Supporting Information For

Concerning the Electronic Coupling of MoMo Quadruple Bonds Linked by 4,4' Azodibenzoate and Comparison With t_{2g}^6-Ru(II) Centers by 4,4' Azodiphenylcyanamido Ligands

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Table S1. Atomic coordinates for the geometry optimized structure of $[(HCO_2)_3Mo_2]_2(\mu\text{-adb})$ in C_{2h} symmetry.

Atom Number	Element	Coordinates / Å		
		x	y	z
1	C	4.515412	0.46654	0.00000
2	C	3.815137	-0.755796	0.00000
3	C	2.429545	-0.770707	0.00000
4	C	1.717606	0.443746	0.00000
5	C	2.414259	1.661784	0.00000
6	C	3.803796	1.676507	0.00000
7	C	-8.736375	-0.482071	2.72173
8	C	5.991649	0.473397	0.00000
9	C	-8.736375	-0.482071	-2.72173
10	C	-11.449683	-0.489398	0.00000
11	C	-5.991649	-0.473397	0.00000
12	C	-4.515412	-0.46654	0.00000
13	C	-3.815137	0.755796	0.00000
14	C	8.736375	0.482071	2.72173
15	C	-3.803796	-1.676507	0.00000
16	C	-2.429545	0.770707	0.00000
17	C	8.736375	0.482071	-2.72173
18	C	-2.414259	-1.661784	0.00000
19	C	-1.717606	-0.443746	0.00000
20	C	11.449683	0.489398	0.00000
21	H	-8.741643	-0.482155	3.81612
22	H	4.377077	-1.683525	0.00000
23	H	1.876101	-1.702523	0.00000
24	H	1.84073	2.583259	0.00000
25	H	4.349413	2.613553	0.00000
26	H	8.741643	0.482155	3.81612
27	H	8.741643	0.482155	-3.81612
28	H	12.54418	0.492568	0.00000
29	H	-8.741643	-0.482155	-3.81612
30	H	-12.54418	-0.492568	0.00000
31	H	-4.377077	1.683525	0.00000
32	H	-4.349413	-2.613553	0.00000
33	H	-1.876101	1.702523	0.00000
34	H	-1.84073	-2.583259	0.00000
35	Mo	8.728229	-0.577651	0.00000
36	Mo	8.721903	1.541436	0.00000
37	Mo	-8.728229	0.577651	0.00000
38	Mo	-8.721903	-1.541436	0.00000
39	N	0.306834	0.551879	0.00000
40	N	-0.306834	-0.551879	0.00000
41	O	-10.845991	-1.609488	0.00000
42	O	6.630715	-0.641407	0.00000
43	O	-10.852402	0.634166	0.00000
44	O	-8.736375	0.639499	-2.12080
45	O	-6.630715	0.641407	0.00000
46	O	-8.729922	-1.603602	-2.12071
47	O	-8.729922	-1.603602	2.12071
48	O	-6.622995	-1.592564	0.00000
49	O	-8.736375	0.639499	2.12080
50	O	6.622995	1.592564	0.00000
51	O	8.729922	1.603602	2.12071
52	O	8.736375	-0.639499	2.12080
53	O	8.729922	1.603602	-2.12071
54	O	8.736375	-0.639499	-2.12080
55	O	10.845991	1.609488	0.00000
56	O	10.852402	-0.634166	0.00000

Table S2. Atomic coordinates for the geometry optimized structure of $[(HCO_2)_3Mo_2]_2(\mu\text{-}O_2CC_6H_4CO_2)$ in D_{2h} symmetry.

