Electronic Supplementary Data

Dalton Transactions

Reactions of Cp_2M (M = Ni, V) with Dilithium Diamido-aryl Reagents; Retention and Oxidation of the Transition Metal Ions

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Computational details

The coordinates of **5a** optimized at the M06-L/6-31+G** level (no solvent model present).

1	6	0	0.042719	-0.843341	3.490971
2	6	0	0.731241	-1.904378	2.873483
3	6	0	0.880944	-3.119599	3.539264
4	6	0	0.370048	-3.270142	4.830572
5	6	0	-0.308057	-2.217675	5.442989
6	6	0	-0.484444	-1.006161	4.769593
7	7	0	1.206511	-1.617964	1.576436
8	28	0	1.420892	0.299586	1.393690
9	7	0	-0.047143	0.320533	2.688242
10	28	0	-1.486895	0.283867	1.343884
11	7	0	-1.442285	2.252914	1.285166
12	6	0	-2.562621	2.900753	0.709325
13	6	0	-2.559282	2.913851	-0.698999
14	6	0	-3.613244	3.506899	-1.390699
15	6	0	-4.652886	4.117346	-0.684030
16	6	0	-4.653471	4.107369	0.708913
17	6	0	-3.615065	3.486192	1.407785
18	7	0	-1.444582	2.268119	-1.281408
19	28	0	-0.000040	2.271440	-0.000173
20	28	0	1.486530	0.282613	-1.343972
21	7	0	2.829853	0.148104	0.049229
22	6	0	3.519390	-1.079120	-0.039576
23	6	0	2.821476	-2.075488	-0.742476
24	6	0	3.382158	-3.343394	-0.894473
25	6	0	4.650611	-3.604092	-0.370365
26	6	0	5.344176	-2.611664	0.321556
27	6	0	4.775251	-1.348381	0.499125
28	7	0	1.559508	-1.663173	-1.220338
29	28	0	-0.000274	-1.708945	0.000603
30	7	0	-1.207019	-1.619757	-1.575672
31	6	0	-0.731190	-1.907206	-2.872247
32	6	0	-0.042557	-0.846611	-3.490379
33	6	0	0.485231	-1.010483	-4.768615
34	6	0	0.309360	-2.222619	-5.441011
35	6	0	-0.368891	-3.274647	-4.827976
36	6	0	-0.880371	-3.123063	-3.537030
37	7	0	0.046891	0.317952	-2.688646
38	28	0	-1.420792	0.297909	-1.393685
39	7	0	-2.830023	0.147833	-0.049203
40	6	0	-3.519533	-1.079267	0.040519
41	6	0	-2.821524	-2.075090	0.744091
42	6	0	-3.382019	-3.342972	0.896857
43	6	0	-4.650433	-3.604175	0.372876
44	6	0	-5.344102	-2.612280	-0.319694
45	6	0	-4.775360	-1.349017	-0.498015
46	7	0	-1.559591	-1.662231	1.221695
47	7	0	1.444996	2.269930	1.280444
48	6	0	2.559446	2.914840	0.696739
49	6	0	2.562159	2.900055	-0.711575
50	6	0	3.614342	3.484423	-1.411276
51	6	0	4.653190	4.106308	-0.713675
52	6	0	4.653239	4.118006	0.679256
53	6	0	3.613842	3.508625	1.387186
54	7	0	1.441426	2.251620	-1.286127
55	1	0	3.612754	3.464084	-2.499149

