Supporting Information for

2,5-Dianilinoterephthalate Bridged MM Quadruply Bonded Complexes of Molybdenum and Tungsten.

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Table S1. Atomic coordinates for the geometry optimized structure of $[(HCO_2)_3Mo_2]_2\{\mu\text{-}1,4\text{-}(CO_2)_2\text{-}2,5\text{-}(NHPh)_2\text{-}C_6H_2\}$ (**1'**) in C_i symmetry.

Atom Number	Element	Coordinates / Å		
		x	y	z
1	C	-1.107931	0.815512	-0.088760
2	C	1.107931	-0.815512	0.088760
3	C	1.328459	0.566028	0.051571
4	C	-1.328459	-0.566028	-0.051571
5	C	-0.166706	-1.396209	0.031102
6	C	0.166706	1.396209	-0.031102
7	C	0.214955	2.869481	-0.042991
8	C	-0.214955	-2.869481	0.042991
9	O	1.343834	3.502741	-0.020008
10	O	-1.343834	-3.502741	0.020008
11	O	-0.882845	3.536447	-0.068065
12	O	0.882845	-3.536447	0.068065
13	Mo	-1.311581	-5.614155	0.041189
14	Mo	1.311581	5.614155	-0.041189
15	Mo	0.805739	-5.630105	0.065782
16	Mo	-0.805739	5.630105	-0.065782
17	O	-0.888434	5.634523	2.056246
18	O	-0.844996	5.632568	-2.185315
19	O	0.888434	-5.634523	-2.056246
20	O	0.844996	-5.632568	2.185315
21	O	1.397467	5.607572	-2.159738
22	O	1.354652	5.618361	2.080003
23	O	-1.397467	-5.607572	2.159738
24	O	-1.354652	-5.618361	-2.080003
25	O	1.389547	7.734440	-0.045009
26	O	-1.389547	-7.734440	0.045009
27	O	-0.853479	7.753202	-0.066632
28	O	0.853479	-7.753202	0.066632
29	H	1.949386	-1.485811	0.187781
30	H	-1.949386	1.485811	-0.187781
31	C	0.226200	5.626610	2.669174
32	C	0.282912	5.617444	-2.774035
33	C	-0.226200	-5.626610	-2.669174
34	C	-0.282912	-5.617444	2.774035
35	C	0.272877	8.345157	-0.056084
36	C	-0.272877	-8.345157	0.056084
37	H	0.295566	5.613471	-3.868219
38	H	0.214755	5.627801	3.763516
39	H	-0.295566	-5.613471	3.868219
40	H	-0.214755	-5.627801	-3.763516
41	H	0.282564	9.439446	-0.056432
42	H	-0.282564	-9.439446	0.056432
43	N	2.599525	1.109636	0.136411
44	N	-2.599525	-1.109636	-0.136411
45	H	-2.617747	-2.110850	-0.281865
46	H	2.617747	2.110850	0.281865
47	C	3.848099	0.468821	0.046643

48	C	4.903819	0.969011	0.829358
49	C	4.105007	-0.597020	-0.832963
50	C	6.177715	0.412329	0.742011
51	H	4.710025	1.788677	1.517423
52	C	5.379539	-1.160372	-0.897799
53	H	3.319362	-0.964654	-1.483997
54	C	6.422817	-0.664442	-0.113359
55	H	6.978363	0.814681	1.357114
56	H	5.558415	-1.984008	-1.584196
57	H	7.413103	-1.106579	-0.171646
58	C	-3.848099	-0.468821	-0.046643
59	C	-4.903819	-0.969011	-0.829358
60	C	-4.105007	0.597020	0.832963
61	C	-6.177715	-0.412329	-0.742011
62	H	-4.710025	-1.788677	-1.517423
63	C	-5.379539	1.160372	0.897799
64	H	-3.319362	0.964654	1.483997
65	C	-6.422817	0.664442	0.113359
66	H	-6.978363	-0.814681	-1.357114
67	H	-5.558415	1.984008	1.584196
68	H	-7.413103	1.106579	0.171646
69	C	-1.107931	0.815512	-0.088760
70	C	1.107931	-0.815512	0.088760

Table S2. Atomic coordinates for the geometry optimized structure of $[(HCO_2)_3W_2]_2\{\mu\text{-}1,4\text{-}(CO_2)_2\text{-}2,5\text{-}(NHPh)_2\text{-}C_6H_2\}$ (**2'**) in C_i symmetry.

