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Supporting Information

Oxalate-bridged heterometallic chains with monocationic dabco derivatives

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Figure S1. ORTEP diagram of complex **1**.

Figure S2. Asymmetric structure of **2**.

Figure S3. Packing structure of **2**.

Figure S4. Asymmetric structure of **3**.

Figure S5. Packing structure of **3**.

Figure S6. ORTEP diagram of complex **4**.

Figure S7. Packing structure of **4** at 130 K.

Figure S8. Magnetic susceptibilities under various dc fields for **1**.

Figure S9. Ac magnetic susceptibilities for **3**.

Figure S10. Arrhenius plot for **3**.

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Figure S12. Calculated potential energy curve and rotation angle of CH_3 moiety of butyl group on Bu-DABCO cation, which is obtained by DFT method (B3LYP, 6-31G*) using Gaussian 03.

Figure S13. DSC data for **4**.

Table S1 Calculated potential energy and rotation angle.

Table S2 Summarized magnetic data of reported Co-Cr oxalate complexes.

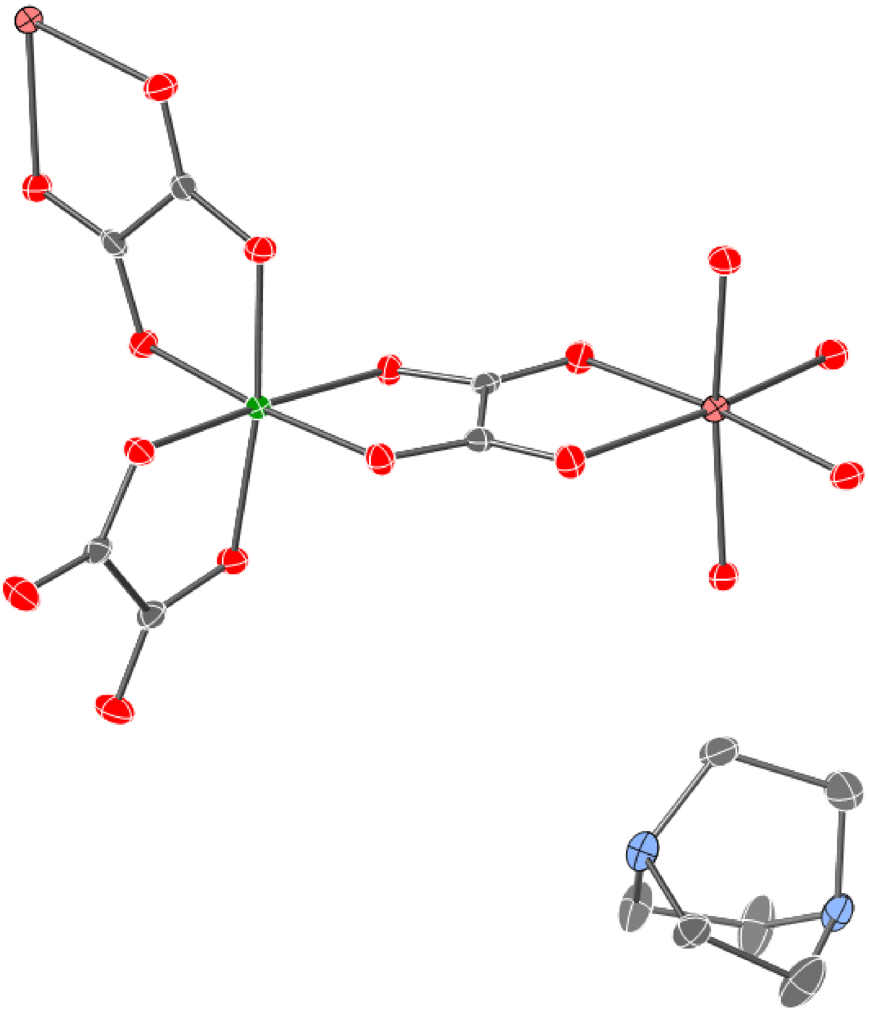

Figure S1. ORTEP diagram of complex 1.

