Supporting information

Theoretical Studies on DNA-photocleavage Efficiencies of Ru(II) polypyridyl Complexes

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Table S1 Calculated thermochemical values in gas and the free energies in aqueous solution for complex $[Ru(bpy)_3]^{n+}$ (n=1~3) in ground states, the lowest-lying triplet/singlet excited state (T_1/S_1) and the lowest triplet state (TR).

	$(S^{o}_{tot})_{gas}$	$(G_{corr})_{gas}$	$(H_{corr})_{gas}$	ε_{ZPE}	ε_{tot}	G_{gas}	G_{aq} [c]
$[Ru(bpy)_3]^{2+}$	188.405	0.426099	0.515617	0.485845	0.514650	-1579.729818	-1579.915085
$[Ru(bpy)_3]^{3+}$	189.517	0.425960	0.516006	0.486124	0.515039	-1579.285627	-1579.705919
$[Ru(bpy)_3]^{1+}$	191.533	0.420027	0.511031	0.480923	0.510064	-1579.965216	-1580.015303
$[Ru(bpy)_3]^{2+}$ (T_1)	186.953	0.425823	0.51465	0.485025	0.513683	-1579.715251	-1579.904537
$[Ru(bpy)_3]^{2+}$ (S_1)	187.454	0.425829	0.514895	0.485219	0.513928	-1579.721347	-1579.906622
$[Ru(bpy)_3]^{2+}$ (TR)	201.898	0.418440	0.514368	0.483216	0.513401	-1579.655661	-1579.840374

[a]All energies values in Hartrees per particle and S^{o}_{tot} in $Cal \cdot M^{-1} \cdot K^{-1}$.
[b]All values were calculated at the level of UB3LYP/LanL2DZ(d)+6-31G(d).
[c]G_{aq} were directly obtained via the single point calculations with UB3LYP/ LanL2DZ(d)+6-31G(d) and CPCM model.

Table S2 Calculated thermochemical values in gas and the free energies in aqueous solution for complexes **1-4** in ground states and the lowest triplet state (TR).

Complex **1**	$(S^{o}_{tot})_{gas}$	$(G_{corr})_{gas}$	$(H_{corr})_{gas}$	ε_{ZPE}	ε_{tot}	G_{gas}	G_{aq} [c]
$[Ru(bpy)_2BPIP]^{2+}$	249.828	0.601456	0.720158	0.678175	0.719182	-2265.706762	-2265.911630
$[Ru(bpy)_2BPIP]^{3+}$	250.167	0.601322	0.720185	0.678093	0.719209	-2265.330306	-2265.698581
$[Ru(bpy)_2BPIP]^{1+}$	253.736	0.595307	0.715865	0.673548	0.714890	-2265.932143	-2266.008609
$[Ru(bpy)_2BPIP]^{2+}$ (TR)	253.071	0.595909	0.716152	0.673661	0.715175	-2265.632477	-2265.820211
Complex **2**							
$[Ru(phen)_2BPIP]^{2+}$	253.951	0.626417	0.747077	0.703864	0.746101	-2418.174849	-2418.376967
$[Ru(phen)_2BPIP]^{3+}$	253.634	0.626619	0.747129	0.703833	0.746152	-2417.799974	-2418.172490
$[Ru(phen)_2BPIP]^{1+}$	257.187	0.620085	0.742283	0.698727	0.741306	-2418.395519	-2418.284552
$[Ru(phen)_2BPIP]^{2+}$ (TR)	257.111	0.554247	0.743008	0.699260	0.742031	-2418.099611	-2418.284552
Complex **3**							
$[Ru(tap)_2BPIP]^{2+}$	252.952	0.577277	0.697462	0.654680	0.696488	-2482.266724	-2482.463411
$[Ru(tap)_2BPIP]^{3+}$	253.113	0.577058	0.697320	0.654413	0.696345	-2481.883853	-2482.251942
$[Ru(tap)_2BPIP]^{1+}$	255.342	0.572957	0.694278	0.651276	0.693303	-2482.519662	-2482.588098
$[Ru(tap)_2BPIP]^{2+}$ (TR)	255.283	0.572163	0.693457	0.650311	0.692482	-2482.200005	-2482.376974
Complex **4**							
$[Ru(tap)_2NO_2\text{-}BPIP]^{2+}$	266.979	0.575702	0.702552	0.657191	0.701578	-2686.757039	-2686.964973
$[Ru(tap)_2NO_2\text{-}BPIP]^{3+}$	267.732	0.574548	0.701756	0.656191	0.700781	-2686.357926	-2686.745184
$[Ru(tap)_2NO_2\text{-}BPIP]^{1+}$	269.076	0.571546	0.699392	0.653819	0.698418	-2687.013101	-2687.089765
$[Ru(tap)_2NO_2\text{-}BPIP]^{2+}$ (TR)	270.182	0.569851	0.698223	0.652393	0.697248	-2686.682547	-2686.874233

[a]All energies values in Hartrees per particle and S^{o}_{tot} in $Cal \cdot M^{-1} \cdot K^{-1}$.
[b]All values were calculated at the level of UB3LYP/LanL2DZ(d)+6-31G(d).
[c]G_{aq} were directly obtained via the single point calculations with UB3LYP/ LanL2DZ(d)+6-31G(d) and CPCM model.