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Development of a gold leaching reagent as an alternative to cyanide: Synthesis and performance evaluation

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Abstract: Cyanide is the most widely used reagent in gold production processes. However, cyanide is highly toxic and poses safety hazards during transportation and use. Therefore, it is necessary to develop gold leaching reagents that can replace cyanide. This paper introduces a method for synthesizing a gold leaching reagent. Sodium cyanate is used as the main raw material, with sodium hydroxide and sodium ferrocyanide used as additives. The gold leaching reagent can be obtained under the conditions of a mass ratio of sodium cyanate, sodium hydroxide, and sodium ferrocyanide of 15:3:1, synthesis temperature of 600°C, and synthesis time of 1 h. This reagent has a good recovery effect on gold concentrate and gold-containing electronic waste. The gold leaching rate of roasted desulfurized gold concentrate can reach 87.56%. For the extraction experiments of three types of gold-containing electronic waste, the gold leaching rate can reach over 90% after 2 h. Furthermore, the reagent exhibits good selectivity towards gold. Component analysis indicates that the effective component in the reagent could be sodium isocyanate.

Keywords: gold leaching reagent; sodium isocyanate; electronic waste; gold leaching rate; selectivity

1. Introduction

Gold, a rare and precious metal, is not only utilized for reserves and investments [1], but also plays a pivotal role in modern industries like telecommunications and aerospace [2]. The extraction of gold primarily relies on hydrometallurgical methods, wherein cyanide leaching significantly dominates the process [3–5]. Cyanide leaching involves employing a cyanide solution as a solvent to extract gold from the ore, followed by the recovery of gold from the resulting pregnant solution. Since the breakthrough discovery in 1887 that cyanide solutions can dissolve gold, cyanidation has a nearly century-long history in gold extraction. This method is well-developed, having the advantage of high gold leaching rates, strong adaptability to ores, and low costs, making it the predominant method in gold production to this day [6].

The process of gold extraction using cyanide primarily involves two steps: cyanide leaching and gold deposition [7]. Cyanide leaching occurs when gold in the ore reacts with cyanide in the presence of an oxidant (typically oxygen), forming gold-cyanide complexes that dissolve into the solution. This process is represented by the chemical reaction (1):

$$4\mathrm{Au(s)} + 8\mathrm{CN^-(aq)} + \mathrm{O_2(g)} + 2\mathrm{H_2O(l)} \rightarrow 4[\mathrm{Au(CN)_2}]^-\mathrm{(aq)} + 4\mathrm{OH^-(aq)} \quad (1)$$

Commonly used cyanide reagents include sodium cyanide, potassium cyanide, ammonium cyanide, calcium cyanide, and cyanide melts. Gold deposition refers to the extraction of gold from the cyanide solution and can be achieved through various methods such as activated carbon adsorption [8–9] (carbon-in-pulp, CIP, and carbon-in-leach, CIL), zinc displacement (zinc wires or zinc powder), electrolytic deposition, ion-exchange resin [10–11] (resin-in-pulp, RIP, and resin-in-leach, RIL), and magnetic carbon method. Among these methods, zinc displacement and activated carbon adsorption are traditional gold deposition techniques widely employed in gold mines [7].

The structure of the cyanide ion is linear, and its highest occupied molecular orbital (HOMO) is a σ bonding orbital formed by the hybridization of the s–p orbitals of carbon and nitrogen atoms. The lowest unoccupied molecular orbital (LUMO) is a π antibonding orbital formed by the p orbitals of carbon and nitrogen atoms [12], as shown in Fig. S1. Therefore, the cyanide ion not only donates a lone pair of electrons during leaching but also has the ability to accept metal π electrons, forming stable coordination compounds with various metal ions [13–14]. Cyanide can form coordination compounds not only with gold ions but also with silver, copper, zinc, nickel, and other metals [15]. Consequently, cyanide ions can quickly bind with trivalent iron in the cytochrome oxidase of living organisms, preventing its reduction to divalent iron and interrupting the electron transfer process,

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leading to cell asphyxiation and respiratory failure, which is the fundamental reason for the high toxicity of cyanide to living organisms [16]. Cyanide is categorized as a highly toxic hazardous chemical. According to literature reports, the lethal dose of sodium cyanide is 1–10 mg/kg [17–19], posing safety risks during use and transportation [20]. Therefore, it is necessary to develop low-toxicity leaching reagents as alternatives to cyanide for gold extraction.

In the past few decades, the development of low-toxicity leaching reagents for gold extraction has been a research hotspot. Thiosulfates are considered to be the most promising alternatives to cyanide. They have fast leaching rates, high leaching rates, low toxicity, and good leaching effects on complex refractory gold ores containing copper, arsenic, carbonaceous matter, and others [21–23]. The thiosulfate leaching process was first applied to the carbonaceous and refractory gold ore at Goldstrike in Nevada, USA, successfully solving the "gold preg-robbing" issue encountered in cyanide leaching [24–25]. However, thiosulfate leaching requires the presence of copper-ammonia complexes [26], and copper ions can accelerate the decomposition of thiosulfate, resulting in a larger dosage of the leaching reagent [23,27]. Currently, Central South University in China is adopting a nickel/cobalt-ammonia catalytic system as a replacement for copper-ammonia catalysis to reduce the decomposition of thiosulfate [28–31]. Additionally, there has been development in the oxygen pressure alkaline leaching technique without the use of a catalyst [27,32]. Another challenge of thiosulfate leaching is that gold in the leaching solution cannot be recovered using traditional activated carbon adsorption technology. Although the resin can adsorb gold in the leaching solution [33], the polysulfate will form competitive adsorption with the resin and reduce the adsorption capacity, and the resin cost is high. In brief, this process has strict conditions, resulting in higher investment and operational costs. Other sulfur-containing leaching reagents, such as thiourea, thiocyanate, polysulfide, and lime sulfur, have issues such as poor stability, requiring large dosages, and difficulties in recovering leached products [34–36]. Halogen leaching agents, represented by iodine and aqua regia, have advantages in refractory ore treatment, reagent stability, and leached product recovery. However, the cost of iodine is higher [37–39], although the cost of chlorine and bromine is lower than that of iodine, but the corrosion resistance of the equipment is high [40]. Organic acids and their derivatives, represented by alkaline glycine and humic acid, have the ability to dissolve gold and are non-toxic and non-corrosive. However, they have low leaching efficiency and poor selectivity [41–43]. In conclusion, there is currently no leaching reagent that can completely replace cyanide [7,44].

In the past decade, China has seen the emergence of a series of new environmentally friendly gold leaching reagents represented by "Jinchan" and "Minjie" [45–46]. These leaching reagents generally contain sodium oxide, nitrogen, ammonia, and iron, and their main raw materials for synthesis are sodium carbonate and urea [47–48]. According to literature reports, the active ingredient of "Jinchan" is carbonated cyanuric acid sodium, while the main component of "Minjie" is polymerized sodium cyanamide [46]. The toxicity of these new environmentally friendly leaching reagents is less than cyanide. However, there are still doubts about the effective ingredients and leaching mechanisms of these new environmentally friendly leaching reagents [45]. Firstly, the core component is detected in the same way as the free cyanide ion detection method [49]. Secondly, the chemical formula of "carbonated cyanuric acid sodium" reported in the literature is questionable. The chemical formula of "carbonated cyanuric acid sodium" in the literature was originally ionically linked but was mistakenly linked by covalent bonds [50–51]. Therefore, there is still much work to be done regarding the leaching mechanisms and analysis of effective ingredients for these new environmentally friendly leaching reagents [45].

Zhang *et al.* [48] used urea, sodium carbonate, and trihydrate potassium ferrocyanide as raw materials, with a mass ratio of 6:2:1. Under the synthesis conditions of 700°C and 1 h, they successfully synthesized a novel eco-friendly synthetic gold lixiviant (NESGL). X-ray diffraction (XRD) tests indicated that the new phase formed in the synthetic reagent is an effective component for gold leaching. Leaching experiments on gold concentrate revealed that the synthetic reagent not only exhibits a comparable gold leaching effect to sodium cyanide but also demonstrates faster leaching kinetics than sodium cyanide. Electrochemical experiments showed that the Coulomb dissolution efficiency of gold is greater than 85.8% in the potential range of −300 to 600 mV. However, at potentials above 600 mV, the Coulomb dissolution efficiency significantly decreases due to the oxidation of the reagent. In comparison with the cyanidation, the synthetic reagent shows no passivation phenomenon during the gold leaching process. At potentials ranging from 150 to 300 mV, gold in the synthetic reagent exhibits a diffusion-controlled leaching process [47].

In this paper, a reagent synthesized at high temperature using sodium cyanate as main raw material is reported. Advanced characterization techniques were utilized to analyze the composition of the synthesized reagent. Subsequently, pure gold foil was used to evaluate the leaching performance of the leaching reagent. The effects of additives, synthesis time, and synthesis temperature on the leaching performance were studied. Finally, the synthesized gold leaching reagent under the optimal conditions was applied to the leaching of gold from gold sulfide ores and electronic waste. The results showed that the synthesized leaching reagent exhibited significant leaching efficiency for gold-containing materials, achieving a high gold leaching rate during the leaching process. Furthermore, the leaching reagent demonstrated good selectivity for gold, minimizing the dissolution of other base metallic elements in the materials.

