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Four related Mixed-Ligand Nickel(II) Complexes: Effect of Steric Encumbrance on the Structure, DNA / BSA binding, DNA cleavage and Cytotoxicity

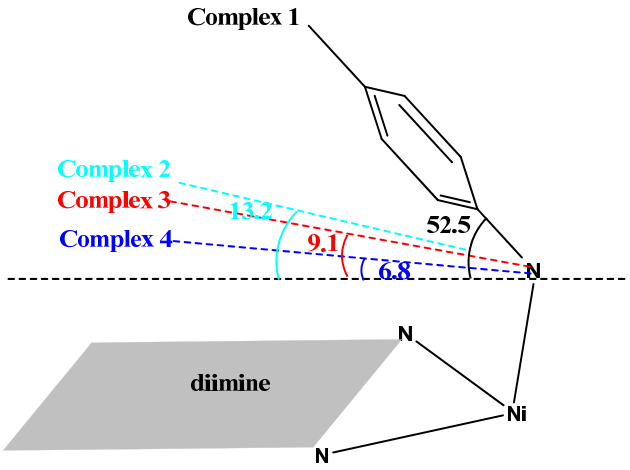
‡ **Chun-Yan Gao[a, b], ‡Zhong-Ying Ma[c], Yong-Po Zhang[b], Si-Tong Li [a,d], Wen Gu[a,d], Xin Liu[a,d], Jin-Lei Tian[a,d*], Jing-Yuan Xu[c*], Jin-Zhong Zhao[b] and Shi-Ping Yan[a]**

[a]*College of Chemistry, Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Nankai University, Tianjin 300071, P. R. China*

[b]*College of Arts and Sciences, Shanxi Agricultural University, Taigu Shanxi 030801, P. R. China*

[c]*College of Pharmacy, Tianjin Medical University, Tianjin 300070, P. R. China*

[d]*Key Laboratory of Advanced Energy Materials Chemistry (MOE), Tianjin 300071, P. R.China*



Scheme S1 Schematic drawing of **1-4** with the dihedral angles between benzene ring of ligand **L** and the plane of the diimine (bpy, phen, dpq or dppz)

* Corresponding authors. E-mail address: tiant@nankai.edu.cn and xujingyuan@tmu.edu.cn.

