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## 十八烷基三甲基氯化铵对钢在三氯乙酸中的 缓蚀作用

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**摘要:**利用失重法和电化学法研究了阳离子表面活性剂十八烷基三甲基氯化铵(OTAC)对冷轧钢在三氯乙酸( $\text{Cl}_3\text{CCOOH}$ )介质中的腐蚀抑制性能,通过扫描电子显微镜(SEM)观察钢片表面的微观形貌,利用接触角测定冷轧钢表面的亲水性和疏水性。结果表明:OTAC对钢在 $0.10 \text{ mol} \cdot \text{L}^{-1} \text{ Cl}_3\text{CCOOH}$ 溶液中具有较好的缓蚀效果,缓蚀率与OTAC浓度变化呈正相关,而与温度变化呈负相关,且在 $20^\circ\text{C}$ 时 $90 \text{ mg} \cdot \text{L}^{-1}$  OTAC的缓蚀率高达92.1%。OTAC在钢片表面的吸附符合Langmuir吸附等温式,吸附类型是以物理吸附为主的吸附;OTAC同时抑制了冷轧钢在三氯乙酸介质中的阴极和阳极反应,Nyquist图高频区的容抗弧随缓蚀剂浓度上升而逐渐增大,电荷转移电阻显著增加;SEM表面微观形貌的分析判断进一步证实OTAC有效抑制钢片表面的腐蚀程度,表现出了良好的缓蚀效果;添加OTAC阳离子表面活性剂后钢表面接触角明显增大,表明OTAC在钢片表面发生定向吸附形成吸附屏障层,使其疏水性增强,有效隔绝 $\text{Cl}_3\text{CCOOH}$ 介质对钢片的腐蚀反应。

**关键词:**十八烷基三甲基氯化铵;缓蚀;三氯乙酸;冷轧钢;吸附

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## Inhibition effect of octadecyl trimethyl ammonium chloride on steel in trichloroacetic acid

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**Abstract:** The inhibition effect of cationic surfactant octadecyl trimethylated ammonium chloride(OTAC) on cold rolled steel(CRS) in trichloroacetic acid( $\text{Cl}_3\text{CCOOH}$ ) media was studied by weight loss method and electrochemical method. The micromorphology of the cold-rolled steel surface was observed by scanning electron microscope(SEM), and the hydrophilicity/hydrophobicity of the cold-rolled steel surface were determined by the contact angle. The results show that OTAC has a good corrosion suppression effect in  $0.10 \text{ mol} \cdot \text{L}^{-1} \text{ Cl}_3\text{CCOOH}$  solution. Inhibition efficiency is positively correlated with the change of OTAC concentration, while



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## Research Article

# Rapeseed cake meal extract as an eco-friendly green sustainable inhibitor for the corrosion of cold rolled steel in trichloroacetic acid solution

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## ABSTRACT

The inhibitory properties of rapeseed cake meal extract (RCME) on the corrosion of cold rolled steel (CRS) in trichloroacetic acid (TCA) were systematically investigated using gravimetric, electrochemical, surface characterizations and theoretical calculations. The results demonstrate that RCME exhibits excellent inhibitory performance with a maximum inhibition efficiency of 92.7 % for 100 mg L<sup>-1</sup> RCME at 20 °C. The adsorption of RCME obeys Langmuir isotherm at 20 and 30 °C, Temkin isotherm at 40 °C, and Freundlich isotherm at 50 °C. RCME acts as a cathodic inhibitor. The charge transfer resistance is increased with the addition of RCME, while the double-layer capacitance decreases. SEM, AFM, CLSM, XPS, XRD and TOF-SIMS analyses confirm that the active components in RCME adsorb onto the surface of CRS, forming a protective film that effectively inhibits the corrosion of CRS by TCA. Along with the increase in the concentration of RCME, the surface tension of the inhibited solution gradually decreases, while the electrical conductivity increases before stabilizing. HPLC-MS and FTIR analyses reveal rutin, linolenic acid, linoleic acid and adenine are the effective substances in RCME. Quantum chemical (QC) calculations and molecular dynamic (MD) simulations indicate that the active centers of the effective inhibitor molecules are predominantly located on benzene rings, O- or N-containing heterocyclic rings, and functional groups such as C=O and C=C. Additionally, their main chains adsorb onto the Fe (001) surface in an approximately flat manner, involving both chemical and physical adsorption processes.

