrow (CH_3)_2C(Cl)C_2H_5 + H_2O$
$3\ C_6H_{11}OH + PBr_3 \rightarrow 3\ C_6H_{11}Br + H_3PO_3 + 3\ HBr$
Kimi Assistant:
(CH3)3C-CH(OH)-CH3+HCl→(CH3)3C-CH=CH-CH3+H2O (△)
C6H11OH+PBr3→C6H11Br+H2O+P(OH)Br2
2025.12：A.$(CH_3)_2C(OH)C_2H_5 + HCl \rightarrow (CH_3)_2CClCH_2CH_3 + H_2O$
B. cyclohexanol + PBr_3 → bromocyclohexane + H_3PO_3
Doubao:
$CH_3CH_2C(OH)(CH_3)_2+HCl \rightarrow CH_3CH_2C(Cl)(CH_3)_2+H_2O$
$C_6H_{11}OH+PBr_3 \rightarrow C_6H_{11}Br+H_3PO_3$
ERNIE Bot:
2-methyl-2-butanol + HCl → 2-methyl-2-butene + H_2O (Note: This is a simplified representation; HCl does not directly catalyze this reaction.)
cyclohexanol + PBr_3 → cyclohexyl bromide + $POBr_3$
2025.12：A. 2-methyl-2-butanol + HCl
Tertiary alcohols undergo acid-catalyzed dehydration or substitution. Here, 2-methyl-2-butanol ($(CH_3)_2C(OH)C_2H_5$) reacts with HCl via an SN1 mechanism:
$(CH_3)_2C(OH)CH_2CH_3 + HCl \rightarrow (CH_3)_2CClCH_2CH_3 + H_2O$
The OH group is protonated, forms a stable tertiary carbocation ($(CH_3)_2C^+CH_2CH_3$), and chloride attacks to yield 2-chloro-2-methylbutane.
B. Cyclohexanol + PBr_3
PBr_3 converts alcohols to alkyl bromides via an SN2 mechanism (for secondary alcohols). Cyclohexanol ($C_6H_{11}OH$) reacts as:
$C_6H_{11}OH + PBr_3 \rightarrow C_6H_{11}Br + HOPBr_2$
The OH group attacks PBr_3, displacing Br^-, which then attacks the carbon, forming bromocyclohexane and pyridinium bromide (byproduct).
Both equations follow standard organic reaction pathways for alcohol conversions.
iFLYTEK Spark:
(CH3)2C−CH2−OH+HCl→(CH3)2C−CH2−Cl+H2O

$C_6H_{11}OH+PBr3 \rightarrow C6H10+P(O)Br_3+HBr$

2025.12：

$$(CH_3)_2C(OH)CH_2CH_3 + HCl \longrightarrow (CH_3)_2C(Cl)CH_2CH_3 + H_2O$$

$$3\,C_6H_{11}OH + PBr_3 \longrightarrow 3\,C_6H_{11}Br + H_3PO_3$$

Student's Judgement:

ChatGPT: × √ (2025.12)

Kimi Assistant: × √ (2025.12)

Doubao: √

ERNIE Bot: × × (2025.12)

iFLYTEK Spark: × √ (2025.12)

13. Propose an equation for the synthesis of hexanal from an alcohol. (within 150 words)

ChatGPT:

To synthesize hexanal (an aldehyde) from an alcohol, the most straightforward approach is the oxidation of 1-hexanol (a primary alcohol) using an oxidizing agent. Here's the equation for this process:

Oxidation of 1-hexanol to hexanal:

$CH_3(CH_2)_4CH_2OH \rightarrow CH_3(CH_2)_4CHO+H_2O$ (by oxidizing Agent)

Explanation:

1. 1-hexanol ($C_6H_{14}O$) is a primary alcohol. Upon oxidation, the hydroxyl group (-OH) is converted into an aldehyde group (-CHO).

2. A suitable oxidizing agent, such as PCC (Pyridinium chlorochromate), DMP (Dess-Martin periodinane), or NaOCl (sodium hypochlorite), will selectively oxidize the primary alcohol to the corresponding hexanal ($C_6H_{12}O$).

3. The reaction produces hexanal and water as the byproduct.

This is a typical oxidation reaction where the primary alcohol is transformed into an aldehyde by the loss of two hydrogen atoms.

Kimi Assistant:

The synthesis of hexanal from an alcohol, such as 1-hexanol, typically involves an oxidation reaction. Here's a brief description of the process:

1. Oxidation of the Alcohol: 1-Hexanol is first oxidized to form an aldehyde. This can be achieved using a strong oxidizing agent like potassium dichromate (K2Cr2O7) in the presence of sulfuric acid (H2SO4) or a more selective reagent like pyridinium chlorochromate (PCC) or Swern's reagent.

2. Formation of Hexanal: The aldehyde group is formed at the end of the hexyl chain, resulting in hexanal.

The chemical equation for the oxidation using PCC as an example is:

$CH_3(CH_2)_4CH_2OH+PCC \rightarrow CH_3(CH_2)_4CHO+H_2O$

In this reaction, the alcohol group (-OH) is converted to an aldehyde group (-CHO), and water (H2O) is produced as a byproduct. The PCC is a reagent that facilitates the oxidation without further oxidizing the aldehyde to a carboxylic acid, which can be a side reaction with less selective oxidizing agents.

Doubao:

1. Starting material:

The alcohol used to synthesize hexanal is 1 - hexanol.

2. Oxidation reaction:

1 - hexanol (C6H13OH) can be oxidized to hexanal (C6H12O). The common oxidizing agent used is pyridinium chlorochromate (PCC).

The reaction equation is: C6H13OH+PCC→ C6H12O + PCC - reduced products

PCC oxidizes the primary alcohol (1 - hexanol) to an aldehyde (hexanal) without further oxidizing it to a carboxylic acid.

ERNIE Bot:

To write an equation for the synthesis of hexanal from an alcohol, we need to consider the type of alcohol involved and the reaction conditions that lead to the formation of hexanal ($C_6H_{12}O$). Hexanal can be synthesized by the oxidation of the corresponding primary alcohol, which in this case is 1-hexanol ($C_6H_{13}OH$).

The oxidation of 1-hexanol to hexanal typically involves the use of a dehydrogenating agent or an oxidizing agent. A common method is the use of a dehydrogenation catalyst, such as copper chromite, under heated conditions. The dehydrogenation process removes two hydrogen atoms from the alcohol molecule, converting it to the aldehyde.

The chemical equation for this reaction can be written as:

$C_6H_{13}OH \rightarrow C_6H_{12}O + H_2$ (Dehydrogenation,Catalyst)

Here, 1-hexanol ($C_6H_{13}OH$) is converted to hexanal ($C_6H_{12}O$) with the release of hydrogen gas (H_2). This equation represents the synthesis of hexanal from 1-hexanol through dehydrogenation.

2025.12：The synthesis of hexanal ($C_6H_{12}O$) from an alcohol involves oxidizing a primary alcohol, such as 1-hexanol ($C_6H_{13}OH$). The balanced equation is:

$(C_6H_{13}OH + [O] \rightarrow C_6H_{12}O + H_2O$

Here, [O] represents an oxidizing agent (e.g., PCC, CrO_3/H_2SO_4 under controlled conditions). Primary alcohols like 1-hexanol ($CH_3(CH_2)_4CH_2OH$) lose two hydrogen atoms during oxidation. Mild oxidizing agents (e.g., PCC in CH_2Cl_2) stop the reaction at the aldehyde stage, preventing further oxidation to hexanoic acid. For example:

$3\ CH_3(CH_2)_4CH_2OH + 2\ CrO_3 + 3\ H_2SO_4 \rightarrow 3\ CH_3(CH_2)_4CHO + Cr_2(SO_4)_3 + 3\ H_2O$

This reaction highlights the role of acidified dichromate in oxidizing 1-hexanol to hexanal. The key is controlling conditions to avoid over-oxidation. The general principle applies to converting any primary alcohol to its corresponding aldehyde using appropriate oxidants.

iFLYTEK Spark:

To synthesize hexanal from an alcohol, you typically use an oxidation reaction. One of the most common methods involves using a reagent like pyridinium dichromate (PDC) or potassium permanganate (KMnO4). Here's how you can write the equation for this synthesis:

If we start with hexan-1-ol, which is the primary alcohol form of hexanol, the reaction can be represented as follows:

$CH_3(CH_2)_4CH_2OH + CrO_3(pyridine)_2 \rightarrow CH_3(CH_2)_4CHO + CrO_3(pyridine) + H_2O$

In this equation:

$CH_3(CH_2)_4CH_2OH$ represents hexan-1-ol.

$CrO3(pyridine)_2$ represents pyridinium dichromate, which acts as the oxidizing agent.

$CH_3(CH_2)_4CHO$ is hexanal, the product formed by oxidation.

CrO3(pyridine) is the reduced form of the oxidizing agent.

H_2O is water, a byproduct of this reaction.

This equation shows the conversion of hexan-1-ol to hexanal through oxidation, highlighting the functional group transformation from an alcohol (-OH) to an aldehyde (-CHO).

Student's Judgement:

ChatGPT: √

Kimi Assistant: √

Doubao: √

ERNIE Bot: × 在实际的实验室或工业合成中，通常采用铜铬催化剂脱氢法进行气相反应，条件比较苛刻，更常用的实验室合成方法是采用温和氧化试剂进行氧化。 √（2025.12）

iFLYTEK Spark: √

14. Explain why the enol form of phenol is more stable than the keto form of phenol.(within 50 words)

ChatGPT:

The enol form of phenol is more stable than the keto form due to resonance stabilization. In the enol form, the lone pair on the oxygen of the hydroxyl group can delocalize into the aromatic ring, creating additional resonance structures that stabilize the molecule. In contrast, the keto form lacks this stabilization.

Kimi Assistant:

The enol form of phenol is more stable than the keto form due to the resonance stabilization of the phenoxide anion. The negative charge is delocalized over the benzene ring, lowering the energy of the enol form. Additionally, the enol form does not have the carbonyl group's electron-withdrawing inductive effect, which would destabilize the keto form.

2025.12：The enol form is aromatic; the keto form loses aromaticity.

Doubao:

The enol form of phenol is more stable due to resonance stabilization of the benzene ring and the hydroxyl group. The keto form lacks this.

ERNIE Bot:

The enol form of phenol is more stable due to intramolecular hydrogen bonding between the hydroxyl group and the oxygen of the enolic double bond. This hydrogen bonding stabilizes the enol form energetically, making it more favorable than the keto form, which lacks such an intramolecular interaction.

2025.12：The enol form of phenol is more stable due to aromatic resonance stabilization. The hydroxyl group's oxygen donates electron density into the ring via resonance, maintaining aromaticity. A keto form would disrupt conjugation, requiring loss of aromatic stabilization, which is energetically unfavorable. Thus, phenol exists predominantly in its enol form.

iFLYTEK Spark:

The enol form of phenol is more stable than the keto form due to resonance stabilization. In the enol form, the negative charge can be delocalized across the aromatic ring, making it more stable compared to the keto form where such resonance is not possible.

2025.12： The enol form of phenol retains aromaticity, providing exceptional stability from delocalized electrons in the benzene ring. Its keto form (a non-aromatic 2,4-cyclohexadienone) loses this aromatic stabilization energy (~150 kJ/mol), making it significantly higher in energy. Resonance in the enol form further enhances stability through oxygen's lone pair delocalization.

Student's Judgement:

ChatGPT: √

Kimi Assistant: × 苯酚的烯醇（正常苯酚的结构），而不是酚氧阴离子。 √（2025.12）

Doubao: √

ERNIE Bot: × 没有提到苯环上存在一个大的π键共轭体系。 √（2025.12）

iFLYTEK Spark: × 烯醇型苯酚（即正常的酚类结构）不带负电荷。 ×（2025.12）酮式名称错误

15. Complete the equation for $CH_3(CH_2)_6CO_2H + SOCl_2 \rightarrow$

ChatGPT: $CH_3(CH_2)_6CO_2H+SOCl_2 \rightarrow CH_3(CH_2)_6COCl+SO_2+HCl$

Kimi Assistant: CH3(CH2)6CO2H+SOCl2→CH3(CH2)6COCl+HCl

2025.12：$CH_3(CH_2)_6CO_2H + SOCl_2 \rightarrow CH_3(CH_2)_6COCl + SO_2 + HCl$

Doubao: CH3(CH2)6CO2H+SOCl2→CH3(CH2)6COCl+HCl+SO2

ERNIE Bot: CH3(CH2)6CO2H+SOCl2→CH3(CH2)6COCl+HCl+SO2

iFLYTEK Spark: CH3(CH2)6CO2H+SOCl2→CH3(CH2)6COCl+HCl+SO2

Student's Judgement:

ChatGPT: √

Kimi Assistant: × 缺乏 SO2 √（2025.12）

Doubao: √

ERNIE Bot: √

iFLYTEK Spark: √

16. Tell me which base is stronger, aniline or p-Cyanoaniline? Why? (within 50 words)

ChatGPT:

Aniline is a stronger base than p-cyanoaniline. The cyano group (-CN) in p-cyanoaniline is electron-withdrawing through both inductive and resonance effects, which decreases the electron density on the nitrogen, making it less available for protonation. In contrast, aniline has no such electron-withdrawing group, enhancing its basicity.

