Ground vs. excited state interaction in ruthenium-thienyl dyads

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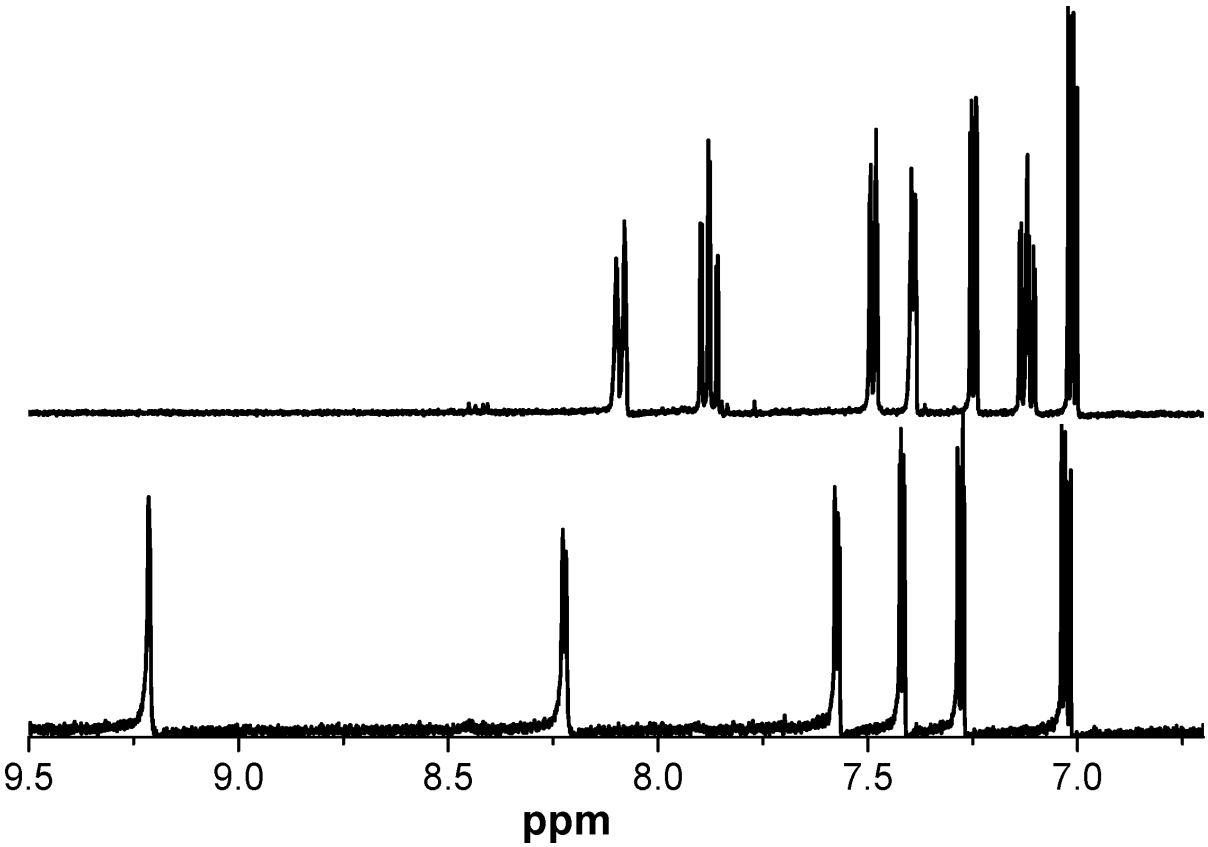

Fig. S1. ^{1}H NMR spectra of **1b** (upper) and **2b** (lower) in CD_3CN (400 MHz).

