Supplementary Materials: Molecularly Engineered Lithium–Chromium Alkoxide for Selective Synthesis of $LiCrO_2$ and Li_2CrO_4 Nanomaterials

Olusola Ojelere, David Graf and Sanjay Mathur *

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Supporting Tables:

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Figure S1 UV-Vis spectra of compound **1** and **2** recorded in THF.

Table S1. Crystallographic data for compounds **1**

Identification code	$[Li_2Cr(O^tBu)_4Cl(THF)_2]$
Empirical formula	$C_{24}H_{52}ClCrLi_2O_6$
Formula weight	537.98
Temperature/K	293(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	25.681(3)
b/Å	8.9889(9)
c/Å	18.4468(18)
α/°	90
β/°	133.511(6)
γ/°	90
Volume/Å^3	3088.3(6)
Z	4
ρ_{calc}g/cm^3	1.157
μ/mm^{-1}	0.488
F(000)	1164.0
Crystal size/mm^3	0.200 × 0.100 × 0.100
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.032 to 53.56
Index ranges	$-32 \leq h \leq 32$, $-10 \leq k \leq 11$, $-23 \leq l \leq 23$
Reflections collected	6874

Table S2: Some selected bond lengths for compounds **1**

Atom	**Atom**	**Length/Å**
Cr1	O4	1.864(3)
Cr1	O5	1.868(3)
Li2	O4	1.922(8)
Li2	O5	1.949(8)
Li2	O2	1.964(8)
Li2	Cl3	2.290(7)

Table S3: Some selected bond Angles for compound **1.**

Atom	Atom	Atom	Angle/°
O4	Cr1	O4	122.51(18)
O4	Cr1	O5	82.97(12)
O4[1]	Cr1	O5	124.58(12)
O4	Cr1	O5[1]	124.58(12)
O4[1]	Cr1	O5[1]	82.97(12)
O5	Cr1	O5[1]	124.85(18)
O4	Cr1	Li2[1]	141.44(18)
O4[1]	Cr1	Li2[1]	41.21(18)
O5	Cr1	Li2[1]	135.55(17)
O5[1]	Cr1	Li2[1]	42.07(17)
O4	Cr1	Li2	41.21(18)
O4[1]	Cr1	Li2	141.44(18)
O5	Cr1	Li2	42.07(17)
O5	Cr1	Li2	135.55(17)
Li2	Cr1	Li2	176.5(3)
O4	Li2	O5	79.4(3)
O4	Li2	O2	116.6(4)
O5	Li2	O2	110.7(3)
O4	Li2	Cl3	116.6(3)
O5	Li2	Cl3	130.6(4)
O2	Li2	Cl3	102.8(3)
O4	Li2	Cr1	39.70(15)
O5	Li2	Cr1	39.95(16)
O2	Li2	Cr1	125.0(3)
Cl3	Li2	Cr1	131.9(3)
Li2	Cl3	Li2	180.0(4)

