

A Molecular Boolean mimic with OR, NOR, YES and INH functions: Dual-ion recognition driven Fluorescence “turn on”

Masood Ayoub Kaloo and Jeyaraman Sankar*

**Department of Chemistry, Indian Institute of Science Education and Research Bhopal,
India – 462 066**

sankar@iiserb.ac.in

Supplementary information

- 1. General Information**
- 2. Synthesis of Schiff base (R)**
- 3. Jobs plot of R with F⁻**
- 4. Jobs plot of R with Cu⁺²**
- 5. ¹H NMR titration of F⁻ with R**
- 6. Combined Absorption of Receptor with F⁻ and OH⁻.**
- 7. Calibration Curve for Cu⁺² Determination**
- 8. Calibration Curve for F⁻ Determination**

1. General Information

All solvents and reagents were purchased from commercial sources and used without further purification except for dry THF which was further distilled. Cations in form of nitrate and Chloride salts and anions in the form of Tetra butyl ammonium (TBA) salts were stored in a desiccator under vacuum containing silica. Mass spectra were recorded on a Bruker HR-MS spectrometer using CH_3CN as solvent. ^{13}C and ^1H nmr spectra were recorded using a Bruker instrument operating at 400 and 500MHz. UV/Vis spectra were recorded on Perkin Elmer spectrophotometer, lambda 25. Fluorescence emission spectra were recorded on a Horiba Jovin Vyon Fluoro log 3-111 spectrophotometer. Titrations were performed on 2.5mL volume of samples of R in dry THF, by addition of THF (dry) stock solutions of the appropriate anions and cations. The synthesis of receptor (R) was carried out openly in the ambient conditions.

2. Synthesis of Schiff base (R)

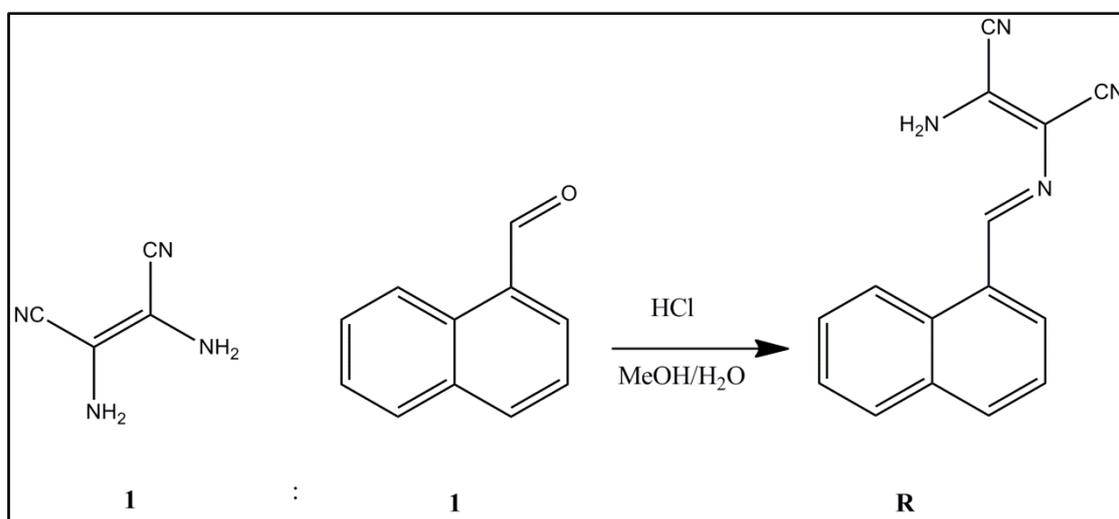


Figure 1. Synthetic Scheme

3. Jobs plot of R with F⁻

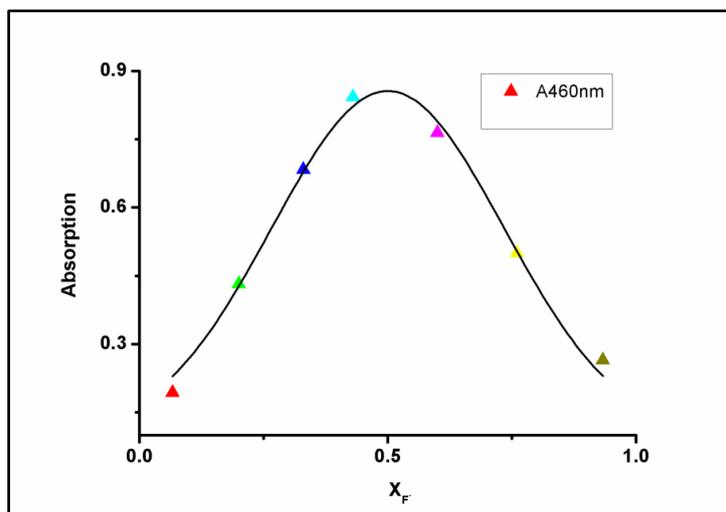


Figure 2. Jobs plot for receptor **R** and F⁻ confirming 1:1stoichiometry. X_F = mole fraction of F⁻.