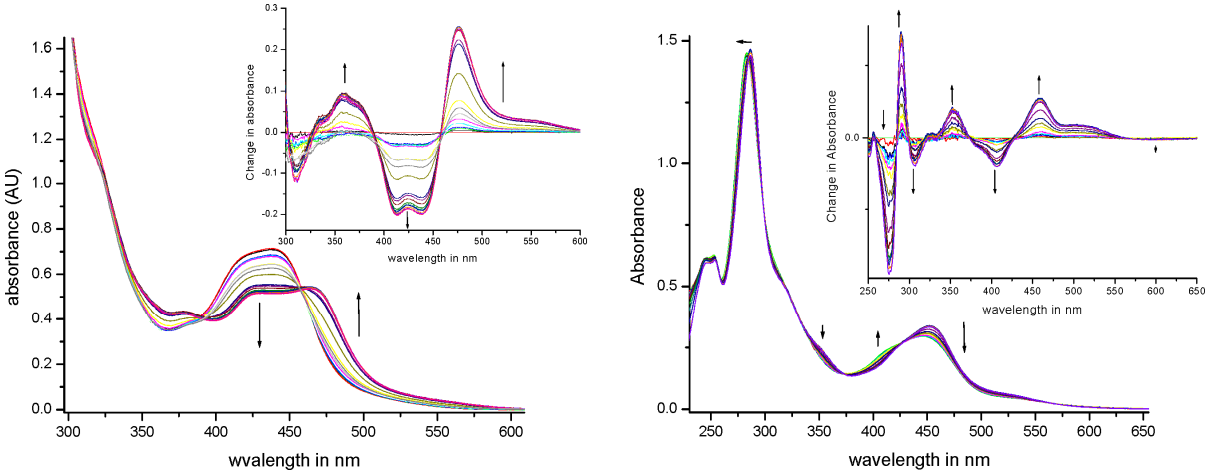

Fig. S2. Changes in UV·vis spectra of **1a** and **2a** between pH 0.5 and 10. (Inset differences spectra compared with completely the protonated complexes).

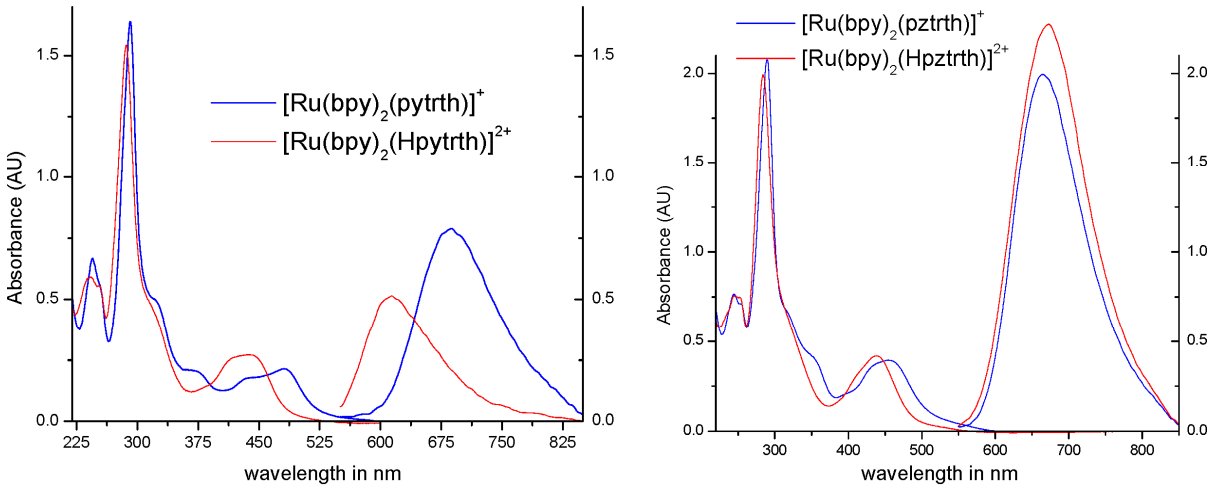

Fig. S3. Absorption and emission spectra for **1a**/**H1a** (left) and **2a**/**H2a** (right) in acetonitrile solution 298 K.

