Supporting Information

Syntheses and solid-state structures of two cofacial (bis)dipyrrin dichromium complexes in different charge states

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A. NMR Spectroscopy

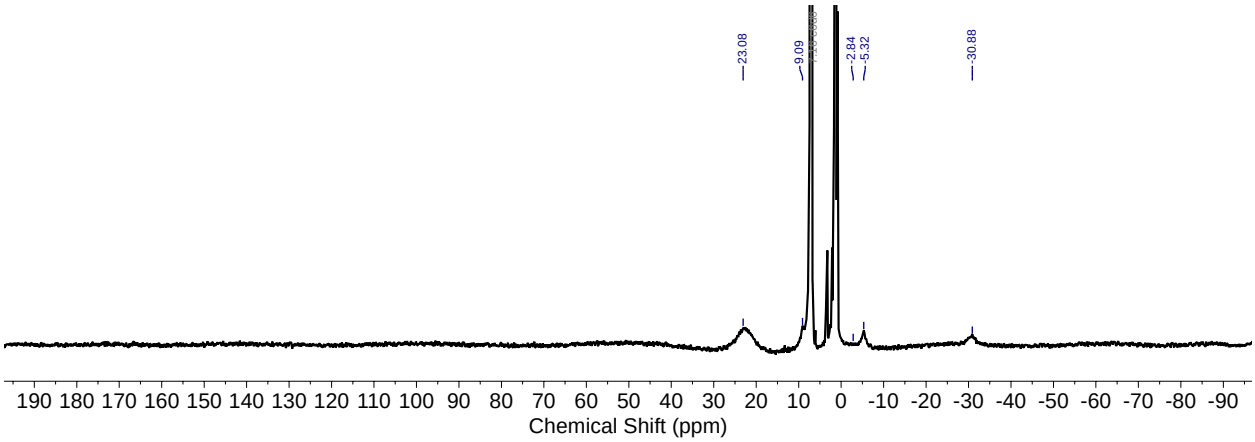

Figure S1. ^{1}H NMR (500 MH_Z, C_6D_6) of **1**.

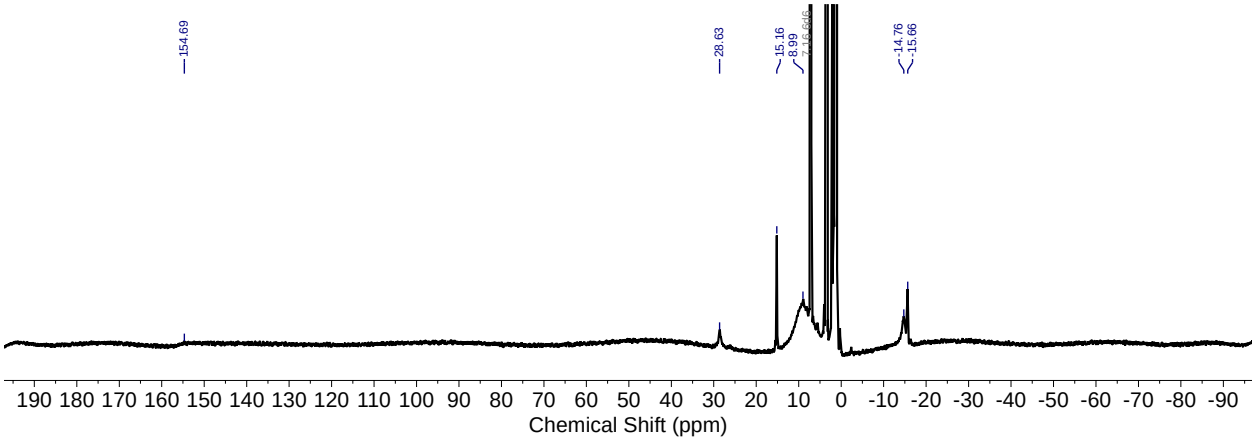

Figure S2. ^{1}H NMR (500 MH_Z, C_6D_6) of **2**.

