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# Synthesis of Naphthalen-2-yl 2-thiocyanatoacetate and Its Application as a Selective Photometric Reagent for Ni(II) Detection

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## INTRODUCTION & AIM

The detection of metal ions, particularly heavy metals that are widely encountered in environmental and industrial processes, occupies an important place in modern analytical chemistry. Nickel (Ni) ions are extensively used in technological processes such as catalysts, alloys, electroplating, and various other applications. However, excessive bioaccumulation of nickel poses significant ecological and toxicological challenges. Elevated concentrations of Ni(II) ions can cause dermatological allergies, respiratory diseases, lung cancer, and other health hazards. Therefore, the development of fast, reliable, selective, and cost-effective methods for Ni(II) determination remains one of the urgent scientific and technical tasks.

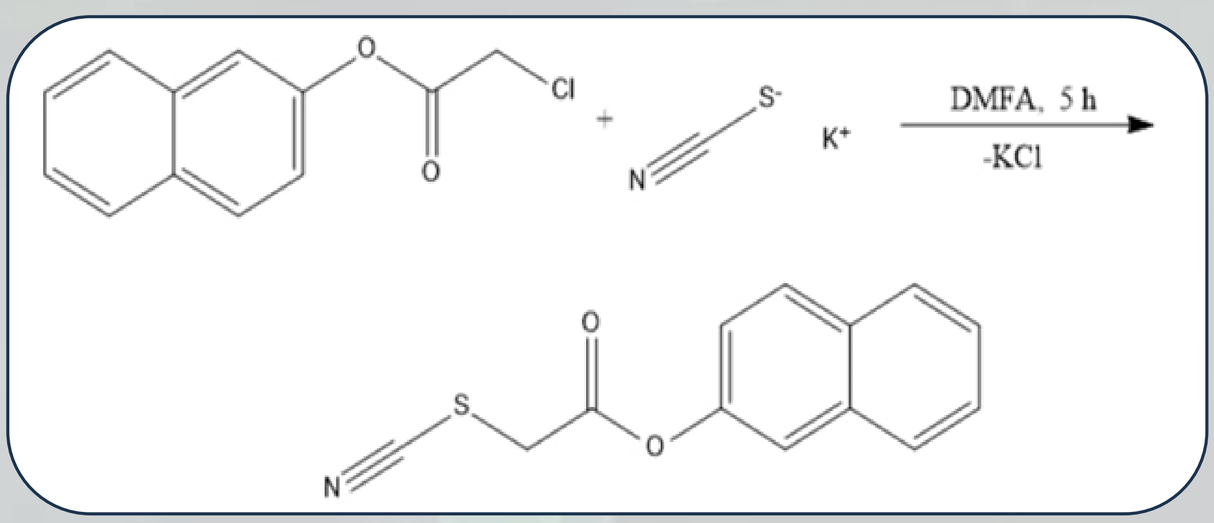
Currently, various advanced techniques are employed for the determination of nickel ions, including atomic absorption spectroscopy (AAS), inductively coupled plasma–optical emission spectroscopy (ICP-OES), voltammetry, and ion chromatography. Although these methods offer high sensitivity, they require expensive instrumentation, skilled operators, and considerable analysis time. In contrast, photometric detection methods are particularly attractive due to their simplicity, rapid execution, low cost, and suitability for a wide range of laboratory conditions.

This research also has an environmental significance. Ni(II) ions are predominantly present in the effluents of metallurgy, electrochemical, and chemical industries; hence, their rapid and inexpensive detection is crucial for effective environmental monitoring

## METHOD

The progression of the reactions and the purity of the synthesized products were monitored by thin-layer chromatography (TLC). The analyses were performed on silica gel 60 F254 aluminum-backed plates (MERCK, India), with a chloroform–ethyl acetate mixture (10:0.3, v/v) serving as the mobile phase. Spot detection was carried out under UV light at 254 nm. Crude reaction products were purified by column chromatography using petroleum ether–ethyl acetate as the eluent. After purification, TLC was repeated to ensure complete separation of components. Upon completion of each reaction, the mixture was quenched by pouring into ice-chilled water, and the resulting solids were isolated via vacuum filtration and subsequently air-dried. Fourier-transform infrared (FT-IR) spectra were recorded on a Specord IR-71 instrument using KBr pellet discs. Nuclear magnetic resonance (NMR) spectra were acquired on a Bruker 400 MHz spectrometer, with tetramethylsilane (TMS) as an internal reference; all chemical shifts are given in ppm. Melting points were measured in open capillaries using an Mvtec melting point apparatus, and the reported values are uncorrected .

**Preparation of Solutions.** a) In this study, a fresh 0.1% solution of *naphthalen-2-yl 2-thiocyanatoacetate* was prepared by accurately weighing 0.25 g of the compound, transferring it into a 250 mL volumetric flask, and dissolving it in distilled water up to the mark. b) Initially, a standard solution of nickel(II) was prepared to be used as the working solution. For this purpose, high-purity $Ni(NO_3)_2{\cdot}6H_2O$ salt was used. An accurately weighed amount of the salt (0.9658 g) was placed into a 250 mL volumetric flask and dissolved in distilled water to obtain a 1 mg/mL solution. Working solutions were prepared freshly before each experiment by diluting aliquots taken from the 1 mg/mL standard solution.