4. Jobs plot of R with Cu⁺²

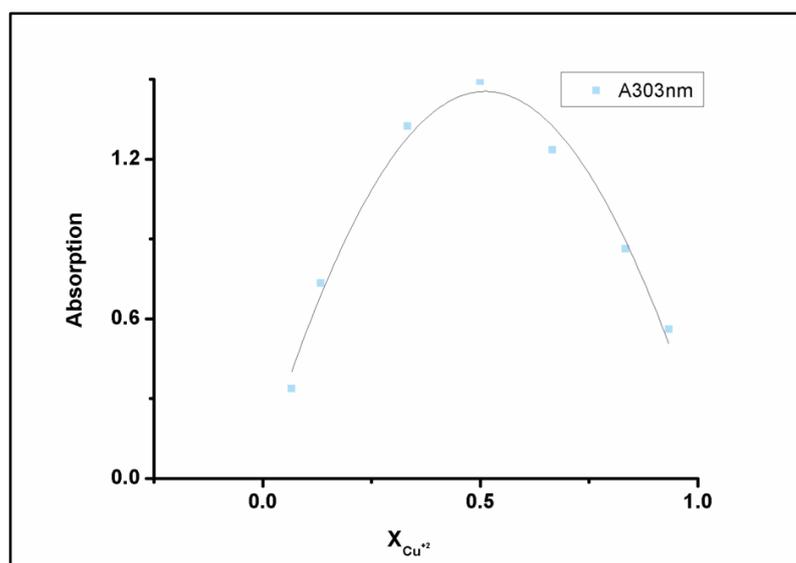


Figure 3. Jobs plot for receptor **R** and Cu⁺² confirming 1:1stoichiometry. X_{Cu⁺²} = mole fraction of Cu⁺².

5. ^1H NMR titration of F^- with **R**

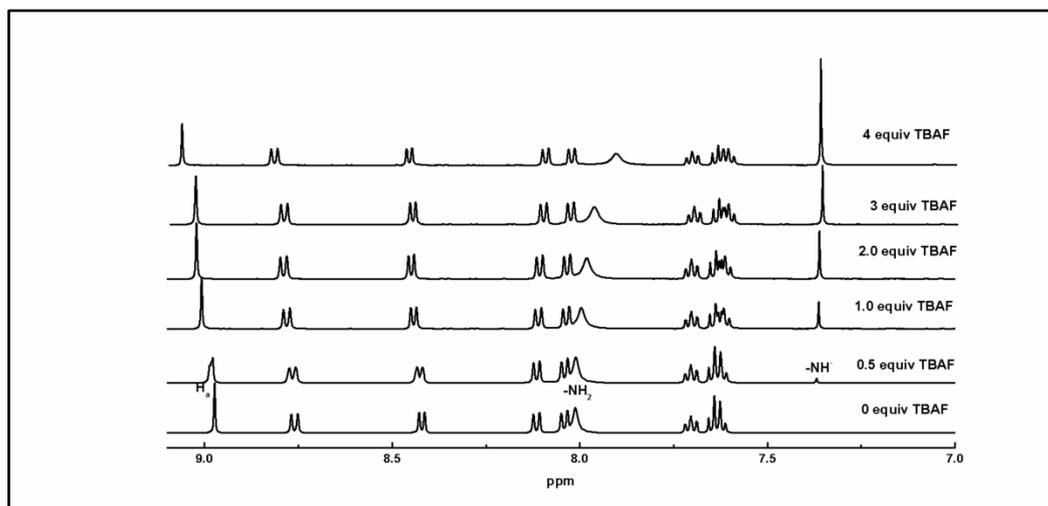


Figure 4. ^1H NMR spectra of **R** (40mM) with different equivalents of 2mM TBAF.