56	1	0	5.460516	4.581780	-1.262620
57	1	0	5.460381	4.602854	1.220233
58	1	0	3.610187	3.508405	2.475338
59	1	0	-3.609035	3.505307	-2.478847
60	1	0	-5.459695	4.601668	-1.225975
61	1	0	-5.460965	4.583654	1.256900
62	1	0	-3.614000	3.467251	2.495686
63	1	0	2.835491	-4.111523	-1.437719
64	1	0	5.098393	-4.583716	-0.509928
65	1	0	6.332465	-2.817344	0.722480
66	1	0	5.308227	-0.568321	1.038648
67	1	0	1.412273	-3.934205	3.051381
68	1	0	0.507661	-4.209879	5.357567
69	1	0	-0.701864	-2.335468	6.448351
70	1	0	-1.018805	-0.184487	5.242340
71	1	0	-5.308421	-0.569372	-1.038054
72	1	0	-6.332352	-2.818345	-0.720520
73	1	0	-5.098078	-4.583779	0.513013
74	1	0	-2.835258	-4.110711	1.440557
75	1	0	-1.411769	-3.937332	-3.048665
76	1	0	-0.506089	-4.214875	-5.354202
77	1	0	0.703653	-2.341256	-6.446081
78	1	0	1.019686	-0.189142	-5.241829
79	1	0	-1.277004	2.633511	-2.215673
80	1	0	-1.269506	2.627100	2.215553
81	1	0	-0.174479	1.136136	3.285168
82	1	0	2.015402	-2.203561	1.370994
83	1	0	-2.015994	-2.205140	-1.369986
84	1	0	0.173973	1.133151	-3.286168
85	1	0	-3.489985	0.914496	-0.173403
86	1	0	-1.306011	-2.208310	2.043944
87	1	0	1.278434	2.635710	2.214729
88	1	0	1.267606	2.625510	-2.216450
89	1	0	1.306006	-2.209817	-2.042223
90	1	0	3.490000	0.914803	0.172235

The coordinates of **5a** optimized at the M06L/6-31+G**with DMSO included via the SMD approach.

1	6	0	0.043954	0.832934	-3.485259
2	6	0	0.725474	1.904674	-2.874009
3	6	0	0.866062	3.118189	-3.546258
4	6	0	0.351735	3.258371	-4.839081
5	6	0	-0.317674	2.195521	-5.446377
6	6	0	-0.482951	0.983849	-4.767204
7	7	0	1.205981	1.628016	-1.577970
8	28	0	1.422360	-0.292874	-1.384111
9	7	0	-0.037846	-0.324842	-2.679228
10	28	0	-1.485475	-0.282204	-1.344348
11	7	0	-1.438194	-2.246907	-1.286200
12	6	0	-2.552795	-2.897329	-0.708765
13	6	0	-2.548083	-2.909941	0.702018
14	6	0	-3.594572	-3.514951	1.396639
15	6	0	-4.630897	-4.134306	0.690062
16	6	0	-4.633742	-4.124357	-0.704483
17	6	0	-3.600591	-3.494638	-1.406873
18	7	0	-1.438878	-2.259242	1.282392
19	28	0	0.000065	-2.250773	-0.000106
20	28	0	1.485512	-0.282442	1.344354
21	7	0	2.840669	-0.147017	-0.041486
22	6	0	3.524638	1.080537	0.042589
23	6	0	2.823280	2.080303	0.741784
24	6	0	3.383024	3.350377	0.888853
25	6	0	4.651772	3.612704	0.362331
26	6	0	5.348207	2.617784	-0.325650
27	6	0	4.781784	1.350707	-0.496238
28	7	0	1.563983	1.669455	1.222229
29	28	0	-0.000023	1.706875	0.000097
30	7	0	-1.205948	1.627620	1.578115
31	6	0	-0.725506	1.904130	2.874225
32	6	0	-0.044001	0.832331	3.485386
33	6	0	0.482839	0.983116	4.767376
34	6	0	0.317522	2.194716	5.446665
35	6	0	-0.351876	3.257622	4.839454
36	6	0	-0.866149	3.117566	3.546595
37	7	0	0.037866	-0.325343	2.679212
38	28	0	-1.422415	-0.293266	1.384177
39	7	0	-2.840652	-0.147124	0.041515
40	6	0	-3.524679	1.080420	-0.042377
41	6	0	-2.823401	2.080323	-0.741465
42	6	0	-3.383244	3.350369	-0.888401
43	6	0	-4.652005	3.612547	-0.361844
44	6	0	-5.348357	2.617503	0.326045
45	6	0	-4.781837	1.350450	0.496497
46	7	0	-1.564090	1.669640	-1.221998
47	7	0	1.438977	-2.258858	-1.282648
48	6	0	2.548230	-2.909650	-0.702461
49	6	0	2.552972	-2.897400	0.708328
50	6	0	3.600795	-3.494879	1.406255
51	6	0	4.633940	-4.124394	0.703676

