Supporting Information

Spontaneous Release of Metalloradicals and Coordinatively Unsaturated Species in Asymmetric Iridium Dimers to Promote C-N Bond Formation

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Table S1. The Atomic Coordinates (angstroms) of Complex **1**

Center Number	Element	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.759466	3.929059	1.656433
2	C	1.123239	3.071809	0.789364
3	C	4.412344	0.483472	3.130124
4	C	3.429838	0.659815	2.157881
5	C	2.915795	-0.401239	1.427138
6	C	3.300296	-1.710078	1.727891
7	C	4.268627	-1.921534	2.729465
8	C	4.837317	-0.825368	3.417039
9	C	2.767394	1.961569	1.764581
10	Cl	4.776036	-3.560012	3.123784
11	C	1.102507	-2.931705	-0.572117
12	C	1.516088	-3.817465	-1.538880
13	C	2.504737	-1.863045	-1.917520
14	C	3.788604	1.621335	-1.603776
15	C	3.072987	0.430515	-1.463184
16	C	3.326953	-0.644964	-2.304887
17	C	4.247624	-0.561919	-3.348246
18	C	4.960270	0.638708	-3.516314
19	C	4.738778	1.724339	-2.638641
20	Cl	5.653428	3.214285	-2.841332
21	C	-1.739991	3.829111	1.685209
22	C	-1.366629	3.075947	0.603416
23	C	-2.327360	1.735105	2.079938
24	C	-2.996322	0.426196	2.443178
25	C	-3.740406	0.158862	3.590722
26	C	-4.368718	-1.094099	3.699467
27	C	-4.241355	-2.043125	2.659707
28	C	-3.454330	-1.757404	1.526490
29	C	-2.802338	-0.524499	1.452242
30	Cl	-5.067149	-3.592435	2.783103
31	N	-1.735491	1.724064	0.912697
32	O	-2.245813	3.007288	2.779248
33	N	1.831017	1.825986	0.863787
34	N	1.725014	-1.678991	-0.883174

35	O	2.486485	-3.217094	-2.451118
36	O	2.959614	3.325484	2.227728
37	C	-0.963312	-2.986621	-0.658178
38	C	-1.381923	-3.862039	-1.632376
39	C	-2.355746	-1.905210	-1.994760
40	C	-3.269486	-0.735436	-2.294014
41	C	-3.047894	0.315047	-1.414133
42	C	-3.826252	1.472513	-1.492002
43	C	-4.814042	1.562811	-2.492406
44	C	-5.010556	0.498515	-3.400816
45	C	-4.229539	-0.666042	-3.302035
46	N	-1.595763	-1.731334	-0.946159
47	O	-2.188289	-3.193036	-2.648220
48	Cl	-5.807801	3.010395	-2.612663
49	Ir	1.604864	0.107694	-0.070861
50	Ir	-1.529499	0.026388	-0.062206
51	Cl	0.005198	0.996670	-1.340679
52	O	0.052605	-0.537469	0.922236
53	H	-5.755796	0.578683	-4.164392
54	H	-4.370185	-1.479940	-3.982201
55	H	-3.673123	2.278171	-0.804661
56	H	-3.353146	-2.474824	0.739124
57	H	-4.946651	-1.328467	4.568985
58	H	-3.835900	0.890079	4.366033
59	H	5.672962	0.730040	-4.309221
60	H	4.410448	-1.392335	-4.003035
61	H	3.615954	2.442119	-0.939371
62	H	2.870906	-2.537653	1.202898
63	H	5.590112	-0.992179	4.158913
64	H	4.828440	1.321873	3.648669
65	C	-0.181152	-5.630863	-0.528190
66	C	0.292095	-4.701098	0.435830
67	C	-1.009916	5.879499	0.460557
68	C	-0.588878	5.024487	-0.599358
69	C	0.100015	5.605578	1.181604
70	C	-0.509847	4.729590	0.244311
71	C	-1.029945	-5.208984	-1.576068
72	C	-0.106665	-3.351168	0.372943

73	C	-1.592246	5.343215	1.625999
74	C	-0.767722	3.618871	-0.532340
75	C	0.009021	3.435116	0.043348
76	C	1.248731	5.202516	1.898940
77	H	-0.439911	2.757513	-0.652524
78	H	-1.366929	5.052734	-0.308799
79	H	-0.312626	6.579275	1.344227
80	H	1.715462	5.857841	2.604337
81	H	-1.911165	5.969700	2.432742
82	H	-0.880695	6.937895	0.371198
83	H	-0.129953	5.452704	-1.465925
84	H	-0.453908	2.989196	-1.338457
85	H	0.232867	-2.636489	1.093207
86	H	0.951039	-5.027191	1.213190
87	H	0.109110	-6.658578	-0.461488
88	H	-1.388207	-5.902729	-2.307678
89	C	1.008515	-5.114918	-1.575172
90	C	0.230697	-3.277124	0.453071
91	C	0.103829	-5.504827	-0.562423
92	C	-0.275179	-4.591858	0.457037
93	H	-0.048277	-2.571464	1.207464
94	H	-0.948176	-4.902607	1.228674
95	H	-0.297842	-6.496563	-0.562773
96	H	1.298601	-5.797745	-2.346180