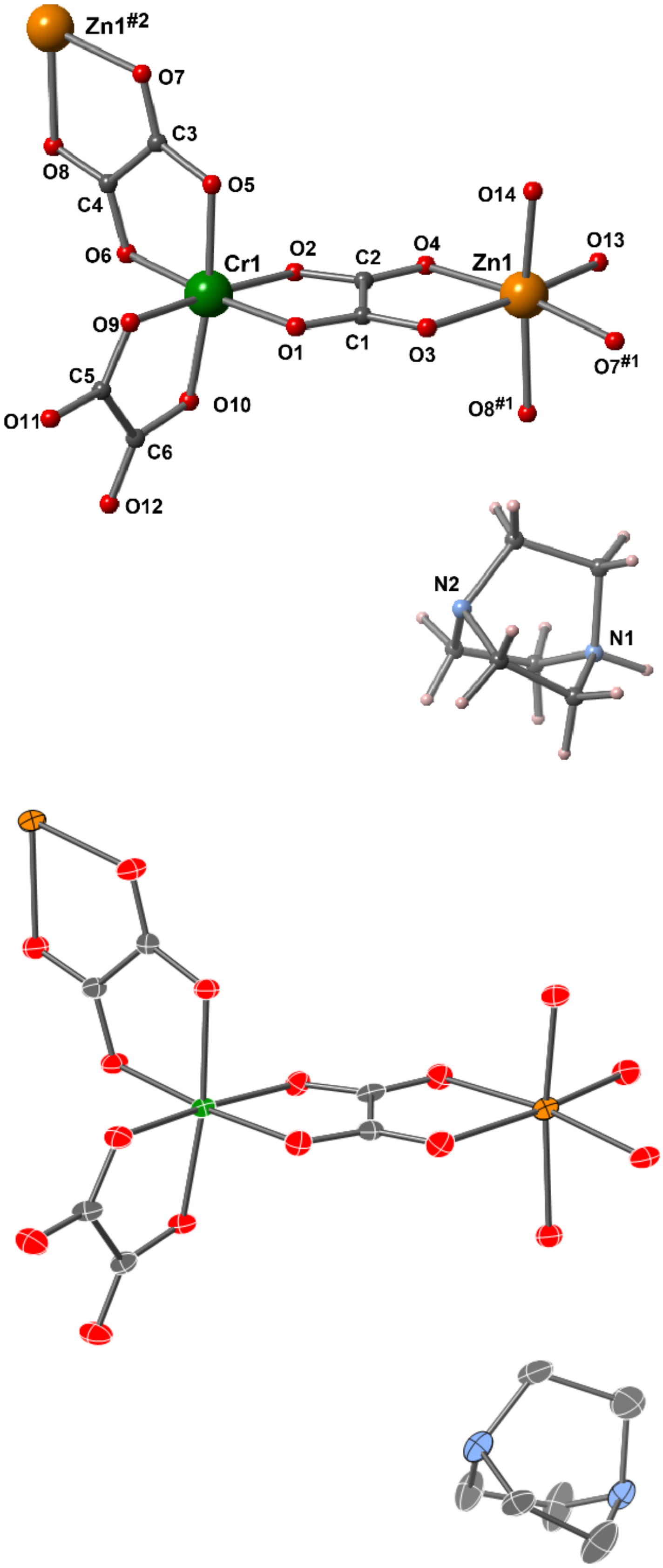

Figure S2. Asymmetric structure (Top: Ball & Stick representation, Bottom; ORTEP diagram) of 2. Solvent molecules omitted for clarity. .Symmetry operation code: #1, +x-1/2, +y-1/2, +z; #2, +x+1/2, +y+1/2, +z

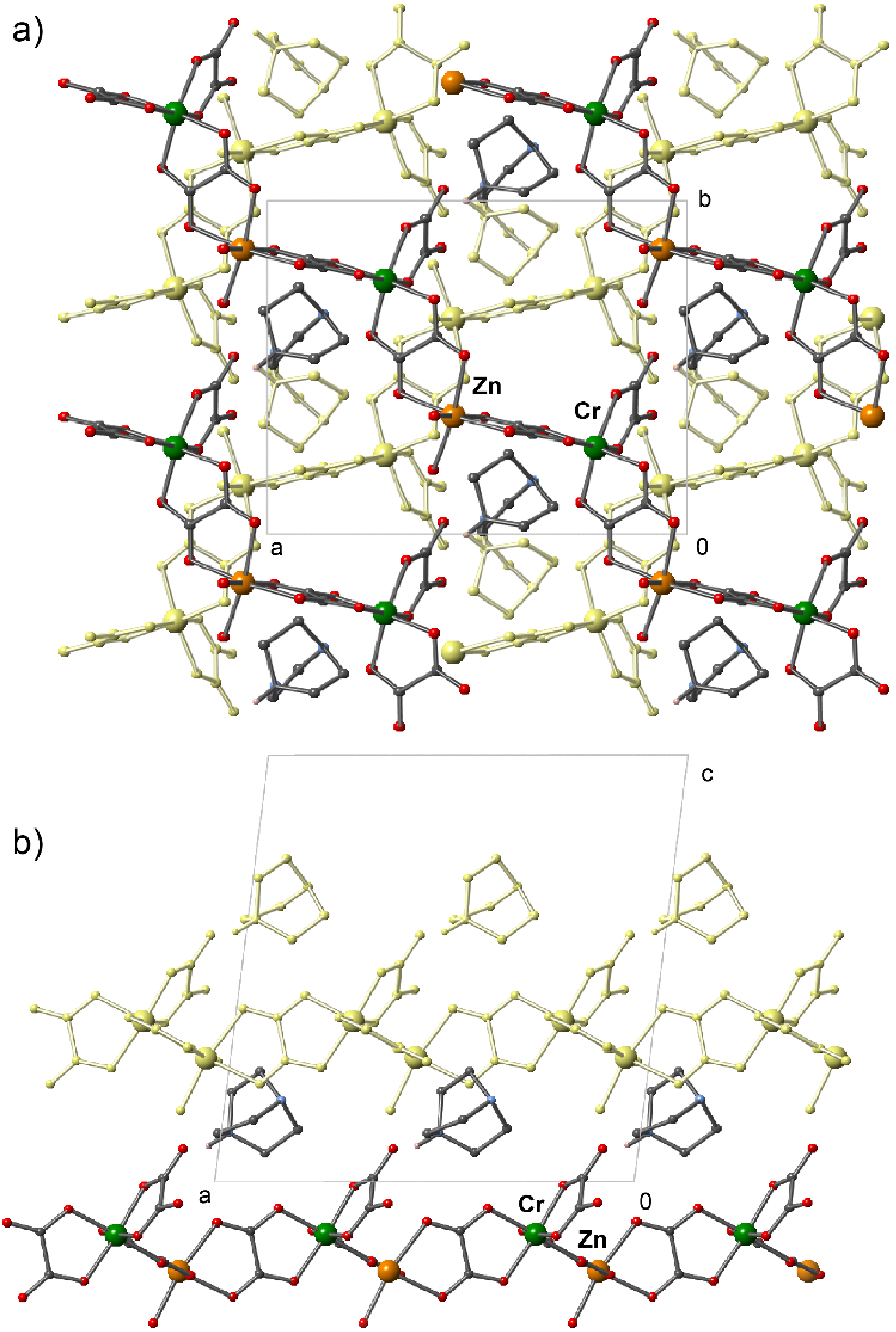

Figure S3. Packing structure of 2. Solvent molecules were omitted for clarity.