B. Structural Metrics

Table S1. Bond lengths (Å) of ($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**1**) and K_2($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**2**).

($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**1**)			K_2($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**2**)		
Atom Numbers		Length	Atom Numbers		Length
Cr1	Cl1	2.3753(9)	Cr1	Cl1	2.420(1)
Cr1	Cl2	2.400(1)	Cr1	Cl2	2.417(1)
Cr1	N1	2.028(2)	Cr1	N1	2.000(4)
Cr1	N2	2.022(2)	Cr1	N2	2.002(4)
Cr2	Cl1	2.376(1)	Cr2	Cl1	2.411(1)
Cr2	Cl2	2.4167(8)	Cr2	Cl2	2.427(1)
Cr2	N3	2.025(2)	Cr2	N3	2.006(4)
Cr2	N4	2.018(3)	Cr2	N4	2.000(4)
O1	C22	1.392(3)	K1	Cl1	3.236(2)
O1	C27	1.395(3)	K1	N3	3.218(4)
N1	C2	1.409(4)	K1	C2	3.203(4)
N1	C5	1.339(4)	K1	C3	2.986(5)
N2	C6	1.407(4)	K1	C4	3.199(5)
N2	C9	1.344(4)	K1	C38	3.199(5)
N3	C37	1.412(4)	K1	C39	3.074(5)
N3	C40	1.336(4)	K1	C40	3.077(5)
N4	C33	1.400(4)	K1	C41	3.172(5)
N4	C36	1.346(4)	K2	Cl2	3.276(9)
C00V	C9	1.515(4)	K2	O1	3.182(9)
C00V	C14	1.545(4)	K2	N2	3.08(1)
C00V	C15	1.529(5)	K2	C6	2.94(1)
C00V	C16	1.535(5)	K2	C7	2.90(1)
C1	C2	1.406(4)	K2	C8	3.07(1)
C1	C6	1.411(4)	K2	C9	3.18(1)
C1	C17	1.499(4)	K2	C34	3.04(1)
C2	C3	1.418(4)	K2	C35	2.94(1)
C3	C4	1.369(5)	K2	C36	3.29(1)
C4	C5	1.415(4)	O1	C23	1.396(6)
C5	C10	1.525(4)	O1	C32	1.406(6)
C6	C7	1.419(4)	N1	C2	1.407(6)
C7	C8	1.373(4)	N1	C5	1.379(6)
C8	C9	1.421(4)	N2	C6	1.399(6)
C10	C11	1.534(4)	N2	C9	1.381(6)
C10	C12	1.535(4)	N3	C38	1.413(6)
C10	C13	1.531(4)	N3	C41	1.374(6)
C17	C18	1.396(4)	N4	C34	1.396(6)
C17	C22	1.399(4)	N4	C37	1.390(6)

Table S1 (cont'd). Bond lengths (Å) of ($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**1**) and K_2($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**2**).

