Supporting Information

The electronic structures of di-ruthenium complexes containing tris(*para*-phenyleneethynylene) links, and related molecular structures.

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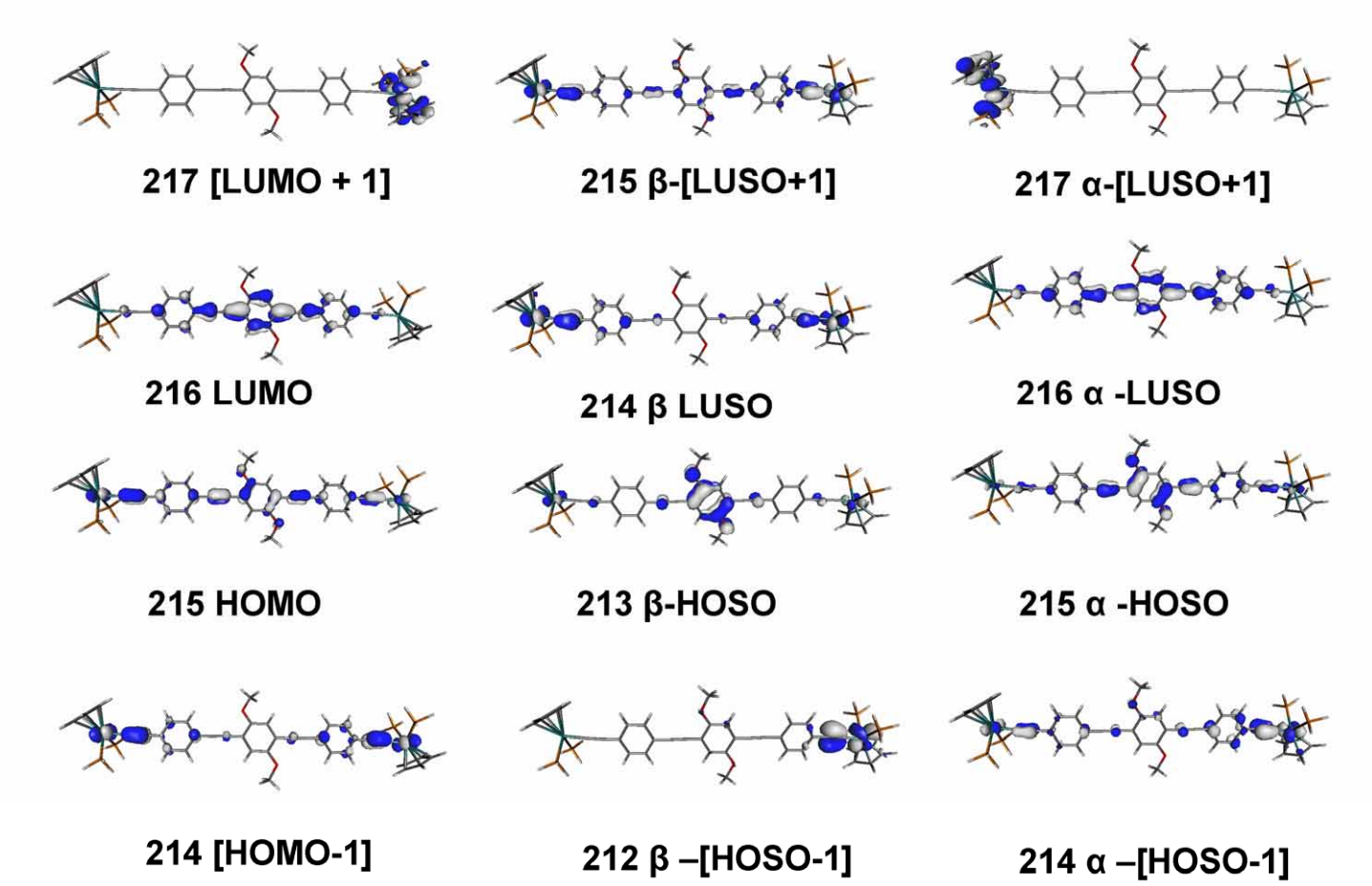

Figure S1: The frontier orbitals of **[4-H]**$^{n+}$ (n = 0, 2) plotted with contour values ± 0.04 (e/bohr^3)$^{1/2}$.