Atom Number	Element	Coordinates / Å		
		x	y	z
1	C	1.39996	0.00000	0.00000
2	C	-1.39996	0.00000	0.00000
3	C	2.87873	0.00000	0.00000
4	C	-2.87873	0.00000	0.00000
5	C	0.69454	0.00000	1.21472
6	C	0.69454	0.00000	-1.21472
7	C	-0.69454	0.00000	1.21472
8	C	-0.69454	0.00000	-1.21472
9	O	3.51222	0.00000	1.11699
10	O	3.51222	0.00000	-1.11699
11	O	-3.51222	0.00000	1.11699
12	O	-3.51222	0.00000	-1.11699
13	Mo	5.61265	0.00000	1.05949
14	Mo	5.61265	0.00000	-1.05949
15	Mo	-5.61265	0.00000	1.05949
16	Mo	-5.61265	0.00000	-1.05949
17	O	7.73574	0.00000	-1.12170
18	O	7.73574	0.00000	1.12170
19	O	-7.73574	0.00000	-1.12170
20	O	-7.73574	0.00000	1.12170
21	O	5.61844	2.12070	1.12154
22	O	5.61844	2.12070	-1.12154
23	O	5.61844	-2.12070	-1.12154
24	O	5.61844	-2.12070	1.12154
25	O	-5.61844	2.12070	1.12154
26	O	-5.61844	2.12070	-1.12154
27	O	-5.61844	-2.12070	-1.12154
28	O	-5.61844	-2.12070	1.12154
29	C	8.33664	0.00000	0.00000
30	C	-8.33664	0.00000	0.00000
31	C	5.62029	-2.72176	0.00000
32	C	5.62029	2.72176	0.00000
33	C	-5.62029	-2.72176	0.00000
34	C	-5.62029	2.72176	0.00000
35	H	1.24711	0.00000	2.14781
36	H	1.24711	0.00000	-2.14781
37	H	-1.24711	0.00000	2.14781
38	H	-1.24711	0.00000	-2.14781
39	H	9.43106	0.00000	0.00000
40	H	-9.43106	0.00000	0.00000
41	H	5.62405	-3.81614	0.00000
42	H	5.62405	3.81614	0.00000
43	H	-5.62405	-3.81614	0.00000
44	H	-5.62405	3.81614	0.00000

Table S3. Atomic coordinates for the geometry optimized structure of the dianion 4,4'-azodi(phenylcyanamido) in C_{2h} symmetry. Atomic labeling scheme is shown in Figure S1.

Atom Number	Element	Coordinates / Å		
		x	y	z
1	C	-0.40290	4.59931	0.00000
2	C	-1.45412	3.63161	0.00000
3	C	-1.20802	2.27237	0.00000
4	C	0.11611	1.77002	0.00000
5	C	1.16336	2.71433	0.00000
6	C	0.92433	4.08014	0.00000
7	H	-2.47407	4.01180	0.00000
8	H	-2.02408	1.55562	0.00000
9	H	2.18197	2.32946	0.00000
10	H	1.75307	4.78483	0.00000
11	N	-0.74373	5.92287	0.00000
12	N	0.48346	0.41889	0.00000
13	C	0.18027	6.85138	0.00000
14	N	0.92433	7.77280	0.00000
15	N	-0.48346	-0.41889	0.00000
16	C	-0.11611	-1.77002	0.00000
17	C	-1.16336	-2.71433	0.00000
18	C	1.20802	-2.27237	0.00000
19	C	-0.92433	-4.08014	0.00000
20	H	-2.18197	-2.32946	0.00000
21	C	1.45412	-3.63161	0.00000
22	H	2.02408	-1.55562	0.00000
23	C	0.40290	-4.59931	0.00000
24	H	-1.75307	-4.78483	0.00000
25	H	2.47407	-4.01180	0.00000
26	N	0.74373	-5.92287	0.00000
27	C	-0.18027	-6.85138	0.00000
28	N	-0.92433	-7.77280	0.00000

Figure S4. Diagram of the 4,4'-azodi(phenylcyanamido) dianion showing the atomic labeling scheme and Cartesian axes.