2. Experimental

2.1. Materials

The leaching material is derived from the Zhaoyuan Gold Mine in Shandong Province, China. It is a gold-bearing sulfide concentrate obtained by flotation. The gold content in the concentrate is 45.71 g/t, and the sulfur content is 32.96wt%. The concentrations of other elements are shown in Table S1. The gold concentrate is a typical high-sulfur gold concentrate. The mineral composition in the ore is shown in Fig. S2(a), mainly composed of pyrite, feldspar, quartz, mica and other minerals. The phase analysis of gold is shown in Fig. S2(b), with free native gold accounting for 44.7%, gold enclosed in carbonate minerals accounting for 7.5%, and gold enclosed in sulfide minerals accounting for 41.2%. Based on the phase analysis results, the enclosed gold accounts for 55.3%. To further dissociate the free native gold, the gold concentrate was subjected to regrinding. After regrinding, the D_{90} (the particle size at which the cumulative distribution percentage reaches 90%) particle size of the material decreased from 147.92 to 56.57 μm. The changes in particle size before and after regrinding are shown in Fig. S3, indicating a significant reduction in particle size of the gold concentrate, which is beneficial for gold leaching.

Gold-containing electronic waste is composed of three different materials, which are sourced from Central Processing Unit (CPU) processors produced by Advanced Micro Devices (AMD), circuit boards from printers, and gold-plated quartz chips. The experimental specimens, as shown in Fig. S4, were only subjected to mechanical dismantling without any other treatments. In order to calculate the leaching rate of metals, the “aqua regia digestion-ICP detection” method was used to determine the metal content in electronic waste. The experimental process is shown in Note S3. The metal content in the three types of electronic waste is shown in Table S2， and the gold content is 0.57wt% (CPU pins), 0.89wt%, and 1.74wt%, respectively.

During the experiment, various chemical reagents were used including sodium cyanate, sodium ferrocyanide, sodium hydroxide, iron powder, ferric chloride, sodium carbonate, hydrochloric acid, nitric acid, activated carbon, and sodium chloride. These reagents are all of analytical grade and were purchased from China National Pharmaceutical Group Corporation and Shanghai Aladdin Bio-Chem Technology Co., Ltd. Pure gold foil (5 mm × 5 mm × 0.1 mm) was used to test the gold leaching performance of the synthesized reagents. Deionized water was used as the solvent throughout the experimental process.

2.2. Lixiviant synthesis and characterization experiments

Using sodium cyanate as the main synthetic raw material, the study investigated the effect of different types and dosages of additives on the gold leaching performance of the reagents. Different mass ratios of chemical reagents were ground uniformly in a mortar, and then transferred to a 100 mL alumina crucible. The crucible was placed in a muffle furnace at room temperature and heated at a rate of 10°C/min until reaching 600°C, where it was held for 1 h. After the insulation period ended, the crucible was removed from the muffle furnace and naturally cooled to room temperature in air. The cooled solid was ground into powder in the mortar and used as the leaching reagent. The synthesized reagent after grinding was characterized using techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy (RS), Ultraviolet–Visible Spectroscopy (UV–Vis), and other analytical methods. Toxicity testing of leaching agents is entrusted to qualified testing institutions.

2.3. Leaching experiments

To eliminate the influence of other substances on the performance of the reagent, the gold leaching performance of the reagent was first tested using pure gold foil (5 mm × 5 mm × 0.1 mm). Before leaching, the gold foil was polished with emery paper, followed by ultrasonic treatment in anhydrous ethanol and ultrapure water for 5 min each, and then air-dried for later use. The gold leaching performance test was conducted under the conditions of a reagent mass of 1.25%, temperature of 25°C, and stirring speed of 180 r/min. After a certain leaching time, 2 mL of leachate was taken, filtered with a 0.22 μm syringe filter, and then the gold content in the leachate was measured using inductively coupled plasma optical emission spectrometer (ICP-OES).

The leaching of the gold concentrate was carried out in a thermostatic oscillation chamber. 40 g of reground gold concentrate was taken, and the effects of reagent dosage, leaching temperature, liquid-to-solid ratio, and oscillation speed on the leaching of gold from the gold concentrate were investigated under the condition of a leaching time of 24 h. Since the gold concentrate is a high-sulfur gold concentrate mainly composed of pyrite, with a large amount of gold encapsulated by pyrite, studies have shown that roasting and desulfurization help to improve the gold leaching rate [52]. In order to improve the gold leaching rate, the gold concentrate was roasted at 750°C for 1 h after grinding to remove sulfur from the gold concentrate and further liberate the gold into monomers. The leaching effect of the reagent on the roasted gold concentrate was tested under the same leaching conditions.

Three different electronic waste samples containing gold were tested for their leaching effects. The experiments were conducted at room temperature (25°C) with an oscillation speed of 80 r/min. The leaching reagent had a mass concentration of 1.5%. Samples were taken every 2 h and filtered using a 0.22 μm syringe filter. The concentrations of various metals in the leachate were measured using ICP-OES.

3. Results and discussion

3.1. Effect of synthesis temperature on synthetic reagent

Experiments on synthesis using sodium cyanate alone were conducted at four different temperatures: 400, 500, 600, and 700°C. The samples were heated to the target temperature and held for 1 h before being taken out and allowed to cool naturally. After grinding into powder, they were subjected to testing. Under the condition of a mass concentration of 1.25%, the synthetic reagent’s ability to leach gold was tested. The experimental results are shown in Fig. 1(a). The results indicated that the reagents synthetic at temperatures below 600°C had almost no leaching effect. However, when the synthesis temperature reaches or exceeds 600°C, the reagents exhibited significant gold leaching capabilities.

XRD patterns of the synthetic reagent (Fig. 1(b)) showed no significant phase transition and no decomposition into sodium carbonate. However, Raman (Fig. 1(c)) and infrared spectrogram results (Fig. 1(d)) indicated the formation of other substances during synthesis. The Raman spectrogram shows that when the synthesis temperature is below 600°C, the symmetric stretching vibration peaks of sodium cyanate (1214.4 and 1303.9 cm^{-1}) gradually intensify, which also correspond to the Fermi vibration peaks of sodium cyanate. When the synthesis temperature reaches or exceeds 600°C, the intensity of the symmetric stretching vibration peaks (1214.4 and 1303.9 cm^{-1}) and the antisymmetric stretching vibration peak (2178.0 cm^{-1}) representing sodium cyanate both weaken. Meanwhile, the bending vibration peak (637.7 cm^{-1}) indicative of sodium cyanate gradually disappears with increasing synthesis temperature. The Raman shift at 136.1 cm^{-1} remains unchanged when the synthesis temperature is below 600°C, but it undergoes a blue shift when the synthesis temperature reaches or exceeds 600°C. Studies have shown that the crystal structure formed by heating sodium cyanate to 527°C within 13 h and holding it at that temperature for 3 h is similar to that of azide ions ($N=N=N^-$) [53]. The above observations indicate that when the synthesis temperature reaches or exceeds 600°C, sodium cyanate undergoes isomerization to form sodium isocyanate. In the literature, characteristic Raman absorption peaks for sodium cyanide are located at around 2100 cm^{-1}, while Raman absorption peaks for sodium carbonate are at around 1081 cm^{-1} [54–55]. No new Raman absorption peaks were observed at around 2100 cm^{-1} at different synthesis temperatures, suggesting the absence of sodium cyanide in the reagent or its content is below the detection limit. With increasing synthesis temperature, the reagents with gold leaching abilities exhibited a Raman shift at 1080.2 cm^{-1}. Infrared spectrogram results showed a weakened absorption peak at 2227.3 cm^{-1}, which represents the triple bond between carbon and nitrogen atoms.

The infrared characteristic absorption peaks of sodium carbonate are located at 1438.6, 881.3, and 702.0 cm^{-1} [54], indicating a gradual conversion of the synthetic reagent to sodium carbonate. In the isocyanate group (–N=C=O), the stretching vibrations of C=N and C=O are strongly coupled due to the different double bond sharing the central C atom, resulting in two split bands around 2220 and 1250 cm^{-1} [56]. The absorption peak at 2220 cm^{-1}, with high intensity, is considered to be the antisymmetric stretching vibration (ν_{as}) of the isocyanate group. Due to the lower stretching vibration frequency of C=N compared to C=O, the C=O stretching vibration component is more pronounced after coupling. The absorption peak at around 1250 cm^{-1} represents the symmetric stretching vibration (ν_{sym}) of the isocyanate group, with a predominant contribution from the C=N stretching vibration. Due to the presence of Fermi resonance, the symmetric stretching vibration peak (ν_{sym}) splits into 1305.5 and 1214.9 cm^{-1}.