Table S1. Energies and compositions of frontier orbitals in the model complex **4-H**

MO		eV	Cp	PH_3	Ru	C1	C2	C_6H_4	C9	C10	$C_6H_2(OMe)_2$	C10'	C9'	C_6H_4'	C2'	C1'	Ru'	Cp'	PH_3'
220	LUMO+4	-0.24	0	0	0	0	0	0	0	0	0	0	0	0	1	8	61	17	13
219	LUMO+3	-0.39	0	1	2	6	0	31	6	1	5	1	6	31	1	6	2	1	1
218	LUMO+2	-0.76	24	27	50	0	0	0	0	0	0	0	0	0	0	0	0	0	0
217	LUMO+1	-0.86	0	0	0	0	0	0	0	0	0	0	0	0	0	0	50	24	27
216	LUMO	-1.34	0	0	1	3	0	16	4	8	37	8	4	16	0	3	1	0	0
215	HOMO	-4.41	1	1	7	5	5	14	4	4	22	4	4	12	4	5	6	1	0
214	HOMO-1	-4.78	3	1	14	6	10	12	3	0	3	0	2	13	10	6	13	3	1
213	HOMO-2	-5.18	4	2	22	4	12	3	0	2	32	2	0	3	4	1	7	2	1
212	HOMO-3	-5.27	4	3	40	7	17	3	0	1	17	1	0	1	1	0	3	1	0
211	HOMO-4	-5.38	0	0	0	0	0	0	0	0	1	0	0	2	24	10	54	5	4

Table S2. Energies and compositions of frontier orbitals in the model complex $[\mathbf{4H}]^{2+}$

MO		eV	Cp	PH_3	Ru	C1	C2	C_6H_4	C9	C10	$C_6H_2(OMe)_2$	C10'	C9'	C_6H_4'	C2'	C1'	Ru'	Cp'	PH_3'
218A	α-LUSO+2	-5.15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	48	26	26
217B	β-LUSO+3	-5.22	25	26	49	0	0	0	0	0	0	0	0	0	0	0	0	0	0
217A	α-LUSO+1	-5.33	26	26	48	0	0	0	0	0	0	0	0	0	0	0	0	0	0
216B	β-LUSO+2	-5.54	0	0	2	4	0	18	4	7	32	7	4	16	0	4	2	0	0
216A	α-LUSO	-5.72	0	0	1	4	0	20	4	6	30	6	4	18	0	4	1	0	0
215B	β-LUSO+1	-7.63	2	1	10	4	6	10	3	2	14	3	2	13	8	5	12	2	1
214B	β-LUSO	-7.96	3	2	17	4	11	13	3	0	4	0	3	10	9	3	14	3	2
215A	α-HOSO	-8.75	1	0	2	3	2	10	4	6	42	6	3	12	2	3	4	1	1
213B	β-HOSO	-8.92	1	1	6	0	3	4	0	4	59	5	0	4	3	0	7	1	1
214A	α-HOSO-1	-9.34	2	1	7	3	5	11	4	1	7	0	3	16	11	5	16	5	3
213A	α-HOSO-2	-9.50	3	2	10	3	7	11	0	0	52	0	2	2	2	1	3	1	1
212B	β-HOSO-1	-9.79	0	0	0	0	0	0	1	0	6	1	0	4	24	8	49	4	3
211B	β-HOSO-2	-9.82	1	1	4	0	1	5	4	3	46	4	3	8	4	2	12	2	1
212A	α-HOSO-3	-9.91	0	0	0	0	0	0	0	0	0	0	0	3	25	9	55	5	3
210B	β-HOSO-3	-9.92	4	3	53	10	27	3	0	0	0	0	0	0	0	0	0	0	0
211A	α-HOSO-4	-10.05	6	3	53	9	25	3	0	0	0	0	0	0	0	0	0	0	0