($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**1**)			K_2($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**2**)		
Atom Numbers		Length	Atom Numbers		Length
C18	C19	1.389(4)	C1	C2	1.429(7)
C19	C20	1.381(4)	C1	C6	1.448(7)
C20	C21	1.399(4)	C1	C18	1.496(6)
C21	C22	1.393(4)	C2	C3	1.419(7)
C21	C23	1.522(4)	C3	C4	1.384(7)
C23	C24	1.549(5)	C4	C5	1.395(7)
C23	C25	1.538(4)	C5	C10	1.518(6)
C23	C26	1.526(4)	C6	C7	1.399(7)
C26	C27	1.395(4)	C7	C8	1.401(7)
C26	C31	1.395(4)	C8	C9	1.396(7)
C27	C28	1.404(4)	C9	C14	1.527(6)
C28	C29	1.393(4)	C10	C11	1.546(8)
C28	C32	1.500(4)	C10	C12	1.540(7)
C29	C30	1.384(5)	C10	C13	1.529(7)
C30	C31	1.382(4)	C14	C15	1.548(7)
C32	C33	1.406(4)	C14	C16	1.521(7)
C32	C37	1.397(4)	C14	C17	1.538(7)
C33	C34	1.426(5)	C18	C19	1.388(7)
C34	C35	1.375(4)	C18	C23	1.388(7)
C35	C36	1.418(4)	C19	C20	1.383(6)
C36	C41	1.515(5)	C20	C21	1.392(8)
C37	C38	1.420(4)	C21	C22	1.398(8)
C38	C39	1.375(4)	C22	C23	1.399(6)
C39	C40	1.421(4)	C22	C24	1.531(7)
C40	C45	1.520(4)	C24	C25	1.557(8)
C41	C42	1.541(5)	C24	C26	1.523(6)
C41	C43	1.527(5)	C24	C27	1.513(7)
C41	C44	1.537(6)	C27	C28	1.382(7)
C45	C46	1.542(4)	C27	C32	1.413(6)
C45	C47	1.529(4)	C28	C29	1.367(7)
C45	C48	1.536(5)	C29	C30	1.388(6)
			C30	C31	1.389(7)
			C31	C32	1.395(7)
			C31	C33	1.490(6)
			C33	C34	1.422(7)
			C33	C38	1.431(7)
			C34	C35	1.417(7)
			C35	C36	1.414(7)
			C36	C37	1.385(7)

Table S1 (cont'd). Bond lengths (Å) of $K_2(^{tBu}dmx)Cr_2Cl_2$ (**2**).

	$K_2(^{tBu}dmx)Cr_2Cl_2$ (**2**)		
	Atom Numbers		Length
	C37	C42	1.516(6)
	C38	C39	1.403(7)
	C39	C40	1.403(7)
	C40	C41	1.397(6)
	C41	C46	1.518(7)
	C42	C43	1.529(7)
	C42	C44	1.534(8)
	C42	C45	1.523(8)
	C46	C47	1.541(7)
	C46	C48	1.524(7)
	C46	C49	1.562(7)

Table S2. Bond angles (°) of ($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**1**) and K_2($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**2**).

($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**1**)				K_2($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**2**)			
Atom Numbers			Angle	Atom Numbers			Angle
Cl1	Cr1	Cl2	85.91(3)	C1	C18	C19	119.5(4)
Cl1	Cr1	N1	89.44(7)	C1	C18	C23	123.0(4)
Cl1	Cr1	N2	163.20(7)	C1	C2	C3	129.5(4)
Cl2	Cr1	N1	166.66(7)	C1	C6	C7	127.1(5)
Cl2	Cr1	N2	94.09(7)	C11	C10	C12	108.4(4)
N1	Cr1	N2	86.8(1)	C11	C10	C13	108.0(4)
Cl1	Cr2	Cl2	85.51(3)	C12	C10	C13	109.7(4)
Cl1	Cr2	N3	90.81(7)	C15	C14	C16	108.1(4)
Cl1	Cr2	N4	166.57(8)	C15	C14	C17	108.7(4)
Cl2	Cr2	N3	163.13(7)	C16	C14	C17	109.7(4)
Cl2	Cr2	N4	93.92(8)	C18	C19	C20	121.4(5)
N3	Cr2	N4	85.9(1)	C18	C23	C22	122.5(5)
Cr1	Cl1	Cr2	86.18(3)	C19	C18	C23	117.4(4)
Cr1	Cl2	Cr2	84.74(3)	C19	C20	C21	120.5(5)
C22	O1	C27	116.4(2)	C2	C1	C18	118.9(4)
Cr1	N1	C2	110.9(2)	C2	C1	C6	124.1(4)
Cr1	N1	C5	135.0(2)	C2	C3	C4	106.8(4)
C2	N1	C5	107.1(2)	C2	N1	C5	107.1(4)
Cr1	N2	C6	110.6(2)	C20	C21	C22	119.5(5)
Cr1	N2	C9	138.0(2)	C21	C22	C23	118.4(5)
C6	N2	C9	107.1(2)	C21	C22	C24	123.0(4)
Cr2	N3	C37	109.8(2)	C22	C24	C25	107.4(4)
Cr2	N3	C40	136.2(2)	C22	C24	C26	112.6(4)
C37	N3	C40	107.0(2)	C22	C24	C27	106.8(4)
Cr2	N4	C33	112.4(2)	C23	C22	C24	118.5(4)
Cr2	N4	C36	136.5(2)	C23	O1	C32	115.1(4)
C33	N4	C36	107.7(2)	C24	C27	C28	124.8(4)
C2	C1	C6	125.3(3)	C24	C27	C32	117.8(4)
C2	C1	C17	117.5(2)	C25	C24	C26	109.0(4)
C6	C1	C17	116.0(2)	C25	C24	C27	109.0(4)
N1	C2	C1	122.5(2)	C26	C24	C27	111.9(4)
N1	C2	C3	108.2(2)	C27	C28	C29	121.8(5)
C1	C2	C3	128.6(3)	C27	C32	C31	122.4(5)
C2	C3	C4	107.0(3)	C28	C27	C32	117.4(4)
C3	C4	C5	107.6(3)	C28	C29	C30	119.6(5)
N1	C5	C4	110.1(2)	C29	C30	C31	121.8(5)
N1	C5	C10	123.8(2)	C3	C4	C5	108.7(4)
C4	C5	C10	125.9(2)	C30	C31	C32	117.0(4)
N2	C6	C1	123.2(2)	C30	C31	C33	119.4(4)