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## 1. Introduction

Metallic corrosion resulting from the interaction between metals or alloys and aggressive media is an inevitable challenge, which has been consistently proven to potential danger to both the economy and the environment [1]. Corrosion, in essence, can detrimentally impact specific components of a metal's parts or the entire structure, gradually diminishing its performance and incurring substantial costs for repairs. According to a survey performed in 2016, corrosion accounts for \$2.5 trillion, or 3.4 % of the gross domestic product (GDP) [2]. Implementing effective corrosion management techniques could potentially save around 15 % to 35 % of costs incurred, translating to annual global savings ranging from \$375 bil-

lion to \$875 billion [3]. Considering the ongoing trajectory of global science and technology around the world, failure to adopt proactive measures for the control and prevention of metal corrosion is anticipated to cause a continued escalation in costs.

The use of inhibitors stands out as a cost-effective and efficient strategy for preventing corrosion [4–8]. During the metal pickling process, the introduction of inhibitors can significantly mitigate metal corrosion induced by acidic mediums through the creation of a protective film via interface adsorption [9–11]. However, commercial industrial inhibitors have been somewhat constrained due to the presence of persistent substances that accumulate the hazardous compounds and pose threats to human health as well as the environment [12]. Therefore, academic attention has turned toward the research of green corrosion inhibitors to achieve sustainable economic and social development [13,14]. Various inhibitors like plant extracts [15,16], oral drugs [17] and flavors [18,19] have

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# Rapeseed cake meal extract as an efficient plant-based inhibitor for the corrosion of steel in $\text{Cl}_2\text{CHCOOH}$ : Experiments and molecular modeling calculations

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## ABSTRACT

In alignment with the principles of environmentally sustainable practices, the inhibition mechanism of rapeseed cake meal extract (RCME) on steel in dichloroacetic acid ( $\text{Cl}_2\text{CHCOOH}$ ) was investigated through the combination of experimental methodologies and molecular modeling calculations. The results indicate that RCME achieves a peak inhibition efficiency of 92.3 % in 0.10 M  $\text{Cl}_2\text{CHCOOH}$  at 40 °C. The adsorption of steel surfaces is consistent with Langmuir adsorption isotherm, which includes both physical and chemical adsorption processes. Theoretical simulations show that amino acids and purine compounds in RCME contain active centers that facilitate the creation of chemical bonds with Fe atoms, thereby collectively exerting inhibitory performance. When these two types of compounds interact in 1:9 ratio within RCME, reduced free volume fraction is observed, effectively diminishing the diffusion rate and mobility of corrosive ions. Microscopic morphological analyses conducted using metallographic microscopy, SEM, AFM, and CLSM reveal noteworthy diminishment in the corrosion degree of steel surface after the introduction of RCME. XPS and TOF-SIMS provide evidence that carbon, nitrogen, and oxygen elements present in RCME can form bonds with Fe atoms. RCME functions as a mixed inhibitor in  $\text{Cl}_2\text{CHCOOH}$  with the electrochemical inhibition mechanism of "active site blocking effect". Following the incorporation of RCME, charge transfer resistance rose, efficiently inhibiting the occurrence of electrochemical corrosion reactions.

## 1. Introduction

Metallic materials are highly susceptible to corrosion due to prolonged exposure to environment during their application in various industrial and manufacturing engineering. In addition to diminishing the operating lifespan of metallic equipment, corrosion results in significant financial losses (Li et al., 2015; Hou et al., 2017). Therefore, it is urgent to do fundamental research on metallic corrosion and protection. In comparison to electrochemical protection and anti-corrosive coatings, the inclusion of inhibitors is currently the most economical anti-corrosion technology, particularly in acidic media (Zhang et al., 2019; Wang et al., 2024). However, in light of the current global advocacy of green development, most traditional inhibitors have been prohibited due to their hard-to-degrade residues (Umoren and Eduok,

2016; Ramezanzadeh et al., 2015; Gharbi et al., 2018). Based on this situation, non-toxic and efficient inhibitors derived from natural plant-based extracts have garnered significant attention from current scholars, owing to the standby merits of widely distribution, large in quantity, easily available, and renewable (Wan et al., 2022a; Tan et al., 2023). Active components such as phenolic compounds, flavonoids, alkaloids, and quinones are abundant in plant extracts. The molecular structures of these active substances possess numerous polar atoms (O, N, S), conjugated double and/or triple bonds, and aromatic rings. Accordingly, they can adsorb on metallic surfaces to create protective barrier film that effectively protects metal substrates from environmental corrosion (Negm et al., 2010; Lebrini et al., 2005; Zhang et al., 2011).

Inorganic acids, being highly acidic, can cause severe corrosion to