Kimi Assistant:

p-Cyanoaniline is a stronger base than aniline due to the electron-withdrawing effect of the cyano group, which increases the availability of the nitrogen's lone pair for protonation, enhancing its basicity.

2025.12：Aniline is stronger. The p-cyano group withdraws electron density via resonance and induction, destabilizing the conjugate acid of p-cyanoaniline and lowering its basicity.

Doubao:

Aniline is a stronger base. The cyano group in p - cyanoaniline is electron - withdrawing, decreasing the electron density on the amino group.

ERNIE Bot:

p-Cyanoaniline (4-Aminobenzonitrile) is the stronger base compared to aniline. The nitrogen in the amino group of p-cyanoaniline is more difficult to protonate due to the electron-withdrawing cyano group, making it less acidic and thus a stronger base.

2025.12： Aniline is stronger than p-Cyanoaniline because the cyano group in p-Cyanoaniline is electron-withdrawing, reducing electron density on the nitrogen and weakening its basicity.

iFLYTEK Spark:

Aniline (C6H5NH2) is a stronger base than p-cyanoaniline (C6H4N(CN)H2). This is because the cyano group (-CN) in p-cyanoaniline is electron-withdrawing by resonance, which destabilizes the lone pair on the nitrogen atom and reduces its ability to donate an electron pair. Aniline, lacking this electron-withdrawing group, has a less destabilized lone pair, making it a stronger base.

Student's Judgement:

ChatGPT: √

Kimi Assistant: × √ （2025.12）

Doubao: √

ERNIE Bot: × √ （2025.12）

iFLYTEK Spark: √

17. When boiled with concentrated aqueous alkali, fats and oils dissolve, but waxes do not. Explain the difference.(within 50 words)

ChatGPT:

Fats and oils are triglycerides (esters of fatty acids and glycerol) that undergo saponification with alkali, producing glycerol and soap. Waxes are esters of fatty acids and long-chain alcohols, which are more resistant to alkali hydrolysis, preventing them from dissolving or reacting under the same conditions.

Kimi Assistant:

Fats and oils are triglycerides with glycerol and unsaturated fatty acids, which can react with alkali to form soap and glycerol, thus dissolving. Waxes, composed of long-chain fatty acids and alcohols, are esters that do not react with alkali and remain insoluble.

Doubao:

Fats and oils are esters of glycerol and fatty acids which can be hydrolyzed by alkali. Waxes have different structures and are less reactive.

ERNIE Bot:

Fats and oils dissolve in concentrated aqueous alkali due to saponification, forming soluble soaps. Waxes do not undergo this reaction and remain insoluble, as they consist mainly of esters of long-chain fatty acids and higher alcohols.

iFLYTEK Spark:

When boiled with concentrated aqueous alkali, fats and oils dissolve because their glycerol backbone undergoes hydrolysis to form glycerol and soap. Waxes do not dissolve as they lack the glycerol backbone; instead, they have long-chain alcohols that do not react similarly under these conditions.

Student's Judgement:

ChatGPT: √
Kimi Assistant: √
Doubao: √
ERNIE Bot: √
iFLYTEK Spark: √

18. Explain why sucrose is a nonreducing sugar but maltose is a reducing sugar. (within 50 words)

ChatGPT:

Sucrose is a nonreducing sugar because both its glucose and fructose units are linked via their anomeric carbons, preventing any free aldehyde or ketone groups. In contrast, maltose has a free anomeric carbon on one glucose unit, allowing it to open and form an aldehyde group, making it a reducing sugar.

Kimi Assistant:

Sucrose is a nonreducing sugar because its glycosidic bond joins glucose's aldehyde group to fructose's carbon, hiding the aldehyde. Maltose is a reducing sugar as it contains a free aldehyde group on one glucose unit, available for redox reactions.

Doubao:

Sucrose has both anomeric carbons involved in glycosidic bond, no free anomeric carbon. Maltose has a free anomeric carbon, making it reducing.

ERNIE Bot:

Sucrose is a nonreducing sugar because its anomeric carbons are involved in glycosidic bonds, lacking free aldehyde/ketone groups. Maltose is reducing due to its free anomeric carbon with an aldehyde group, capable of undergoing reduction reactions.

iFLYTEK Spark:

Sucrose is a nonreducing sugar because its glucose and fructose units are joined by an α,β-1,2-glycosidic bond, eliminating free aldehyde or ketone groups. Maltose is a reducing sugar as it has a free aldehyde group on one of its glucose units due to an α,1→4-glycosidic bond.

Student's Judgement:

ChatGPT: √
Kimi Assistant: √
Doubao: √
ERNIE Bot: √
iFLYTEK Spark: √

19. Find literature related to glycerol as a food additive.

ChatGPT:

To find literature related to glycerol (glycerin) as a food additive, we can refer to scientific journals, databases, and authoritative sources that discuss its uses, safety, and regulations in food applications. Below are some key areas to explore and sources where you can find relevant literature:

Key Areas to Explore:

1. Glycerol as a Humectant: Glycerol is commonly used in food products as a humectant, which helps retain moisture and maintain the texture of the product. It is used in products like baked goods, candies, and ice cream.
2. Glycerol as a Sweetener: Glycerol is sometimes used as a low-calorie sweetener in food and beverages. It is less sweet than sugar but provides a sweet taste with fewer calories.
3. Glycerol in Pharmaceutical and Food Grade Quality: Literature discussing the safety, purity, and production processes of glycerol for food and pharmaceutical use is important for understanding regulatory standards.
4. Glycerol's Role in Food Preservation: Glycerol can be used to preserve the quality of food by preventing spoilage, as it has antimicrobial properties when used in appropriate concentrations.
5. Regulations and Safety: Literature discussing the acceptable daily intake (ADI) and safety regulations for glycerol as a food additive is essential for understanding how it is used in the food industry.

Key Databases and Journals to Explore:

1. PubMed (NCBI)

PubMed is a reliable database for peer-reviewed scientific articles. Search for terms like "glycerol food additive," "glycerin in food," or "glycerol as humectant" to find studies on its application, safety, and usage.

[PubMed](https://pubmed.ncbi.nlm.nih.gov/)

2. Google Scholar

Google Scholar provides access to a wide range of scholarly articles, theses, and books. It’s an excellent resource for finding research papers, reviews, and citations on glycerol in food.

[Google Scholar](https://scholar.google.com/)

3. ScienceDirect

ScienceDirect hosts peer-reviewed journal articles and books in a wide array of scientific fields, including food science. You can find articles specifically related to glycerol as a food additive.

[ScienceDirect](https://www.sciencedirect.com/)

4. Food and Chemical Toxicology Journal

This journal often publishes articles on food safety and additives. You can find studies discussing the safety and toxicity of glycerol as a food additive.

[Food and Chemical Toxicology Journal](https://www.journals.elsevier.com/food-and-chemical-toxicology)

5. Journal of Food Science

This journal covers a wide range of food science topics, including food additives. You can find articles that discuss glycerol’s role in food processing, preservation, and formulation.

[Journal of Food Science](https://onlinelibrary.wiley.com/journal/20421332)

6. Regulatory Agencies

Websites of organizations like the FDA (U.S. Food and Drug Administration) and EFSA (European Food Safety Authority) provide valuable information on food additives, including glycerol.

[FDA GRAS Substances (Glycerol)](https://www.fda.gov/food/food-additives-petitions)

[EFSA on Food Additives](https://www.efsa.europa.eu/en/topics/topic/food-additives)
Sample Search Terms for Literature:
"Glycerol as a food additive"
"Glycerol humectant in food"
"Safety of glycerol as food ingredient"
"Glycerol use in beverages and confectionery"
"Glycerol in food preservation"
"Glycerol sweetener in low-calorie foods"
Example Studies or Articles:
1. Glycerol as a food ingredient: Physicochemical properties and technological applications
This review article may cover the diverse applications of glycerol, including its role as a humectant and sweetener in various food products.
2. Evaluation of glycerol as a sweetener and its effects on human health
This article could focus on the use of glycerol as a low-calorie sweetener and its impact on health, metabolism, and its regulatory status.
3. Glycerol in food processing: Its functions and safety considerations
This type of article might examine the functional properties of glycerol in food manufacturing, as well as its safety, including recommended concentrations and regulatory limits.
Conclusion:
Glycerol is widely used as a food additive, primarily as a humectant, sweetener, and preservative. By exploring the sources above and searching for the relevant terms in these databases, you should be able to find a comprehensive range of literature regarding its uses, safety, and regulatory status.
Kimi Assistant:
Here are some academic papers and articles related to glycerol as a food additive:
1. "Re‐evaluation of glycerol (E 422) as a food additive" published in the EFSA Journal. This paper discusses the re-evaluation of glycerol as a food additive, providing insights into its safety and regulatory status.
2. "Re‐evaluation of glycerol esters of wood rosin (E 445) as a food additive" available on PMC. This article focuses on the re-evaluation of glycerol esters of wood rosin as a food additive, which is related to the use of glycerol in food products.
3. "Re‐evaluation of mono‐ and di‐glycerides of fatty acids (E 471) as food additives" on PMC. Although this paper specifically discusses mono- and diglycerides, it is relevant to the broader context of glycerol's role in food additives.
These resources can provide a comprehensive understanding of glycerol's application, safety, and regulatory status as a food additive.
Doubao:
To find literature related to glycerol as a food additive, you can follow these steps:
1. Scientific Databases
PubMed:
This is a widely - used database for biomedical literature. You can search for terms like "glycerol as a food additive" or "glycerol food applications".
Many of the articles are peer - reviewed, providing reliable scientific information on the safety, usage, and properties of glycerol in food.
Web of Science:

It indexes a wide range of scientific journals across different fields. A search using relevant keywords can yield research articles, reviews, and case studies related to glycerol in food.

ScienceDirect:

This database contains a large number of scientific and technical research papers. You can access full - text articles on food chemistry, food technology, and related areas that mention glycerol as a food additive.

2. Regulatory Agencies

FDA (Food and Drug Administration):

The FDA website has documents regarding food additives. You can search for glycerol in their food additive database or relevant regulations.

They provide information on the approved uses, maximum allowable levels, and safety evaluations of glycerol as a food additive.

EFSA (European Food Safety Authority):

EFSA conducts risk assessments for food additives in the European Union. Their reports and scientific opinions on glycerol are available on their website.

These documents provide insights into the safety of glycerol for consumers and any restrictions on its use in food products.

3. Industry Publications

Food Technology Magazines and Journals:

Publications like "Food Technology" by the Institute of Food Technologists often have articles on food ingredients, including glycerol.

These articles may discuss new applications, manufacturing processes, and consumer - facing aspects of using glycerol in food.

Food Industry Reports:

Market research firms produce reports on food ingredients. These reports can provide information on the market trends of glycerol usage in the food industry, consumer preferences, and emerging applications.

4. University Theses and Dissertations

ProQuest Dissertations & Theses Global:

This database contains graduate - level research from universities around the world. You may find theses or dissertations related to the use of glycerol in food, such as studies on its impact on food texture, shelf - life, or nutritional aspects.

By using these resources, you can gather a comprehensive collection of literature related to glycerol as a food additive, ranging from its scientific properties to its regulatory status and industrial applications.

ERNIE Bot:

Literature related to glycerol as a food additive includes various studies and reviews that examine its use, safety, and effects in food products. Here are some key references:

Safety Evaluation:

A comprehensive review titled "Re-evaluation of glycerol (E422) as a food additive" discusses the safety of glycerol as a food additive. This evaluation includes information on its toxicity, genotoxicity, and carcinogenicity studies, as well as its use in various food products.

Use in Food Products:

Glycerol is commonly used as a food additive for its humectant and emulsifying properties. It can be found in a wide range of food products, including egg yolk sauce and salad dressing.

Specific Applications:

Studies have explored the use of glycerol monolaurate (GML), a derivative of glycerol, in specific food applications. For example, one study investigated the effects of dietary glycerol monolaurate on the growth, activity of digestive enzymes, and gut microbiota in zebrafish. Another study focused on the use of GML as a feed additive in poultry and its impact on production performance and flesh quality.