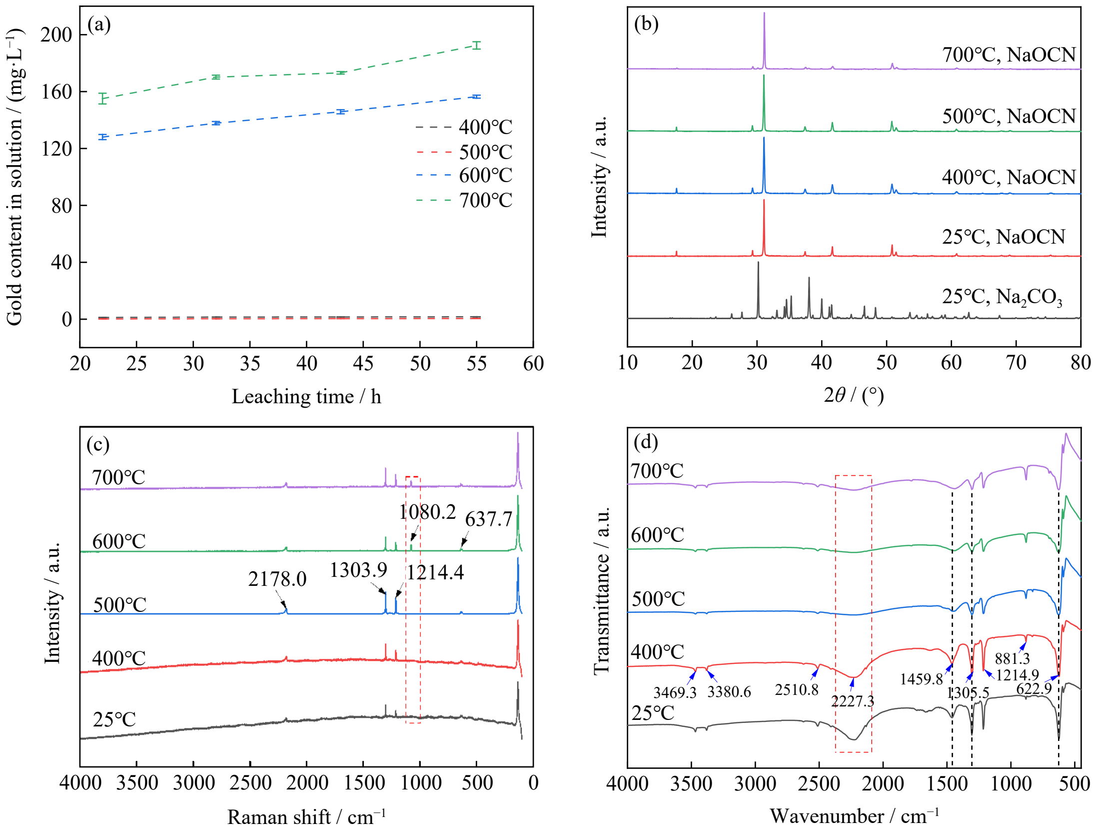

Fig. 1. Characterization results of compounds synthesized at different temperatures: (a) leaching results; (b) XRD patterns; (c) Raman spectra; (d) infrared spectra.

Additionally, the infrared absorption peaks at 1305.5 and 1214.9 cm^{-1} weaken. However, the infrared absorption peak at 881.3 cm^{-1} gradually strengthens. These experimental results indicate the formation of new compounds during the synthesis process of sodium cyanate. The infrared spectrum is a molecular vibration spectrum, and its production condition is that coupling occurs between infrared light and molecules when the dipole moment changes during molecular vibration. Therefore, observable infrared absorption only occurs when there is a change in the dipole moment due to molecular vibration, and this change is closely linked to the inherent dipole moment of the molecule itself. Consequently, molecules with higher symmetry exhibit smaller changes in dipole moment during vibration, resulting in weaker infrared absorption peaks. Conversely, molecules with greater polarity undergo more significant changes in dipole moment during vibration, leading to stronger infrared absorption peaks. For instance, the isocyanate group (–N=C=O) has stronger symmetry compared to the cyanate group (–O–C≡N), causing minimal dipole moment change during vibration and resulting in weaker infrared absorption peaks compared to the cyanate group.

According to the results of the experiments on synthesis using sodium cyanate alone at different temperatures, it can be observed that the synthesis reagent exhibits gold leaching ability when the temperature reaches or exceeds 500°C, and the leaching ability becomes stronger with higher ftemperatures (Fig. 1(a)). Therefore, further exploratory tests were conducted on synthesis time at higher temperatures, and the results are shown in Fig. 2. From Fig. 2(a), it can be seen that at 750°C, with the increase in synthesis time, the leaching ability of the reagent gradually decreases. When the synthesis time reaches 3 h, the synthesis reagent loses its gold leaching ability. The effective component measured by the argentometry decreases gradually with the increase in synthesis time. The XRD patterns (Fig. 2(c)) and infrared spectrogram (Fig. 2(d)) results of the synthesized reagent indicate that with the extension of the synthesis time, the reagent gradually transforms into sodium carbonate. It is well known that sodium carbonate does not have the ability to leach gold. Literature reports [57] that sodium cyanate decomposes into sodium carbonate, sodium cyanide, carbon dioxide, and nitrogen gas under the catalysis of nickel and iron at 700°C in a vacuum, as shown in reaction (2). This suggests that if the chemical reaction shown in reaction (2) occurs, there should be a large amount of cyanide present in the synthesized reagent, especially under the condition of a synthesis time of 180 min. However, according to the gold leaching ability test results in Fig. 2(a), the reagent does not possess gold leaching ability at a synthesis time of 180 min. Additionally, the occurrence of the chemical reaction shown in reaction (2) requires a vacuum condition, indicating that the effective component of the reagent is not cyanide. Therefore, the sodium carbonate in the reagent comes from the reaction of sodium cyanate and sodium isocyanate with oxygen, and the chemical reaction occurs as shown in reactions (3) and (4).

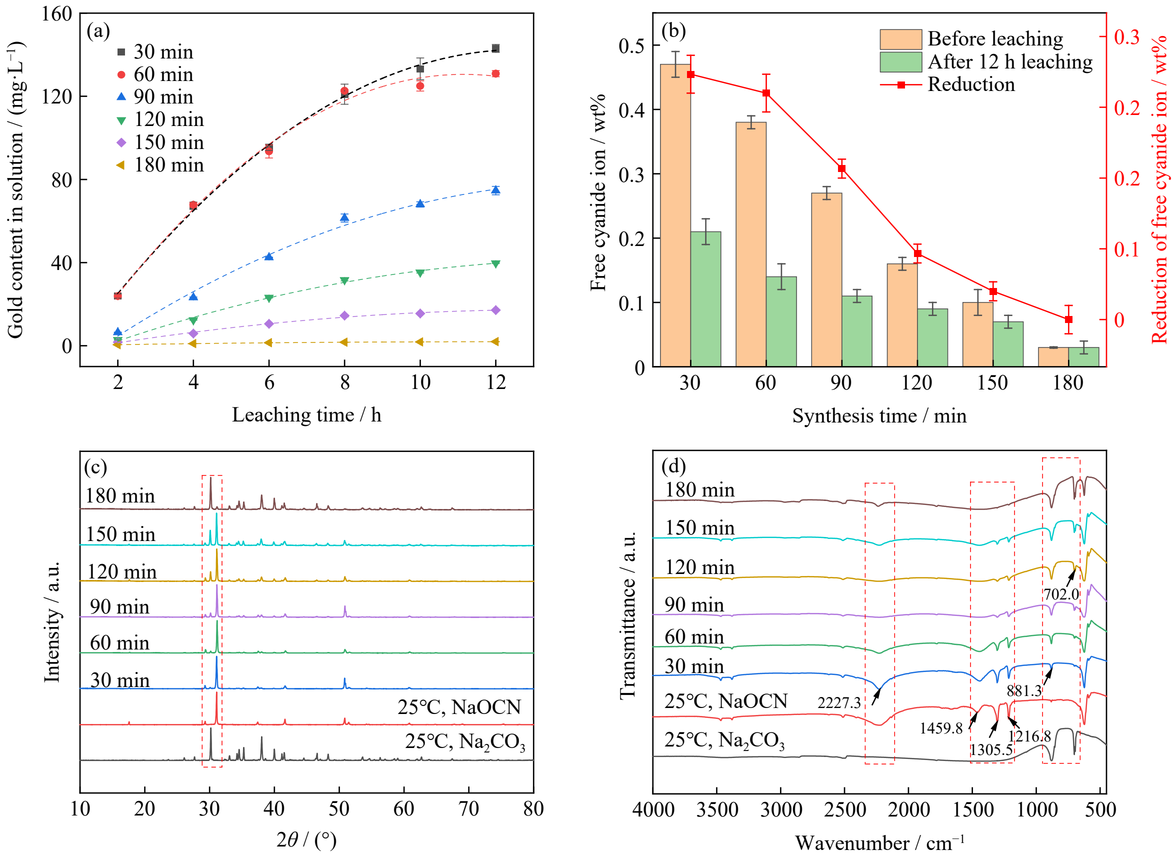

Fig. 2. Results for different synthesis time periods at 750°C: (a) gold content in solution at different leaching time periods; (b) change of free cyanide ion; (c) XRD patterns; (d) infrared spectra.

$$5NaOCN(s) \rightarrow Na_2CO_3(s) + 3NaCN(s) + CO_2(g) + N_2(g) \tag{2}$$

$$4NaOCN(s) + 3O_2(g) \rightarrow 2Na_2CO_3(s) + 2CO_2(g) + 2N_2(g) \tag{3}$$

$$4NaNCO(s) + 3O_2(g) \rightarrow 2Na_2CO_3(s) + 2CO_2(g) + 2N_2(g) \tag{4}$$

To explore the gold leaching capability of synthesis reagents at relatively low temperatures, the gold leaching capability of sodium cyanate reagents at 600°C with different synthesis time periods was tested. From Fig. 3(a), it can be observed that at a synthesis temperature of 600°C, the gold leaching capability of the synthesis reagent initially increases and then decreases with prolonged time. When the synthesis time is 60 min, the reagent exhibits the strongest gold leaching capability. UV–visible light testing was conducted on the solution before and after gold foil dissolution, as shown in Fig. 3(b) and (c). The experimental results show that regardless of the change in synthesis time, two new absorption peaks appear at 229 and 239 nm in the solution after gold foil dissolution. The intensity of these absorption peaks is consistent with the gold concentration in the solution. These two UV absorption peaks are attributed to the formation of coordination compounds between the reagent and gold.

