

Supporting Information

White light emitting soft materials from off-the-shelf ingredients

Raju Laishram, Sandip Bhowmik, Uday Maitra*

Department of Organic Chemistry, Indian Institute of Science, Bangalore-560012, Karnataka, India

Job plots

Titration of Tb^{3+} , Eu^{3+} and Zn^{2+} with DHN (2 mM solutions were used) were studied by absorption spectroscopy in HEPES-Acetic Acid buffer (pH 7). From these job plots it was observed that all metal ions formed 1:1 complex with DHN.

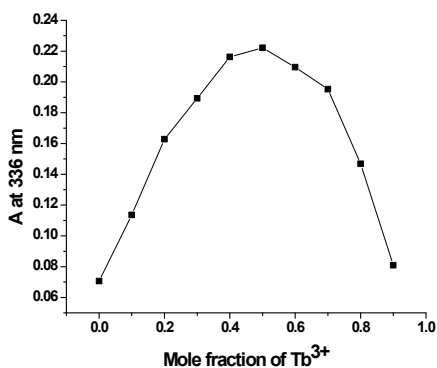


Figure S1 Job's plot for Tb^{3+} and DHN

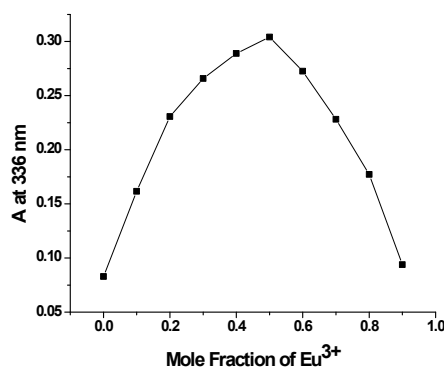


Figure S2 Job's plot for Eu^{3+} and DHN

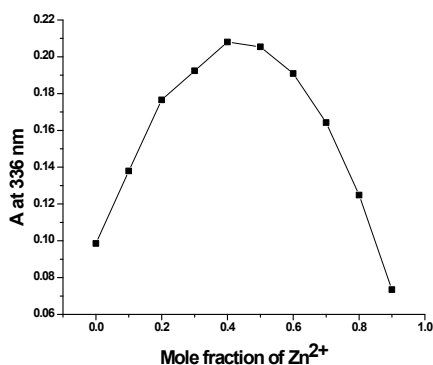
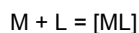


Figure S3 Job's plot for Zn^{2+} and DHN

Binding constant determination

Binding constants of metals and DHN were determined by fluorescence titration,¹ in which fixed concentrations of DHN was taken with increasing metal ion concentration (in HEPES-Acetic Acid buffer, pH 7)

As the binding is 1:1 mode, the binding reaction can be represented as



Where L is DHN and M is Metal ion (Tb^{3+} , Eu^{3+} or Zn^{2+})

The Binding Constant will be given by

$$K = \frac{[ML]}{[M][L]}$$

$$[M] = [M_0] - [ML]; [L] = [L_0] - [ML]$$

$[M_0]$ and $[L_0]$ are concentrations before formation of the complex.

So,

$$K = \frac{[ML]}{[M_o] - [ML]} \frac{[L_o] - [ML]}{[ML]}$$

For fluorescence measurements the following equation is followed

$$F = F_L[L] + F_M[M] + F_{ML}[ML]$$

F is the intensity of total fluorescence observed, F_L for DHN, F_M for the metals and F_{ML} for the Metal-DHN complex which can be substituted by the maximum F i.e., F_{max} . Since the metals are not fluorescent at 380 nm (wavelength under study) the equation can be simplified as

$$F = F_L[L] + F_{max}[ML]$$

$$\text{Using } [L] = [L_o] - [ML]$$

$$F = F_L + (F_{max} - F_L) \frac{[ML]}{[L_o]}$$

$$[ML] = \frac{(F - F_L) [L_o]}{(F_{max} - F_L)} = \frac{\Delta F [L_o]}{\Delta F_{max}}, \text{ where } \Delta F = (F - F_L); \Delta F_{max} = (F_{max} - F_L)$$

Then,

$$K = \frac{\{\Delta F \times [L_o] / \Delta F_{max}\} / \{[L_o] - \Delta F \times [L_o] / \Delta F_{max}\} \{[M_o] - \Delta F \times [L_o] / \Delta F_{max}\}}$$

Using this equation K value of the complexes was determined.

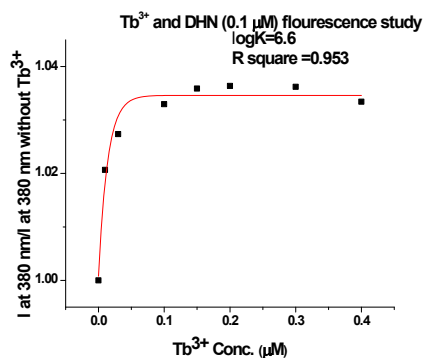


Figure S4 Fluorescence titration curve of Tb^{3+} and DHN

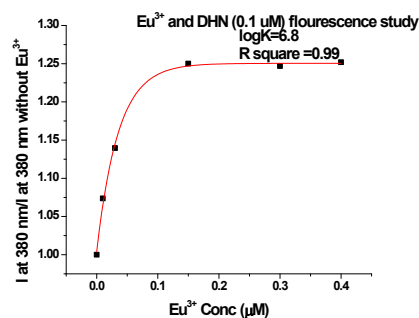


Figure S5 Fluorescence titration curve of Eu^{3+} and DHN

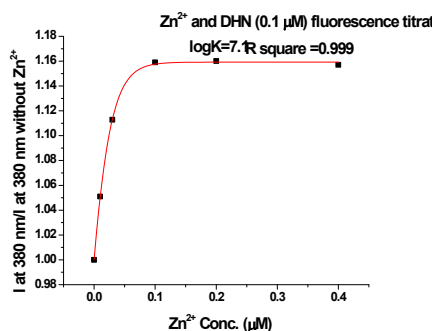


Figure S6 Fluorescence titration curve of Zn^{2+} and DHN

(1) C. Xu, C. Zhao, J. Ren and X. Qu, *Chem. Commun.*, 2011, **47**, 8043.