Safety and Health Benefits:

Glycerol and its derivatives have been evaluated for their safety in human consumption. Studies have shown that glycerol and certain derivatives, such as diacylglycerol, are safe for human consumption and may even have health benefits, such as promoting weight loss and reducing body fat.

In summary, the literature on glycerol as a food additive includes studies on its safety, use in various food products, specific applications, and potential health benefits. These studies provide valuable insights into the role of glycerol in the food industry and its impact on human health.

iFLYTEK Spark:

Glycerol, also known as glycerin or glycerine, is a versatile compound used in various industries, including food and beverage. When used as a food additive, it serves multiple purposes such as a sweetener, humectant, and texturizer. Here are some key aspects and references related to glycerol as a food additive:

Key Uses of Glycerol in Food Industry:

1. Humectant: Glycerol helps retain moisture in food products, preventing them from becoming dry and hard. This is particularly useful in baked goods, candies, and chewing gum.
2. Sweetener: While not as sweet as sugar, glycerol provides a mild sweetness and can be used in combination with other sweeteners to reduce overall sugar content.
3. Texture Improver: It can improve the texture of foods, making them softer and more pliable.
4. Solvent: Glycerol can dissolve other substances, which can be useful in creating emulsions and blending flavors.
5. Carrier: Often used as a carrier for flavors and colors in processed foods.

Regulatory Status:

In many countries, glycerol is generally recognized as safe (GRAS) by regulatory agencies such as the U.S. Food and Drug Administration (FDA).

The Codex Alimentarius Commission has established standards for glycerol used in food.

Literature and References:

1. Books:

"Food Additives Handbook" by Phillip A. Schweitzer and John W. Murray provides comprehensive information about various food additives, including glycerol.

"Handbook of Enzymes: Science, Technology, and Applications" by R.L. Madroneo might include sections on enzymes that can interact with glycerol in food processing.

2. Scientific Articles:

"Glycerol as a Humectant in Food Products" by M.A. Khan et al., published in Journal of Food Science, discusses the role of glycerol in maintaining moisture in different types of food products.

"Application of Glycerol in Baked Goods" by J. Smith et al., published in Cereal Chemistry, explores how glycerol affects the texture and shelf life of baked goods.

3. Regulatory Guidelines:

The FDA's website offers detailed information on the regulatory status and guidelines for using glycerol in food.

Codex Alimentarius Standards provide international regulations regarding the use of glycerol in food

products.
4. Industry Reports:
Market research reports from firms like Grand View Research or MarketsandMarkets often contain sections on trends and usage of glycerol in the food industry.
Reports from trade organizations such as the Food and Agriculture Organization (FAO) may also cover the topic.
5. Online Databases:
PubMed and Google Scholar are valuable resources for finding scientific articles on glycerol's applications and safety in food.
The National Institutes of Health (NIH) database provides access to studies and reviews on the health effects and uses of glycerol.
By exploring these sources, you can gather detailed information on the uses, benefits, and regulatory aspects of glycerol as a food additive.

Student's Judgement:

ChatGPT: √ 无法打开某些链接。
Kimi Assistant: √
Doubao: √
ERNIE Bot: √
iFLYTEK Spark: √
本文开展的文献检索只能提供较为宽泛的概要信息。这类信息仅涵盖文献的基本要素，例如标题、作者、期刊名称等。若将其应用于严谨的学术研究，其信息的完整性和深度都远远不够。学术研究需要对文献进行综合分析。仅依赖此类概要信息，难以全面把握研究全貌，可能导致关键内容的遗漏，从而影响研究的准确性和深度。

20. Explain the definition of osmosis.

ChatGPT:
Osmosis is the process by which water molecules move across a semipermeable membrane from an area of lower solute concentration to an area of higher solute concentration. This movement continues until equilibrium is reached, meaning the concentrations of solute on both sides of the membrane become equal.
Kimi Assistant:
Osmosis is a biological and physical process that involves the movement of solvent molecules (usually water) across a selectively permeable membrane from an area of lower solute concentration to an area of higher solute concentration. This movement continues until the concentration of solute is equal on both sides of the membrane, a state known as equilibrium.
Doubao:
Osmosis is the spontaneous net movement of solvent molecules through a semi - permeable membrane from a region of lower solute concentration to a region of higher solute concentration. The solvent is usually water in biological systems.
ERNIE Bot:
In a physical or chemical context, osmosis refers to the process by which a liquid passes through a semi-permeable membrane (or a thin piece of solid substance) from a region of higher concentration (or

higher water potential) to a region of lower concentration (or lower water potential), until an equilibrium in concentration (or water potential) is established on both sides of the membrane.

iFLYTEK Spark:

Osmosis is a fundamental biological and physical process that describes the movement of water molecules from an area of lower solute concentration to an area of higher solute concentration, through a semipermeable membrane. This movement occurs until equilibrium is reached, meaning the concentrations of solutes on either side of the membrane become equalized.

Student's Judgement:

ChatGPT: √

Kimi Assistant: √

Doubao: √

ERNIE Bot: √

iFLYTEK Spark: √

21. We want to prepare a buffer solution of pH 5.10, calculate the volume of 0.1 mol/L NaOH we should add to the solution of 100 mL 0.1 mol/L HAc. (Concise text output)

ChatGPT:

To prepare a buffer solution with pH 5.10 using acetic acid (HAc) and sodium hydroxide (NaOH), we can use the Henderson-Hasselbalch equation:

pH = pKa + log([A-]/[HA])

For acetic acid, the pKa is approximately 4.76.

Step 1: Set up the equation

5.10 = 4.76 + log([A-]/[HA])

log([A-]/[HA]) = 5.10 - 4.76 = 0.34

[A-]/[HA] = 10^{0.34}≈2.19

Step 2: Determine the moles of A- (acetate) needed

Let's assume the initial moles of HAc are:

moles of HAc=0.1mol/L×0.1L= 0.01mol

Let x be the moles of NaOH added. When NaOH is added, it converts HAc to acetate (A-) according to the reaction:

HAc +OH- →A- + H_2O

The moles of acetate will be x, and the remaining moles of HAc will be 0.01 - x. The ratio of acetate to acetic acid is:

X/(0.01 - x) = 2.19

Step 3: Solve for x

x = 2.19 × (0.01 - x)

x = 0.0219 - 2.19x

3.19x = 0.0219

x ≈ 0.00687 mol

Step 4: Calculate the volume of NaOH required

The concentration of NaOH is 0.1 mol/L, so the volume needed is:

Volume of NaOH = 0.00687 mol÷0.1mol/L = 0.0687L= 68.7mL

Final Answer:

To prepare the buffer solution of pH 5.10, 68.7 mL of 0.1 mol/L NaOH should be added to 100 mL of 0.1 mol/L HAc.

Kimi Assistant:

To prepare a buffer solution of pH 5.10 using 100 mL of 0.1 mol/L acetic acid (HAc) and 0.1 mol/L NaOH, we need to calculate the volume of NaOH to add. The Henderson-Hasselbalch equation is used:

pH= pKa + log{[A-]/[HA]}

For acetic acid, pKa = 4.74. We want the pH to be 5.10, so:

5.10 = 4.74 + log{[A-]/[HA]}

Solving for the ratio [A-]/[HA]:

log{[A-]/[HA]} = 5.10 - 4.74 = 0.36

[A-]/[HA] = 10^{0.36}≈2.26

This means we need slightly more acetate ion than acetic acid. Let V be the volume of NaOH in liters. The moles of NaOH added will be 0.1V , and the moles of HAc initially present are 0.1 × 0.1 = 0.01 moles. The moles of A- will also be 0.1V . Setting up the equation:

0.1V/(0.01 - 0.1V) = 2.26

Solving for V:

0.1V = 2.26(0.01 - 0.1V)

0.1V = 0.00226 - 0.226V

0.326V = 0.00226

V = 0.00226/0.326≈0.0069L

Converting to milliliters:

V = 0.0069×1000 = 6.9mL

The Final Answer is: 6.9mL

2025.12： Use the Henderson–Hasselbalch equation:

$pH = pK_a + \log([Ac^-]/[HAc])$

$5.10 = 4.76 + \log([Ac^-]/[HAc])$

$\Rightarrow [Ac^-]/[HAc] = 2.19$

Let V (mL) be the volume of 0.10 M NaOH added; it converts V mmol HAc $\rightarrow Ac^-$.

Remaining HAc = (10 – V) mmol.

2.19 = V / (10 – V) ⇒ V = 6.9 mL.

Add 6.9 mL of 0.1 M NaOH.

Doubao:

First, we know that for a buffer solution of acetic acid (HAc) and its conjugate base acetate (Ac-), the Henderson - Hasselbalch equation is:

pH = pKa+log{[Ac-]/[HAc]}

The pKa of acetic acid is 4.74. Given pH = 5.10.

So, 5.10 = 4.74+log{[Ac-]/[HAc]}

log{[Ac-]/[HAc]}=5.10 - 4.74 = 0.36

[Ac-]/[HAc] = 10^0.36≈2.29

Let V be the volume of NaOH added.

The initial amount of HAc is nHAc=0.1×0.1=0.01 mol.

After adding NaOH, the amount of HAc is nHAc=0.01 - 0.1V

The amount of Ac- formed is nAc-= 0.1V.

Since[Ac-]/[HAc]=nAc-/nHAc=0.1/(0.01 - 0.1V}=2.29.

0.1V = 2.29×(0.01 - 0.1V).

0.1V = 0.0229 - 0.229V.

0.1V+0.229V = 0.0229.

0.329V = 0.0229.

V=0.0229/0.329≈70mL.

ERNIE Bot:

To prepare a buffer solution of pH 5.10 using 100 mL of 0.1 mol/L HAc, we need to calculate the volume of 0.1 mol/L NaOH to add.

Using the Henderson-Hasselbalch equation:

$pH=pKa+\log_{10}([A^-]/[HA])$

Given:

pH=5.10

pKa(HAc)=4.76

[HA]=0.1 mol/L (initial concentration of HAc)

We solve for [A−] (acetate ion concentration):

$5.10=4.76+\log_{10}([A^-]/0.1)$

Rearranging and solving for [A−]:

$\log_{10}([A^-]/0.1)=0.34$

$[A^-]/0.1=10^{0.34}$

$[A^-]=0.1\times10^{0.34}\approx0.22$ mol/L

Assuming the total volume of the solution remains approximately constant (100 mL + V mL of NaOH), we can calculate the volume of NaOH (V) needed to achieve this acetate ion concentration:

$M_{total}\times V_{total}=[A^-]\times V_{total}l+[HA]\times V_{HA}$

0.22 mol/L×(100 mL+V mL)=0.1 mol/L×100 mL+0.1 mol/L×V mL (since NaOH adds OH- which reacts with HAc to form acetate)

Solving for V:

0.22(100+V)=10+0.1V

22+0.22V=10+0.1V

0.12V=−12

V=−12/0.12=−100 (not possible as we add NaOH)

However, we need to consider the reaction:

$HAc+NaOH\rightarrow NaAc+H_2O$

For each mL of NaOH added, 0.1 mmol of HAc reacts to form 0.1 mmol of NaAc.

Let x be the mmol of NaOH added:

X/(100+x)=(0.22−0.1)/1

(since initial [HA] = 0.1 mol/L and final [A-] desired = 0.22 mol/L)

Solving for x:

x=22 mmol

V=22 mmol÷0.1 mol/L=22 mL

Thus, add 22 mL of 0.1 mol/L NaOH to 100 mL of 0.1 mol/L HAc to prepare the buffer solution.

2025.12：

1. **Henderson-Hasselbalch Equation**:
   pH = pKa + log([A^-]/[HA])
   Given pH = 5.10 and pKa (acetic acid) = 4.76:
   5.10 = 4.76 + log([A^-]/[HA]) → log([A^-]/[HA]) = 0.34 → [A^-]/[HA] = $10^{0.34}$ ≈ 2.187.
2. **Initial Moles of HAc**:
   Moles of HAc = 0.1 L × 0.1 mol/L = 0.01 mol.
3. **Let V = Volume of NaOH (L)**:
   Moles of NaOH added = 0.1 × V.
   Moles of HAc remaining = 0.01 - 0.1V.
   Moles of A^- (acetate) = 0.1V.
4. **Ratio [A^-]/[HA]**:
   (0.1V) / (0.01 - 0.1V) = 2.187.
   Solving:
   0.1V = 2.187(0.01 - 0.1V) → 0.1V = 0.02187 - 0.2187V → 0.3187V = 0.02187 → V ≈ 0.0686 L.
5. **Convert to mL**:
   0.0686 L × 1000 = **68.6 mL**.

iFLYTEK Spark:

To prepare a buffer solution with pH 5.10 using 100 mL of 0.1 mol/L acetic acid (HAc), we calculate the volume of 0.1 mol/L NaOH needed to achieve this pH.

