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## **Electronic supplementary information(ESI)**

## Efficient DNA Condensation by Ruthenium(II) Polypyridyl Complexes Containing Triptycenyl Functionalized 1,10-phenanthroline

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**Table 1**: Calculated MOs of  $[Ru(bpy)_3]^{2+}$  and 1–4 complexes (isovalue = ±0.03). Energies in eV with respect of HOMO are given in bracket.







**Table 2:** The orbital contribution (in %) on the molecular fragments estimated using the sphericalized atomic densities in free state by Hirshfeld method.

Orbital		1		2			3			4		
	Ru	tet-phen	bpy	Ru	tet-phen	phen	Ru	tet-phen	dppz	Ru	tet-phen	tet-phen
HOMO-4	15.4	41.4	1.7	17.2	40.5	1.8	23.8	36.9	2.5	20.6	12.9	16.9
НОМО-3	11.0	43.3	2.4	6.4	45.8	2.0	14.9	40.6	4.0	0.0	34.1	31.4
НОМО-2	56.0	16.1	11.9	48.4	23.3	5.0	50.1	18.6	12.8	43.8	21.1	29.9
HOMO-1	50.0	22.4	5.2	57.2	13.1	16.6	41.6	27.1	4.3	44.6	15.9	8.0
НОМО	74.7	8.3	8.6	74.6	8.5	8.4	74.6	8.5	8.3	74.7	8.4	8.5
LUMO	0.3	49.5	0.7	0.3	49.7	0.4	0.2	8.0	83.8	0.3	34.0	32.5
LUMO+1	0.3	49.7	0.2	0.3	49.6	0.4	0.3	42.0	15.7	0.3	27.7	64.7
LUMO+2	1.2	30.2	38.4	1.3	36.6	25.5	0.3	49.6	0.4	0.3	38.0	2.5
LUMO+3	6.3	18.9	56.0	6.7	46.2	1.0	1.2	29.6	39.6	1.2	34.0	31.7
LUMO+4	6.7	46.2	0.9	6.5	12.3	68.9	6.7	19.3	54.6	6.6	23.8	61.2

## ospray ionisation -MS

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· 8 (0.224) AM (Cen,4, 100.00, Ar,8500.0,556.28,0.40,LS 10); Sm (SG, 2x5.00); Sb (10,1.00 ); Cm (7:14-1:3) 587,1353



Fig. S1 ESI-MS spectrum of 1.



Fig. S2 ESI-MS spectrum of 2.



Fig. S3 ESI-MS spectrum of 3, inset shows the isotopic distribution for  $[M-2Cl=]^{2+}$  peak (650).



## WATERS Q-TOF Premier-HAB213



**Fig. S4** ESI-MS spectrum of **4**, inset shows the isotopic distribution for  $[M-2Cl=]^{2+}$  peak (738).



**Fig. S5** Geometrically optimized molecular structures of complexes by DFT studies (a) 1, (b) 2, (c) 3 and (d) 4.



Fig. S6 Fluorescence microscopy bright field images of CT-DNA condensate adduct induced by (a) 1, (b) 2, (c) 3 and (d) 4 images are captured after mixing DNA (200  $\mu$ M) and complex (50  $\mu$ M)solutions.



**Fig. S7.** Agarose gel (1%) electrophoresis of plasmid DNA, [DNA] = 200 ng,  $[complex] = 5-20 \mu$ M, Incubation time 15 min at 37 °C, Light irradiation ( $\lambda$ =327 nm) for 20 min.



Fig. S9 <sup>1</sup>H-NMR spectra of complex 2 in DMSO-d<sub>6</sub>.



Fig. S11 <sup>1</sup>H-NMR spectra of complex 4 in DMSO-d<sub>6</sub>.