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# Study of 4-(1*H*-Benzo[*d*] oxazole-2-yl)-2-methoxyphenol for Cyanide Ion Detection

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ABSTRACT

Benzoxazole containing moiety **S3** was productively synthesized and functional for detection of $CN^-$ion. The **S3** moleculealtereditscolourfordarkbrowntodarkgreenonaccumulationofthe$CN^-$iononlyinDimethylSulfoxidesolvent.Thelimitofdetectionand association constant ($K_a$) were $0.4 \times 10^{-6}$ M and $1.0 \times 10^{7}$ $M^{-1}$; and $0.46 \times 10^{-4}$ M and $1.0 \times 10^{5}$ $M^{-1}$ resolute by UV-visible spectroscopic titration and fluorescence titration,correspondingly.

**Benzoxazole, Cyanide ion.**

## INTRODUCTION

Ecologicalcontaminationbyorganicchemicalscontinues tobeoneoftheworld'sleadingchallengestosustainabledevelopment.In current Scenario,thedevelopmentsofopticalchemo-sensors for discerning detection of environmentally important ionic species, such as cyanide ion, have gained attentions in research community.

Cyanide as one of the most lethal anions exists in many naturalsourcesanditsknownasoneofthemostrapidlyacting and powerful poisons, various industrial processes release of cyanidetotheenvironment.Therefore,recognitionanddetection of cyanide have also received significantconsideration. The rationalsynthesisdesignofhighlyselectiveandsensitiveefficient chemo-sensors for $CN^-$anion recognitionhave attracted great attentionduetotheiroperationalsimplicity,goodconvenience, low cost, and excellent selectivity and high sensitivity.

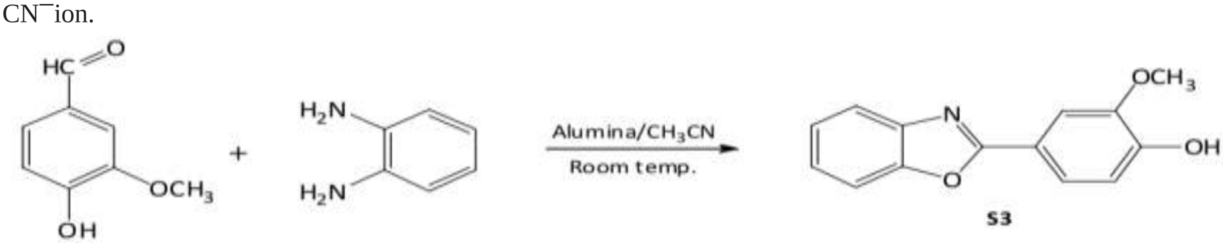
Inpreviousstudy,wedesignedachemo-sensorcompound derivedfrombenzimidazole(S1), whichisactiveasfluorescence receptor and selectively to detect $CN^-$ion. However, S1moleculesuffersfromseveralparameterslikelongresponse time,lowdetectionlimit,*etc*.henceinthisstudy,anewchemo-sensor compound (**S3**) based on benzoxazole molecule is designed and tested for optical properties for detecting the presence of $CN^-$ion.

## EXPERIMENTAL

Meltingpointwasmeasuredusingа IA-9100 (electro thermal apparatus), theInfraredspectrameasuredusingaFTIRspectroscopy, Massspectrawereanalyzedbyusinggaschromatograph-mass spectrometer(GCMS-QP2010S),$^{1}$Hand$^{13}$CNMRweremeasured using a JOEL JNM ECA-500 MHz while fluorescent was conducted using a Spectroflourophotometer

All the solvents and materials obtained commercially in this work were of analytical purity grade quality and used without further purification. The anions wereadded intheformofsodiumcyanide,sodiumfluoride,sodiumiodide, sodiumdihydrogenphosphate and sodiumbromide.

**Synthesis:** The synthesis procedure for **S3** molecule is adoptedfromReyes*etal*.methodwithsomealterations. Vanillin (1.6 g), 2-aminophenol (1.1 g) and alumina (0.75 g) in25mlacetonitrylwerestirredatroomtemperaturefor4.25hrs. The progress of the reaction was checked with Thin Layer Chromatography, and then the mixture was poured into 300 ml cold distilled water andleft thesolutionatroomtemperaturefor24h.Theprecipitateformed was recrystallized with methanol and then characterized (**Pic.1**). Greenish-brown powder, Yield: 68 %, m.p 178- 180 ºC.