The Henderson-Hasselbalch equation is used:

$pH=pKa+\log([A^-]/[HA]\quad)$

For acetic acid, $Ka\approx1.8\times10^{-5}$, so $pKa=-\log(1.8\times10^{-5})\approx4.74$.

Given pH 5.10:

$5.10=4.74+\log([A^-]/[HA])$

$\log([A^-]/[HA])=5.10-4.74=0.36$

$[A^-]/[HA]=10^{0.36}\approx2.24$

Starting with 100 mL of 0.1 mol/L HAc:

$nHAc=0.1\ mol/L\times0.1\ L=0.01\ mol$

For a 2.24:1 ratio:

$nNaAc=2.24\times0.01\ mol=0.0224\ mol$

With 0.1 mol/L NaOH:

$VNaOH=0.0224\ mol\div0.1\ mol/L=0.224\ L=224\ mL$

Add 224 mL of 0.1 mol/L NaOH to the 100 mL of 0.1 mol/L HAc to achieve a pH of 5.10.

2025.12：

To prepare a pH 5.10 buffer from 100 mL of 0.1 mol/L acetic acid (HAc):

- **pKa of HAc** = 4.74
- **Henderson-Hasselbalch equation**:

$$\mathrm{pH} = \mathrm{pKa} + \log\left(\frac{[\mathrm{Ac}^-]}{[\mathrm{HAc}]}\right)$$
$$5.10 = 4.74 + \log\left(\frac{[\mathrm{Ac}^-]}{[\mathrm{HAc}]}\right)$$
$$\log\left(\frac{[\mathrm{Ac}^-]}{[\mathrm{HAc}]}\right) = 0.36$$
$$\frac{[\mathrm{Ac}^-]}{[\mathrm{HAc}]} = 10^{0.36} \approx 2.29$$

Let V = volume (L) of 0.1 mol/L NaOH added.

- Moles of HAc initially = $0.1 \times 0.1 = 0.01$ mol
- Moles of NaOH added = $0.1V$ mol
- After reaction:

$$[\mathrm{Ac}^-] = 0.1V \text{ mol}$$
$$[\mathrm{HAc}] = 0.01 - 0.1V \text{ mol}$$

Substitute into ratio:

$$\frac{0.1V}{0.01-0.1V} = 2.29$$
$$0.1V = 2.29(0.01 - 0.1V)$$
$$0.1V = 0.0229 - 0.229V$$
$$0.329V = 0.0229$$
$$V = \frac{0.0229}{0.329} \approx 0.0696\mathrm{L} = 69.6\mathrm{mL}$$

Answer: Add **69.6 mL** of 0.1 mol/L NaOH.

Student's Judgement:

ChatGPT: √

Kimi Assistant: × × (2025.12)

Doubao: √

ERNIE Bot: × √ (2025.12)

iFLYTEK Spark: × √ (2025.12)

22. The rate constant of a first-order reaction is $3.46 \times 10^{-2} s^{-1}$ at 298 K. What is the rate constant at 350 K if the activation energy for the reaction is 50.2 kJ/mol?(Concise text output)

ChatGPT:

To find the rate constant at 350 K, we use the Arrhenius equation:

$$k2 = k1 \times e\text{^}[\frac{Ea}{R}(\frac{1}{T1} - \frac{1}{T2})]$$

Step 1: Calculate the exponential factor

$$\text{exponential factor} = e\text{^}[\frac{50200}{8.314} \times (\frac{1}{298} - \frac{1}{350})] \approx 20.085$$

Step 2: Calculate k2

K2=3.46×10^{-2}×20.085≈0.694s^{-1}

Final Answer:

The rate constant at 350 K is 0.694 s^{-1}.

Kimi Assistant:

Using the Arrhenius equation: $k = Ae^{\wedge}(-\frac{Ea}{RT})$

Given: k1=3.46×$10^{-2}$$s^{-1}$,T1=298K,T2=350K,Ea=50.2kJ/mol=50200J/mol,R=8.314J/(mol·K)

First, find A: 3.46×10^{-2}=Ae^$(-\frac{50200}{8.314\times298})$

Now, find k2: k2=Ae^$(-\frac{50200}{8.314\times350})$

The Final Answer is: 3.54×10^{-2} s^{-1}

2025.12:

- $k_1 = 3.46 \times 10^{-2}\,\mathrm{s}^{-1}$ 在 $T_1 = 298\,\mathrm{K}$
- $T_2 = 350\,\mathrm{K}$
- $E_a = 50.2\,\mathrm{kJ/mol} = 50200\,\mathrm{J/mol}$

使用两点形式的阿累尼乌斯方程：

$$\ln\left(\frac{k_2}{k_1}\right) = \frac{E_a}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

$$\ln\left(\frac{k_2}{3.46 \times 10^{-2}}\right) = \frac{50200}{8.314}\left(\frac{1}{298} - \frac{1}{350}\right)$$

$$\ln\left(\frac{k_2}{3.46 \times 10^{-2}}\right) = 3.02 \Rightarrow \frac{k_2}{3.46 \times 10^{-2}} = e^{3.02} \approx 20.5$$

$$k_2 = 3.46 \times 10^{-2} \times 20.5 \approx \mathbf{0.71\,s^{-1}}$$

Doubao:

Use the Arrhenius equation: $\ln\frac{k2}{k1} = \frac{Ea}{R}(\frac{1}{T1} - \frac{1}{T2})$

Given k1=3.46×$10^{-2}$$s^{-1}$,T1=298K,T2=350K,Ea=50.2kJ/mol=50200J/mol,R=8.314J/(mol·K)

Calculate $\frac{1}{T1} - \frac{1}{T2}$ and substitute into the equa ion to find $\ln\frac{k2}{k1}$.
t

Then find k2 using k2=k1× $e \wedge (\ln \frac{k2}{k1})$. The result is k2≈ 0.739s^(− 1).

ERNIE Bot:

The rate constant at 350 K a first-order reaction, given the rate constant at 298 K is 3.46x10^-2 s^-1 and the activation

energy is 50.2 kJ/mol, can be calculated using the Arrhenius equation. The result is approximately 231 s^-1.

2025.12:

The rate constant at 350 K is calculated using the two-point form of the Arrhenius equation:

$$\ln\left(\frac{k_2}{k_1}\right) = \frac{E_a}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

Given $k_1 = 3.46 \times 10^{-2}\,\mathrm{s}^{-1}$ at $T_1 = 298\,\mathrm{K}$, $T_2 = 350\,\mathrm{K}$, and $E_a = 50.2\,\mathrm{kJ/mol}$ (converted to $50200\,\mathrm{J/mol}$), the calculation proceeds as follows:

1. Compute $\frac{1}{T_1} - \frac{1}{T_2} = \frac{1}{298} - \frac{1}{350} \approx 0.0004986\,\mathrm{K}^{-1}$.
2. Calculate $\frac{E_a}{R} = \frac{50200}{8.314} \approx 6038.008$.
3. Multiply these results: $6038.008 \times 0.0004986 \approx 3.0103$.
4. Exponentiate to find $k_2 = k_1 \cdot e^{3.0103} = 3.46 \times 10^{-2} \cdot 20.294 \approx 0.702\,\mathrm{s}^{-1}$.

Final Answer:

The rate constant at 350 K is $\boxed{0.702\,\mathrm{s}^{-1}}$.

iFLYTEK Spark:

To determine the rate constant at 350 K, we use the Arrhenius equation:

$k = Ae\wedge(-\frac{Ea}{RT})$

Given k1=3.46×10^{-2}s^{-1},T1=298K,T2=350K,Ea=50.2kJ/mol=50200J/mol,R=8.314J/(mol·K)

Calculate the ratio of the rate constants at the two temperatures:

$\frac{k2}{k1} = e\wedge[\frac{50200}{8.314}\times(\frac{1}{298}-\frac{1}{350})] = e\wedge(20.67\times\frac{52}{104300})$ =e^0.1041=1.109

Calculate k2 : k2=k1×1.109=3.46×10^{-2}×1.109=3.84×10^{-2}

The rate constant at 350 K is approximately 3.84×10^{-2} s^{-1}.

2025.12:

To determine the rate constant k_2 at 350 K for a first-order reaction, we apply the **two-point form of the Arrhenius equation**:

$$\ln\left(\frac{k_2}{k_1}\right) = \frac{E_a}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

Given:

- $k_1 = 3.46 \times 10^{-2}\,\mathrm{s}^{-1}$
- $T_1 = 298\,\mathrm{K}$
- $T_2 = 350\,\mathrm{K}$
- $E_a = 50.2\,\mathrm{kJ/mol} = 50200\,\mathrm{J/mol}$
- $R = 8.314\,\mathrm{J/(mol\cdotpK)}$

Step 1: Compute the temperature difference term

$$\frac{1}{T_1} - \frac{1}{T_2} = \frac{1}{298} - \frac{1}{350} = 0.0033557 - 0.0028571 = 0.0004986\,\mathrm{K}^{-1}$$

Step 2: Calculate $\frac{E_a}{R}$

$$\frac{E_a}{R} = \frac{50200}{8.314} \approx 6038.0\,\mathrm{K}$$

Step 3: Multiply to find $\ln\left(\frac{k_2}{k_1}\right)$

$$\ln\left(\frac{k_2}{k_1}\right) = 6038.0 \times 0.0004986 \approx 3.0103$$

Step 4: Solve for k_2

$$\frac{k_2}{k_1} = e^{3.0103} \approx 20.29$$

$$k_2 = k_1 \times 20.29 = (3.46 \times 10^{-2}) \times 20.29 \approx 0.702\,\mathrm{s}^{-1}$$

Final Answer:

$$\boxed{0.702}\,\mathrm{s}^{-1}$$

Student's Judgement:

ChatGPT: √

Kimi Assistant: × √ (2025.12)

Doubao: √

ERNIE Bot: × √ (2025.12)

iFLYTEK Spark: × √ (2025.12)

23. Explain the definition of electronegativity.

ChatGPT:

Electronegativity is a measure of an atom's ability to attract and hold onto electrons when it forms a chemical bond with another atom. In simpler terms, it indicates how strongly an atom "pulls" electrons towards itself in a bond.

Kimi Assistant:

Electronegativity is a chemical property that describes the tendency of an atom to attract a bonding pair of electrons towards itself in a chemical bond. It is a measure of how strongly an atom will pull electrons towards itself in a covalent bond.

Doubao:

Electronegativity is a measure of the tendency of an atom to attract a shared pair of electrons (in a covalent bond). It reflects the ability of an atom to pull electron density towards itself.

ERNIE Bot:

Electronegativity is a property of atoms that reflects their ability to attract electrons, especially in the context of forming chemical bonds.

iFLYTEK Spark:

Electronegativity is a chemical property that quantifies the ability of an atom to attract a shared pair of electrons in a covalent bond. It reflects how strongly an atom can pull electrons towards itself within a molecule.

Student's Judgement:

ChatGPT: √

Kimi Assistant: √

Doubao: √

ERNIE Bot: √

iFLYTEK Spark: √

24. Elucidate the main contents of molecular orbital theory.(Within 100 words)

ChatGPT:

Molecular Orbital (MO) theory explains how atomic orbitals combine to form molecular orbitals, which are the regions where electrons are most likely to be found in a molecule. According to MO theory, when atoms bond, their atomic orbitals overlap to create bonding orbitals (lower energy) and antibonding orbitals (higher energy). Electrons fill these molecular orbitals based on the Aufbau principle, with bonding orbitals being filled first. The bond order is calculated by the difference between electrons in bonding and antibonding orbitals. MO theory also explains magnetic properties, bond strength, and the electronic structure of molecules.

Kimi Assistant:

Molecular Orbital (MO) Theory is a method for describing the electronic structure of molecules using quantum mechanics. It focuses on the combination of atomic orbitals to form molecular orbitals, which can be bonding (lower energy, stable) or antibonding (higher energy, less stable). Key points include:

1. Atomic orbitals combine to create molecular orbitals.
2. Pauli Exclusion Principle and Aufbau Principle apply.
3. Bond order (number of bonding electrons minus antibonding electrons) predicts bond strength.
4. Molecular orbitals can be visualized using diagrams and energy levels.
5. Theory explains magnetic properties and bond lengths.

Doubao:

Molecular orbital theory states that atomic orbitals combine to form molecular orbitals. These orbitals can be bonding, antibonding, or non - bonding. Electrons are distributed among these molecular orbitals following the Aufbau principle, Pauli exclusion principle, and Hund's rule. It helps to explain the stability, bond order, and magnetic properties of molecules.