Table S2 (cont'd). Bond angles (°) of ($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**1**) and K_2($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**2**).

($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**1**)				K_2($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**2**)			
Atom Numbers			Angle	Atom Numbers			Angle
N2	C6	C7	108.6(2)	C31	C33	C34	115.7(4)
C1	C6	C7	126.4(3)	C31	C33	C38	117.1(4)
C6	C7	C8	106.7(3)	C32	C31	C33	123.4(4)
C7	C8	C9	107.7(3)	C33	C34	C35	126.8(5)
N2	C9	C00V	124.1(3)	C33	C38	C39	128.7(5)
N2	C9	C8	109.8(3)	C34	C33	C38	124.3(4)
C5	C10	C11	107.7(2)	C34	C35	C36	105.8(4)
C5	C10	C12	110.1(2)	C34	N4	C37	107.1(4)
C5	C10	C13	112.1(2)	C35	C36	C37	108.5(4)
C11	C10	C12	109.1(3)	C36	C37	C42	127.8(4)
C11	C10	C13	108.1(2)	C37	C42	C43	108.1(4)
C12	C10	C13	109.7(2)	C37	C42	C44	111.2(4)
C1	C17	C18	117.5(2)	C37	C42	C45	111.3(4)
C1	C17	C22	124.1(3)	C38	C39	C40	107.2(4)
C18	C17	C22	118.3(3)	C38	N3	C41	106.7(4)
C17	C18	C19	121.0(3)	C39	C40	C41	107.4(4)
C18	C19	C20	119.6(3)	C4	C5	C10	128.0(4)
C19	C20	C21	121.1(3)	C40	C41	C46	126.3(4)
C20	C21	C22	118.4(3)	C41	C46	C47	107.8(4)
C20	C21	C23	122.4(3)	C41	C46	C48	112.3(4)
C22	C21	C23	119.2(2)	C41	C46	C49	111.0(4)
O1	C22	C17	117.2(2)	C43	C42	C44	108.3(4)
O1	C22	C21	121.3(2)	C43	C42	C45	108.5(4)
C17	C22	C21	121.5(3)	C44	C42	C45	109.3(5)
C21	C23	C24	108.4(2)	C47	C46	C48	108.3(4)
C21	C23	C25	112.5(2)	C47	C46	C49	107.1(4)
C21	C23	C26	107.5(2)	C48	C46	C49	110.1(4)
C24	C23	C25	108.4(2)	C5	C10	C11	107.9(4)
C24	C23	C26	107.2(2)	C5	C10	C12	110.5(4)
C25	C23	C26	112.6(2)	C5	C10	C13	112.2(4)
C23	C26	C27	119.0(2)	C6	C1	C18	114.6(4)
C23	C26	C31	122.4(3)	C6	C7	C8	106.5(4)
C27	C26	C31	118.5(3)	C6	N2	C9	106.5(4)
O1	C27	C26	121.1(2)	C7	C8	C9	107.9(4)
O1	C27	C28	117.6(2)	C8	C9	C14	126.5(4)
C26	C27	C28	121.3(3)	C9	C14	C15	107.5(4)
C27	C28	C29	118.2(3)	C9	C14	C16	112.3(4)
C27	C28	C32	124.4(3)	C9	C14	C17	110.3(4)
C29	C28	C32	117.5(2)	Cl1	Cr1	Cl2	82.83(4)