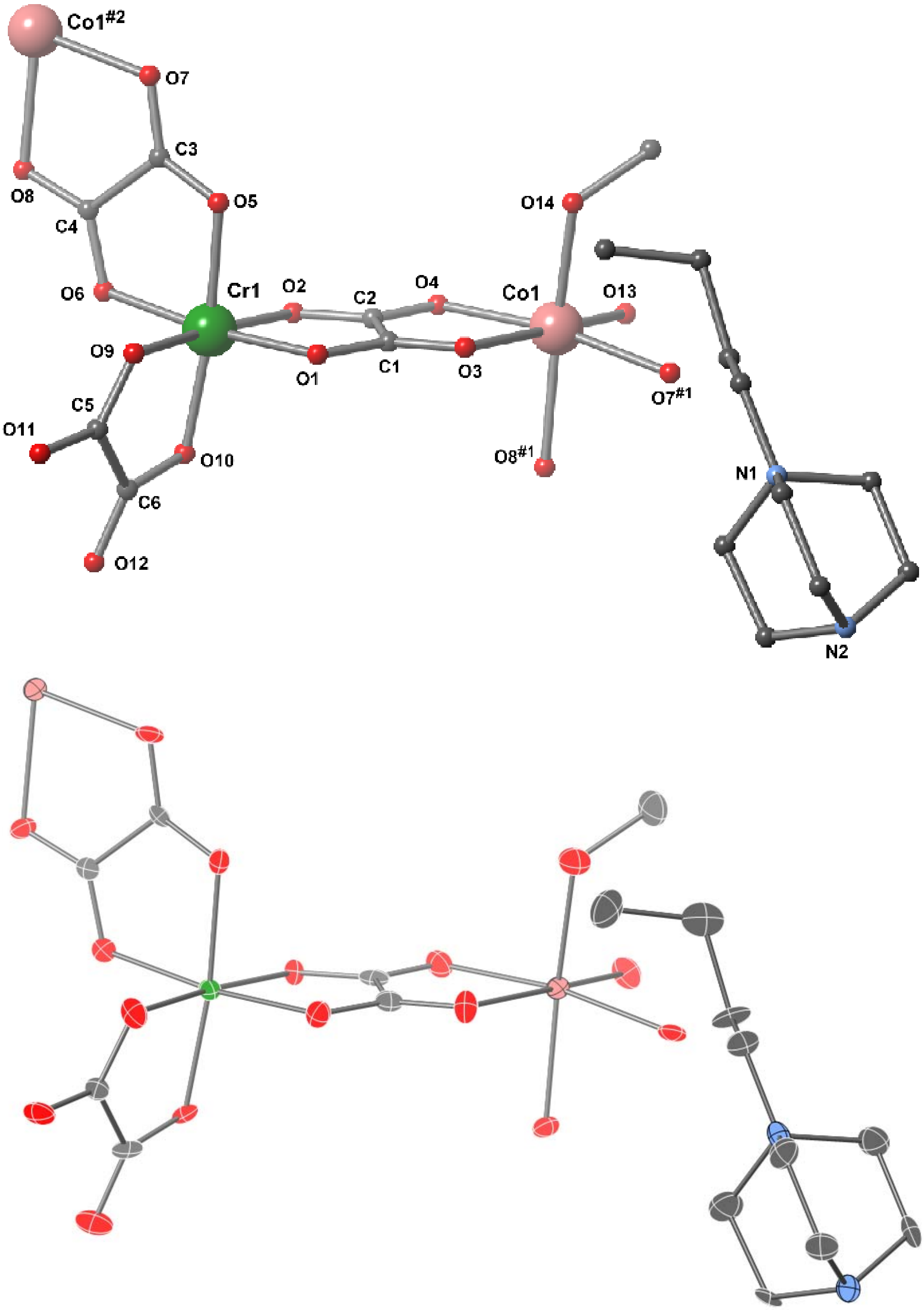

Figure S4. Asymmetric structure (Top: Ball & Stick representation, Bottom; ORTEP diagram) of 3. Solvent molecules were omitted for clarity. Symmetry operation code: #1, +x+1, +y, +z; #2, +x-1, +y, +z.

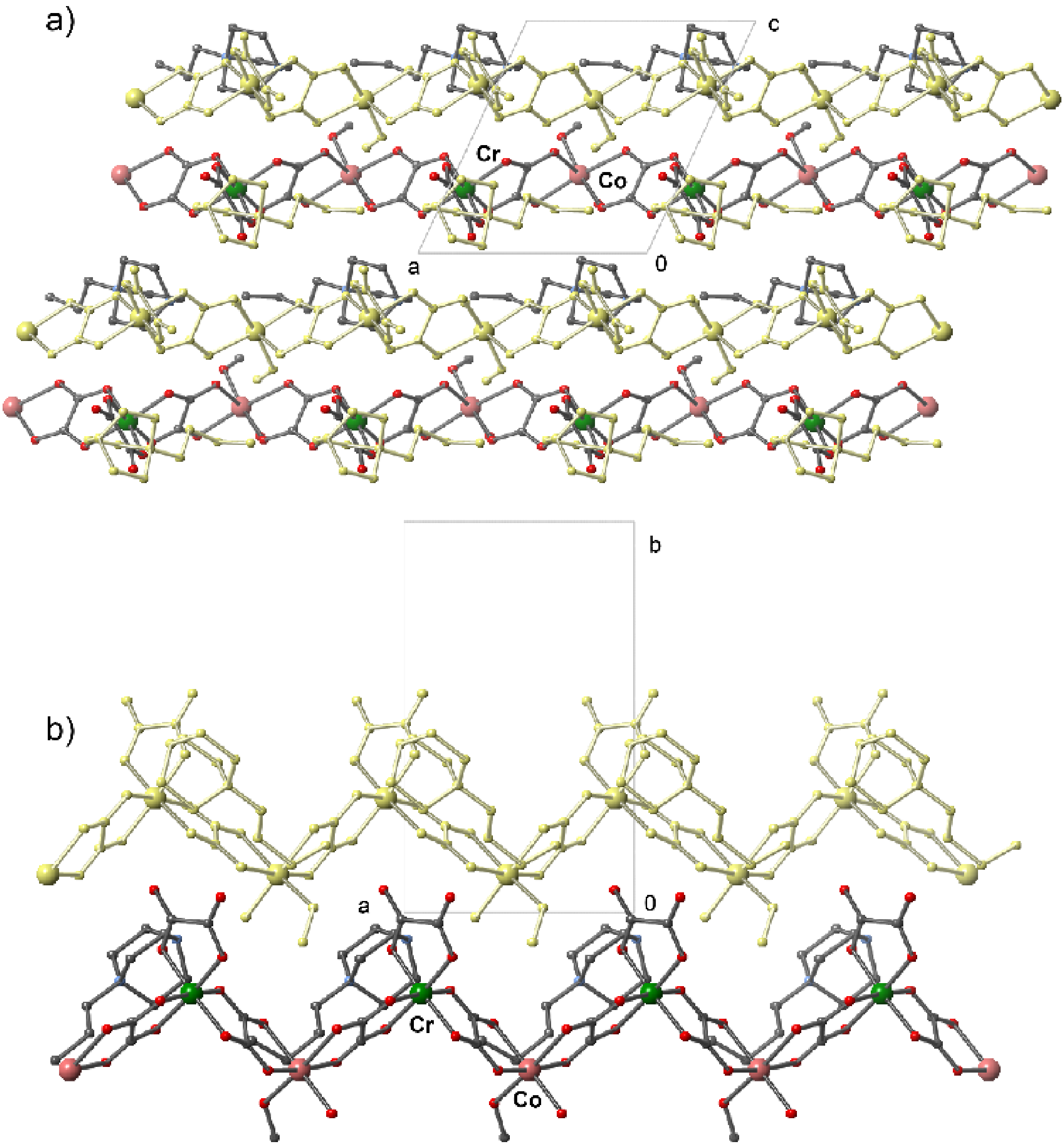

Figure S5. Packing structure of 3. Solvent molecules were omitted for clarity.