ERNIE Bot:

Molecular orbital theory is a fundamental concept in chemistry that explains the bonding and properties of molecules. It suggests that electrons in a molecule are not confined to individual atoms, but are instead delocalized and shared between the atomic nuclei. The theory uses mathematical functions, called molecular orbitals, to describe the probable locations of these electrons. These orbitals can be bonding, which stabilize the molecule, or antibonding, which destabilize it. The shape and energy of

these orbitals determine the overall structure and reactivity of the molecule. In essence, molecular orbital theory provides a comprehensive framework for understanding the electronic structure and bonding in molecules.

iFLYTEK Spark:

Molecular Orbital Theory (MOT) explains the behavior of electrons in molecules by describing their distribution in molecular orbitals, which are regions around nuclei where the probability of finding an electron is high. The theory states that atomic orbitals combine to form these molecular orbitals, leading to bonding or anti-bonding interactions. Bonding MOs stabilize the molecule, while anti-bonding MOs destabilize it. The energy levels of these orbitals can be predicted using principles like symmetry and overlap, and electrons fill them following the Aufbau principle, Hund's rule, and the Pauli exclusion principle. MOT helps predict molecular geometry, bond strength, and reactivity.

Student's Judgement:

ChatGPT: √

Kimi Assistant: √

Doubao: √

ERNIE Bot: √

iFLYTEK Spark: √

25. Calculate the electrode potential of the following electrode in pH = 5 solution? Pt | MnO_4^-(1.0mol/L),Mn^{2+}(1.0mol/L),H^+(10^{-5}mol/L) (Concise text output)

ChatGPT:

To calculate the electrode potential, we use the Nernst equation:

$E = E° - 0.0592 \div n \times \log Q$

For the half-reaction:

$MnO_4^- + 8H^+ + 5e^- \rightarrow Mn^{2+} + 4H_2O$

$E° = +1.51V$

$n = 5$ (number of electrons)

$Q = [Mn^{2+}] \div \{[MnO_4^-][H^+]^8\}$

Given:

$[MnO_4^-] = 1.0$ mol/L

$[Mn^{2+}] = 1.0$ mol/L

$[H^+] = 10^{-5}$mol/L

Now apply the Nernst equation:

$E = 1.038V$

Final Answer:

The electrode potential is 1.038 V.

Kimi Assistant:

Using the Nernst equation for the half-reaction:

$MnO_4^- + 8H^+ + 5e^- \rightarrow Mn^{2+} + 4H_2O$

Given:

E = 1.67V

$[MnO_4^-]$ = 1.0 mol/L

$[Mn^{2+}]$= 1.0 mol/L

$[H^+]$ = 10^{-5}mol/L

The reaction quotient Q is:

$$Q = \frac{[Mn2+]}{[MnO4-][H+]^8} = 1.0 \div 1.0 \div (10^{-5})^8 = 10^{40}$$

The electrode potential E is:

$$E = 1.67 - \frac{0.0592}{5}\ln(10^{40}) = 1.67 - 0.0592 \times 40 = 1.67 - 2.368 = -0.698V$$

The Final Answer is: -0.698V

2025.12:

To calculate the electrode potential, we use the Nernst equation for the MnO_4^-/Mn^{2+} half-reaction:

$MnO_4^- + 8H^+ + 5e^- \rightarrow Mn^{2+} + 4H_2O$

$E° = +1.51$ V

Nernst equation:

$E = E° - (0.0591/5)\log([Mn^{2+}] / ([MnO_4^-][H^+]^8))$

Given:

$[MnO_4^-] = 1.0$ M

$[Mn^{2+}] = 1.0$ M

$[H^+] = 10^{-5}$ M

$E = 1.51 - (0.0591/5)\log(1 / (1 \times (10^{-5})^8))$

$E = 1.51 - (0.0591/5)\log(10^{40})$

$E = 1.51 - (0.0591/5) \times 40$

$E = 1.51 - 0.4728 =$ **1.037 V**

Answer: 1.04 V

Doubao:

1. The half-reaction is $MnO_4^-+8H^++5e^-\leftrightharpoons Mn^{2+}+4H_2O$.
2. The Nernst equation is $E = E°+\frac{0.0592}{n}\log\frac{[MnO4-]\times[H+]^8}{[Mn2+]}$.
3. For this electrode, E°=1.51V, n=5

4.Substitute values: $[MnO_4^-]$ = 1.0 mol/L, $[Mn^{2+}]$= 1.0 mol/L, $[H^+]$ = 10^{-5}mol/L

5.Calculate: $E = 1.51+\frac{0.0592}{5}\log\frac{1.0\times[10^{(-5)}]^8}{1.0}$ = 1.04V.

ERNIE Bot:

The electrode potential E for the electrode Pt | MnO_4^-(1.0mol/L),Mn^{2+}(1.0mol/L),H^+(10^{-5}mol/L) in a pH=5 solution can be calculated using the Nernst equation. Assuming a standard electrode potential E° =1.51V for the reaction $MnO_4^-+8H^++5e^-\rightarrow Mn^{2+}+4H_2O$:

$$E=1.51V-\frac{0.02306V}{5}\ln\left(\frac{1.0mol/L}{1.0mol/L\times[10^{(-5)}mol/L]^8}\right)=1.3255V$$

Thus, the electrode potential is 1.3255V.

2025.12:

The electrode potential is calculated using the Nernst equation for the reaction:
MnO_4^- + 8H^+ + 5e^- → Mn^{2+} + 4H_2O

Nernst Equation:

$$E = E^\circ - \frac{0.0592}{n} \log Q$$

Where:

- $E^\circ = 1.51\,\text{V}$ (standard reduction potential)
- $n = 5$ (electrons transferred)
- $Q = \frac{[\text{Mn}^{2+}]}{[\text{MnO}_4^-][\text{H}^+]^8} = \frac{1.0}{(1.0)(10^{-5})^8} = 10^{40}$

Calculation:

$$E = 1.51 - \frac{0.0592}{5} \log(10^{40}) = 1.51 - 0.01184 \times 40 = 1.51 - 0.4736 = 1.0364\,\text{V}$$

Final Answer:
The electrode potential at pH = 5 is **1.04 V** (rounded to two decimal places).

iFLYTEK Spark:

To calculate the electrode potential of the given redox reaction in a pH = 5 solution, we use the Nernst equation:

E = E°- RT/(nF)×lnQ

where:

E° is the standard electrode potential for $MnO_4^-+8H^++5e^-\rightarrow Mn^{2+}+4H_2O$, which is 1.51V.

R is the universal gas constant (8.314 J/mol·K),

T is the temperature in Kelvin (assuming room temperature, T=298 K),

n is the number of electrons transferred (5 in this case),

F is the Faraday constant (96485 C/mol),

Q is the reaction quotient, calculated as:

$Q=[Mn^{2+}]^{1/5}\div\{[MnO_4^-][H^+]^{8/5}\}=10^4$

Substituting these values into the Nernst equation: E = 1.505 V

Therefore, the electrode potential at pH=5 is approximately E = 1.505V

2025.12:

To determine the electrode potential of the Pt|MnO_4^-(1.0 M), Mn^{2+}(1.0 M), H^+(10^{-5} M) system at pH = 5, we apply the **Nernst equation** for the reduction half-reaction:

$$MnO_4^- + 8H^+ + 5e^- \rightarrow Mn^{2+} + 4H_2O$$

Step 1: Standard Potential and Reaction Quotient

- **Standard reduction potential**: $E^\circ = 1.51\,V$
- **Number of electrons transferred**: $n = 5$
- **Concentrations**:
  - $[MnO_4^-] = [Mn^{2+}] = 1.0\,M$
  - $[H^+] = 10^{-5}\,M$ (from pH = 5)

The **reaction quotient** Q is:

$$Q = \frac{[Mn^{2+}]}{[MnO_4^-][H^+]^8} = \frac{1.0}{1.0 \cdot (10^{-5})^8} = 10^{40}$$

Step 2: Apply the Nernst Equation

$$E = E^\circ - \frac{0.0592}{n} \log Q$$

Substitute values:

$$E = 1.51 - \frac{0.0592}{5} \cdot \log(10^{40}) = 1.51 - \frac{0.0592}{5} \cdot 40$$

$$E = 1.51 - (0.01184 \cdot 40) = 1.51 - 0.4736 = 1.0364\,V$$

Final Answer

$$\boxed{1.04}\,V$$

Student's Judgement:

ChatGPT: √

Kimi Assistant: × √ (2025.12)

Doubao: √

ERNIE Bot: × √ (2025.12)

iFLYTEK Spark: × √ (2025.12)

26. Determine the ground-state electron configuration and bond order of the F_2 molecule.

ChatGPT:

Ground-state electron configuration of F_2: $(\sigma_{1s})^2(\sigma^*_{1s})^2(\sigma_{2s})^2(\sigma^*_{2s})^2(\pi_{2px})^2(\pi_{2py})^2(\pi^*_{2py})^2(\pi^*_{2pz})^2(\sigma_{2pz})^2$

Bond order of F_2: 1 (indicating a single bond between the two fluorine atoms).

2025.12：Ground-State Electron Configuration of F_2:

$[(\sigma_{1s})^2 (\sigma_{1s}^*)^2 (\sigma_{2s})^2 (\sigma_{2s}^*)^2 (\sigma_{2p_z})^2 (\pi_{2p_x})^2 (\pi_{2p_y})^2]$

Bond Order of F_2:[1]

In conclusion, the bond order of F2 is actually 1, which indicates a single bond between the two fluorine atoms.

Kimi Assistant:

The ground-state electron configuration of F2 molecule is: $(\sigma 1s)^2(\sigma\ 1s)^2(\sigma 2s)^2(\sigma 2s)^2(\sigma 2pz)^2(\pi 2px)^2(\pi 2py)^2(\pi\ 2px)^2(\pi 2py)^2$. The bond order of F2 is calculated as (Nb - Na)/2, where Nb is the number of electrons in bonding molecular orbitals and Na is the number of electrons in antibonding molecular orbitals. For F2, Nb = 10 and Na = 8, so

the bond order is (10 - 8)/2 = 1

2025.12：F_2

$\sigma(1s)^2$ $\sigma^*(1s)^2$ $\sigma(2s)^2$ $\sigma^*(2s)^2$ $\sigma(2p_z)^2$ $\pi(2p_x)^2$ $\pi(2p_y)^2$ $\pi^*(2p_x)^2$ $\pi^*(2p_y)^2$

Bond order = ½(10 − 8) = 1

Doubao:

The electron configuration of F_2 is $(\sigma_{1s})^2(\sigma^*_{1s})^2(\sigma_{2s})^2(\sigma^*_{2s})^2(\sigma_{2px})^2(\pi_{2py})^2(\pi_{2pz})^2(\pi^*_{2px})^2(\pi^*_{2py})^2$

Bond order BO=0.5×(10-8)=1

ERNIE Bot:

Ground-state electron configuration for F_2:(1 σ g)2(1 σ u)2(2 σ g)2(1 π u)4(3 σ g)2(2 π u)4(1 π g*)2

The bond order of F2 molecule (considering all electrons) is 5, but the more accurate bond order (only considering valence electrons) is 3.

2025.12：The ground-state electron configuration of F_2 is:

$(\sigma_2 s)^2$ $(\sigma_2 s)^2$ $(\pi_2 p)^4$ $(\sigma_2 p)^2$ $(\pi_2 p)^4$

Using crystal field theory (or MO theory), bonding electrons = 8 (σ_2 s, σ_2 p, π_2 p), antibonding electrons = 6 (σ_2 s, π_2 p).

Bond order = (8 - 6)/2 = 1.

F_2 has a single bond, consistent with its diatomic stability.

iFLYTEK Spark:

Ground-state electron configuration for F_2: The individual fluorine atoms have the electron configuration $[1s^2][2s^2][2p^6][3s^2][3p^5]$, but in the context of the F_2 molecule, the focus is on the bonding between the two atoms, specifically involving the 3p electrons.

Bond order: 1

2025.12：Ground-state electron configuration of F_2 :

KK(σ_2 s)^2 (σ_2 s)^2 (σ_2 p)^2 (π_2 p)^4 (π_2 p)^4

(KK denotes filled K-shell core orbitals; σ_2 p = $\sigma(2p_x)$ bonding orbital)

Bond order calculation:

Bonding electrons: σ_2 s^2 (2), σ_2 p^2 (2), π_2 p^4 (4) → 8

Antibonding electrons: σ_2 s^2 (2), π_2 p^4 (4) → 6

Bond order = ½ × (8 − 6) = 1

Explanation:

Fluorine (atomic number 9) has 9 electrons; F_2 has 18 total electrons. After accounting for core orbitals (KK, 4e⁻), 14 valence electrons fill MOs in the order: σ_2 s → σ_2 s → σ_2 p → π_2 p → π_2 p. The π^*_2 p orbitals hold 4 electrons (fully occupied, all paired). Bond order 1 confirms a single bond, consistent with F_2 's stability and diamagnetism.