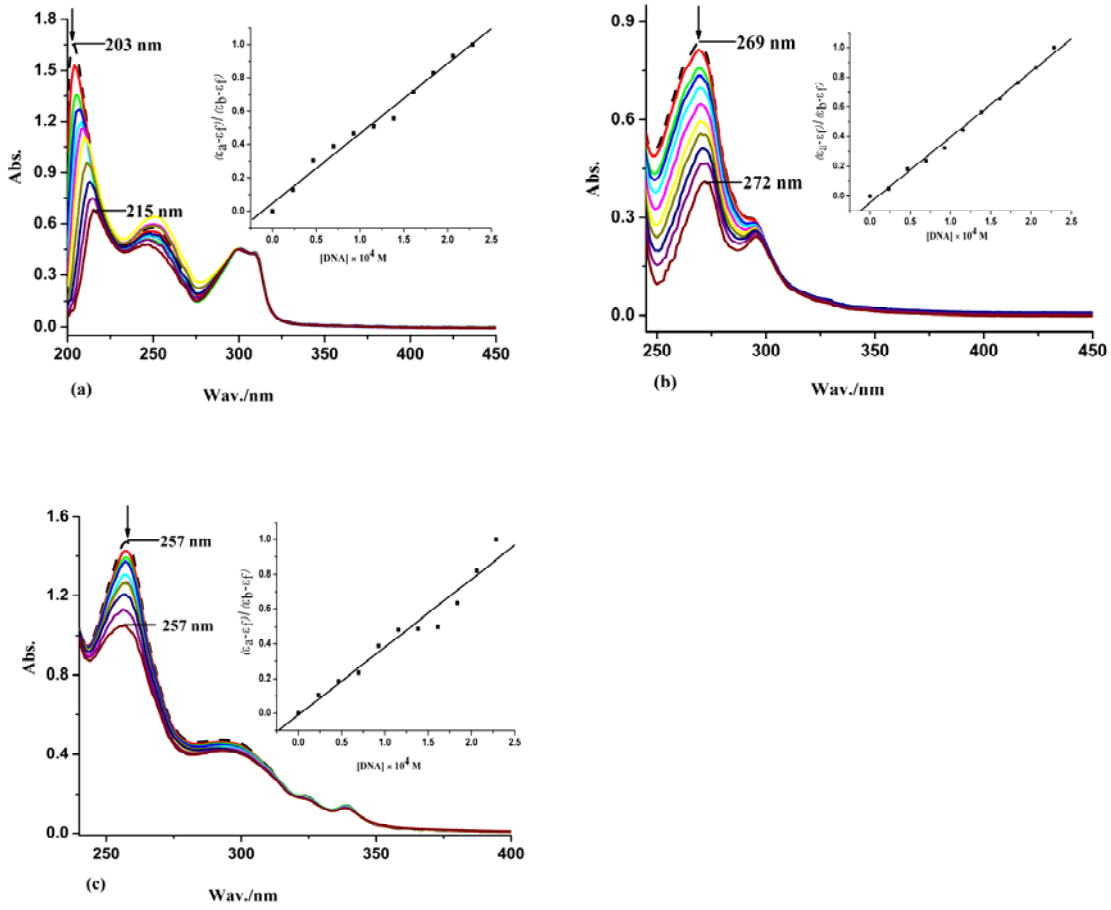
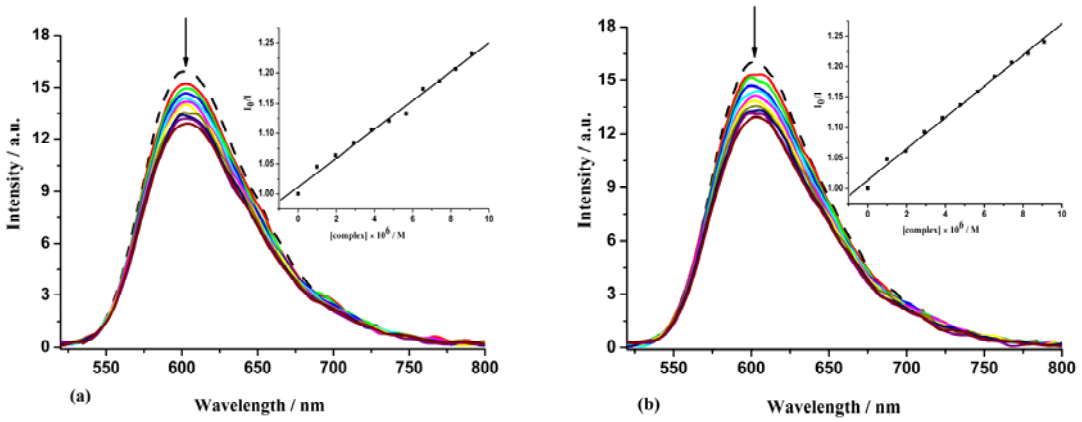


Fig. S1(a-c) Absorption spectra of complexes **1-3** (24.39μM, 0.24% DMF) in the absence (dashed line) and presence (solid line) of increasing amounts of CT-DNA (23.4, 46.6, 69.7, 92.8, 115.7, 138.5, 161.2, 183.7, 206.2, and 228.6 μM) in 5 mM Tris-HCl/50 mM NaCl buffer (pH = 7.2). The arrow shows the absorbance changes on increasing DNA concentration. Insert: Plot of $(\varepsilon_a - \varepsilon_f)/(\varepsilon_b - \varepsilon_f)$ versus [DNA] for the titration of DNA to complex.



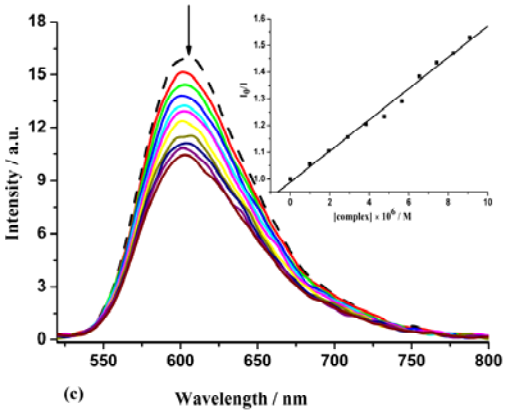


Fig. S2(a-c) Fluorescence emission spectra of the EB (2.4 μM) bound to CT-DNA (48 μM) system in the absence (dashed line) and presence (solid lines) of complexes **1-3** (0.99, 0.1.96, 2.91, 3.85, 4.76, 5.66, 6.54, 7.41, 8.26 and 9.09 μM). Inset: the plot of I_0/I versus the complex concentration.