52	6	0	4.631074	-4.133969	-0.690872
53	6	0	3.594725	-3.514439	-1.397263
54	7	0	1.438378	-2.247152	1.285964
55	1	0	3.593903	-3.483867	2.494337
56	1	0	5.437174	-4.610950	1.250251
57	1	0	5.432292	-4.627249	-1.234382
58	1	0	3.582572	-3.517207	-2.485395
59	1	0	-3.582444	-3.518003	2.484771
60	1	0	-5.432121	-4.627736	1.233429
61	1	0	-5.436963	-4.610778	-1.251198
62	1	0	-3.593679	-3.483333	-2.494952
63	1	0	2.834759	4.119371	1.430012
64	1	0	5.096851	4.594852	0.497082
65	1	0	6.336587	2.823647	-0.727901
66	1	0	5.317514	0.567204	-1.028723
67	1	0	1.392440	3.939116	-3.062947
68	1	0	0.480891	4.197316	-5.370904
69	1	0	-0.711012	2.303730	-6.453758
70	1	0	-1.002520	0.151005	-5.236824
71	1	0	-5.317509	0.566853	1.028899
72	1	0	-6.336747	2.823249	0.728329
73	1	0	-5.097163	4.594672	-0.496497
74	1	0	-2.835043	4.119455	-1.429495
75	1	0	-1.392509	3.938539	3.063342
76	1	0	-0.481060	4.196513	5.371364
77	1	0	0.710820	2.302828	6.454073
78	1	0	1.002405	0.150233	5.236930
79	1	0	-1.263649	-2.614801	2.220140
80	1	0	-1.262875	-2.610831	-2.221046
81	1	0	-0.156977	-1.149902	-3.265661
82	1	0	1.999012	2.236251	-1.374701
83	1	0	-1.999050	2.235808	1.374976
84	1	0	0.157009	-1.150475	3.265547
85	1	0	-3.504586	-0.908822	0.176906
86	1	0	-1.306633	2.235228	-2.030033
87	1	0	1.263647	-2.614312	-2.220416
88	1	0	1.263200	-2.611182	2.220794
89	1	0	1.306475	2.234906	2.030344
90	1	0	3.504619	-0.908652	-0.177132

The coordinates of **5b**$^{2-}$ at the M06-L/6-31+G** level (the one THF solvent molecule bound to Li is included, but no other solvent effects are included).

1	6	0	5.155244	1.722450	0.887467
2	8	0	4.767379	0.629407	1.724770
3	6	0	5.459608	-0.525076	1.231177
4	6	0	5.715463	-0.289934	-0.263963
5	6	0	5.192192	1.131969	-0.508785
6	3	0	2.655062	0.331819	1.586196
7	7	0	0.892007	0.051846	2.327160
8	6	0	0.085761	-0.085194	3.429660
9	6	0	-1.220681	0.483367	3.358359
10	6	0	-2.075689	0.476715	4.458908
11	6	0	-1.664727	-0.112286	5.662582
12	6	0	-0.410560	-0.727688	5.732132
13	6	0	0.444413	-0.735565	4.628885
14	7	0	-1.522938	0.982554	2.080329
15	28	0	0.148948	1.405662	1.185103
16	7	0	1.918473	1.698209	0.370422
17	6	0	2.070958	2.866677	-0.318584
18	6	0	1.648203	2.904944	-1.688223
19	6	0	1.873592	4.020191	-2.489243
20	6	0	2.498392	5.159287	-1.959408
21	6	0	2.840441	5.179088	-0.604889
22	6	0	2.606058	4.067140	0.208374
23	7	0	0.980666	1.729115	-2.072113
24	28	0	1.610705	0.281894	-0.916826
25	7	0	2.334818	-1.065808	0.267516
26	6	0	2.777285	-2.120871	-0.481846
27	6	0	2.401042	-2.160868	-1.864422
28	6	0	2.936284	-3.108639	-2.734122
29	6	0	3.827000	-4.082342	-2.257677
30	6	0	4.119406	-4.129206	-0.891672
31	6	0	3.578383	-3.187407	-0.012927
32	7	0	1.435303	-1.193866	-2.179942
33	28	0	-0.424054	-1.437524	-1.508794
34	7	0	0.110152	-2.838666	-0.245496
35	6	0	-0.886168	-3.670146	0.272904
36	6	0	-1.644910	-3.089846	1.320229
37	6	0	-2.650896	-3.836727	1.939017
38	6	0	-2.892736	-5.158789	1.550453
39	6	0	-2.144431	-5.730689	0.521836
40	6	0	-1.151499	-4.983443	-0.122500
41	7	0	-1.278650	-1.784565	1.653277
42	28	0	0.586442	-1.394480	1.059850
43	28	0	-1.958058	-0.259785	0.575301
44	28	0	-0.852397	1.462194	-1.361788
45	7	0	-0.699898	2.837218	-0.004472
46	6	0	-1.945524	3.320723	0.384744
47	6	0	-3.019341	2.447060	0.093290
48	6	0	-4.323480	2.804941	0.431605
49	6	0	-4.579065	4.041735	1.037566
50	6	0	-3.521196	4.903987	1.326798