Student's Judgement:

ChatGPT: × × (2025.12)

Kimi Assistant: × √ (2025.12)

Doubao: √

ERNIE Bot: × × (2025.12)

iFLYTEK Spark: × × (2025.12)

27.Describe the distribution of d electrons in the complex ions $[Co(H2O)_6]^{2+}$

and $[Co(CN)_6]^{4-}$ using crystal field theory. The hexaaquacobalt(Ⅱ) ion is a high-spin complex, and the hexacyanocobaltate(Ⅱ) ion is a low-spin complex. How many unpaired electrons are there in each ion?

ChatGPT:

1. $[Co(H_2O)_6]^{2+}$ (Hexaaquacobalt(II) Ion) – High Spin Complex

Oxidation State of Co: In $[Co(H_2O)_6]^{2+}$, cobalt is in the +2 oxidation state, so the central cobalt ion has an electron configuration of [Ar] $3d^7$.

Geometry: The complex is octahedral, meaning that the 6 water molecules are arranged around the cobalt ion in an octahedral geometry.

Crystal Field Splitting: In an octahedral field, the five degenerate d-orbitals split into two sets due to the ligand field:

The eg set (higher energy): d_{z2} and d_{x2-y2}

The t2g set (lower energy): d_{xy}, d_{xz}, and d_{yz}

The energy gap between the e_g and t_{2g} orbitals is denoted by Δo.

High Spin Complex: Since water is a weak field ligand, the crystal field splitting energy (Δo) is small. As a result, $[Co(H_2O)_6]^{2+}$is a high-spin complex, meaning electrons will occupy the higher-energy eg orbitals before pairing up in the lower-energy t2g orbitals.

Electron Configuration: Cobalt has 7 d-electrons in total. The distribution of these electrons in the t2g and eg orbitals for a high-spin octahedral complex is as follows:

3 electrons in the t2g orbitals

4 electrons in the eg orbitals

This results in 3 unpaired electrons.

Number of Unpaired Electrons: There are 3 unpaired electrons in the $[Co(H_2O)_6]^{2+}$complex.

2. $[Co(CN)_6]^{4-}$ (Hexacyanocobaltate(II) Ion) – Low Spin Complex

Oxidation State of Co: In $[Co(CN)_6]^{4-}$, cobalt is in the +2 oxidation state, so the electron configuration of the central cobalt ion is also [Ar] $3d^7$.

Geometry: The complex is also octahedral, but here, cyanide (CN^-) is a strong field ligand, which leads to a larger crystal field splitting energy (Δo).

Crystal Field Splitting: In an octahedral field, the d-orbitals split into eg and t2g sets, with eg being higher in energy and t2g being lower.

Low Spin Complex: Since cyanide is a strong field ligand, the crystal field splitting energy is large enough that the complex is low-spin. This means that electrons will pair up in the lower-energy t2g orbitals before occupying the higher-energy eg orbitals.

Electron Configuration: With 7 d-electrons, the electron configuration in the t2g and eg orbitals for a low-spin octahedral complex is:

6 electrons in the t2g orbitals (fully paired)

1 electron in one of the eg orbitals

This results in 1 unpaired electron.

Number of Unpaired Electrons: There is 1 unpaired electron in the $[Co(CN)_6]^{4-}$ complex.

Kimi Assistant:

Crystal field theory describes the splitting of d orbitals in a complex ion due to the interaction with ligands. For $[Co(H_2O)_6]^{2+}$, a high-spin complex, the d orbitals split into two groups: a lower energy group (t_2g) and a higher energy group (eg). The electron configuration for Co2+ is [Ar] 3d7. In a high-spin complex, the electrons fill the orbitals according to Hund's rule, resulting in 2 electrons in the t_2g orbitals and 5 in the eg orbitals. Therefore, there are 5 unpaired electrons in $[Co(H_2O)_6]^{2+}$.

For $[Co(CN)_6]^{4-}$, a low-spin complex, the d orbitals also split into t2g and eg groups, but the splitting is larger due to the stronger field of the CN- ligands. The electron configuration for Co2+ remains [Ar] 3d7. In a low-spin complex, the electrons pair up in the t2g orbitals before filling the eg orbitals. This results in 6 electrons in the t2g orbitals and 1 in the eg orbitals. Therefore, there is 1 unpaired electron in [Co(CN)6]4-.

The Final Answer is: 5 unpaired electrons in $[Co(H_2O)_6]^{2-}$ and 1 unpaired electron in $[Co(CN)_6]^{4-}$

2025.12：$[Co(H_2O)_6]^{2+}$ (high-spin, weak-field H_2O)

t_2g ↑ ↑ （3） eg ↑ ↑ （2） 5 unpaired e^-

$[Co(CN)_6]^{4-}$ (low-spin, strong-field CN^-)

t_2g ↑ ↓ ↑ ↓ ↑ ↓ （6） eg（0） 0 unpaired e^-

Doubao:

$[Co(H_2O)_6]^{2+}$

In crystal field theory, for an octahedral complex, the d orbitals split into two sets: t2g and eg.

The Co^{2+} ion has a d^7 electron configuration.

In $[Co(H_2O)_6]^{2+}$, since H_2O is a weak field ligand, it forms a high-spin complex. The electrons will first fill the t2g orbitals singly and then the eg orbitals. So, the electron distribution is $t2g^5eg^2$, and there are 3 unpaired electrons.

$[Co(CN)_6]^{4-}$

The Co^{2+} ion still has a d^7 electron configuration.

In $[Co(CN)_6]^{4-}$, CN^- is a strong field ligand, leading to the formation of a low-spin complex. Electrons will first fill the t2g orbitals completely before starting to fill the eg orbital. Thus, the electron distribution is $t2g^6eg^1$, and there is 1 unpaired electron.

ERNIE Bot:

To describe the distribution of d electrons in the complex ions $[Co(H2O)6]^{2+}$ and $[Co(CN)6]^{4-}$ using crystal field theory, we need to consider the effect of the ligands ($H2O$ and CN^-) on the energy levels of the cobalt (Co) d orbitals.

Crystal Field Theory Basics

Crystal field theory (CFT) simplifies the complex interactions between metal ions and ligands in coordination compounds by focusing on the electrostatic interactions between the positively charged metal ion and the negatively charged ligands or their dipole moments. The ligands create a crystal field that splits the energy levels of the metal ion's d orbitals into two sets: lower-energy t2g and higher-energy eg orbitals.

High-Spin vs. Low-Spin Complexes

The distribution of electrons in these orbitals determines whether the complex is high-spin or low-spin:
High-spin complex: More electrons are in singly occupied orbitals, leading to a higher total spin.

Low-spin complex: Electrons pair up in the lower-energy orbitals, reducing the total spin.

$[Co(H2O)6]2+$: High-Spin Complex

Cobalt Ion: Co^{2+} has a $[Ar]\ 3d^7$ configuration.

Ligand Field Strength: Water ($H2O$) is a weak field ligand.

Electron Distribution: In a high-spin complex, the electrons prefer to remain unpaired and occupy as many orbitals as possible. Therefore, the electrons in Co^{2+} will distribute themselves as follows:
$t2g^3$ (three electrons in the lower-energy t2g orbitals)

eg^4 (four electrons in the higher-energy eg orbitals, each singly occupied to maximize spin)

Unpaired Electrons: There are four unpaired electrons in the eg orbitals.

$[Co(CN)6]^{4-}$: Low-Spin Complex

Cobalt Ion: Again, Co^{2+} has a $[Ar]\ 3d^7$ configuration.

Ligand Field Strength: Cyanide (CN^-) is a strong field ligand.

Electron Distribution: In a low-spin complex, the electrons pair up in the lower-energy orbitals to minimize energy. Therefore, the electrons in Co^{2+} will distribute themselves as follows:
$t2g^6$ (six electrons in the lower-energy t2g orbitals, all paired)

eg^1 (one electron in the higher-energy eg orbital, singly occupied but not contributing to unpaired electron count due to pairing in t2g)

Unpaired Electrons: Although there is one electron in the eg orbital, it is considered paired with respect to the overall complex because all lower-energy t2g orbitals are filled and paired. However, traditionally when discussing unpaired electrons in low-spin complexes, we focus on the fact that there are no additional unpaired electrons beyond those necessary to fill the lower-energy orbitals. Thus, for practical purposes in this context, we can say there are effectively zero unpaired electrons in the sense that no additional spins are available for pairing (all available spins are already paired).

Summary

$Co(H2O)6]^{2-}$: High-spin complex with four unpaired electrons.

$[Co(CN)6]^{4-}$: Low-spin complex with effectively zero unpaired electrons beyond those in the filled and paired t2g orbitals (traditionally considered as zero unpaired electrons in this context).

2025.12：In crystal field theory, the ligand field strength determines electron pairing. For $[Co(H_2O)_6]^{2+}$ (high-spin, weak field ligand H_2O):

d^7 configuration: Electrons occupy t_2g^4 eg^3, maximizing unpaired electrons.

Unpaired electrons: 3 (t_2 g: 2 unpaired; eg: 1 unpaired).

For $[Co(CN)_6]^{4-}$ (low-spin, strong field ligand CN^-):

d^7 configuration: Electrons pair in t_2g^6 eg^1, minimizing unpaired electrons.

Unpaired electrons: 1 (eg: 1 unpaired).

Crystal field splitting energy (Δ) dictates these arrangements, with high-spin favoring unpaired electrons and low-spin favoring pairing.

iFLYTEK Spark:

To describe the distribution of d electrons in the complex ions $[Co(H_2O)_6]2+$ and $[Co(CN)_6]^{4-}$ using crystal field theory, we first need to understand the electronic configuration of the cobalt(II) ion (Co^{2+}). Cobalt is a transition metal with an atomic number of 27. The electron configuration of Co^{2+} (cobalt losing two 4s electrons) is:

[Ar] 3d^7

This means there are seven 3d electrons in the cobalt ion.

Crystal Field Theory

In crystal field theory, the d orbitals of a transition metal ion split into different energy levels when the ion is placed in a ligand field. The extent of this splitting depends on the nature of the ligand. Water (H_2O) is a weak field ligand, while cyanide (CN^-) is a strong field ligand. This difference affects whether the complex ion will be high-spin or low-spin.

$[Co(H_2O)_6]2+$ (High-Spin)

1. Weak Field Ligand (H_2O): In a weak ligand field like water, the crystal field splitting is smaller than the electron-electron pairing energy. Therefore, the 3d electrons remain unpaired to maximize the number of unpaired electrons.

2. Electronic Configuration: All seven 3d electrons remain unpaired, filling the orbitals singly from lower to higher energy.

3. Magnetic Moment: Since all electrons are unpaired, there are 7 unpaired electrons.

$[Co(CN)_6]^{4-}$ (Low-Spin)

1. Strong Field Ligand (CN^-): In a strong ligand field like cyanide, the crystal field splitting is larger than the electron-electron pairing energy. This causes the electrons to pair up in the lower energy orbitals before occupying higher energy orbitals.

2. Electronic Configuration: The d orbitals split into t_2g (lower energy, triplet) and eg (higher energy, doublet) sets. The stronger ligand field stabilizes the lower energy t_2g orbitals more, causing the electrons to pair up and fill these orbitals first.

3. Filling the Orbitals: The seven 3d electrons fill the t_2g orbitals completely (three electrons each in two of the t_2g orbitals and one electron in the third), leaving no unpaired electrons in the lower energy set. The remaining two electrons go into the eg orbitals, also pairing up due to the strong ligand field.

4. Magnetic Moment: There are no unpaired electrons in $[Co(CN)_6]^{4-}$ because all electrons are paired in the presence of the strong ligand field.

Summary

$[Co(H_2O)_6]^{2-}$ (High-Spin):7 unpaired electrons.

$[Co(CN)_6]^{4-}$ (Low-Spin): 0 unpaired electrons.

These differences in electron configuration and spin states arise from the varying strengths of the ligand fields, which influence the balance between crystal field splitting energy and electron pairing energy.

2025.12：$[Co(H_2O)_6]^{2+}$ (d^7, high-spin):

Weak-field H_2O ligands cause small Δ_0. Electrons occupy orbitals to maximize spin: $t_2g^5 e_g^2$. t_2g^5 has 1 unpaired electron (one paired orbital, two half-filled); e_g^2 has 2 unpaired electrons. Total unpaired electrons: 3.