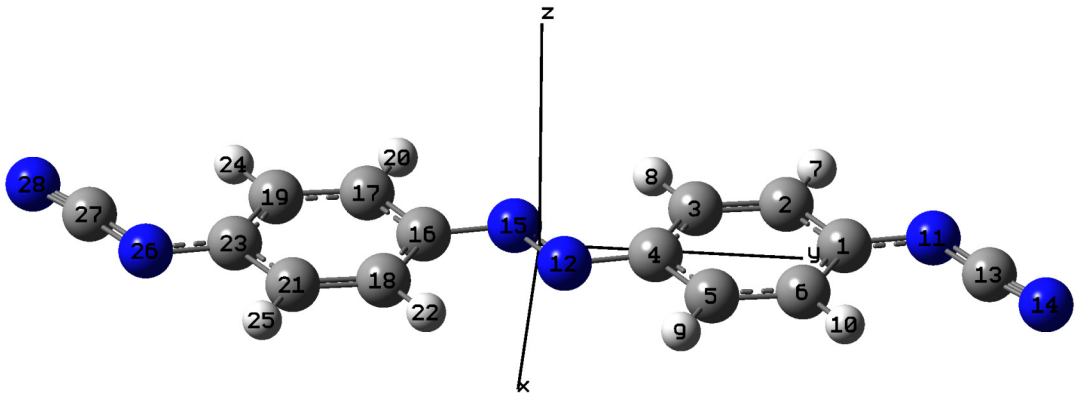

Figure S5. HOMO-5, HOMO-6, HOMO-7, HOMO-8 and HOMO-9 molecular orbital plots for $[(trpy)(bpy)Ru]_2(\mu\text{-adpc})^{2+}$. Orbital plots were generated from a single point calculation on the crystallographically obtained geometry using GaussView, with an isosurface value of 0.02. Hydrogen atoms have been omitted for clarity.

