Electronic Supplementary Information for Dalton Transactions

Synthesis and DNA Binding Properties of a Newly Synthesized Ru(II)-polypyridyl complex

Amrita Ghosh[a], Amit Mandoli[a], D. Krishna Kumar[a], Narendra Singh Yadav,[a] Tamal Ghosh[b], Bhavanath Jha[a] Jim A Thomas*[c] Amitava Das[a]**

[a] *Central Salt and Marine Chemicals Research Institute (CSIR), Bhavnagar:364002, Gujarat, India*

[b] *Motilal Nehru National Institute of Technology Allahabad 211004, India.*

[c] *Department of Chemistry, University of Sheffield, Sheffield, S3 7H, UK.*

E-Mail: bjha@csmcri.org (BJ), james.thomas@sheffield.ac.uk (JAT), amitava@csmcri.org (AD)

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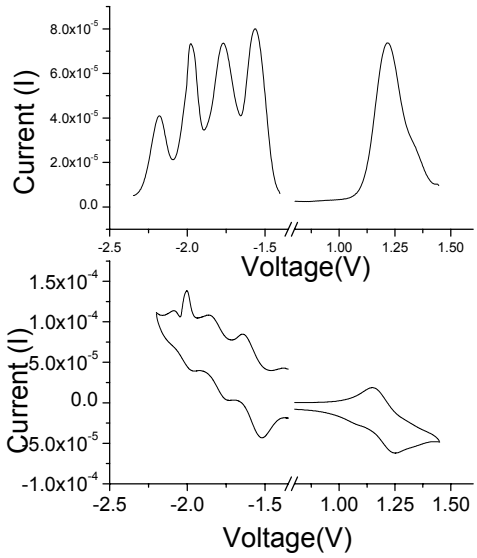
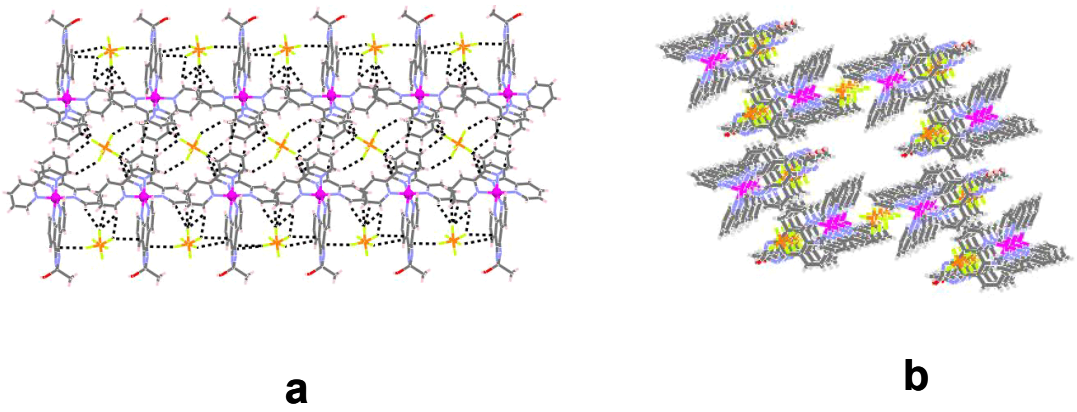
1. Square wave and Cyclic voltammogram of complex 1:



SI Figure 1: Square wave and Cyclic voltammogram of **1**. Experiments were performed in CH_3CN and 0.1M $But^t_4NBF_4$. CV was recorded at 200 mVs^{-1}.