3.2. Influence of additive types on the synthesis of reagents

First, the effects of sodium carbonate and sodium hydroxide as additives on the leaching ability of the reagent were tested at different temperatures, as shown in Fig. 4. According to the results in Fig. 1(a), When there is no sodium hydroxide or sodium carbonate in the synthetic raw material, the higher the synthesis temperature, the stronger the leaching ability after 1 h of synthesis. However, when sodium carbonate or sodium hydroxide was added, the leaching ability of the reagent at 600°C was found to be higher than that at 700°C (Fig. 4(a) and 4(c)). Additionally, the effect of sodium hydroxide was better than that of sodium carbonate. After 55 h of leaching of gold foil, the gold concentration in the reagent solution with sodium hydroxide added at 600°C reached as high as 300 mg/L, while with sodium carbonate added, it was only 92 mg/L. This indicates that an alkaline environment can enhance the leaching ability of the reagent, and the stronger the alkalinity, the more significant the effect.

Under the addition of different alkalis, the infrared spectra of the synthesized reagent (Fig. 4(b)) showed the same phenomenon. With the increase in temperature, the absorption peak at 2227.3 cm^{-1} representing cyanide ions gradually disappeared, while absorption peaks appeared at 881.3 and 702 cm^{-1}. The XRD patterns of the reagent synthesized with sodium hydroxide (Fig. 4(d)) shows that the addition of alkali promotes the formation of the new substance, and its diffraction peak is 30°. Literature studies have indicated that sodium hydroxide can facilitate the generation of the isothiocyanate group [58]. Notably, the oxygen atom in the isocyanate group and the sulfur atom in the isothiocyanate group both belong to group VI A elements. As a result, sodium hydroxide can also support the formation of sodium isocyanate. Astronomers found that sodium cyanate and sodium isocyanate formed in the star-forming region, while sodium hydroxide was also found in this region, so they thought that sodium isocyanate may be formed by sodium hydroxide reacting with cyanide radicals or cyanogen gas [59]. Based on the experimental observations and the characterization results of the reagent, it is inferred that the effective leaching component in the reagent is sodium isocyanate. Sodium cyanate melts at above 550°C, and the molten state facilitates the transfer of electrons, leading to linkage isomerism of the π bond in sodium cyanate, changing the triple bond into a polymerized double bond structure. This is consistent with the above test results.

In addition to the influence of alkali on the conversion of sodium cyanate, the effects of reducing agents represented by iron powder and oxidizing agents represented by ferric chloride on the synthesized reagent were tested. The experimental results are shown in Fig. 5. A small amount of iron powder helps improve the gold leaching ability of the reagent. When the mass ratio of sodium cyanate to iron powder is 100:1, the reagent exhibits the best gold leaching ability (Fig. 5(a)). As the amount of iron powder increases, sodium cyanate gradually converts into other substances predominantly composed of sodium carbonate (Fig. 5(b) and (c)), resulting in a decrease in the gold leaching ability of the corresponding reagent. However, after the addition of ferric chloride, two ab-

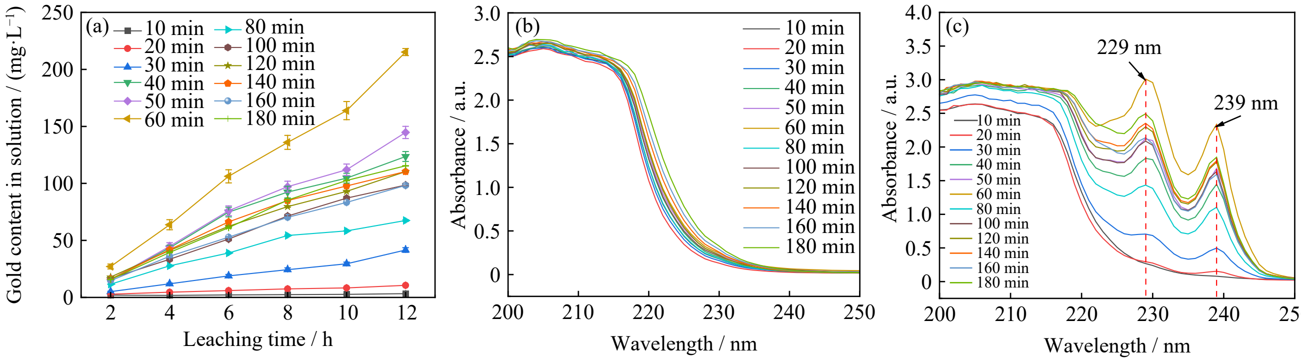

Fig. 3. Results for different synthesis time periods at 600°C: (a) gold content in solution for different leaching time periods; (b) UV–visible spectra of the reagents before gold foil leaching; (c) UV–visible spectra of the reagents after gold foil leaching.

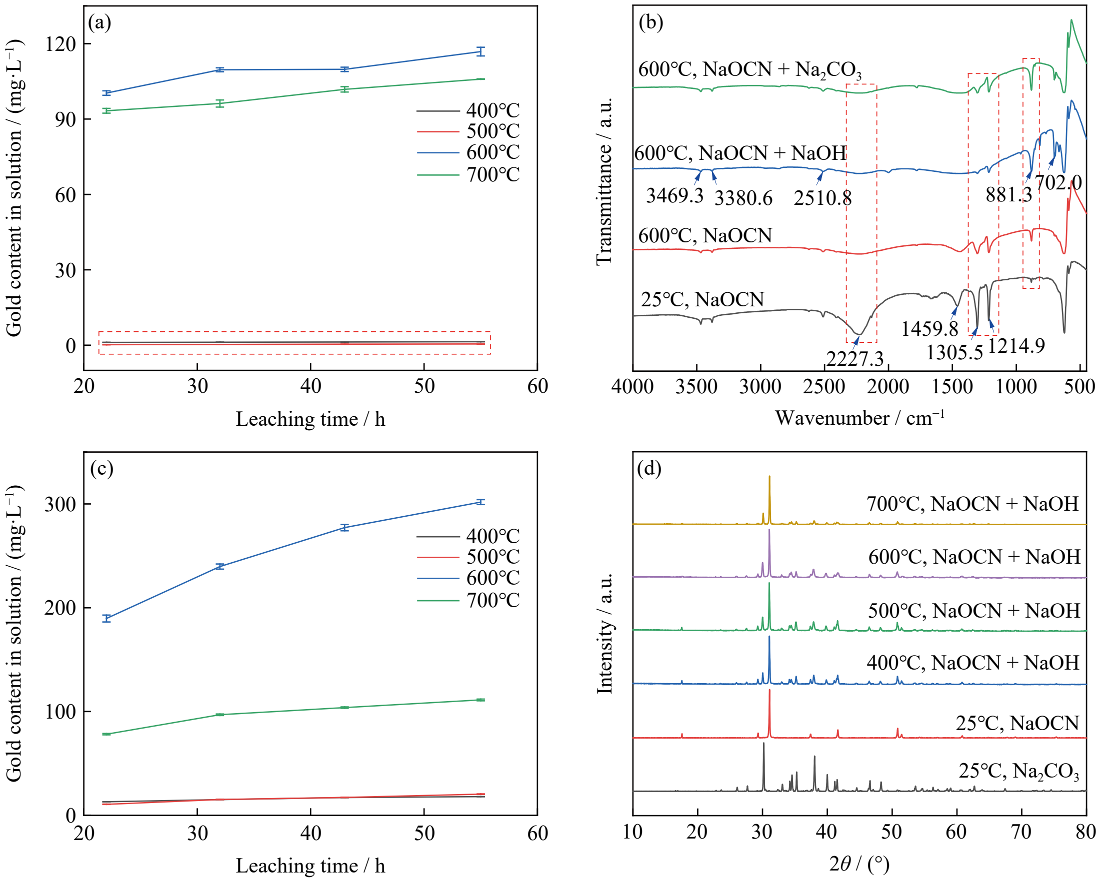

Fig. 4. Characterization results of synthetic reagent with a mass ratio of sodium cyanate to additive of 10:3: (a) gold leaching ability after adding sodium carbonate; (b) infrared spectra of different additives; (c) gold leaching ability and (d) XRD patterns of the reagent after adding sodium hydroxide.

sorption peaks appear at 229 nm and 239 nm after leaching the gold foil (Fig. 5(e) and (f)). The intensity of these absorption peaks decreases with increasing dosage of ferric chloride. The generation of these two absorption peaks is caused by the coordination compounds formed between the reagent and gold. In general, the addition of ferric chloride reduces the gold leaching ability of the reagent (Fig. 5(d)).

In addition to iron powder and ferric chloride, the effects of other additives such as sodium ferrocyanide, ferric oxide, manganese dioxide, potassium ferrocyanide, and potassium ferricyanide on the gold leaching ability of the synthesized reagent were tested. The experimental results are shown in Fig. 6. Iron salts (sodium ferrocyanide, potassium ferrocyanide, and potassium ferricyanide) greatly improve the gold leaching ability of the reagent, while other additives such as manganese dioxide and ferric oxide show minimal improvement in the reagent's gold leaching ability (Fig. 6(a)). An interesting phenomenon is that the reagent synthesized by adding only sodium ferrocyanide does not exhibit significant gold leaching ability, but when sodium hydroxide is added, the gold leaching ability of the synthesized reagent significantly improves. In conclusion, the additives sodium ferrocyanide and sodium hydroxide have a significant impact on enhancing the gold leaching ability of the synthesized reagent. Therefore, sodium ferrocyanide and sodium hydroxide are selected as the additives for the synthesized reagent.