Table S2 (cont'd). Bond angles (°) of ($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**1**) and K_2($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**2**).

($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**1**)

Atom Numbers			Angle
C28	C29	C30	121.3(3)
C29	C30	C31	119.6(3)
C26	C31	C30	121.1(3)
C28	C32	C33	117.5(2)
C28	C32	C37	116.4(2)
C33	C32	C37	124.7(3)
N4	C33	C32	122.3(2)
N4	C33	C34	108.1(2)
C32	C33	C34	127.9(3)
C33	C34	C35	106.8(3)
C34	C35	C36	107.6(3)
N4	C36	C35	109.7(3)
N4	C36	C41	122.8(3)
C35	C36	C41	127.4(3)
N3	C37	C32	123.5(3)
N3	C37	C38	108.4(2)
C32	C37	C38	127.0(3)
C37	C38	C39	106.8(3)
C38	C39	C40	107.3(3)
N3	C40	C39	110.4(3)
N3	C40	C45	124.6(3)
C39	C40	C45	125.0(3)
C36	C41	C42	108.1(3)
C36	C41	C43	110.0(3)
C36	C41	C44	112.3(3)
C42	C41	C43	110.6(3)
C42	C41	C44	107.1(3)
C43	C41	C44	108.7(3)
C40	C45	C46	108.1(3)
C40	C45	C47	111.9(2)
C40	C45	C48	109.8(3)
C46	C45	C47	108.4(3)
C46	C45	C48	108.1(3)
C47	C45	C48	110.4(3)

K_2($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**2**)

Atom Numbers			Angle
Cl1	Cr1	N1	91.7(1)
Cl1	Cr1	N2	164.0(1)
Cl1	Cr2	Cl2	82.81(4)
Cl1	Cr2	N3	92.9(1)
Cl1	Cr2	N4	168.0(1)
Cl2	Cr1	N1	169.2(1)
Cl2	Cr1	N2	93.9(1)
Cl2	Cr2	N3	164.5(1)
Cl2	Cr2	N4	91.9(1)
Cr1	Cl1	Cr2	84.34(4)
Cr1	Cl2	Cr2	84.05(4)
Cr1	N1	C2	112.1(3)
Cr1	N1	C5	133.8(3)
Cr1	N2	C6	112.8(3)
Cr1	N2	C9	138.0(3)
Cr2	N3	C38	113.2(3)
Cr2	N3	C41	137.6(3)
Cr2	N4	C34	111.3(3)
Cr2	N4	C37	135.8(3)
K2	O1	C23	123.4(3)
K2	O1	C32	117.4(3)
N1	C2	C1	122.0(4)
N1	C2	C3	108.2(4)
N1	C5	C10	122.7(4)
N1	C5	C4	109.1(4)
N1	Cr1	N2	88.8(1)
N2	C6	C1	122.8(4)
N2	C6	C7	109.6(4)
N2	C9	C14	124.0(4)
N2	C9	C8	109.4(4)
N3	C38	C33	122.4(4)
N3	C38	C39	108.5(4)
N3	C41	C40	109.9(4)
N3	C41	C46	123.6(4)
N3	Cr2	N4	89.4(1)
N4	C34	C33	123.6(4)
N4	C34	C35	109.2(4)
N4	C37	C36	109.3(4)
N4	C37	C42	122.8(4)

Table S2 (cont'd). Bond angles (°) of $K_2(^{tBu}dmx)Cr_2Cl_2$ (**2**).