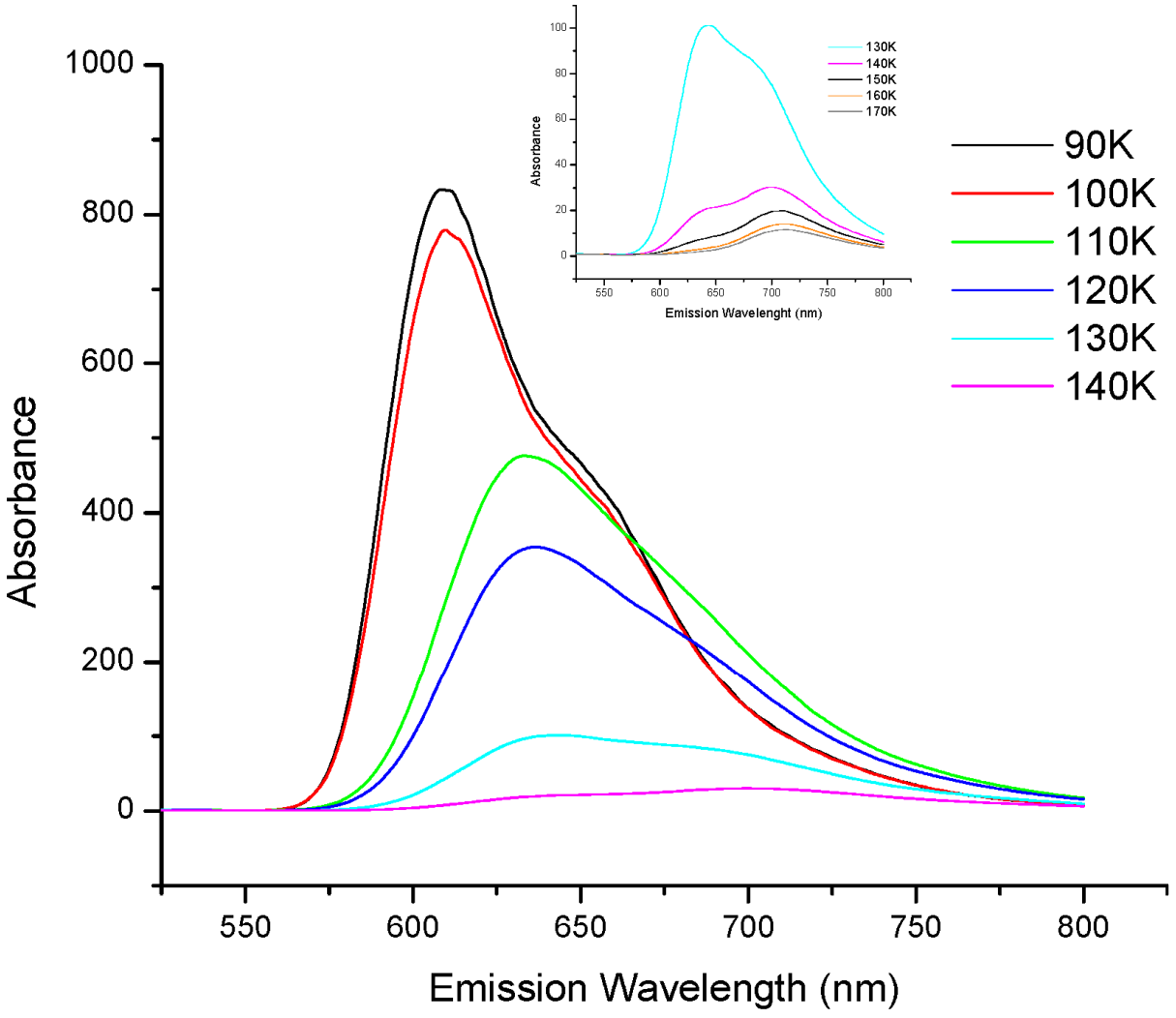

Fig. S4. Temperature dependent emission of **2a** in EtOH:MeOH (4:1).