3.3. Effects of additive dosage on the synthesized reagent

Based on experiments with different additive types, sodium ferrocyanide and sodium hydroxide have a promoting effect on the gold leaching performance of the reagent. Experiments were conducted to determine the optimal dosage of sodium hydroxide and sodium ferrocyanide, and the results are shown in Fig. 7. The best gold leaching effect of the synthesized reagent is achieved when the mass ratio of sodium cyanate to sodium hydroxide is 3:1. The gold leaching ability of the synthesized reagent significantly decreases when the mass ratio is less than 3 (Fig. 7(a)). According to the XRD spectra (Fig. 7(b)) and infrared spectra (Fig. 7(c)) of the reagent, a change in the main phase of the synthesized reagent occurs when the mass ratio of sodium ferrocyanide to sodium hydroxide is less than 3. When the mass ratio is 1.2, the main component of the synthesized reagent is sodium carbonate, which is the reason for the decrease in gold leaching ability.

The effect of sodium ferrocyanide addition on the gold solubility of the reagent is shown in Fig. 7(e), sodium ferrocyanide can enhance the gold leaching ability of the reagent to varying degrees. However, when the mass ratio of sodium cyanate, sodium hydroxide, and sodium ferrocyanide is 15:3:1, the gold leaching ability of the reagent is significantly stronger compared to other conditions. The XRD spectra of the reagent (Fig. 7(d)) shows a shift of the main peak of

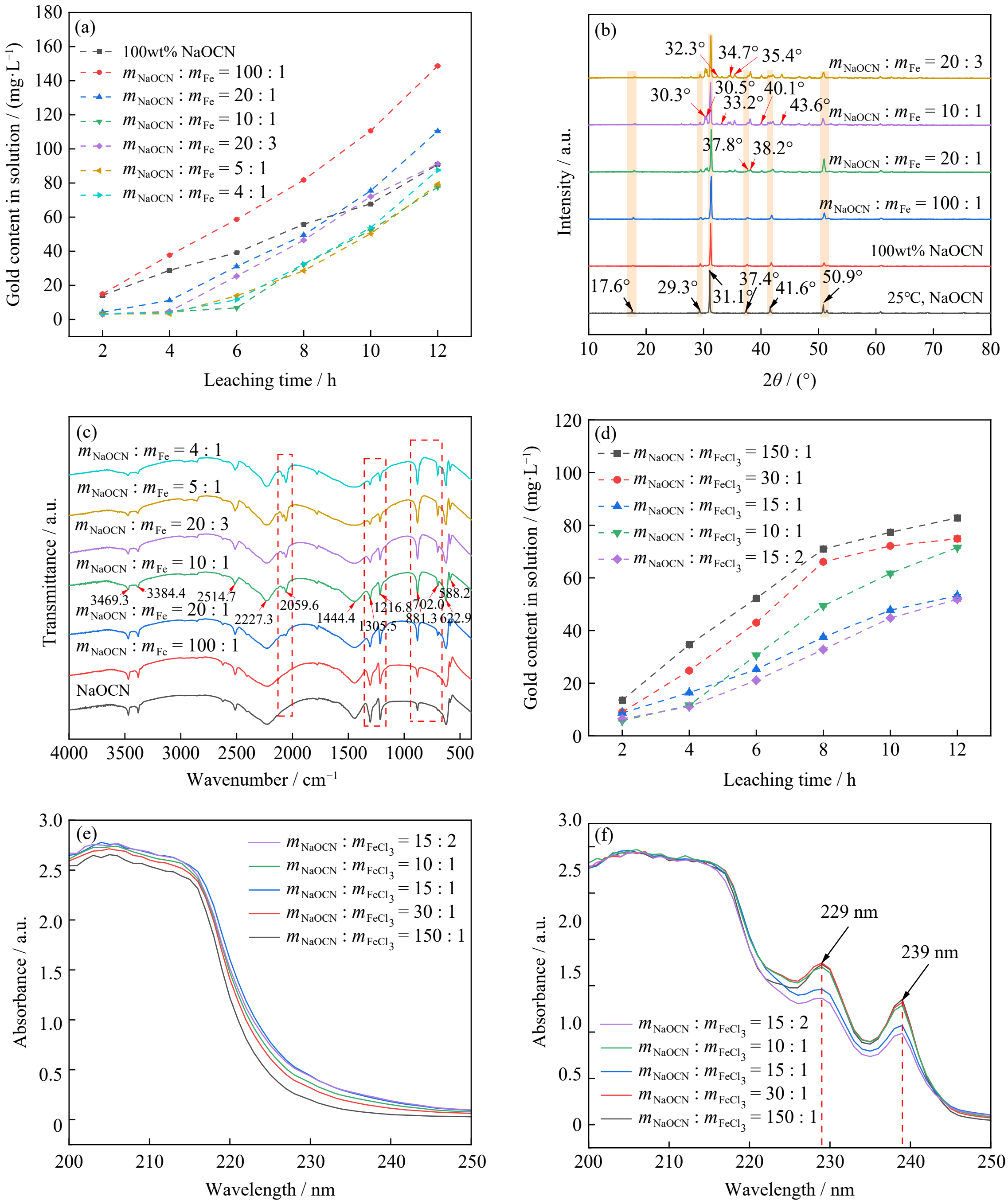

Fig. 5. The results of characterization of different additives of iron: (a) results of gold leaching ability of different proportion of iron powder; (b) XRD patterns; (c) infrared spectrogram; (d) results of gold leaching ability of different proportion of ferric chloride; UV–visible spectra before (e) and after (f) leaching. m_i—Mass of chemical reagent *i*.

sodium cyanate from 31.1° to 31.5°, while the infrared spectra of the reagent (Fig. 7(f)) show no significant change. Based on the experimental results mentioned above, it is speculated that the component in the reagent with gold leaching ability is the isomer of sodium cyanate, known as sodium isocyanate.

3.4. Optimal conditions for reagent synthesis experiment

Based on the experimental results of additives types and dosages, when the mass ratio of sodium cyanate, sodium hydroxide, and sodium ferrocyanide is 15:3:1, and the reagent is synthesis at 600°C for 1 h, the reagent exhibits the strongest gold leaching ability. Under these conditions, the effects of different combinations of synthesized reagents on gold dissolution ability were tested, and the corresponding reagents were characterized. The experimental results are shown in Fig. 8.

From Fig. 8(a), it can be seen that the synthesized reagents have varying degrees of gold leaching ability in the presence of sodium cyanate. When the synthetic raw material is only sodium ferrocyanide, the reagent still has gold leaching ability. According to the XRD spectra (Fig. 8(b)) and Raman spectra (Fig. 8(c)), this is due to the cyanides formed by the high-temperature decomposition of sodium

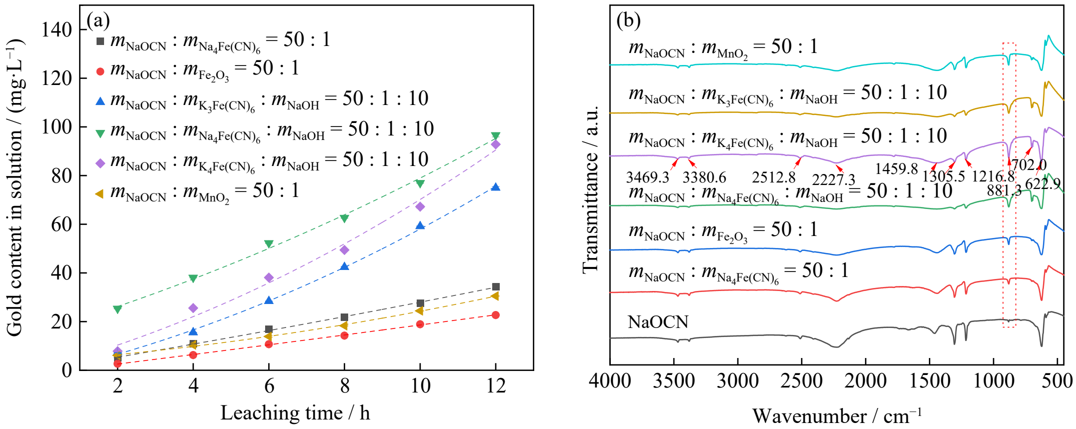

Fig. 6. Effects of different additives on the synthesized reagent at 600°C: (a) experimental results of gold leaching ability; (b) infrared spectrogram.