	$K_2(^{tBu}dmx)Cr_2Cl_2$ (**2**)			
	Atom Numbers			Angle
	O1	C23	C18	118.1(4)
	O1	C23	C22	119.3(4)
	O1	C32	C27	120.0(4)
	O1	C32	C31	117.6(4)

C. Computational Results

Table S3. Mulliken charges and spin densities for ($^{t\text{Bu}}$dmx)Cr_2Cl_2 (**1**).

Atom	Mulliken Charge	Spin Density	Atom	Mulliken Charge	Spin Density
1 Cr	0.324333	4.134156	38 H	0.160660	0.000065
2 Cr	0.326641	4.137313	39 H	0.156737	0.000296
3 Cl	–0.193505	–0.059001	40 H	0.158624	0.000071
4 Cl	–0.212064	–0.056078	41 C	–0.464409	–0.019185
5 O	–0.113969	0.000446	42 H	0.153522	0.003543
6 N	–0.079321	–0.100777	43 H	0.161401	0.002082
7 N	–0.078575	–0.101137	44 H	0.174434	0.004438
8 N	–0.078192	–0.099752	45 C	–0.432086	0.000054
9 N	–0.081878	–0.103327	46 H	0.153734	–0.000016
10 C	–0.089012	0.007875	47 H	0.153814	0.000362
11 C	–0.009149	0.012764	48 H	0.177801	0.002237
12 C	–0.012637	–0.014632	49 C	–0.240332	0.002889
13 C	–0.196082	0.034209	50 C	–0.169525	–0.000749
14 H	0.189749	–0.001603	51 H	0.146351	–0.000137
15 C	–0.154278	–0.011705	52 C	0.005010	–0.000106
16 H	0.166136	–0.000094	53 H	0.129791	0.000036
17 C	–0.011495	0.045496	54 C	–0.239336	0.000016
18 C	0.105046	–0.013754	55 H	0.143222	–0.000004
19 C	–0.194337	0.033495	56 C	0.038959	0.000000
20 H	0.187180	–0.001677	57 C	0.122938	–0.000905
21 C	–0.150586	–0.009342	58 C	0.011095	–0.000200
22 H	0.169602	–0.000035	59 C	–0.344696	0.000004
23 C	–0.000238	0.044597	60 H	0.155191	0.000003
24 C	–0.066677	0.009390	61 H	0.153703	0.000001
25 C	–0.445027	0.000582	62 H	0.171964	0.000016
26 H	0.158397	0.000071	63 C	–0.513799	0.000006
27 H	0.156630	0.000330	64 H	0.191345	0.000000
28 H	0.159708	0.000069	65 H	0.170259	–0.000003
29 C	–0.434155	–0.001689	66 H	0.168591	–0.000002
30 H	0.170681	0.003961	67 C	–0.036063	–0.000015
31 H	0.158079	0.000414	68 C	0.212274	–0.000102
32 H	0.153831	0.000037	69 C	–0.317981	0.001601
33 C	–0.472249	–0.019398	70 C	–0.151730	–0.000629
34 H	0.175911	0.004829	71 H	0.134542	0.000134
35 H	0.162823	0.002206	72 C	0.009649	–0.000392
36 H	0.159878	0.002906	73 H	0.129313	0.000023
37 C	–0.451257	0.000676	74 C	–0.234228	0.000107

Table S3 (cont'd). Mulliken charges and spin densities for (^{tBu}dmx)Cr_2Cl_2 (**1**).