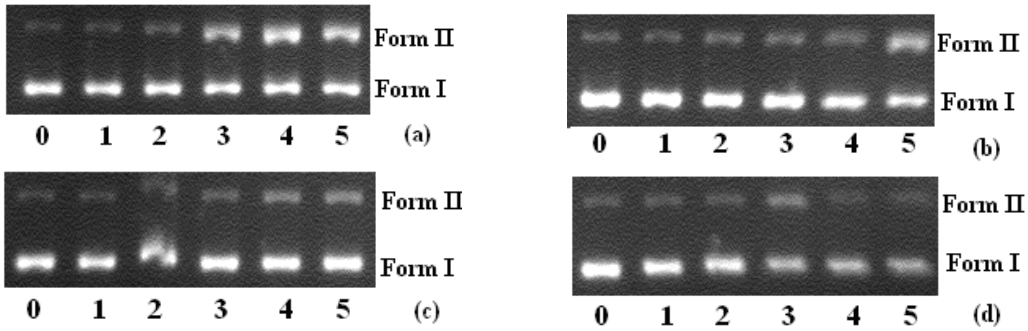


Fig. S3(a-d) Gel electrophoresis diagram showing the cleavage of pBR322 DNA (0.1μg/μL) for complexes **1-4** at different concentrations in Tris-HCl/NaCl buffer (pH = 7.2) and 37 °C. Lane 0: DNA control (3 h); Lane 1-5: DNA + **complex** (5, 20, 35, 50, 65 μM)

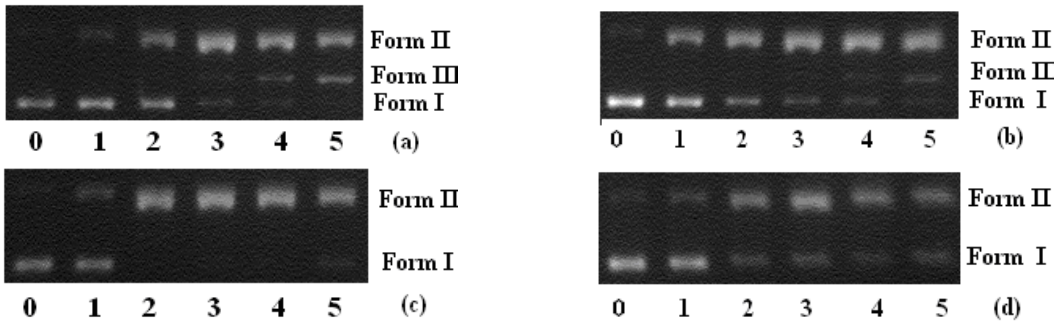
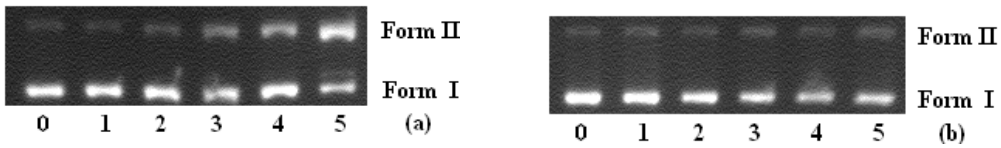


Fig. S4(a-d) Gel electrophoresis diagrams showing the cleavage of pBR322 DNA (0.1 μg/μL) for **complexes 1-4** at different concentrations in Tris-HCl/NaCl buffer (pH = 7.2) and 37 °C. Lane 0: DNA control (3 h); Lane 1: DNA + 0.25 mM GSH; Lane 2-5: DNA + GSH + **complex** (5, 20, 35, 50 μM), respectively.



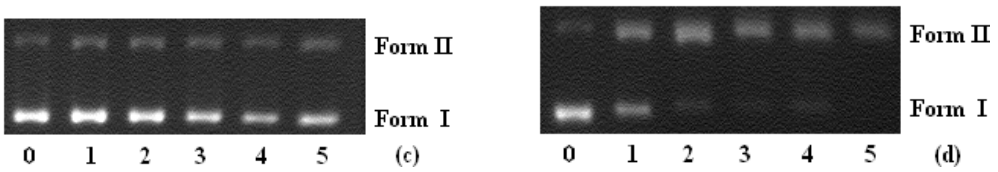


Fig. S5 (a-d) Gel electrophoresis diagram showing the cleavage of pBR322 DNA (0.1μg/μL) for complexes **1-4** with different concentrations on photoirradiation at 365 nm in Tris-HCl/NaCl buffer (pH = 7.2). Lane 0: DNA control (3 h); Lane 1-5: DNA + **complex** (5, 20, 35, 50, 65 μM)