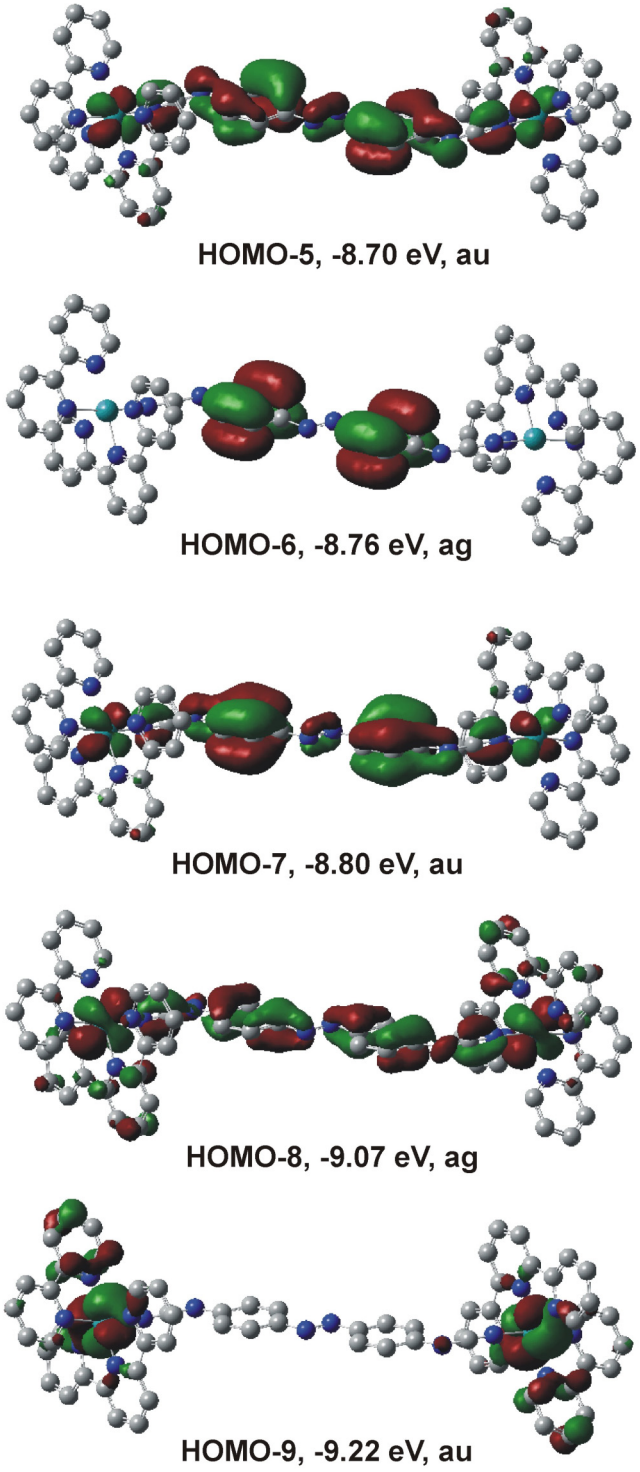
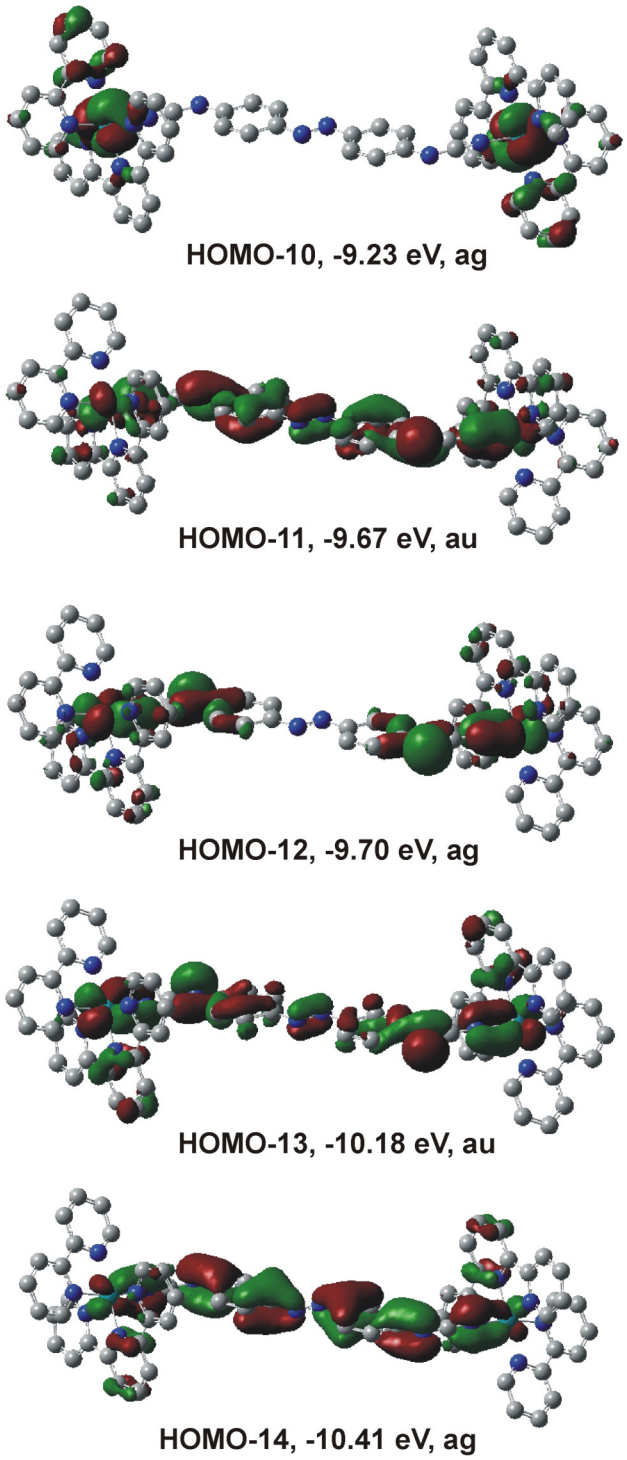
Figure S6. HOMO-10, HOMO-11, HOMO-12, HOMO-13 and HOMO-14 molecular orbital plots for $[(trpy)(bpy)Ru]_2(\mu\text{-adpc})^{2+}$. Orbital plots were generated from a single point calculation on the crystallographically obtained geometry using GaussView, with an isosurface value of 0.02. Hydrogen atoms have been omitted for clarity.