51	6	0	-2.206796	4.542638	1.011494
52	7	0	-2.626914	1.254568	-0.531889
53	7	0	-2.313644	-1.493668	-0.984360
54	6	0	-3.094529	-1.096269	-2.074995
55	6	0	-2.423812	-0.277303	-3.017835
56	6	0	-3.103583	0.175079	-4.147343
57	6	0	-4.437135	-0.192411	-4.366208
58	6	0	-5.100133	-0.993162	-3.438277
59	6	0	-4.433346	-1.432221	-2.288432
60	7	0	-1.085407	-0.008162	-2.683879
61	1	0	6.150124	2.089914	1.204864
62	1	0	4.413677	2.513002	1.016299
63	1	0	5.811570	1.713110	-1.200025
64	1	0	4.167624	1.095474	-0.902292
65	1	0	6.785811	-0.372788	-0.489837
66	1	0	5.186472	-1.026490	-0.876287
67	1	0	4.817640	-1.388615	1.424698
68	1	0	6.402628	-0.641993	1.792455
69	1	0	3.794285	-3.238208	1.053814
70	1	0	4.778620	-4.906452	-0.505625
71	1	0	4.260664	-4.808510	-2.942530
72	1	0	2.644410	-3.095373	-3.785950
73	1	0	1.423442	-1.209735	4.682788
74	1	0	-0.091529	-1.199744	6.661274
75	1	0	-2.321841	-0.098345	6.530068
76	1	0	-3.063670	0.931134	4.370295
77	1	0	-1.376252	5.210635	1.234753
78	1	0	-3.714755	5.864974	1.800158
79	1	0	-5.601047	4.324762	1.281425
80	1	0	-5.137957	2.118118	0.202537
81	1	0	1.545179	4.005053	-3.530339
82	1	0	2.692317	6.022876	-2.592697
83	1	0	3.296709	6.070666	-0.174616
84	1	0	2.862580	4.090563	1.267521
85	1	0	-0.557853	-5.422991	-0.923210
86	1	0	-2.327727	-6.759799	0.218259
87	1	0	-3.663137	-5.738429	2.055614
88	1	0	-3.221272	-3.379910	2.746993
89	1	0	-4.941596	-2.058200	-1.556058
90	1	0	-6.136957	-1.279262	-3.603469
91	1	0	-4.952510	0.152251	-5.260460
92	1	0	-2.580395	0.810005	-4.861688
93	1	0	-2.285215	1.657648	2.131800
94	1	0	1.370957	-1.059242	-3.186915
95	1	0	0.959350	1.651263	-3.087675
96	1	0	-1.571482	-1.579420	2.607537
97	1	0	0.833604	-3.395974	-0.698501
98	1	0	-2.694778	-2.349286	-0.583002
99	1	0	-0.557890	0.245449	-3.517070
100	1	0	-3.404447	0.881452	-1.073760
101	1	0	-0.028716	3.593912	-0.120220