6. Combined Absorption of Receptor with F^- and OH^- .

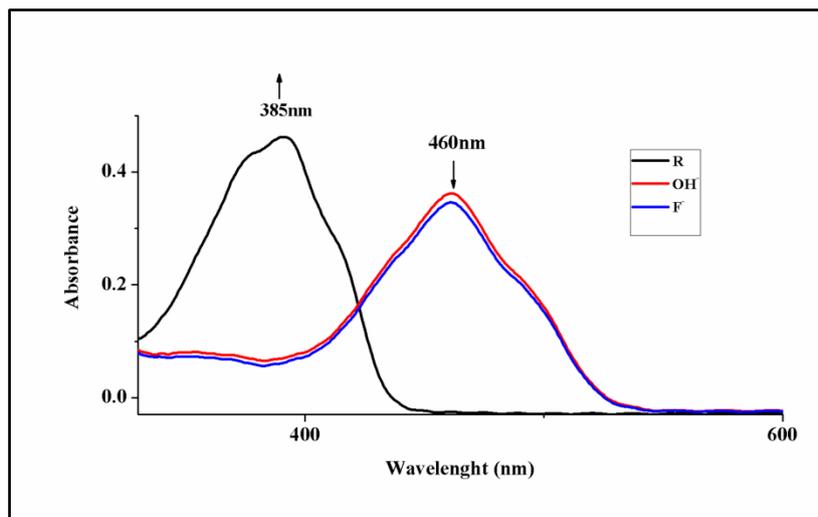


Figure 5. Combine absorption spectra of **R** (5×10^{-6} M) with different equivalents of 0.03 ml's of 1mM TBAF and TBAOH.

7. Calibration Curve for Cu^{2+} determination

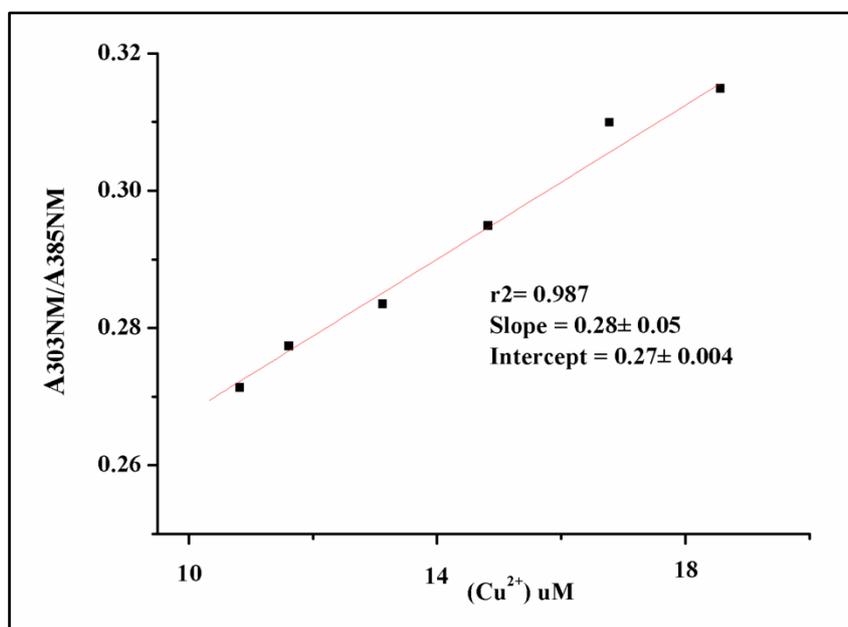


Figure 6. Absorption ratiometric response of **R** (7×10^{-6} M) with different concentrations of Cu^{2+} in dry THF. Measurements at 298K.

8. Calibration Curve for F^- Determination

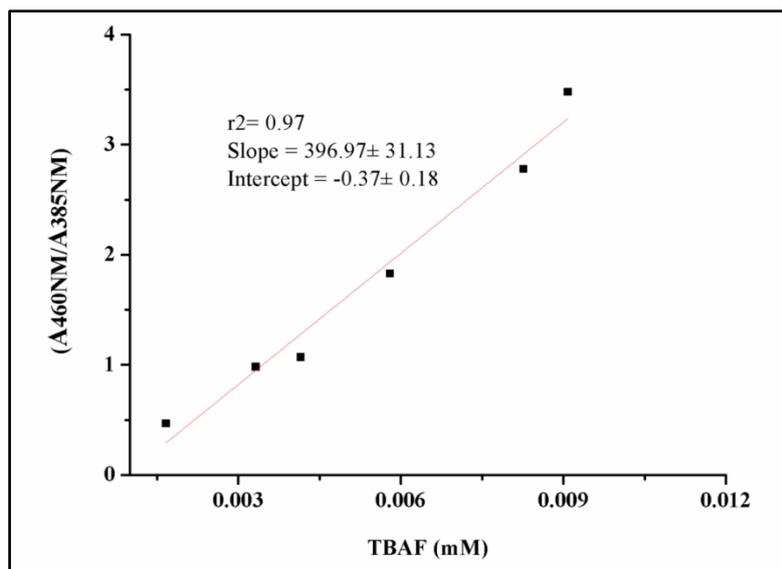


Figure 7. Absorption ratiometric response of **R** (3.5×10^{-7} M) with different concentrations of TBAF in dry THF. Experimental conditions 298K.