Atom Number	Element	Coordinates / Å		
		x	y	z
1	C	-1.165213	0.738564	0.064197
2	C	1.165213	-0.738564	0.064197
3	C	1.283425	0.654015	0.017367
4	C	-1.283425	-0.654015	0.017367
5	C	-0.066396	-1.409855	0.052386
6	C	0.066396	1.409855	0.052386
7	C	0.023640	2.876327	0.095857
8	C	-0.023640	-2.876327	0.095857
9	O	1.121859	3.572025	0.130626
10	O	-1.121859	-3.572025	0.130626
11	O	-1.111542	3.491949	0.096537
12	O	1.111542	-3.491949	0.096537
13	W	-1.033997	-5.661959	0.138895
14	W	1.033997	5.661959	0.138895
15	W	1.165213	-5.578011	0.122422
16	W	-1.165213	5.578011	0.122422
17	O	-1.203005	5.570719	2.233360
18	O	-1.176944	5.596232	-1.988194
19	O	1.176944	-5.596232	-1.988194
20	O	1.203005	-5.570719	2.233360
21	O	1.071784	5.674221	-1.972445
22	O	1.045623	5.652265	2.249440
23	O	-1.045623	-5.652265	2.249440
24	O	-1.071784	-5.674221	-1.972445
25	O	0.988400	7.770898	0.147785
26	O	-0.988400	-7.770898	0.147785
27	O	-1.260823	7.692843	0.132563
28	O	1.260823	-7.692843	0.132563
29	H	2.060177	-1.342327	0.125129
30	H	-2.060177	1.342327	0.125129
31	H	2.491793	2.266683	0.205052
32	H	-2.491793	-2.266683	0.205052
33	C	-0.083480	5.607796	2.845948
34	C	-0.048487	5.638487	-2.584694
35	C	0.048487	-5.638487	-2.584694
36	C	0.083480	-5.607796	2.845948
37	C	-0.157926	8.335884	0.142921
38	C	0.157926	-8.335884	0.142921
39	H	-0.041127	5.645439	-3.676995
40	H	-0.091233	5.601871	3.938214
41	H	0.091233	-5.601871	3.938214
42	H	0.041127	-5.645439	-3.676995
43	H	-0.195771	9.427603	0.147909
44	H	0.195771	-9.427603	0.147909
45	C	-3.771594	-0.764757	-0.381445
46	C	-3.936606	0.261971	-1.327666
47	C	-4.918592	-1.368074	0.166839

48	C	-5.217019	0.678572	-1.692383
49	H	-3.069739	0.711380	-1.799263
50	C	-6.191475	-0.955614	-0.218033
51	H	-4.798979	-2.156226	0.906973
52	C	-6.351907	0.078140	-1.143989
53	H	-5.322933	1.471517	-2.428347
54	H	-7.061943	-1.438931	0.217929
55	H	-7.344875	0.406542	-1.436514
56	C	3.771594	0.764757	-0.381445
57	C	3.936606	-0.261971	-1.327666
58	C	4.918592	1.368074	0.166839
59	C	5.217019	-0.678572	-1.692383
60	H	3.069739	-0.711380	-1.799263
61	C	6.191475	0.955614	-0.218033
62	H	4.798979	2.156226	0.906973
63	C	6.351907	-0.078140	-1.143989
64	H	5.322933	-1.471517	-2.428347
65	H	7.061943	1.438931	0.217929
66	H	7.344875	-0.406542	-1.436514
67	N	2.521506	1.276590	0.000177
68	N	-2.521506	-1.276590	0.000177
69	C	-1.165213	0.738564	0.064197
70	C	1.165213	-0.738564	0.064197

Figure S1. Diagram of the calculated structures for $[(HCO_2)_3Mo_2]_2\{\mu\text{-}1,4\text{-}(CO_2)_2\text{-}2,5\text{-}(NHPh)_2\text{-}C_6H_2\}$ (**1'**) in C_i symmetry. The structure of the tungsten analogue (**2'**) is qualitatively similar.