**Pic.1:** Synthesis of benzoxazole containing compound (**S3**)

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## RESULTSANDDISCUSSION

**Ionochromictest:**preliminarytestofmolecule**S3**sensoractivity was performed at concentration of 1 × $10^{-1}$ M Dimethyl Sulfoxide in the presence of several anions ($CN^-$, $F^-$, $Br^-$, $I^-$and $H_2PO_4^-$). Adding 50µLCN⁻in**S3**-Dimethyl Sulfoxidesolutionresultscolour transformtogreen.Moreover,fluorescenceoccursonlyin**S3**-$CN^-$solutionsasindicatedbyUVspectrumatλ366nm,which means that molecule **S3** has a high selectivity for $CN^-$ion.

**UV-visible spectroscopic titration:** The **S3** solution in Dimethyl Sulfoxideat the concentration of 1 × $10^{-6}$ M was brownishclear solutionintheabsenceofions.TitrationofCN⁻ionswiththe **S3**-Dimethyl Sulfoxide was done at the analogous intensityoftheionandsensor.Itisfoundthatthediscolouration of **S3**- Dimethyl Sulfoxidesolution after the addition of 50 µL $CN^-$ions wasoccurred.Theaugmentationincolourcontrastoccurredas the concentration of $CN^-$ionsincrease.

Thedeterminationof**S3**-$CN^-$interactionwasquantitatively preceded by measuring the absorbance of complex solutions usingUV-visiblespectroscopy.TheUV-visiblespectraof**S3** titration with $CN^-$ions is presented in Fig. a. The **S3**solution showstheabsorbanceatλ320nmhavingapeakat390nmin absenceofCN⁻ion.AddingCN⁻resultedtheabsorbance spectra to steadilydiminish, it means that the interactionof**S3**withCN⁻occurs.Thecolourofthesolutionbeing turned to green-yellow was indicated by the appearance of a newpeakatλ420nm.Theisosbesticpeakcreatedat340nm showschemical relations between **S3** and $CN^-$.

**Fluorometry titration:** The fluorescent titrations were carriedataconcentrationof1×$10^{-6}$Msolutionyieldedpoorly spectral results. So further dilute solution was recommended (1 × $10^{-7}$ M) for performing the fluorescenttitration,

Thecolourof**S3**solutionwasclearbrowncoloursolution in absence of ions and it absorbed the light at $\lambda_{max}$ 410 nm. TitrationsofCN⁻ionswith**S3**-DMSOsolutionwereperformed at the equivalent concentration of ion and sensor. It is found that the fluorescence colour of **S3** solution changed after the addition of 50 µL $CN^-$ions. Thus, more the concentration of $CN^-$ion added, the more intense of fluorescent strength. The titrationspectraofUV-visibleshowninFig.2.The**S3**emitted lightatλ365nmwithanintensityof224000.Theaccumulationof CN⁻tothe3rdcorrespondent(2×$10^{-5}$M)outcomeinreduced emission strength, and from the addition of 4th correspondent (4 × $10^{-5}$ M) λstimulatedto λ 431 nm with the significance of Stoke's shift 66 nm.