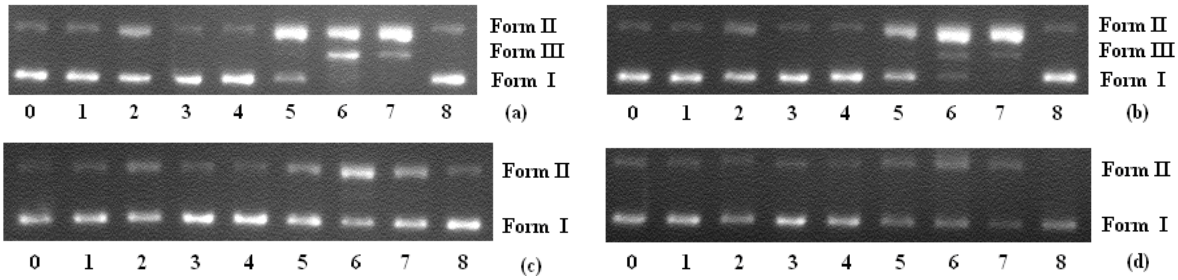
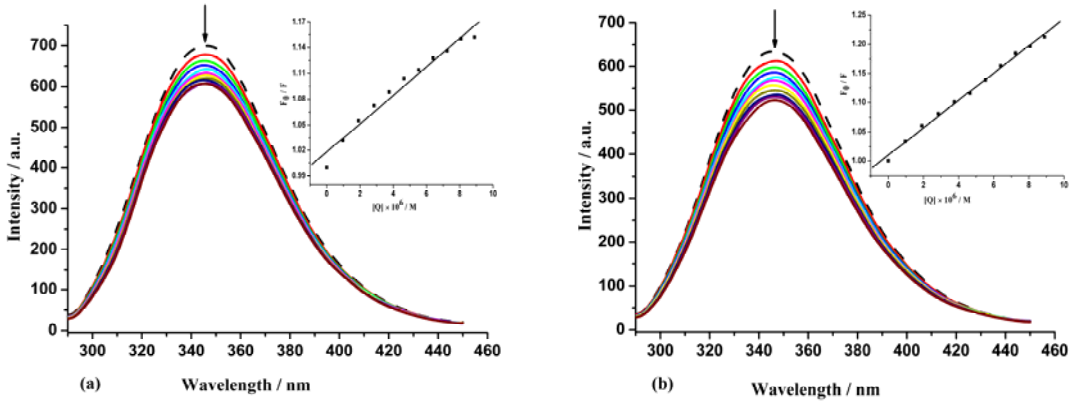


Fig. S6 (a-d) Cleavage of plasmid pBR322 DNA (0.1 μg/μL) in presence of 15 μM complexes **1-4** and different inhibitors after 3 h incubation at 37 °C . Lane 0: DNA control; Lane 1: DNA + 0.25 mM GSH; Lane 2: DNA + 0.25 mM GSH + complex; Lane 3-8: DNA + 0.25 mM GSH + complex + inhibitors (0.1M NaN_3, 0.1M KI, 25% (V/V) D_2O, 2 U/mL SOD, 0.2 U/mL Catalase, 0.5mM EDTA).



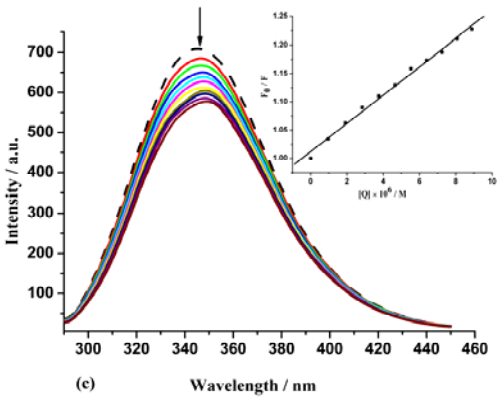


Fig. S7(a-c) Fluorescence emission spectra of the BSA (36.6 μM) system in the absence (dashed line) and presence (solid lines) of complexes **1 - 3** (0.97, 1.91, 2.84, 3.76, 4.65, 5.53, 6.39, 7.24, 8.07 and 8.89 μM, respectively). Inset: the plot of F_0/F versus the complex concentration.