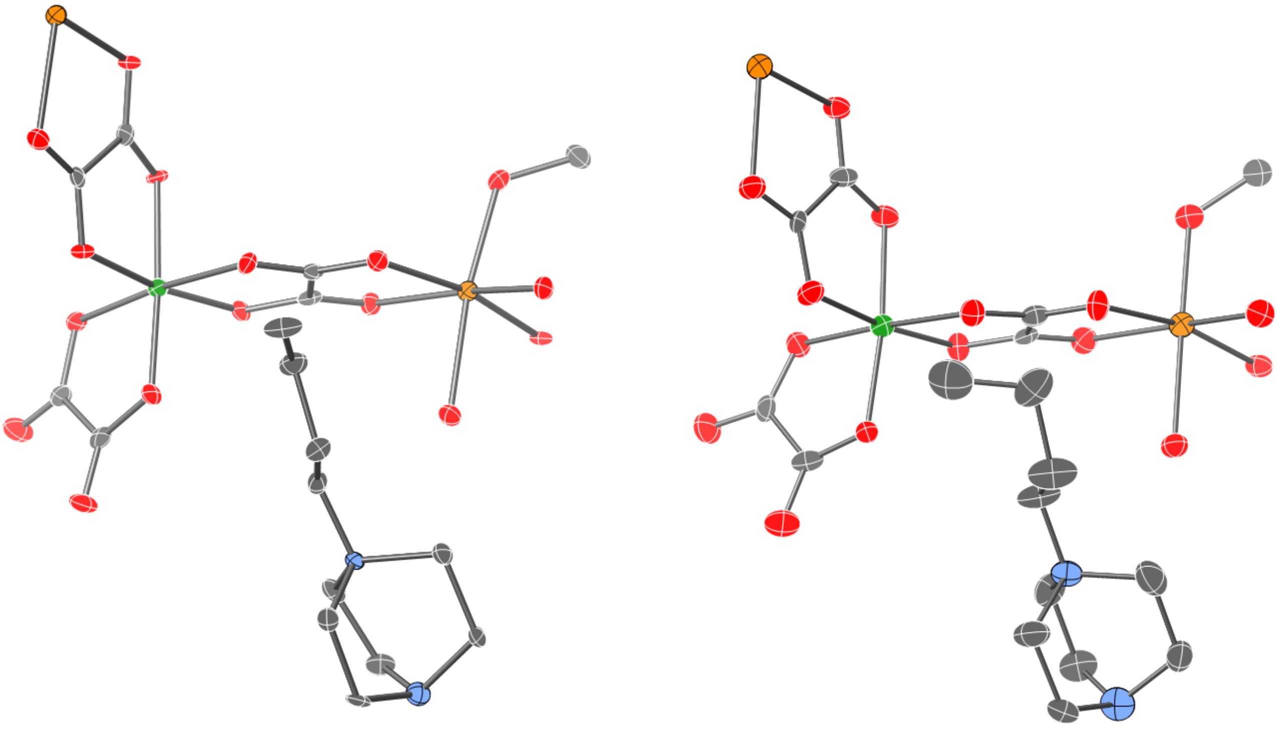

Figure S6. ORTEP diagram of complex 4 at100 K (left) and 130 K (right)

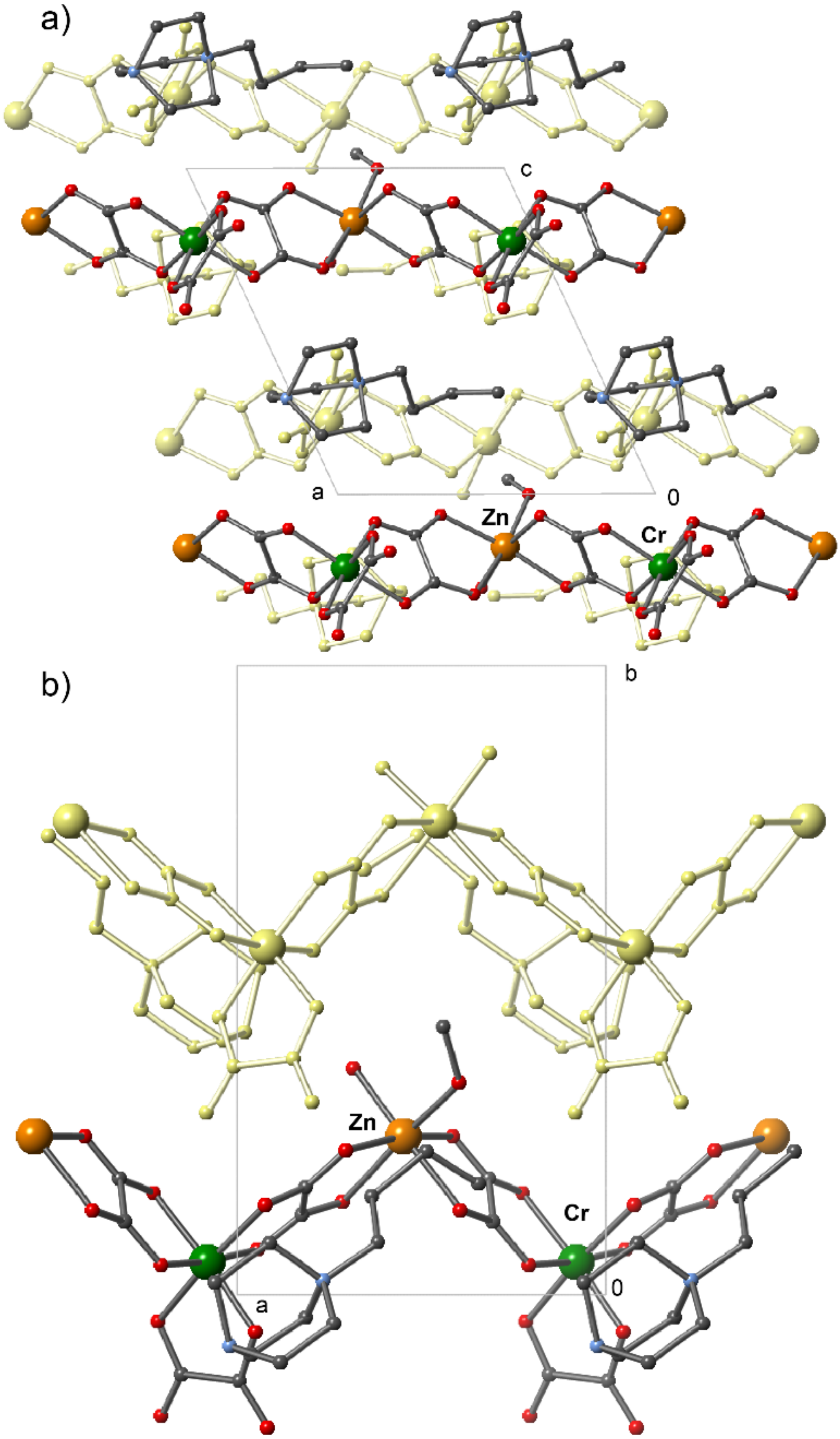

Figure S7. Packing structure of 4 at 130 K. Solvent molecules were omitted for clarity.