Atom	Mulliken Charge	Spin Density	Atom	Mulliken Charge	Spin Density
75 H	0.143934	0.000006	95 H	0.177870	0.001626
76 C	–0.008446	0.012546	96 H	0.154315	0.000344
77 C	0.064706	–0.011945	97 H	0.154829	0.000036
78 C	–0.206625	0.034647	98 C	–0.511521	–0.034606
79 H	0.178012	–0.001798	99 H	0.187151	0.008053
80 C	–0.143514	–0.009526	100 H	0.165343	0.002878
81 H	0.164586	–0.000004	101 H	0.165844	0.006380
82 C	–0.011384	0.040779	102 C	–0.071373	0.006099
83 C	0.020048	–0.015599	103 C	–0.445777	0.000560
84 C	–0.190371	0.034619	104 H	0.159191	0.000113
85 H	0.185483	–0.001596	105 H	0.157448	0.000306
86 C	–0.152056	–0.011861	106 H	0.158172	0.000063
87 H	0.170060	–0.000053	107 C	–0.463839	–0.015671
88 C	–0.011103	0.046822	108 H	0.160307	0.003432
89 C	–0.050128	0.016746	109 H	0.160217	0.001907
90 C	–0.440916	0.000857	110 H	0.169920	0.003489
91 H	0.157816	0.000052	111 C	–0.437787	–0.000678
92 H	0.155219	0.000330	112 H	0.156212	–0.000011
93 H	0.000018	0.159431	113 H	0.156667	0.000320
94 C	–0.437781	0.000130	114 H	0.177082	0.002852

Table S4. Mulliken charges and spin densities for $K_2(^{tBu}dmx)Cr_2Cl_2$ (**2**).

Atom	Mulliken Charge	Spin Density	Atom	Mulliken Charge	Spin Density
1 Cr	0.304088	4.091886	40 H	0.180204	–0.000015
2 Cr	0.307110	4.087832	41 C	–0.139764	0.000465
3 K	1.069719	0.004171	42 H	0.152619	0.000080
4 O	–0.377979	–0.000122	43 H	0.155593	–0.000058
5 C	–0.109412	0.000147	44 Cl	–0.254933	–0.056134
6 H	0.153039	0.000009	45 Cl	–0.250505	–0.056322
7 H	0.149975	0.000458	46 O	–0.133322	0.003477
8 C	–0.365240	0.000048	47 N	–0.073742	–0.121594
9 H	0.175339	0.000000	48 N	–0.055951	–0.121151
10 H	0.172803	–0.000003	49 N	–0.085996	–0.123954
11 C	–0.387680	0.000045	50 N	–0.065953	–0.126662
12 H	0.190608	–0.000002	51 C	0.179113	–0.470658
13 H	0.180335	–0.000008	52 C	–0.181208	0.114765
14 C	–0.120516	–0.000553	53 C	–0.374351	–0.179042
15 H	0.155147	0.000827	54 H	0.110565	0.007807
16 H	0.156015	0.000048	55 C	–0.191242	0.005224
17 O	–0.341512	0.000055	56 H	0.137778	0.001614
18 C	–0.153425	–0.000198	57 C	–0.007568	–0.130995
19 H	0.136174	–0.000021	58 C	–0.316024	0.101801
20 H	0.145029	–0.000145	59 C	–0.223460	–0.151875
21 C	–0.337180	0.000076	60 H	0.143524	0.006714
22 H	0.168602	–0.000039	61 C	–0.169914	0.022161
23 H	0.165347	0.000002	62 H	0.137922	–0.000354
24 C	–0.403806	–0.000320	63 C	–0.063309	–0.109881
25 H	0.171201	0.000001	64 C	–0.030690	0.027159
26 H	0.190125	–0.000102	65 C	–0.447872	–0.007632
27 C	–0.074456	0.000106	66 H	0.147928	0.000594
28 H	0.187959	–0.001400	67 H	0.151737	–0.002063
29 H	0.160313	0.002272	68 H	0.158780	0.001141
30 K	1.045357	0.004531	69 C	–0.469979	–0.007000
31 O	–0.372187	–0.000060	70 H	0.175797	0.003253
32 C	–0.146726	–0.000589	71 H	0.156564	–0.002722
33 H	0.168865	–0.000040	72 H	0.158176	0.000027
34 H	0.163272	–0.000009	73 C	–0.491495	–0.023912
35 C	–0.351088	0.000052	74 H	0.182647	0.005765
36 H	0.179291	0.000013	75 H	0.159335	0.002662
37 H	0.179324	–0.000017	76 H	0.165719	0.003997
38 C	–0.355463	0.000016	77 C	–0.043785	0.018665
39 H	0.174006	0.000005	78 C	–0.463449	–0.006755