$[Co(CN)_6]^{4-}$ (d^7, low-spin):

Strong-field CN^- ligands cause large Δ_0. Electrons pair in t_2g: $t_2g^6 e_g^1$. t_2g^6 is fully paired; e_g^1 has 1 unpaired electron. Total unpaired electrons: 1.

Student's Judgement:

ChatGPT: √

Kimi Assistant: × × (2025.12)

Doubao: √

ERNIE Bot: × × (2025.12)

iFLYTEK Spark: × √ (2025.12)

28.Use the VSEPR model to predict the geometry of AsH_3 and OF_2.

ChatGPT:

The VSEPR (Valence Shell Electron Pair Repulsion) model helps predict the shapes of molecules based on the repulsion between electron pairs around a central atom. To apply the VSEPR model, we first need to determine the number of electron pairs around the central atom and then use this to predict the molecular geometry.

1. AsH_3 (Arsine)

Step 1: Count the Valence Electrons

Arsenic (As) is in Group 15, so it has 5 valence electrons.

Hydrogen (H) has 1 valence electron, and there are 3 hydrogen atoms, so the total number of electrons from hydrogen is 1×3=31 \times 3 = 31×3=3.

Total valence electrons for AsH_3 = 5+3=85 + 3 = 85+3=8 electrons.

Step 2: Determine the Electron Pair Geometry

In AsH_3, arsenic is the central atom, and it forms 3 single bonds with hydrogen atoms.

There are no lone pairs on the arsenic atom (since the 8 valence electrons are used in bonding, with 2 electrons per bond).

As a result, arsenic has 3 bonding pairs of electrons around it and no lone pairs. According to the VSEPR model, 3 bonding pairs of electrons arrange themselves in a trigonal pyramidal geometry.

Step 3: Predict the Molecular Geometry

Since there are no lone pairs on the central atom, the geometry is based on the 3 bonding pairs.

The shape of AsH_3 is trigonal pyramidal, with bond angles slightly less than 109.5° due to the repulsion between the bonding pairs.

Geometry of AsH_3: Trigonal pyramidal.

2. OF_2 (Oxygen Difluoride)

Step 1: Count the Valence Electrons

Oxygen (O) is in Group 16, so it has 6 valence electrons.

Fluorine (F) is in Group 17, so each fluorine atom has 7 valence electrons, and there are 2 fluorine atoms, so the total number of electrons from fluorine is 7×2=147 \times 2 = 147×2=14.

Total valence electrons for OF_2 = 6+14=206 + 14 = 206+14=20 electrons.

Step 2: Determine the Electron Pair Geometry

Oxygen is the central atom and forms single bonds with the two fluorine atoms.

Oxygen has 6 valence electrons, and 2 are used for bonding with the fluorines. This leaves 4 electrons (or 2 lone pairs) on oxygen.

So, oxygen in OF_2 has 2 bonding pairs and 2 lone pairs of electrons.

Step 3: Predict the Molecular Geometry

With 2 bonding pairs and 2 lone pairs around oxygen, the electron pair geometry is tetrahedral (since there are 4 regions of electron density).

However, because lone pairs take up more space than bonding pairs, the molecular geometry is modified by the lone pairs. The lone pairs will push the bonding pairs closer together, reducing the bond angle.

Thus, the shape of OF_2 is bent (also called angular), with bond angles less than 109.5° due to the lone pairs on oxygen.

Geometry of OF_2: Bent.

Summary:

AsH_3: Trigonal pyramidal geometry.

OF_2: Bent geometry.

Kimi Assistant:
Using the Valence Shell Electron Pair Repulsion (VSEPR) model, we can predict the molecular geometries of AsH3 and OF2 as follows:

AsH3 (Arsine) Geometry:

The central atom in AsH3 is arsenic (As), which has 5 valence electrons. Each hydrogen (H) atom contributes 1 valence electron. This results in a total of 5 + 3(1) = 8 valence electrons, which form 3 bonding pairs and 1 lone pair on the central arsenic atom.

According to VSEPR theory, the lone pair of electrons will repel the bonding pairs, causing a distortion from the ideal tetrahedral geometry. Therefore, the predicted geometry for AsH3 is trigonal pyramidal, not tetrahedral, due to the presence of the lone pair on the central atom.

OF2 (Oxygen Difluoride) Geometry:

The central atom in OF2 is oxygen (O), which has 6 valence electrons. Each fluorine (F) atom contributes 7 valence electrons. This results in a total of 6 + 2(7) = 20 valence electrons, which form 2 bonding pairs and 2 lone pairs on the central oxygen atom.

According to VSEPR theory, the two lone pairs and the two bonding pairs will arrange themselves to minimize repulsion, which leads to a linear geometry for OF2. The electron pairs are as far apart as possible, which is consistent with a linear arrangement.

In summary, the predicted geometry for AsH3 is trigonal pyramidal, and the predicted geometry for OF2 is linear.

2025.12：AsH_3 : 4 electron domains (3 bonds, 1 lone pair) → trigonal-pyramidal, ≈ 92° .

OF_2 : 4 electron domains (2 bonds, 2 lone pairs) → bent, ≈ 103° .

Doubao:

AsH_3 (Arsenic Trihydride)

Central Atom and Valence Electrons:

The central atom is arsenic (As). Arsenic has 5 valence electrons. Each hydrogen atom contributes 1 valence electron. So, the total number of valence electrons in AsH_3 is valence electrons.

Electron - Domain Geometry:

According to the VSEPR (Valence - Shell Electron - Pair Repulsion) theory, the electron - domain geometry is determined by the number of electron domains around the central atom. In AsH_3, there are 3 bonding pairs and 1 lone pair of electrons around the As atom. So, the total number of electron domains is .

The electron - domain geometry for 4 electron domains is tetrahedral.

Molecular Geometry:

The molecular geometry, which describes the arrangement of only the atoms, takes into account the lone pairs. In AsH_3, due to the presence of 1 lone pair, the molecular geometry is trigonal pyramidal. The lone pair of electrons on the As atom repels the bonding pairs, causing the hydrogen atoms to be pushed downwards, giving a trigonal pyramidal shape.

OF_2 (Oxygen Difluoride)

Central Atom and Valence Electrons:

The central atom is oxygen (O). Oxygen has 6 valence electrons, and each fluorine atom contributes 7 valence electrons. The total number of valence electrons in OF_2 is valence electrons.

Electron - Domain Geometry:

In OF_2, there are 2 bonding pairs and 2 lone pairs of electrons around the O atom. The total number of electron domains is .

The electron - domain geometry for 4 electron domains is tetrahedral.

Molecular Geometry:

Considering the molecular geometry, due to the presence of 2 lone pairs, the shape of the molecule is bent or V - shaped. The lone pairs of electrons on the O atom repel the bonding pairs more strongly than the bonding pairs repel each other, causing the fluorine atoms to be pushed closer together and the molecule to have a bent shape

ERNIE Bot:

To predict the geometry of *AsH*3 and *OF*2 using the Valence Shell Electron Pair Repulsion (VSEPR) model, we need to follow these steps:

Step 1: Determine the Central Atom

For *AsH*3:

The chemical formula *AsH*3 indicates that arsenic (As) is the central atom, and hydrogen (H) atoms are bonded to it.

For *OF*2:

The chemical formula *OF*2 indicates that oxygen (O) is the central atom, and fluorine (F) atoms are bonded to it.

Step 2: Calculate the Number of Electron Pairs

For *AsH*3:

1.Arsenic (As) has a valence of 5.

2.Each hydrogen (H) atom contributes 1 valence electron.

3.Thus, the total number of valence electrons is 5+3×1=8.

4.These 8 electrons form 4 electron pairs (since each pair consists of 2 electrons).

For *OF*2:

1.Oxygen (O) has a valence of 6.

2.Each fluorine (F) atom contributes 1 valence electron (but since F is more electronegative than O, it will take an electron from O to form the bond, but we still consider the bonding electrons as part of the central atom's valence shell for VSEPR purposes).

3.Thus, the total number of valence electrons around O (considering bonding and lone pairs) is 6+2×1=8 (note that each F atom formally takes 1 electron from O, but we count the shared electrons as part of O's valence shell).

4.These 8 electrons form 4 electron pairs (since each pair consists of 2 electrons).

Step 3: Determine the Electron Pair Geometry

The electron pair geometry is determined by the number of electron pairs around the central atom.

For both *AsH*3 and *OF*2, there are 4 electron pairs.

The electron pair geometry for 4 electron pairs is tetrahedral.

Step 4: Determine the Molecular Geometry

The molecular geometry is determined by the arrangement of the atoms around the central atom, considering only the bonded atoms (ignoring lone pairs).

For *AsH*3:

There are 3 bonded atoms (H) and 1 lone pair.

The bonded atoms (H) arrange themselves around the central atom (As) in a trigonal pyramidal geometry, with the lone pair pushing the bonded atoms down to form a pyramid.

For *OF*2:

There are 2 bonded atoms (F) and 2 lone pairs.

The bonded atoms (F) and the lone pairs repel each other, causing the bonded atoms to arrange themselves in a bent (or angular) geometry around the central atom (O).

Conclusion

The geometry of *AsH*3 is trigonal pyramidal.

The geometry of *OF*2 is bent (or angular).

iFLYTEK Spark:

The VSEPR (Valence Shell Electron Pair Repulsion) model is a useful tool for predicting the molecular geometry of molecules based on the arrangement of their valence electrons. Let's apply this model to predict the geometries of AsH3 and OF2.

Arsenic Trihydride (AsH3)

Identify the central atom and its valence electrons:

Arsenic (As) has an electronic configuration of Ne*Ne* 3s^2 3p^3.

The valence electrons are those in the outermost energy level, which are the 3p electrons.

Count the number of valence electron pairs:

There are three 3p orbitals, each capable of holding two electrons.

Since there are three p electrons, they will occupy one 3p orbital fully (paired) and the other two 3p orbitals partially (one with one electron).

This gives us three pairs of electrons: one pair from the fully occupied 3p orbital and two pairs from the partially occupied 3p orbitals.

Determine the geometry using the VSEPR model:

For three pairs of electrons, the predicted geometry is trigonal planar (T-shaped).

So, AsH3 is expected to have a trigonal planar geometry.

Oxygen Difluoride (OF2)

Identify the central atom and its valence electrons:

Oxygen (O) has an electronic configuration of Ne*Ne* 2s^2 2p^4.

The valence electrons are those in the outermost energy level, which are the 2p electrons.

Count the number of valence electron pairs:

There are three 2p orbitals, each capable of holding two electrons.

Since there are four p electrons, they will occupy two 2p orbitals fully (each with two electrons) and one 2p orbital partially (with one electron).

This gives us three pairs of electrons: two pairs from the fully occupied 2p orbitals and one pair from the partially occupied 2p orbital.

Determine the geometry using the VSEPR model:

For three pairs of electrons, the predicted geometry is trigonal planar (T-shaped).

So, OF2 is expected to have a trigonal planar geometry.

Summary

Arsenic Trihydride (AsH3): Trigonal Planar (T-shaped)

Oxygen Difluoride (OF2): Trigonal Planar (T-shaped)

2025.12：AsH_3 : Central As has 4 electron domains (3 bonding pairs, 1 lone pair). Electron geometry: tetrahedral. Molecular geometry: trigonal pyramidal (bond angle ~92°). Lone pair repulsion reduces angle from 109.5° .

OF_2 : Central O has 4 electron domains (2 bonding pairs, 2 lone pairs). Electron geometry: tetrahedral. Molecular geometry: bent (bond angle ~103°). Strong lone pair repulsion compresses angle below tetrahedral.

Student's Judgement:

ChatGPT: √

Kimi Assistant: × √ (2025.12)

Doubao: √

ERNIE Bot: √

iFLYTEK Spark: × √ (2025.12)

29. Locate relevant literature on the application of acid-base theory in medicine.

ChatGPT:

The application of acid-base theory in medicine is crucial in understanding various physiological processes and treating medical conditions. Acid-base balance impacts numerous biological functions, and the clinical importance is reflected in managing conditions like metabolic acidosis, alkalosis, respiratory disturbances, and drug formulation. Below are several areas where acid-base theory is applied in medicine, along with some relevant literature suggestions:

1. Blood pH and Acid-Base Balance

The body maintains a tight regulation of blood pH (around 7.4) through buffer systems (e.g., bicarbonate), respiratory compensation, and renal regulation. Disruptions in this balance can lead to disorders such as:

- Acidosis (low blood pH)
- Alkalosis (high blood pH)

Relevant Literature:

- "Acid-Base Disorders: A Primer on Their Diagnosis and Management" by David G. H. B. Hering, The American Journal of Medicine (2018).
- "Clinical Assessment of Acid-Base Status: Concepts and Applications" by T. L. Brunette et al., American Journal of Kidney Diseases (2016).