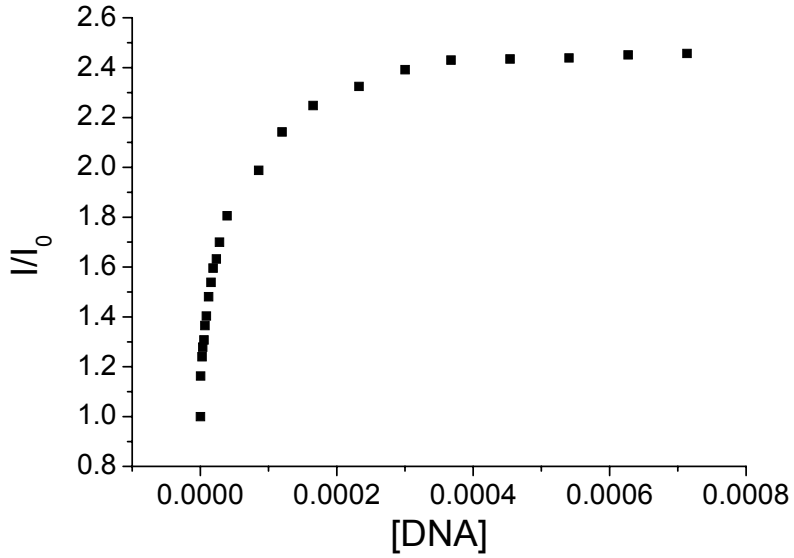
Cyclic and square wave voltammogram for **1** are shown in SIFigure 1. Electrochemical studies reveal that oxidation of Ru(II)-center to the corresponding Ru(III)-state in **1** is easier by about 40 mV as compared to that of $Ru(2,2'\text{-bpy})_3^{2+}$; whereas reduction of L to $L^{\bullet-}$ as compared to the 2,2'-bpy unit(s) present in **1** is easier by ~ 200 mV. Thus the lowest energy MLCT band (~ 2.78 V) is expected to be dominated by the $Ru(d\pi) \rightarrow L(\pi^*)$ transition and thus corroborate our earlier presumption. Lower reduction potential for L as compared to 2,2'-bpy can be explained on the basis of the extended conjugation that is present in the molecule. Similar argument can also be offered for the observed blue shift of ~ 7 nm for **1**, as compared to $Ru(2,2'\text{-bpy})_3^{2+}$.

2. Packing Diagram for 1.



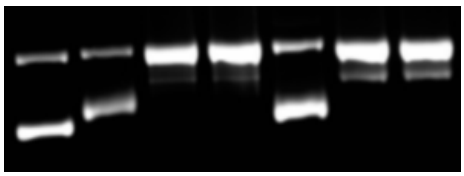
SI Figure 2: (a) One dimensional tape like architecture formed along a-axis *via* C-H…F interactions between the benzene ring of $Ru(bpy)_2$(**L**) and the anion; (b) Packing of the such one dimensional tape in a two dimensional fashion resulting in continuous channels along a-axis within which the disordered anion and solvent molecules are located.

3. Luminescence data



SI Figure 3: Plot of I/I_o *vs.* [DNA] for **1**

4. Photocleavage experiment with $Ru(phen)_3Cl_2$ as standard :



Form II Open circular
Form III Linear

Form I Closed circular

SI Figure 4: Lane1: control plasmid DNA, Lanes 2 and 5: DNA with **1** and Std.**,** respectively (dark reaction), Lanes 3 and 4: DNA incubated with **1** for 1h and then irradiated (Light experiments) at 450 nm for 1 h, Lanes 6 and 7: DNA incubated with $Ru(phen)_3^{2+}$ for 1h and then irradiated (Light experiments) at 450 nm for 1h. For all experiments [DNA] = 0.8 μg, [**1**] and [std.] = 10 μM.

5. Hydrolysis study of phosphodiester of paranitrophenyl phosphate by Complex 1:

To investigate the ability of the complex **1** to hydrolyse the phosphoester bond, we have carried out the hydrolysis study with the model system, *p*-nitro phenyl phosphate disodium salt. *p*-nitrophenol phosphate (pnpp). Hydrolysis, generates *p*-nitrophenolate ion with a distinctive absorption at 420 nm.

To establish that complex **1** generates p-nitrophenolate ion on hydrolysis of the ester linkage, the following procedure was followed.

Experimental Procedure

In a UV-Vis cuvette, complex **1** and pnpp (both of known concentration) were taken to pH ~ 7.5. Electronic spectra were then recorded at 420 nm over the time period of 1.5 h. A similar experiment was repeated without the addition of complex **1**, to account for any effect of the sightly basic pH towards hydrolysis.

6. T4 DNA ligase experiment:

An enzymatic assay was performed using T4 DNA ligase to determine whether the cleaved product (open circular form II) was consistent with hydrolysis of the phosphodiester linkage in DNA. For the religation experiment, pBR 322 was incubated with **1** for 18 h at room temperature, prior to gel electrophoresis. The open circular form II obtained from the hydrolytic cleavage reaction was recovered from agarose gel by phenol chloroform extraction method and purified by ethanol precipitation. This was dissolved in 10µl of tris buffer, which was followed by the addition of 10X ligation buffer and T4 DNA ligase (5 units) to the gel purified Form II for overnight at 16 ºC. Electrophoresis gel profile of the treated plasmid DNA is shown in figure 11 in the manuscript.