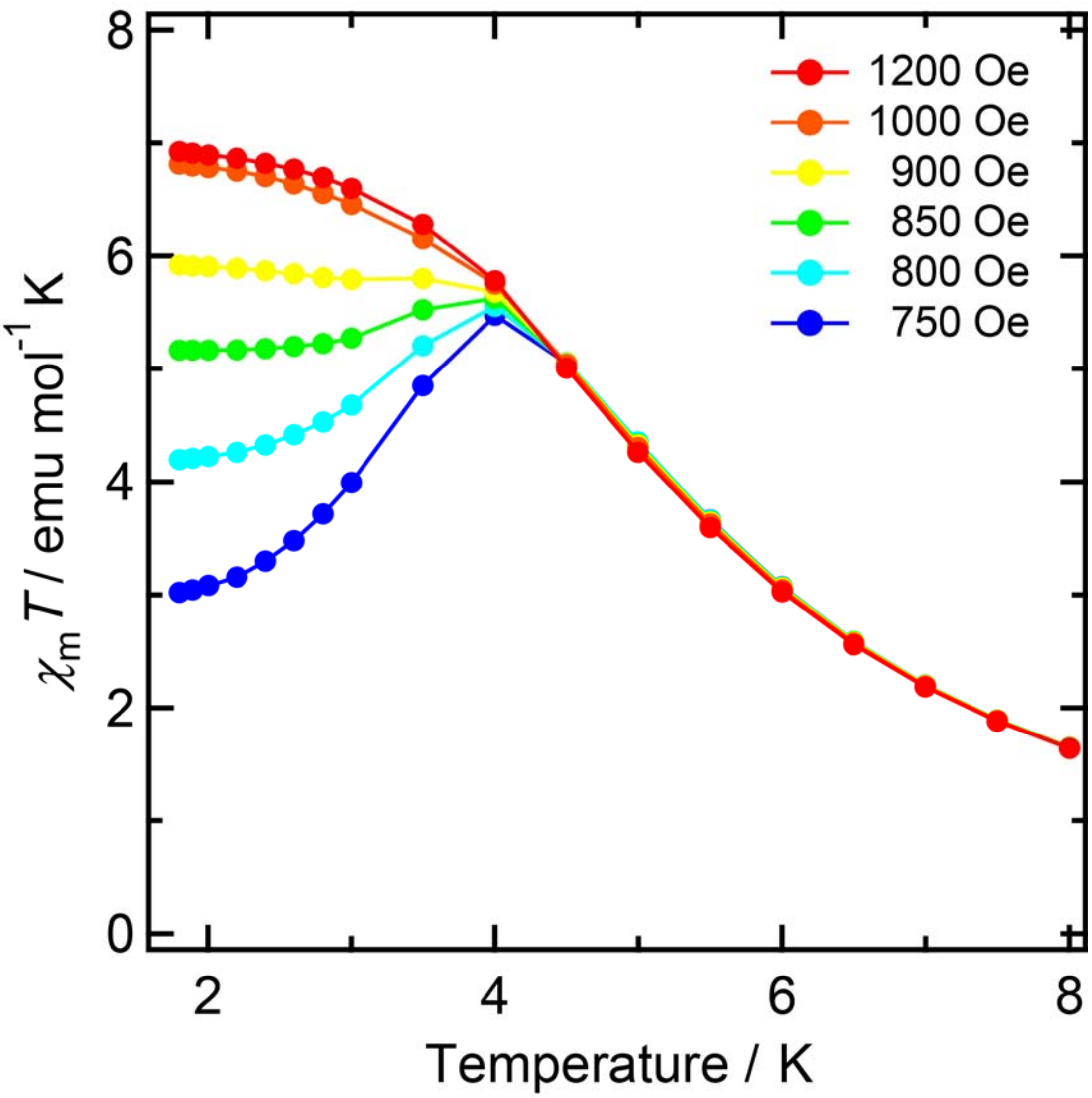

Figure S8. Magnetic susceptibilities under various dc fields for 1.