2. Respiratory and Metabolic Acidosis/Alkalosis

Acid-base disorders related to respiratory and metabolic systems are often seen in conditions like:

- Chronic obstructive pulmonary disease (COPD) and asthma can cause respiratory acidosis.
- Diabetic ketoacidosis (DKA) and chronic kidney disease are associated with metabolic acidosis.
- Hyperventilation or vomiting can result in metabolic alkalosis.

Relevant Literature:

- "Diagnosis and Management of Acute and Chronic Acid-Base Disorders" by W. B. Gennari et al., Clinical Journal of the American Society of Nephrology (2009).
- "Acid-Base and Electrolyte Disorders in Critical Care" by C. S. Kraut, Critical Care Clinics (2017).

3. Renal Physiology and Acid-Base Homeostasis

The kidneys play a critical role in maintaining acid-base balance by regulating the excretion of hydrogen ions (H^+) and bicarbonate (HCO_3^-). Impairment in kidney function can lead to various acid-base disturbances.

Relevant Literature:

- "Renal Regulation of Acid-Base Balance" by K. L. Wall et al., The New England Journal of Medicine (2018).

- "The Role of the Kidney in Acid-Base Homeostasis" by K. R. Dunn et al., Kidney International (2016).

4. Acid-Base Theory in Pharmacology

The acid-base properties of drugs affect their absorption, distribution, and excretion. For instance, the pH of the gastrointestinal tract influences drug solubility, and the pH of urine can affect drug elimination. The application of acid-base theory in drug formulation is critical for optimizing the efficacy and safety of medications.

Relevant Literature:

- "Acid-Base Considerations in Drug Therapy" by R. L. Taylor, Journal of Clinical Pharmacology (2019).
- "The Influence of pH on Drug Absorption and Distribution" by A. S. Lawrence et al., Pharmaceutical Research (2017).

5. Acid-Base Theory in Gastrointestinal Diseases

Disorders like gastroesophageal reflux disease (GERD), ulcers, and peptic acid disorders are influenced by acid-base imbalances. The use of proton-pump inhibitors (PPIs) and antacids directly correlates with acid-base theory in medicine.

Relevant Literature:

- "Acid-Base Physiology of Gastrointestinal Tract and Implications for Therapy" by J. H. Sutherland et al., World Journal of Gastroenterology (2017).
- "Acid-Base Disorders in Gastrointestinal Disease" by M. A. Johnson et al., Gastroenterology Clinics of North America (2018).

6. Acid-Base Theory in Critical Care and Anesthesia

In critical care, acid-base disturbances are common, and managing these imbalances is a key aspect of patient care. Anesthesiologists also need to consider the effects of anesthesia drugs on the acid-base balance during surgeries.

Relevant Literature:

- "Acid-Base Disorders in Intensive Care" by R. M. Ueda, Critical Care Medicine (2016).
- "Anesthesia and Acid-Base Balance: Implications for Clinical Practice" by L. B. Boehme et al., Anesthesia & Analgesia (2017).

Conclusion

Acid-base theory plays an essential role in diagnosing and treating many medical conditions, ranging from respiratory disorders to critical care. The listed references provide an in-depth understanding of how acid-base balance is managed in the body and applied in various medical contexts. These articles can be accessed for further study or clinical insights.

Kimi Assistant:

Here are two relevant literature pieces on the application of acid-base theory in medicine:

Clinical Approach to Assessing Acid-Base Status: Physiological vs Stewart

This article examines the attributes and drawbacks of the physiological and physicochemical approaches to acid-base status assessment, offering a rationale for the preference of the physiological approach due to its rigor, simplicity, and ease of application.

Analysis of acid–base disorders in an ICU cohort using a computer script

This study discusses the use of different approaches to acid-base derangement to predict mortality in critically ill patients, providing insights into the practical application of acid-base theory in intensive care settings.

These articles provide a good starting point for understanding the application of acid-base theory in medical practice, particularly in the assessment and management of acid-base disorders.

Doubao:

"Application of the Hard and Soft Acid and Base Principle in Medical Science" by Zhang Qinsheng：This paper points out that the classification of acids and bases as hard and soft is applicable in certain areas of medical science. It introduces the hard and soft acid-base principle, which states that any molecule, ion, or atomic group that can donate an electron pair is called a base, and any that can accept an electron pair is called an acid.

"100 years of blood gas and acid-base analysis in clinical medicine"：The author reviews the development of acid-base theory in clinical medicine since the first mention of acidosis in 1898, including Henderson's mass action law for carbonic acid/bicarbonate balance in 1907 and Hasselbalch's improvement of the Henderson equation in 1917. These theories and equations are of great significance for understanding blood acid-base balance and the diagnosis and treatment of related diseases.

"Acid-Base Theories and Their Applications"：This article briefly introduces the establishment and basic concepts of modern acid-base theories, such as the Brønsted-Lowry acid-base theory, the Lewis acid-base theory, the HSAB theory, and the superacid theory. It also gives examples of their wide applications in fields such as physical organic chemistry, organic synthesis, and organic catalysis, including relevant applications in the medical field, such as the importance of acid-base balance in human physiology and diseases.

"Treatment of Various Gynecological Inflammations by Acid-Base Balance Method"：This paper introduces the "Acid-Base Balance Therapy" introduced by Nanjing Military Hospital. The therapy combines modern fine detection techniques with Chinese and Western medical theories. It first determines the cause of "acid-base imbalance" in female patients through the bacterial and toxic cell perspective detection system, and then uses a variety of technical means to restore the body's acid-base balance, thereby achieving the purpose of treating gynecological inflammations such as vulvitis, vaginitis, cervicitis, and pelvic inflammatory disease.

ERNIE Bot:

A relevant literature on the application of acid-base theory in medicine is "软硬酸碱原则在医学科学中的应用" by Zhang Qinsheng. This literature discusses the application of the soft and hard acid-base principle in medical science. The soft and hard acid-base principle, proposed in the early 1960s by Pearson, categorizes Lewis acids and bases into soft, hard, and borderline types, and suggests that hard acids prefer to combine with hard bases and soft acids prefer to combine with soft bases.

This principle has found applications in various fields, including medicine. In medical science, it can be used to explain and predict the biological activity and pharmacological effects of certain compounds, as well as to guide drug design and synthesis. For example, the interaction between metal ions and ligands in biological systems can be understood in terms of the soft and hard acid-base principle. This understanding can help in the development of new drugs that target specific metal ions or ligands involved in disease processes.

Overall, the application of the soft and hard acid-base principle in medical science provides a useful tool for understanding and manipulating biological systems at the molecular level, with potential implications for drug discovery and development.

iFLYTEK Spark:

Stewart's pH Formula and Quantitative Acid-Base Physiology

Reference: Stewart, P. (1978). "A new approach to the quantitative understanding of acid-base balance." Annals of Internal Medicine, 88(5), 647-653.
Summary: This seminal paper introduces the Stewart approach to acid-base balance, which emphasizes the independent regulation of strong ion difference (SID) and the effective strong ion difference at constant PCO2 and total weak acid concentration.
Physiologic Basis for the Stewart Approach to Acid-Base Physiology
Reference: Fencl, V. F., & Leibfritz, D. A. (1989). "The physiologic basis for the Stewart approach to acid-base physiology." American Journal of Physiology, 257(1 Pt 1), R11-R22.
Summary: This article provides a detailed explanation of the physiological principles underlying the Stewart approach, discussing how it differs from traditional approaches and its advantages in clinical practice.
Clinical Application of Acid-Base Theory in Anesthesia and Intensive Care Medicine
Reference: Vincent, J. L., & Abraham, E. (2014). "Acid-Base Disorders in Critical Illness." Critical Care Clinics, 30(4), vii-viii, 577-592.
Summary: This review discusses the practical application of acid-base theory in managing critically ill patients, focusing on common disorders and their correction in anesthesia and intensive care settings.
Practical Guide to Acid-Base Disorders
Reference: McArdle, M. D. (2018). "Practical approach to acid-base disorders." BMJ Learning, BMJ 361.
Summary: This resource offers a practical guide for clinicians on diagnosing and managing acid-base disorders, emphasizing the importance of understanding basic principles and their application in real-world scenarios.
These references cover foundational theories, physiological mechanisms, and practical applications of acid-base theory in medical practice.

Student's Judgement:

Most of the literatures in this topic can be found in the corresponding journal websites, and only a few literatures are difficult for researchers to find, which may be related to the limitations of network platforms. However, this does not prevent us from evaluating AI chatbots, and our evaluation results are as follows:

ChatGPT: √

Kimi Assistant: √

Doubao: √

ERNIE Bot: √

iFLYTEK Spark: √

需要说明的是，我们可以通过增加额外限制条件来使 AI 聊天机器人输出更符合我们的需求。研究人员也测试过这个想法，但这里没有列出。

Ⅲ. 2025.12 再次评估

2025 年 12 月的更新数据(见表 SI1)显示，五款 GAI 模型在大学化学教学问题解决中的能力实现显著提升，整体准确率从 2024 年的“48%-86%”跃升至“83%-100%”。核心变化体现在以下两方面：

1. GAI 模型间差距显著收窄：2024 年各模型准确率极差为 38%（豆包 86%， Kimi 智能助手 48%），而 2025 年极差仅为 17%，豆包以 100%全对占据首位，Kimi 智能助手、文心一言、讯飞星火均稳定在 83%，整体表现更趋均衡。

2. 低准确率模型消失：2024 年 Kimi 智能助手、文心一言、讯飞星火三款 GAI 模型的准确率低于 60%，而 2025 年所有模型均高于 80%，达到实用化水平。

表 SI1 AI 聊天机器人在所有问题上的准确率对比（2025.12）

Table SI1 Accuracy Comparison of AI Chatbots Across All Questions（2025.12）

AI 聊天机器人	$n_{正确}$	$n_{错误}$	$n_{全部}$	准确率（%）
ChatGPT	25	4	29	86
Kimi 智能助手	24	5	29	83
豆包	29	0	29	100
文心一言	24	5	29	83
讯飞星火	24	5	29	83

此次全面评估延续了原有的五大问题类型（概念型、解释型、机理型、计算型、综合型）及 29 道测试题（见表 SI2），评估结果显示 GAI 模型在处理各种类型化学问题的准确率均较 2024 年实现针对性提升。其中豆包再度以全题型满分占据首位，讯飞星火作为增幅最为明显的模型，短板题型的改善效果突出。

表 SI2 按问题类型划分的人工智能聊天机器人的准确率（2025.12）

Table SI2 Accuracy of AI Chatbots by Question Type（2025.12）

问题类型	$n_{全部}$	ChatGPT	Kimi 智能助手	豆包	文心一言	讯飞星火
概念型	6	5 (83%)	4 (67%)	6 (100%)	5 (83%)	5 (83%)
解释型	9	8 (89%)	8 (89%)	9 (100%)	7 (78%)	7 (78%)
机理型	4	3 (75%)	4 (100%)	4 (100%)	4 (100%)	3 (75%)
计算型	3	3 (100%)	2 (67%)	3 (100%)	3 (100%)	3 (100%)
综合型	7	6 (86%)	6 (86%)	7 (100%)	5 (71%)	6 (86%)

综合来看，从 2024 年 11 月到 2025 年 12 月，五款 GAI 模型的大学化学问题解决能力实现质的飞跃：整体准确率大幅提升，模型间差距明显缩小，此前的薄弱题型（如化学计算、多步骤反应机理分析）改善显著。迭代后的 GAI 逐渐不再是“可能踩坑”的辅助工具，而是能切实减轻学习负担、深化化学概念理解的“好帮手”，后续再优化复杂合成、高阶计算等少数短板，其教学实用性将进一步增强——以准确性持续提升为标志的 GAI 在化学教育领域正从“能用”稳步走向“好用”。

Ⅳ. 补充声明

DeepSeek R1 于 2025 年 1 月正式发布，其问世迅速引发广泛关注。

DeepSeek R1 性能强劲且具备诸多优势，它采用强化学习进行后期训练，仅需少量标注数据就能显著提升推理能力，在数学、代码、自然语言推理等复杂任务中表现出色。

多家教育企业已与 DeepSeek R1 达成合作，推动教育领域的转型。例如，有道的 AI 全科学习助手“有道小 P”借助该模型优化了个性化问答功能；猿辅导集团的相关产品也基于这一大模型推出了 AI 问答服务。

DeepSeek R1 的持续发展与完善，或将与本研究中的 5 款 AI 聊天机器人协同作用，更好地辅助学生理解化学概念、解决化学问题。同时，其开源属性有望吸引更多开发者参与，共同探索如何将其优势与化学教育需求相结合，从而推动化学教育的创新与发展。