Table S4: Crystal data and structure refinement for compound **2.**

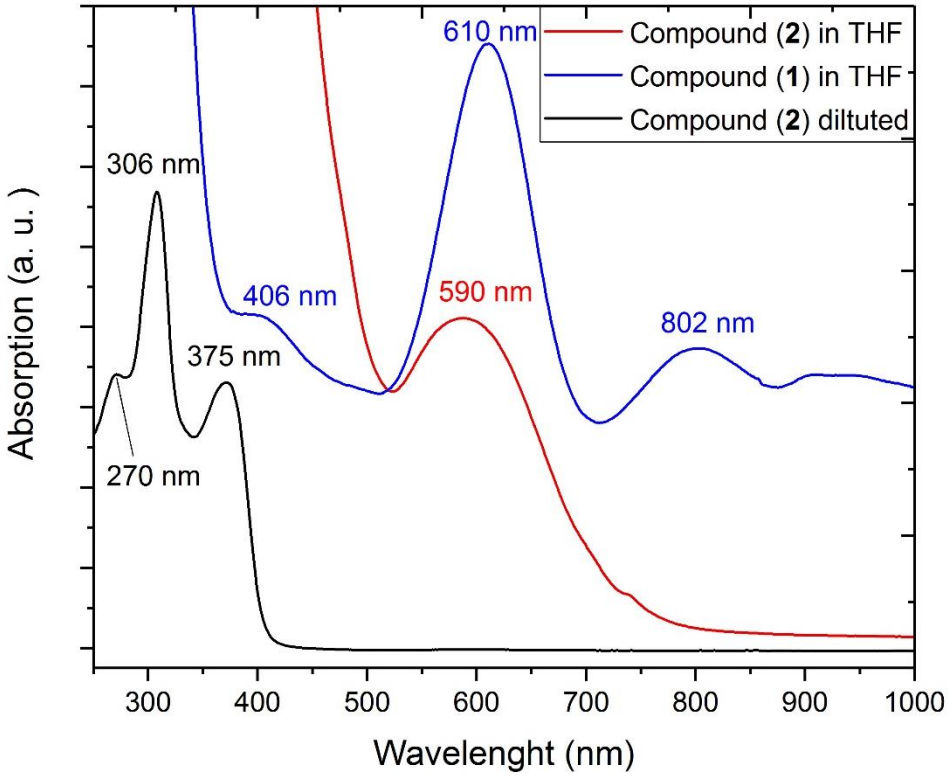
Formula	$C_{32}H_{44}CrF_6LiN_2O_6$
Formula weight	725.63
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.8499(6)
b/Å	10.7574(5)
c/Å	22.6334(11)
α/°	90
β/°	90.059(4)
γ/°	90
Volume/Å^3	3615.6(3)
Z	4
ρ_{calc}g/cm^3	1.333
μ/mm^{-1}	0.390
F(000)	1516.0
Crystal size/mm^3	0.3 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
Reflections collected	32116
Independent reflections	7685 [R_{int} = 0.0931, R_{sigma} = 0.0772]
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0679, wR_2 = 0.1627
Final R indexes [all data]	R_1 = 0.1149, wR_2 = 0.1826

Table S5: Some selected bond lengths for compound **2.**

Atom	**Atom**	**Length/Å**
Cr1	O1	1.949(3)
Cr1	O2	1.950(3)
Cr1	O4	1.954(3)
Cr1	O3	1.971(4)
Cr1	N2	2.087(5)
Cr1	N1	2.112(5)
Cr1	Li1	2.900(7)
Li1	O2	1.897(9)
Li1	O4	1.912(9)
Li1	O5	2.006(12)
Li1	O6	2.095(13)

Table S6: Some selected bond angles for compound **2.**

Atom	Atom		Angle/°
O1	Cr1	O2	96.12(15)
O1	Cr1	O4	176.18(18)
O2	Cr1	O4	81.10(13)
O1	Cr1	O3	86.78(15)
O2	Cr1	O3	176.85(16)
O4	Cr1	O3	96.06(15)
O1	Cr1	N2	84.3(2)
O2	Cr1	N2	93.0(2)
O4	Cr1	N2	93.2(2)
O3	Cr1	N2	88.47(18)
O1	Cr1	N1	88.6(2)
O2	Cr1	N1	93.7(2)
O4	Cr1	N1	94.2(2)
O3	Cr1	N1	85.16(18)
N2	Cr1	N1	170.73(19)
O1	Cr1	Li1	136.5(2)
O2	Cr1	Li1	40.4(2)
O4	Cr1	Li1	40.9(2)
O3	Cr1	Li1	136.7(2)
N2	Cr1	Li1	96.9(3)
N1	Cr1	Li1	92.4(3)
O2	Li1	O4	83.6(3)
O2	Li1	O5	118.7(7)
O4	Li1	O5	121.6(6)
O2	Li1	O6	120.6(6)
O4	Li1	O6	115.2(6)
O5	Li1	O6	98.9(4)
O2	Li1	Cr1	41.78(18)
O4	Li1	Cr1	41.96(18)
O5	Li1	Cr1	135.2(6)
O6	Li1	Cr1	125.9(5)
C24	O1	Cr1	125.8(4)
C9	O2	Li1	130.9(4)
C9	O2	Cr1	130.5(3)
Li1	O2	Cr1	97.8(3)
C18	O3	Cr1	124.3(4)
C1	O4	Li1	131.5(4)
C1	O4	Cr1	131.0(3)
Li1	O4	Cr1	97.2(3)
C29	O5	Li1	122.3(5)
C30	O5	Li1	130.7(6)



FigureS1: UV-Vis spectra of compound **1** and **2**.