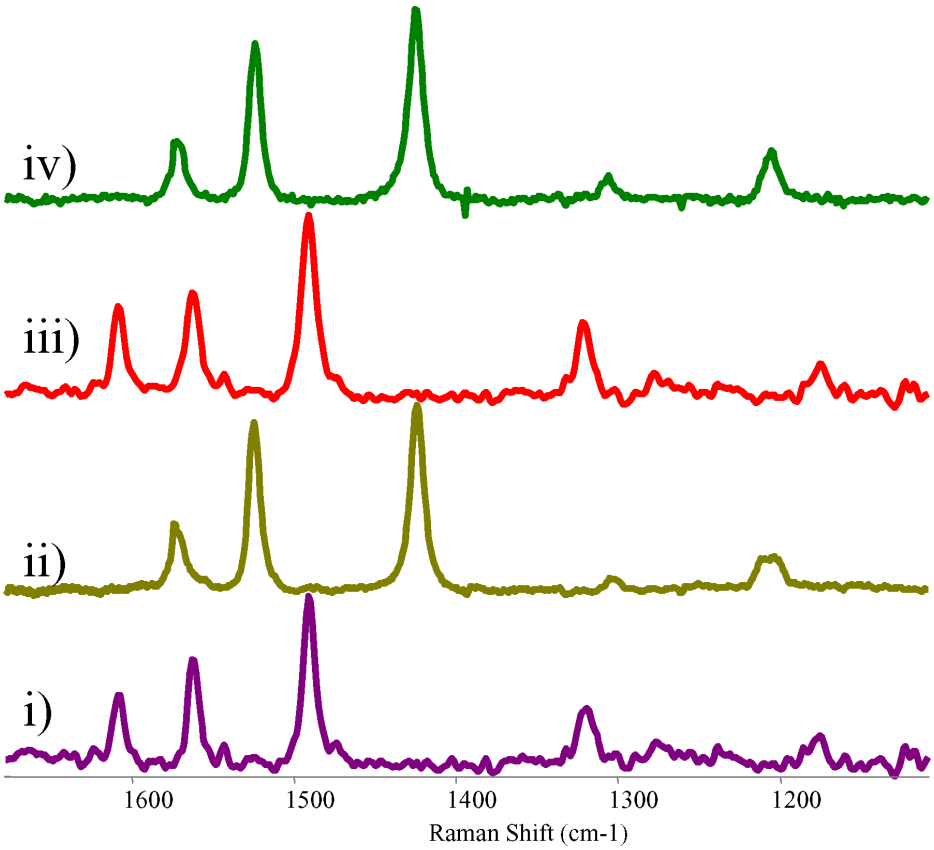

Fig. S5. Resonance Raman spectra of (i) **1a** (ii) **1b** (iii) **H1a** (iv) **H1b** in H_2O at $\lambda_{exc.}$ 457 nm.