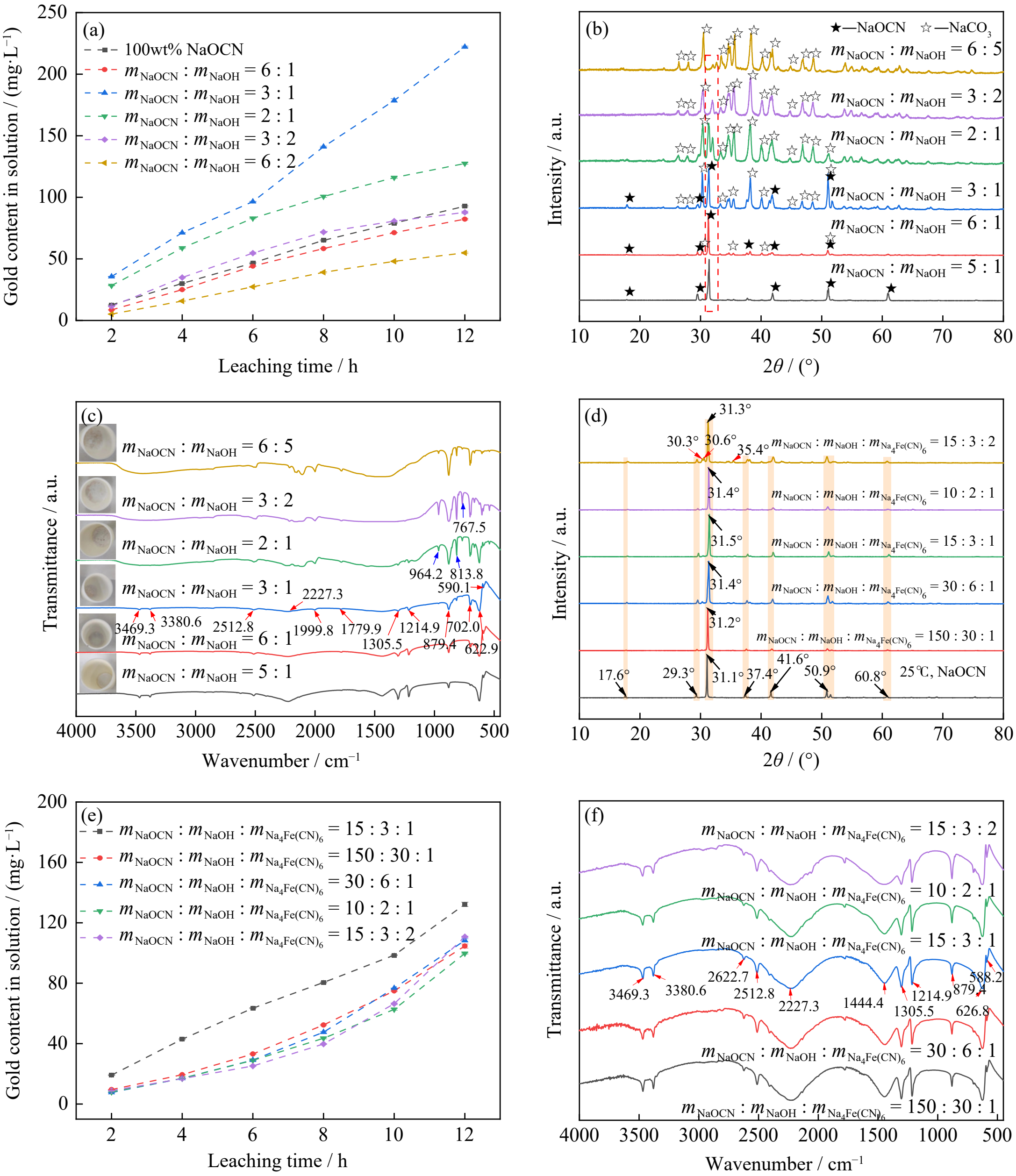

Fig. 7. Characterization of sodium hydroxide and sodium ferrocyanide in different proportions: (a) gold leaching ability results, (b) XRD patterns, and (c) infrared spectra in the presence of sodium hydroxide; (d) XRD patterns, (e) gold leaching ability results, and (f) infrared spectra in the presence of sodium hydroxide and sodium ferrocyanide.

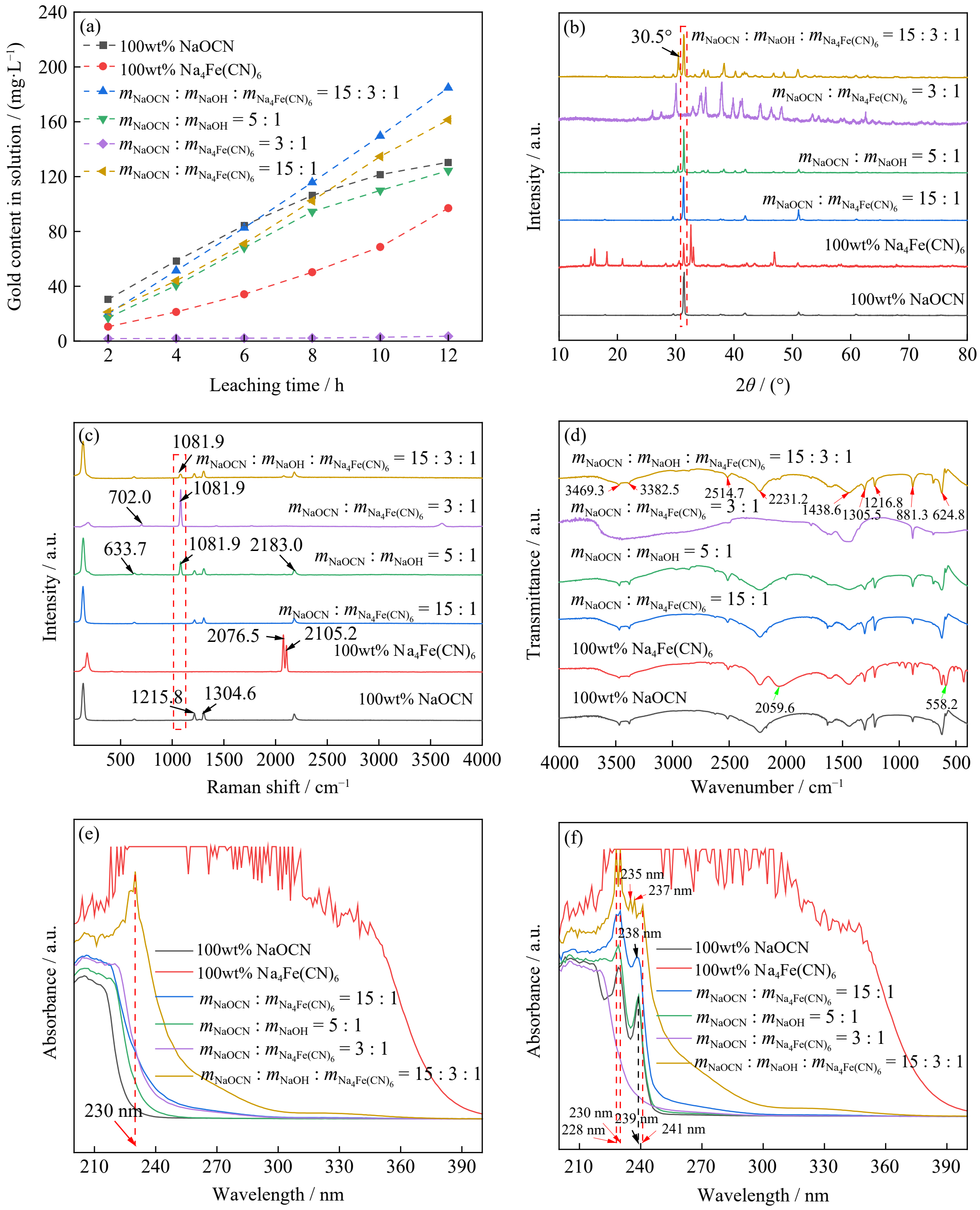

Fig. 8. Experimental results of different combinations under the optimal composition ratio: (a) gold leaching ability results; (b) XRD patterns; (c) Raman spectrogram; (d) infrared spectrogram; (e) and (f) UV–visible spectroscopy before and after leaching.

ferrocyanide. According to the UV–visible spectra before and after dissolving gold foil (Fig. 8(e) and (f)), it can also be observed that the absorption peak position after dissolving gold foil is significantly different from that of other reagents. This indicates a possible chemical reaction as shown in Eq. (1). However, an interesting phenomenon is that the reagent produced by calcining sodium ferrocyanide alone has gold leaching ability, but the reagent produced by the combination of sodium ferrocyanide and sodium hydroxide after synthesis has almost no gold leaching ability. Analysis of the XRD spectra (Fig. 8(b)), Raman spectra (Fig. 8(c)), and infrared spectra (Fig. 8(d)) reveals that no cyanides are generated in the product, and no absorption peak indicating interaction between the reagent and gold is observed in the UV–visible spectra. This indicates that sodium hydroxide can inhibit the decomposition of sodium ferrocyanide.

Another noteworthy phenomenon is that when sodium cyanate, sodium hydroxide, and sodium ferrocyanide are synthesized in a mass ratio of 15:3:1 and subjected to synthesis, the properties of the resulting reagent differ from those of other combinations. From the analysis of the XRD spectra (Fig. 8(b)), a new peak at 30.5° is observed in the reagent. Compared to the Raman spectrum of sodium cyanate (Fig. 8(c)), the reagent synthesized under the optimal ratio shows new peaks at 1081.9 and 2183 cm^{-1}, which attributed to the absorption peak of the isocyanate group. Furthermore, from the UV–visible spectra before and after leaching gold foil (Fig. 8(e) and (f)), it can be observed that the UV absorption peak position and shape of the reagent synthesized under the optimal conditions are different from those of the reagents synthesized under other combinations. This could be due to the reaction of the synthetic agent with gold.

To further validate the synthesis temperature under the optimal ratio, the leaching ability of sodium cyanate, sodium hydroxide, and sodium ferrocyanide with a mass ratio of 15:3:1 was tested at different temperatures, as shown in Fig. 9. The test results indicate that when the synthesis temperature is 500°C, the reagent exhibits weak leaching ability. However, the melting point of sodium cyanate is 550°C, indicating that some sodium cyanate bond isomerization forms sodium isocyanate before reaching the melting point. As the temperature increases to 600°C (Fig. 9(a)), complete melting of the reagent accelerates the isomerization reaction, resulting in the reagent with the highest leaching ability being synthesized under this condition. However, as the temperature continues to rise, the leaching ability of the reagent decreases, which may be attributed to the decomposition of sodium isocyanate caused by high temperature, thereby affecting the leaching ability of the reagent. UV–visible spectrogram of the solution before leaching gold foil with the synthesized reagent (Fig. 9(b)) shows a UV absorption peak at 229 nm for all the reagents, indicating that they have the same chemical structure. However, the UV–visible spectra of the solutions after leaching gold foil show differences (Fig. 9(c)). Except for the reagent synthesized at 900°C, the other reagents exhibit a new peak at 241 nm, which may be due to the formation of a coordination compound between the isocyanate ion and the gold ion.