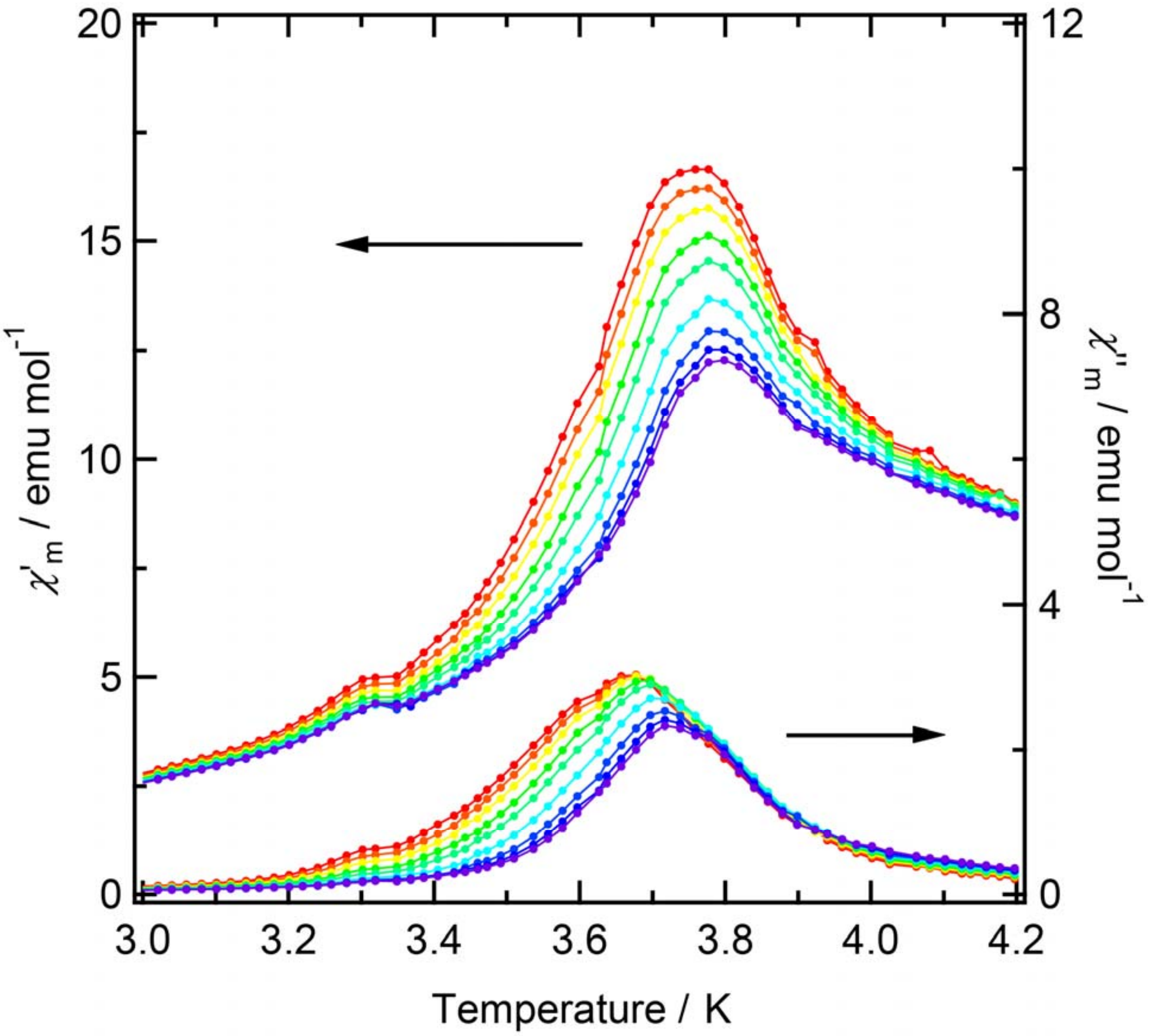

Figure S9. Ac magnetic susceptibilities for 3.

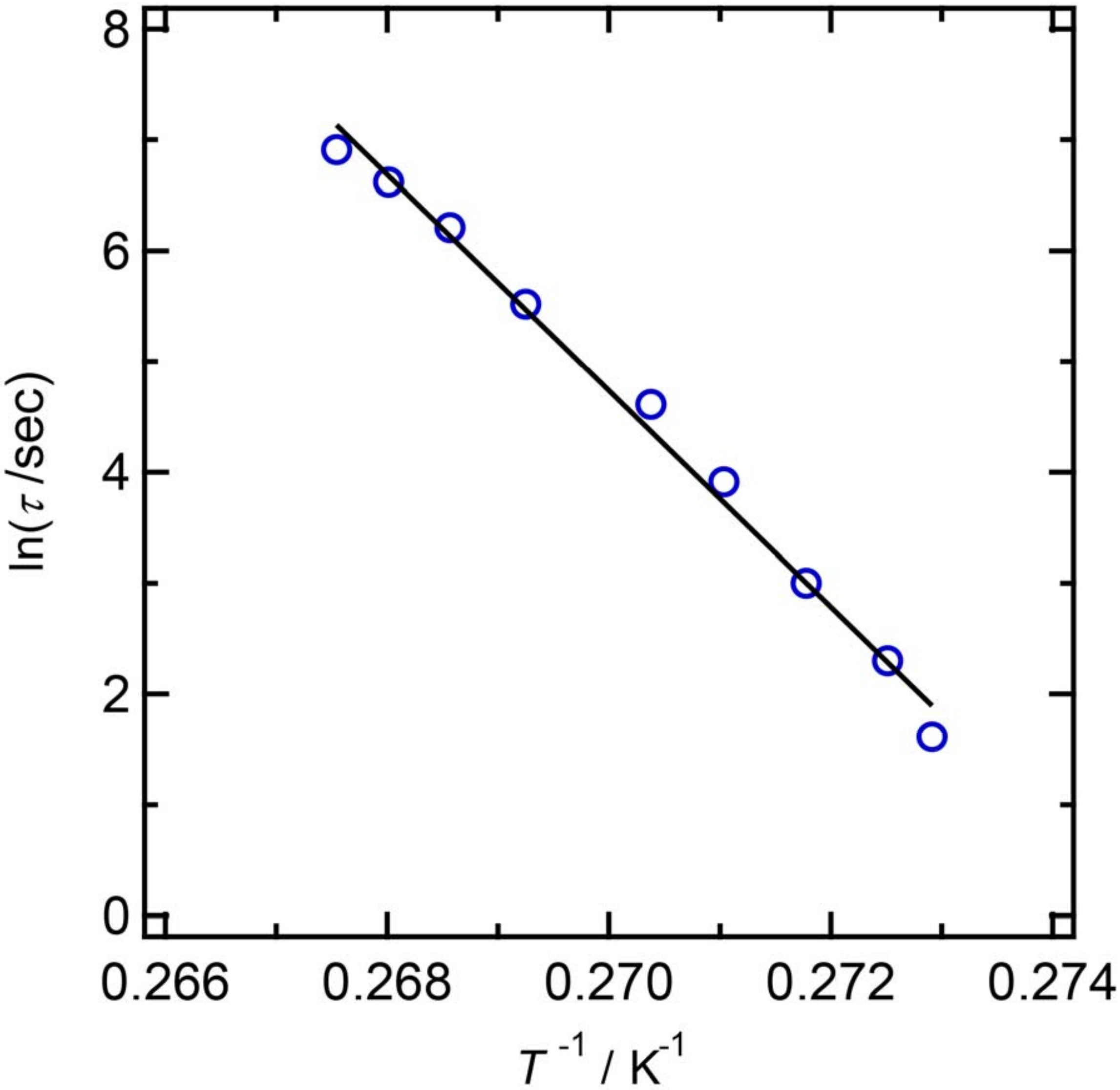

Figure S10. Arrhenius plot for 3.