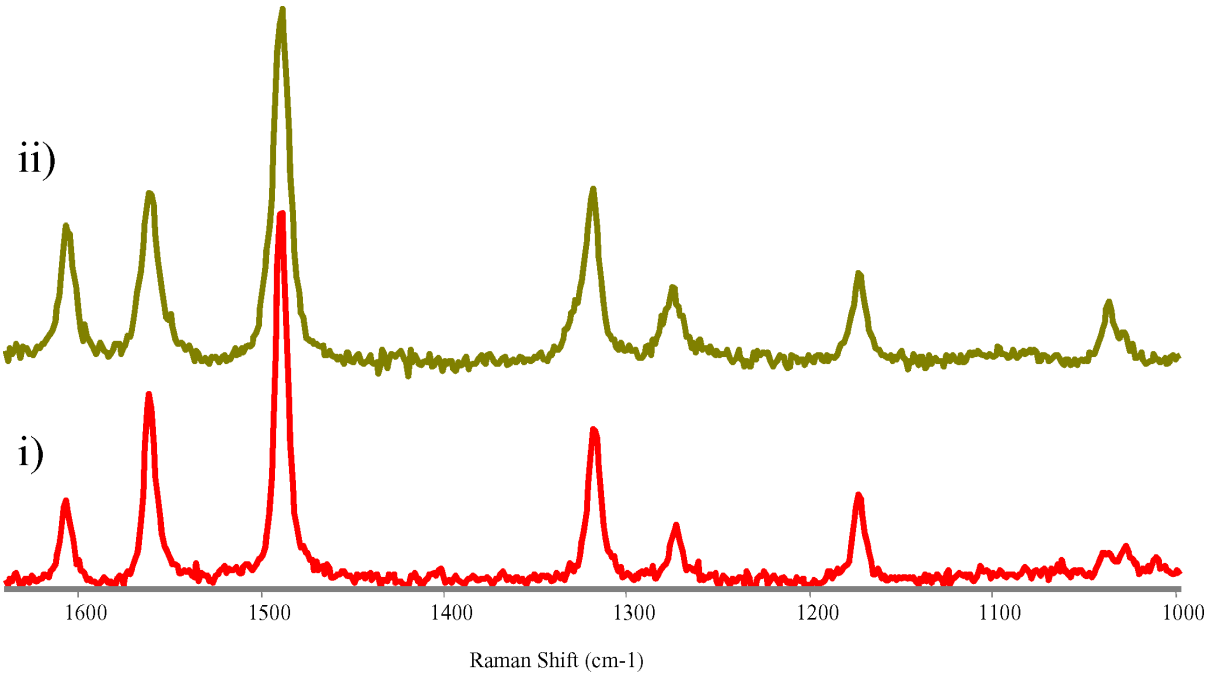

Fig. S6. Resonance Raman spectra of (i) **1a** (ii) **H1a** in H_2O at $\lambda_{exc.}$ 488 nm.

MO		eV	Symmetry	Ru	bpy1	bpy2	pz	tr	th
154	L+10	-2.77	A	0	92	7	0	0	0
153	L+9	-2.78	A	1	1	1	0	33	63
152	L+8	-3.01	A	1	7	91	0	1	1
151	L+7	-3.86	A	1	5	2	80	11	1
150	L+6	-4.08	A	2	90	4	3	0	0
149	L+5	-4.23	A	3	75	21	1	0	0
148	L+4	-4.27	A	2	9	89	0	0	0
147	L+3	-4.53	A	3	14	70	11	3	0
146	L+2	-4.68	A	3	4	11	72	9	0
145	L+1	-5.13	A	5	91	3	1	0	0
144	LUMO	-5.35	A	4	4	91	1	0	0
143	HOMO	-7.45	A	7	1	0	5	29	58
142	H-1	-8.41	A	2	0	0	0	1	96
141	H-2	-8.46	A	72	6	5	1	5	11
140	H-3	-8.56	A	70	11	4	2	7	6
139	H-4	-8.66	A	73	4	12	6	4	2
138	H-5	-9.21	A	5	0	1	26	52	16
137	H-6	-9.24	A	1	1	0	0	97	2
136	H-7	-9.58	A	2	1	1	89	8	0
135	H-8	-10	A	0	94	1	0	4	1
134	H-9	-10.18	A	4	5	4	7	74	6
133	H-10	-10.21	A	1	1	95	1	2	0

MO		eV	Symmetry	Ru	bpy1	bpy2	pz	tr	th
154	L+10	-5.19	A	63	17	12	8	0	0
153	L+9	-5.29	A	4	12	82	1	1	0
152	L+8	-6.4	A	2	91	6	0	1	1
151	L+7	-6.52	A	2	18	33	3	20	25
150	L+6	-6.57	A	1	19	31	6	20	23
149	L+5	-6.63	A	2	42	56	0	0	0
148	L+4	-6.78	A	1	24	66	7	1	0
147	L+3	-7.19	A	1	3	6	75	11	5
146	L+2	-7.51	A	4	92	2	1	0	0
145	L+1	-7.65	A	5	2	90	2	1	0
144	LUMO	-7.97	A	5	2	4	64	22	3
143	HOMO	-11.01	A	39	3	2	5	17	34
142	H-1	-11.27	A	70	9	8	3	3	7
141	H-2	-11.4	A	75	4	11	7	1	1
140	H-3	-11.45	A	50	7	2	0	9	31
139	H-4	-11.87	A	0	0	0	0	1	99
138	H-5	-12.36	A	1	96	2	0	0	0
137	H-6	-12.5	A	1	2	92	5	0	0
136	H-7	-12.56	A	1	1	5	91	2	0
135	H-8	-13.07	A	1	2	0	46	33	18
134	H-9	-13.55	A	2	2	4	2	88	2
133	H-10	-13.61	A	1	68	31	0	1	0

Fig. S7. Molecular orbital data for **2a** (top) and **H2a** (bottom).