*Schematic representation of the synthesis of naphthalen-2-yl 2-thiocyanatoacetate via nucleophilic substitution of naphthalen-2-yl 2-chloroacetate with potassium thiocyanate in dimethylformamide (DMF).*

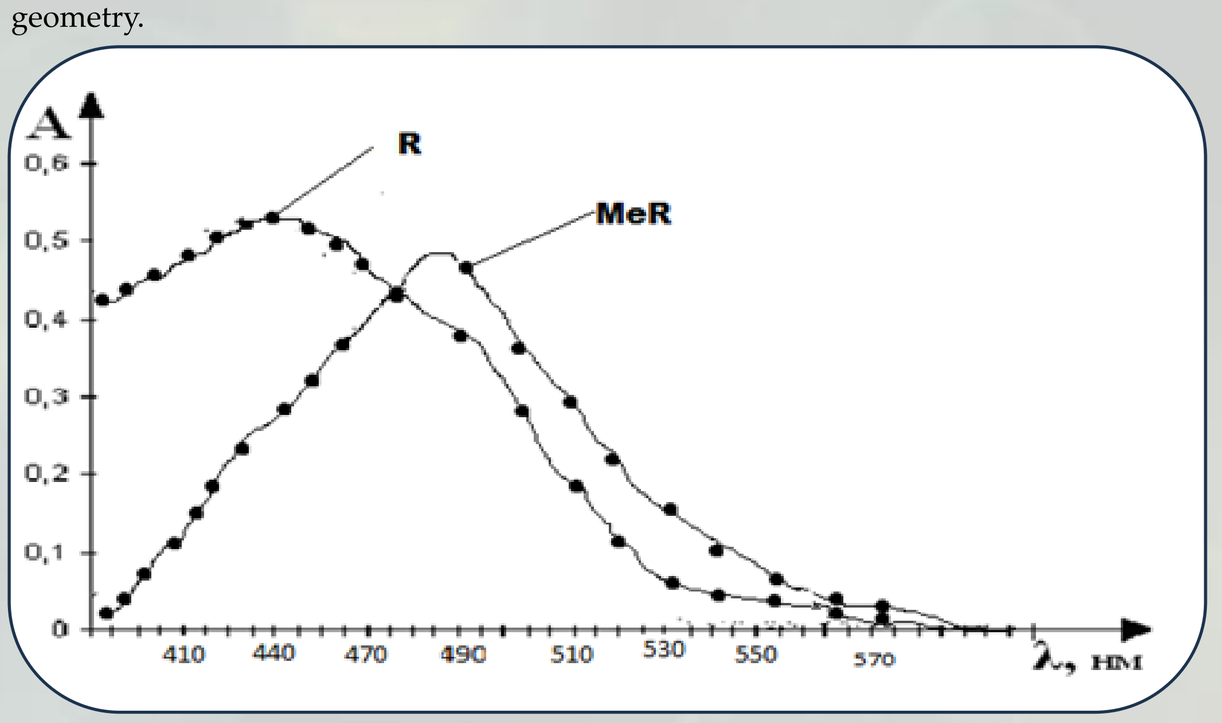
## RESULTS & DISCUSSION

The synthesis of *naphthalen-2-yl 2-thiocyanatoacetate* was accomplished via a nucleophilic substitution reaction of *naphthalen-2-yl 2-chloroacetate* with potassium thiocyanate (KSCN) in dimethylformamide (DMF) as the reaction medium. The transformation proceeds predominantly through a bimolecular nucleophilic substitution (SN2) pathway, which is facilitated by the use of a polar aprotic solvent and elevated temperature.

Upon coordination with Ni(II) ions, a distinct shift in the absorption maximum toward longer wavelengths (red shift) is observed. The Ni(II)–ligand complex (MeR) shows a new absorption maximum in the region of 490–500 nm, with an absorbance value close to that of the free ligand (A ≈ 0.50). The bathochromic shift is indicative of electronic structure reorganization caused by complex formation, most likely involving ligand-to-metal charge transfer (LMCT) as well as d–d transitions within the Ni(II) coordination sphere.

The observed spectral changes confirm the successful formation of a stable Ni(II)–ligand complex. The red shift of λmax to approximately 490 nm provides a distinct analytical advantage, as it offers a spectral window with minimal interference from the free ligand, thereby improving measurement selectivity. This wavelength was therefore selected as the optimal analytical wavelength for all subsequent photometric determinations.

These results are in agreement with previous findings on thiocyanate-based ligands, where coordination with transition metal ions results in significant bathochromic shifts due to alterations in the ligand's electron density distribution and coordination geometry.




**Absorption spectra of naphthalen-2-yl 2-thiocyanatoacetate reagent (R) and its complex with nickel (II) (MeR).**

The Ni(II)–*naphthalen-2-yl 2-thiocyanatoacetate* complex shows a reddish-green color with a maximum absorption at **490 nm** (Δλ = 50 nm compared to the free reagent), optimal at **pH 6.55**. Using 35 μg Ni(II) ($5.96 \times 10^{-4}$ mol/L) in a 2.0 cm cell, the method achieves high sensitivity with a Sandell's value of **0.0060 μg/cm²**, indicating suitability for trace nickel determination. Overall, the data confirm that the Ni(II)–naphthalen-2-yl 2-thiocyanatoacetate complex is stable, exhibits a well-defined absorption maximum, and demonstrates high analytical sensitivity, making it suitable for precise photometric determination of nickel ions.

## CONCLUSION

In this work, *naphthalen-2-yl 2-thiocyanatoacetate* was successfully synthesized via a nucleophilic substitution reaction under optimized conditions, and its structure was confirmed by IR and NMR spectroscopy. The synthesized reagent was subsequently applied as a selective ligand for the spectrophotometric determination of Ni(II) ions.

## FUTURE WORK / REFERENCES

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