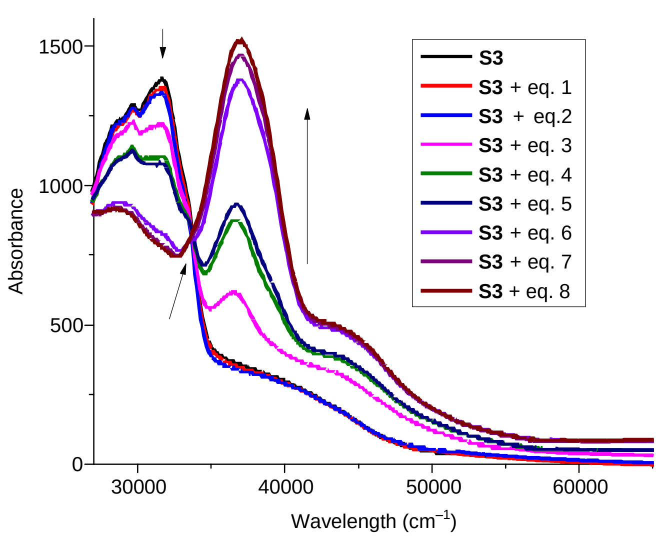


Fig. a. UV-visible spectra of **S3** titration with $CN^-$

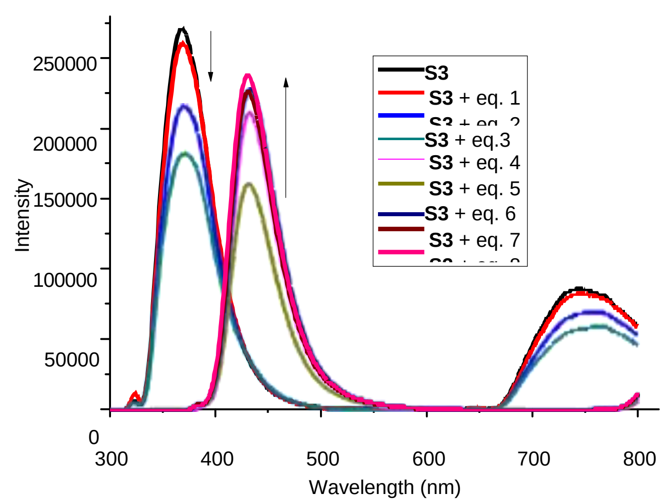


Fig. b. Spectrophotometer fluorescent titration of **S3** with $CN^-$

**Host-guestinterface:**Thequantitativeanalysisofhost-guest interface of complex **S3**-$CN^-$was done by measuring the limit of detection and $K_a$ values; and their interaction mechanisms. The limit of detection of **S3**-$CN^-$complex was calculated using 3σ/K equation. On the basis of their stoichiometry ratio,thecorresponding$K_a$ of**S3**-CN⁻wereconsidered.

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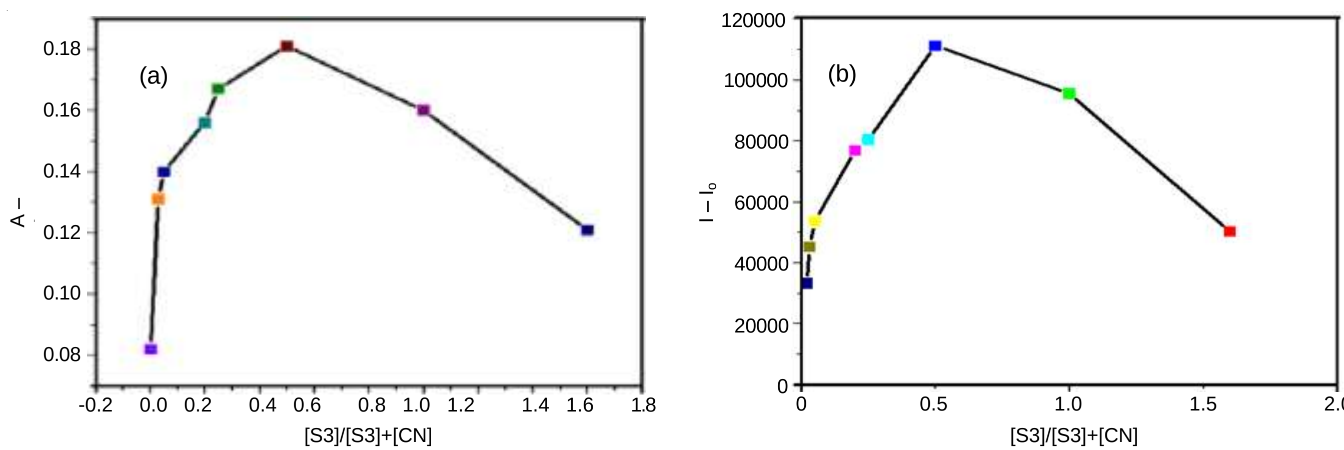


Fig. c. Job's plotted curve titration of **S3**-$CN^-$ on: (a) UV-visible and (b) fluorescent

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