Table S4 (cont'd). Mulliken charges and spin densities for $K_2(^{tBu}dmx)Cr_2Cl_2$ (**2**).

Atom	Mulliken Charge	Spin Density	Atom	Mulliken Charge	Spin Density
79 H	0.165030	0.001164	118 C	–0.329682	0.116672
80 H	0.153478	–0.001478	119 C	–0.361616	–0.191460
81 H	0.150051	0.000629	120 H	0.149407	0.007637
82 C	–0.475869	–0.021272	121 C	–0.115346	0.011482
83 H	0.158986	0.005509	122 H	0.126616	0.000575
84 H	0.159194	0.002336	123 C	0.011245	–0.119217
85 H	0.176598	0.004603	124 C	–0.199445	0.115422
86 C	–0.472399	–0.004225	125 C	–0.233544	–0.168019
87 H	0.154107	–0.000364	126 H	0.119639	0.008389
88 H	0.157970	–0.002444	127 C	–0.213630	0.019620
89 H	0.172254	0.002235	128 H	0.130785	0.000131
90 C	–0.148803	0.036278	129 C	–0.102596	–0.116227
91 C	–0.215595	–0.024212	130 C	–0.044604	0.021464
92 H	0.181005	0.001365	131 C	–0.452321	–0.007445
93 C	–0.026220	0.009087	132 H	0.150468	0.000689
94 H	0.126381	–0.001078	133 H	0.151244	–0.001810
95 C	–0.229440	–0.025255	134 H	0.159909	0.001230
96 H	0.136364	0.001872	135 C	–0.452681	–0.006006
97 C	–0.068198	0.008722	136 H	0.173416	0.003200
98 C	0.022747	–0.021103	137 H	0.152904	–0.002475
99 C	0.079707	–0.002942	138 H	0.149809	–0.000274
100 C	–0.374805	0.000331	139 C	–0.478209	–0.017866
101 H	0.171461	–0.000135	140 H	0.178105	0.004414
102 H	0.157278	0.000053	141 H	0.157201	0.002137
103 H	0.155587	–0.000023	142 H	0.158618	0.002945
104 C	–0.536054	0.000132	143 C	–0.025818	0.021150
105 H	0.174067	–0.000175	144 C	–0.464551	–0.006977
106 H	0.174584	–0.000054	145 H	0.160367	0.001055
107 H	0.191318	0.000014	146 H	0.153355	–0.001733
108 C	0.013645	0.000868	147 H	0.150529	0.000708
109 C	–0.272409	–0.005520	148 C	–0.479232	–0.022075
110 H	0.140818	0.000379	149 H	0.159259	0.005068
111 C	0.043637	0.002774	150 H	0.159965	0.002522
112 H	0.123420	–0.000526	151 H	0.180298	0.004959
113 C	–0.232785	–0.013954	152 C	–0.477977	–0.006551
114 H	0.143629	0.000908	153 H	0.164097	–0.000124
115 C	–0.102643	0.032023	154 H	0.157515	–0.002409
116 C	–0.005625	–0.010305	155 H	0.167832	0.002344
117 C	0.214341	–0.476923			