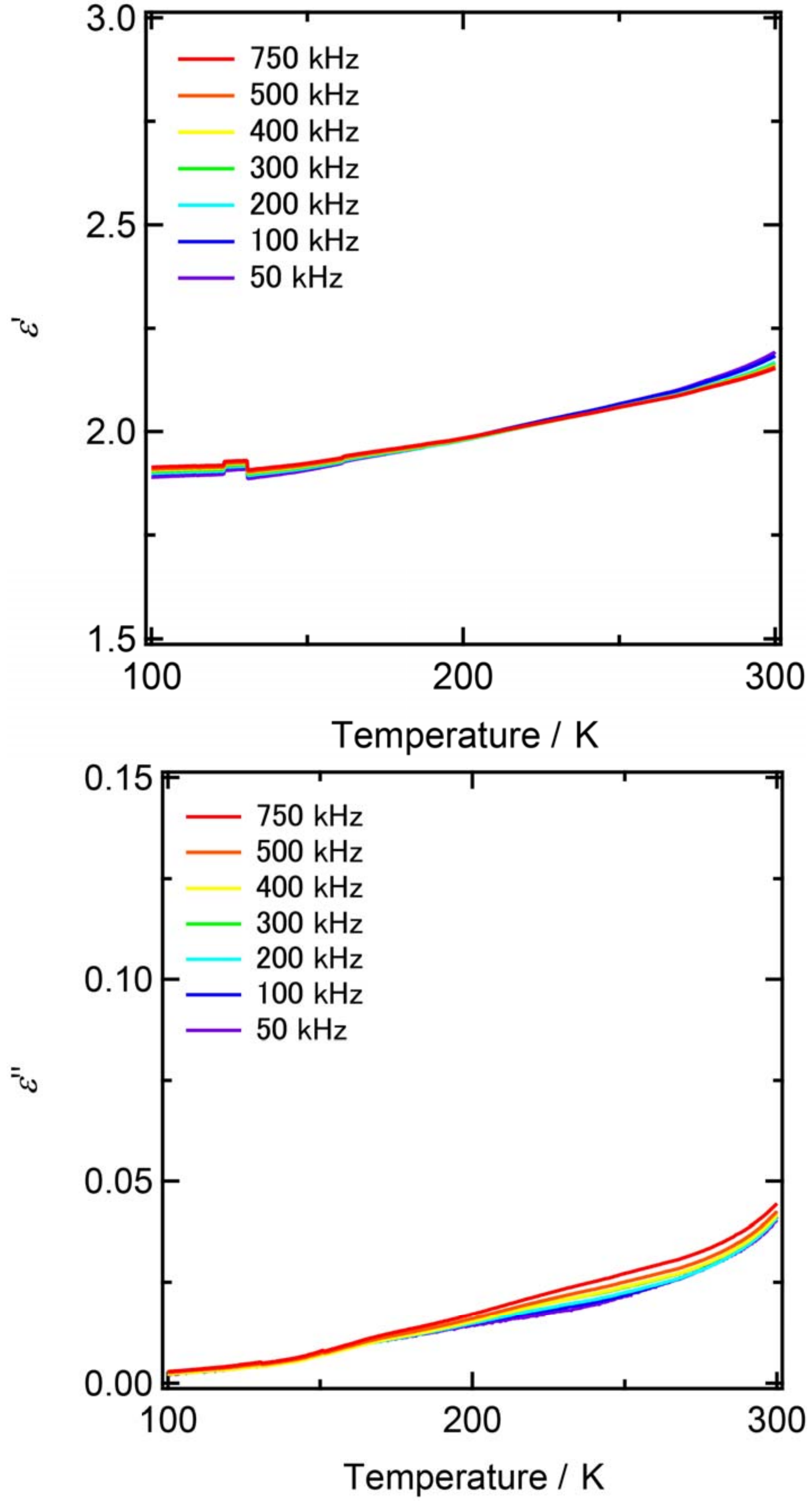

Figure S11. Permittivity data for 3. Top: real part. Bottom: imaginary part.

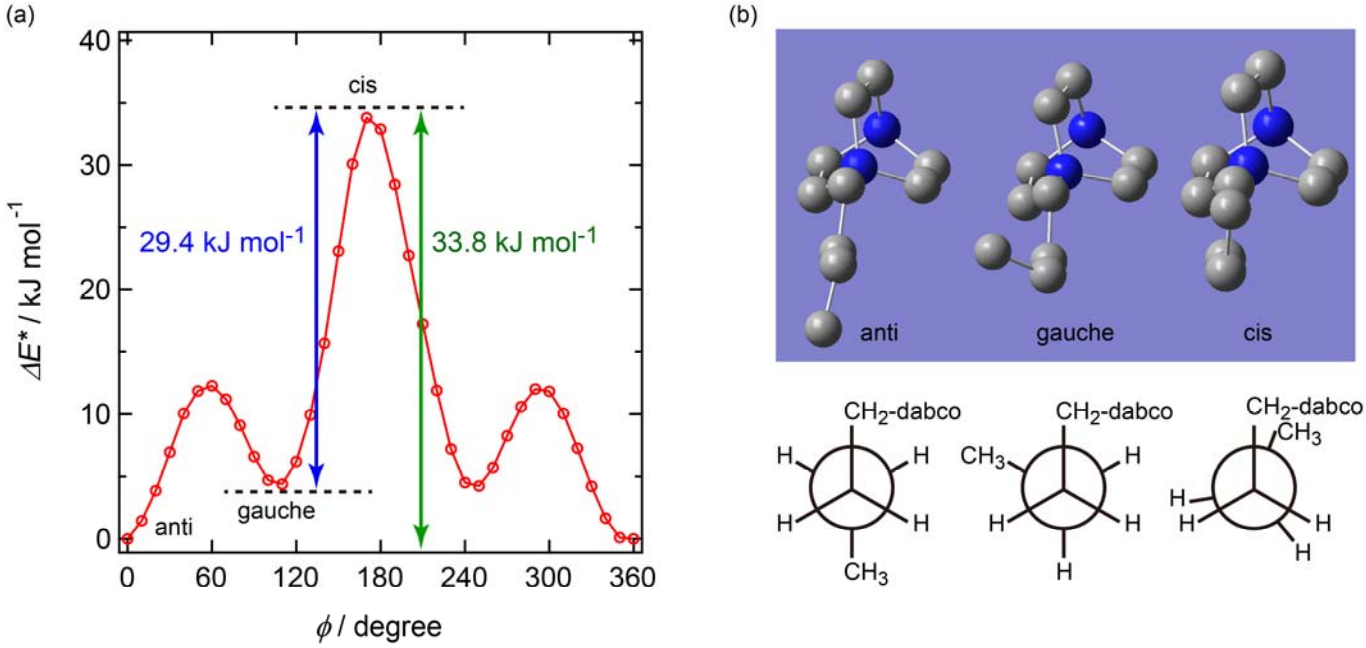

Figure S12. (a) Calculated potential energy curve and rotation angle of CH_3 moiety of butyl group on Bu-dabco cation, obtained by DFT method (B3LYP, 6-31G*) using Gaussian 03. The structure of Bu-dabco cation was modeled based on the crystal structure data determined by single crystal X-ray structural analyses. (b) Structure model used in the calculation.