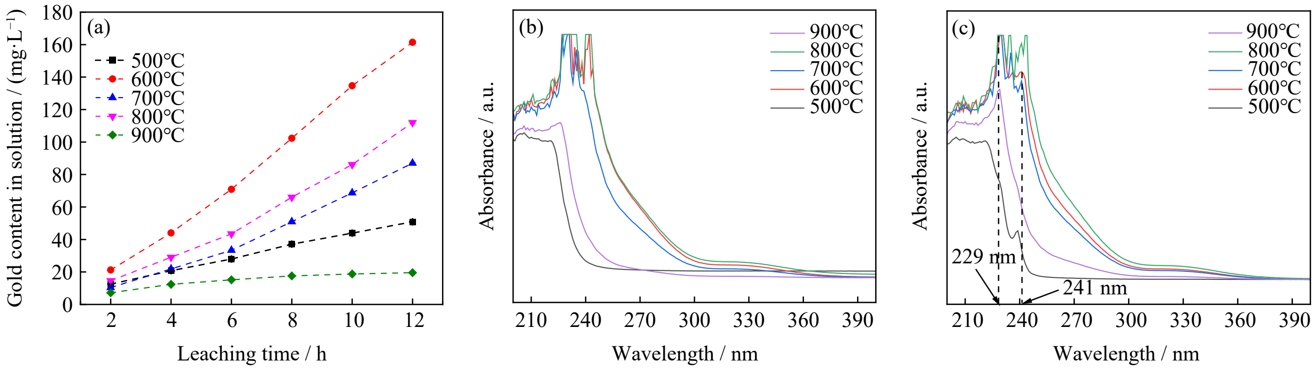

Fig. 9. Synthesis temperature experimental under optimal ratio: (a) gold leaching ability results; (b) and (c) UV–visible spectroscopy before and after leaching.

3.5. Toxicity testing and environmental safety assessment of synthetic reagents

Toxicity testing of the synthetic leaching agent was conducted in accordance with the GB/T 21603—2008 method for acute oral toxicity testing of chemicals, using the Horn method. Forty ICR mice, evenly divided between males and females, were organized into groups and administered samples at doses of 21.5, 46.4, 100.0, and 215 mg/kg, once within a 24-h period, with a gastric intubation volume of 20 mL/kg. Continuous observation was carried out for 14 d, and the test results are presented in Table S3. The results of the test indicate that the synthetic leaching agent has an oral median lethal dose (LD_{50}) 68.1 mg/kg in ICR mice, whereas the LD_{50} value for sodium cyanide is 1–10 mg/kg [17–19], suggesting a toxicity level is much lower than that of sodium cyanide.

In this study, we conducted an environmental safety assessment of gases and solids generated during the reagent synthesis process, with a focus on gases and solids produced during the reagent synthesis process, as well as liquids and residues generated during the leaching process. Sodium cyanate was used as the main synthetic raw material, supplemented with small amounts of sodium hydroxide and sodium ferrocyanide as catalysts. The synthesis process generates minimal waste gas, with only sodium carbonate, carbon dioxide, and nitrogen produced under excess reaction conditions. These gases are predominantly atmospheric constituents with low concentrations, thus posing no significant impact on the atmosphere. Additionally, efficient gas filtration and purification equipment were installed on the calcination device to prevent incomplete reactions from producing nitrogen oxides and carbon monoxide.

Solid substances produced during the calcination process include cyanates and isocyanates, which have very low toxicity, as well as catalysts such as sodium ferrocyanide, sodium hydroxide, and sodium carbonate. These substances are present in low concentrations and have minimal environmental impact. Sodium ferrocyanide is commonly used as an anti-caking agent in table salt, sodium hydroxide reacts with carbon dioxide in the air to form sodium carbonate, and sodium carbonate is a commonly used weak alkaline substance. Therefore, the solid substances and residues produced during calcination will not adversely affect the environment and can be treated together with the leaching residues.

Gold in the leaching solution is typically recovered using activated carbon adsorption, which also absorbs some harmful substances during the gold adsorption process. Additionally, we neutralize the leaching solution through recycling and chlorination, further reducing its environmental impact. Through these measures, we have effectively minimized the environmental impact, ensuring the environmental friendliness and sustainability of the research process.

3.6. Leaching of gold-bearing materials by synthetic reagent

The synthetic reagent synthesized under the optimal conditions, with a mass ratio of sodium cyanate, sodium hydroxide, and sodium ferrocyanide of 15:3:1, and the synthesis temperature and time of 600°C and 1 h, respectively, was applied for the extraction of gold from the gold concentrate. The experimental results are shown in Fig. S6. It can be observed that when the leaching agent dosage is constant, the gold leaching rate initially increases and then decreases with increasing leaching temperature. When the leaching temperature is 45°C, the gold leaching rate is higher than those at 35 and 55°C. Although a higher leaching temperature favors the leaching reaction of gold, the hydrolysis reaction and evaporation of sodium cyanate accelerate when the leaching temperature exceeds 45°C, resulting in the formation of cyanate and polymerization. Therefore, the gold leaching rate at 55°C is consistently lower than 10%. When the reagent dosage is 3000 g/t, the gold leaching rates at 35, 45, and 55°C are 49.9%, 66.15%, and 4.42%, respectively. Further increasing the reagent dosage does not effectively enhance the gold leaching rate.

The gold leaching rate of gold concentrate increases slowly with the decrease of leaching concentration (Fig. S6(b)). When the liquid-to-solid ratio is 3:1, the gold leaching rate is the highest. Further reducing the leaching concentration does not affect the gold leaching rate. Within the range of agitation speed from 120 to 180 r/min, the gold leaching rate increases with increasing agitation speed. Further increasing the agitation speed has no significant effect on the gold leaching rate.

As shown above, under the conditions of leaching temperature of 45°C, liquid-to-solid ratio of 3:1, reagent dosage of 3000 g/t, and agitation speed of 180 r/min, the maximum gold leaching rate from the high-sulfur gold concentrate can reach 66.15%. However, there is still 33.85% of gold unrecovered. Based on the analysis of process mineralogy, the gold encapsulated content accounts for 55.3%, with 41.2% of gold encapsulated in sulfide minerals. Although regrinding of the gold ore dissociates some of the encapsulated gold particles, a significant amount of gold remains undissociated. Therefore, it is necessary to perform roasting desulfurization treatment on the high-sulfur gold concentrate. The roasting temperature for the high-sulfur gold concentrate is 750°C, and the roasting time is 1 h. Air is continuously introduced during the roasting process, and the generated sulfur dioxide gas is discharged.

The leaching behavior of the roasted gold concentrate follows the same trend as before roasting (Fig. S7). However, compared with the gold concentrate before roasting desulfurization, the gold leaching rate is obviously higher. When the reagent dosage is 3000 g/t, the gold leaching rates at 35, 45, and 55°C are 83.01%, 87.56%, and 34.72%, respectively. The results of the liquid-to-solid ratio and agitation speed experiments show the same trend as before roasting. Therefore, under the optimal leaching conditions, namely a leaching temperature of 45°C, liquid-to-solid ratio of 3:1, reagent dosage of 3000 g/t, agitation speed of 180 r/min, and roasting of the gold concentrate at 750°C for 1 h, the gold leaching rate can be increased from 66.15% to 87.56%. This indicates that the reagent can effectively recover gold from the gold concentrate.

To evaluate the process economics and efficiency of the synthesized reagent for this ore, we conducted a cost analysis, revenue analysis, and economic feasibility analysis. The price of gold is calculated at the current rate of 560 RMB per gram, and the leaching rate of gold after roasting has increased by 21.41 percentage points, so 9.79 grams of gold can be extracted per ton of ore, equivalent to 5482.4 RMB. Energy costs were calculated at an average rate of 0.85 RMB/kWh. The results are shown in Table S4. Given the current high price of gold, the economic benefits are significant. After deducting material costs, energy costs, labor, and other expenses, the profit per ton is 4057.53 RMB.

In this study, the raw material utilization rate exceeded 95%, and the energy utilization rate reached over 80%. By improving the calcination process, the gold leaching rate increased from 66.15% to 87.56%. Further improvements in raw material handling and leaching conditions are expected to enhance gold leaching rates even more. The recycling rate of the leaching solution reached 90%, significantly reducing environmental impact. The equipment utilization rate was 85%. Overall, this process demonstrates high efficiency.

In order to investigate the leaching effect of the synthetic reagent under optimal conditions on gold-plated electronic waste, three different types of gold-containing electronic waste were studied, and the experimental results are shown in Fig. S8. The gold in all three types of electronic waste can achieve a leaching rate of over 90% within 2 h of leaching, and the gold leaching rate is significantly higher than that of other metals during the leaching process. It is worth noting that for copper-containing electronic waste (Fig. S8(a) and (b)), copper is leached to some extent, but its leaching rate is much lower than that of gold, and the leaching rate of copper gradually increases only after the leaching of gold is completed. The iron content in the leachate of the three types of electronic waste is approximately 17 mg/L, and the concentration of iron in the solution does not change over time. This indicates that the iron in the solution is due to the presence of sodium ferrocyanide in the reagent, rather than iron being leached from the electronic waste. Another piece of evidence is that the iron concentration in the gold-plated quartz chips is also about 17 mg/L (Fig. S8(c)), while there is no iron in the gold-plated quartz chips. After 12 h of leaching, the gold-plated layer in the three types of electronic waste was completely stripped (Fig. S8(d)), and the gold leaching rates reached 98.89%, 99.19%, and 99.88% respectively.

The relatively lower leaching rate of other metals in electronic waste by synthetic reagents may be attributed to the gold plating on the surfaces of these metals. Therefore, individual metals were used to verify the solubility of synthetic reagents to these metals, the experimental results are illustrated in Fig. S9.

From Fig. S9, it is evident that the reagent demonstrates superior leaching efficiency for copper-group metals compared to other metals. Among the copper-group metals, the leaching efficiency for gold surpasses that for silver and copper. Another noteworthy observation is that, under identical leaching conditions, an increase in leaching temperature hinders gold leaching. This contrasts with the general expectation that higher temperatures facilitate metal leaching in typical leaching reactions. The occurrence of this phenomenon is attributed to the more pronounced hydrolysis reaction of sodium isocyanate at elevated leaching temperatures, as illustrated in Eq. (5).

$$2NCO^{-}(aq) + 3H_2O(l) \rightarrow CO_3^{2-}(aq) + 2NH_3(g) + CO_2(g) \tag{5}$$

3.7. Mechanism analysis

The experimental procedure is shown in Fig. 10. The gold in the leaching solution can be extracted by adsorption on activated carbon or by zinc displacement. Then, the gold can be obtained by smelting after the extraction process. The active ingredient in the reagent is the isocyanate anion. Isocyanic acid (HNCO), cyanic acid (HOCN), and fulminic acid (HCNO) are isomers with different structures. Among these three structures, the isocyanate anion and fulminate anion satisfy the conditions for forming coordination compounds with gold, as they can provide lone pair electrons and accept π electrons. However, the cyanate ion does not meet these conditions. In fact, the cyanate ion does not possess the ability to dissolve gold. For example, in cyanide leaching process, the treatment of wastewater containing cyanide ions usually involves adding hypochlorite to oxidize cyanide ions into cyanate ions with low toxicity.

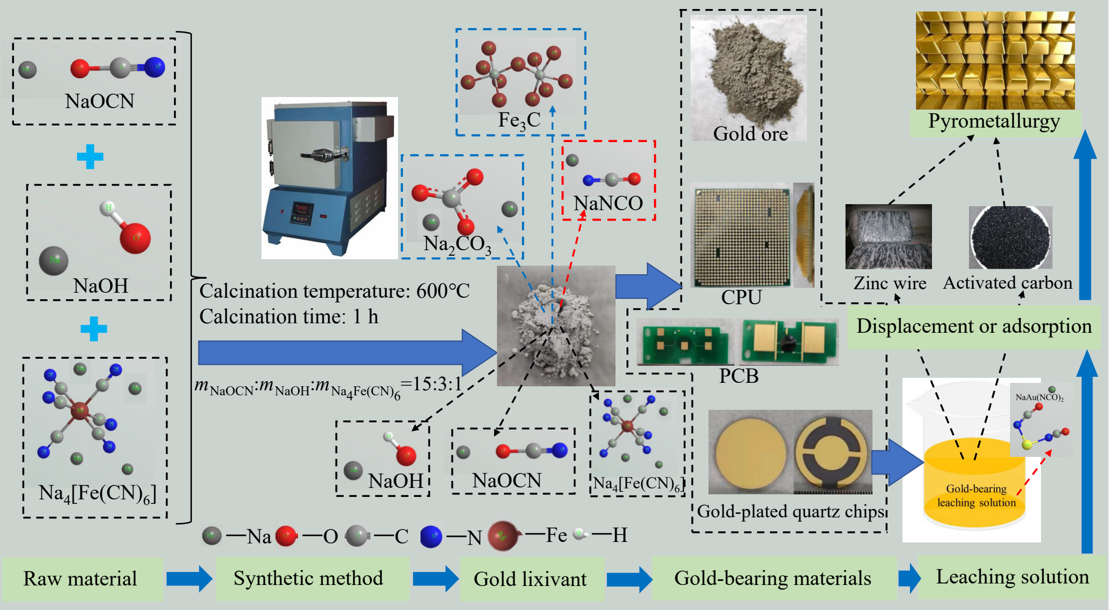

Fig. 10. Schematic diagram of synthesis and gold leaching process for gold leaching reagent.

The gold-leaching capabilities of thiocyanate (MSCN) have been confirmed in practical production, whereas cyanate salts (MOCN) in group VI A do not possess gold-leaching abilities. Researchers generally attribute this difference to the sulfur atom in the thiocyanate group, which is in the third period and has an empty d orbital in its valence layer. This allows it to form a *d–d* feedback π bond with gold, whereas the oxygen atom, which is in the second period and lacks a valence layer d orbital, cannot effectively interact with gold. However, it's important to note that the thiocyanate group has a bonding isomer known as the isothiocyanate group, which not only forms a *d–d* feedback π bond with gold but also creates a d–π^* feedback π bond. Consequently, the cyanate group within the same chemical family also exhibits the isocyanate structure. Although the use of sodium isocyanate has not been extensively documented in the literature, some researchers have suggested, based on computational chemistry, that the stability of isocyanate (–N=C=O) is greater than that of cyanate (–O–C≡N) [59–61]. Additionally, the coordination ability of isocyanate, with nitrogen as the coordinating atom, is stronger than that of basic glycine, which relies on oxygen as the coordinating atom [62].

The possible bonding mode analysis between the isocyanate anion and gold ion is shown in Fig. S10. The carbon atom in the isocyanate anion forms bonds through sp hybridization. The nitrogen atom and carbon atom each have two lone pairs of electrons and two unpaired p electrons. The nitrogen atom forms a σ bond with the carbon atom through one of its p electrons and the sp hybrid orbital of the carbon atom. The remaining unpaired p electron of the nitrogen atom forms a π bond with the unhybridized p orbital of the carbon atom. Therefore, the structure of the isocyanate anion is characterized by a conjugated double bond, and it is linear in shape.

The possible bonding between the isocyanate anion and the gold ion is illustrated in Fig. S10(b). The empty orbitals of gold’s 6s and 6p are involved in bonding through sp hybridization, while the lone pair electrons on the nitrogen atom in the isocyanate anion fill the hybrid orbitals of gold. The electrons from the gold’s 5d orbitals feed back into the π orbitals of the isocyanate anion, forming a “σ–π” bond, similar to the bonding mode in cyanide compounds.

4. Conclusions

This paper proposes a method for synthesizing a gold leaching reagent, which has been successfully applied to the extraction of gold from gold-containing materials. The main conclusions of the paper are summarized as follows.

(1) Sodium cyanate is used as the main raw material for synthesis, with sodium hydroxide and sodium ferrocyanide as additives. A gold leaching reagent is obtained by synthesis at 600°C for 1 h. The mass ratio of sodium cyanate, sodium hydroxide, and sodium ferrocyanide is 15:3:1.

(2) The synthesized leaching reagent is a mixture, which consists of unreacted raw materials and generated sodium isocyanate, sodium carbonate, and iron carbide. The effective component in the leaching reagent with gold leaching ability is sodium isocyanate. The toxicity of the gold leaching reagent is lower than that of sodium cyanide.

(3) The leaching reagent synthesized under optimal conditions exhibits significant effects on gold concentrates and gold-containing electronic waste. Under the best leaching conditions, the gold leaching rate from high-sulfur gold concentrate can reach 66.15%. After desulfurization by roasting, the gold leaching rate increases to 87.56%. Leaching experiments on three types of gold-containing electronic waste show that under the conditions of leaching temperature of 25°C, agitation speed of 80 r/min, and leaching reagent concentration of 1.5wt%, the leaching agent has significant dissolving effect on gold plating in electronic waste. More than 90% of gold can be dissolved after 2 h of leaching, and the gold leaching rates in the three types of electronic waste can reach 98.89%, 99.19%, and 99.88% after 12 h of leaching, respectively.

(4) The effective gold leaching component in the leaching reagent is sodium isocyanate, whose molecular structure meets the basic requirements of a gold leaching reagent, i.e., it can form a “σ–π” coordination bond. This bonding mode is similar to that of cyanides, thiosulfates, halogens, and other gold-leaching agents with similar structures, indicating that the reagent can replace cyanide as a new gold leaching reagent.

In summary, the gold leaching reagent synthesized in this paper not only simple to prepare but also has remarkable effect on gold leaching. It has broad application prospects and commercial value not only for gold extraction from gold mines but also for gold extraction from electronic waste.

Acknowledgement

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Ethics declarations

The animal experiment was conducted by Shanghai Micro-spectrum Detection Technology Group Co., Ltd. The experimental mice were from Shanghai Shengchang Biotechnology Co., Ltd. The animal experiment production license: SCXK (Shanghai) 2021-0002; Quality Certificate: 20210002004851; Experimental animal use license: SYXK (Shanghai) 2021-0023. All animal experiments complied with the National Research Council’s Guide for the Care and Use of Laboratory Animals.

Conflict of Interest

Chunbao Sun is an editorial board member for this journal and was not involved in the editorial review or the decision to publish this article. The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Supplementary Information

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