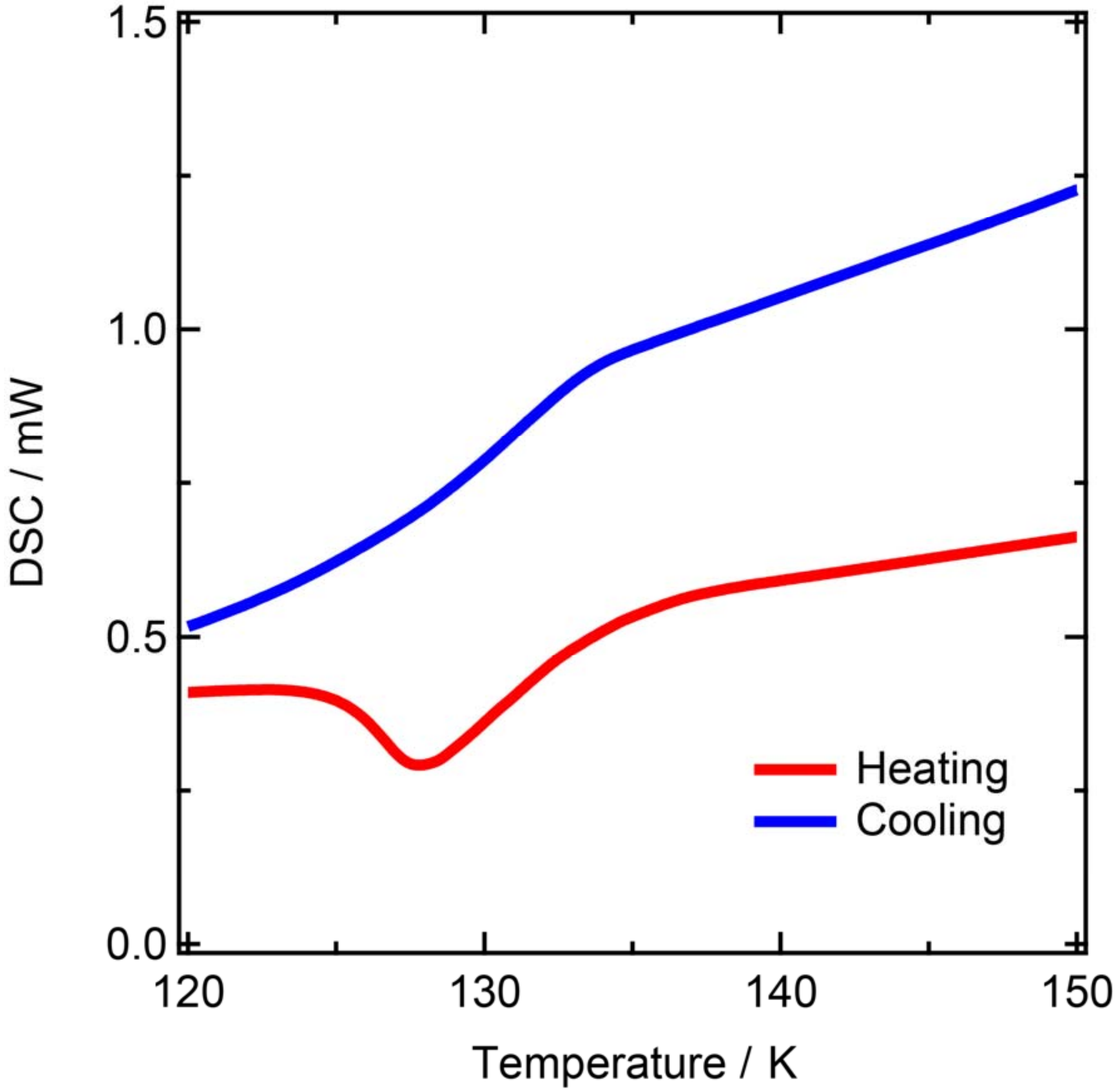

Figure S13. DSC data for 4.

Table S1. Calculated potential energy and rotation angle.

Angle / degree	ΔE / kJ mol^{-1}	Angle / degree	ΔE / kJ mol^{-1}
0	0.00	180	32.88
10	1.45	190	28.42
20	3.86	200	22.72
30	6.96	210	17.22
40	10.04	220	11.88
50	11.84	230	7.20
60	12.25	240	4.51
70	11.17	250	4.24
80	9.09	260	5.71
90	6.60	270	8.26
100	4.72	280	10.56
110	4.40	290	11.99
120	6.19	300	11.81
130	9.91	310	10.03
140	15.68	320	7.26
150	23.08	330	4.23
160	30.10	340	1.65
170	33.82	350	0.09

Table S2. Summarized magnetic data of reported Co-Cr oxalate complexes.

Compound name	J (cm^{-1})	θ (K)	T_c (K)	reference
3-D compound				
$[Ir(ppy)_2(bpy)][CoCr(ox)_3]\cdot 0.5H_2O$	–	5.2	5.2	a
2-D compounds				
$[FeCp^*{}_2][CoCr(ox)_3]$	–	–	9	b
$[CoCp^*{}_2][CoCr(ox)_3]$	–	9.9	8.2	c
$[XR_4^+][CoCr(ox)_3]$	–	–	10	c
$[BEDT\text{-}TTF]_3[CoCr(ox)_3]\cdot(CH_2Cl_2)$	–	–	9.2	d
m-rad$[CoCr(ox)_3].H_2O$	–	–	10	d
$[BEDS\text{-}TTF]_3[CoCr(ox)_3]\cdot(CH_2Cl_2)$	–	–	10.8	d
$[BET\text{-}TTF]_3[CoCr(ox)_3]\cdot(CH_2Cl_2)$	–	–	13	d
$[BEDT\text{-}TSF]_3[CoCr(ox)_3]\cdot(CH_2Cl_2)$	–	–	9.2	d
$[Bu_3MeN][CoCr(ox)_3]$	–	–	15	e
$[Bu_3EtN][CoCr(ox)_3]$	–	–	12	e
$[Bu_3PrN][CoCr(ox)_3]$	–	–	10	e
$[Bu_4N][CoCr(ox)_3]$	–	–	10	e
$[Ph_3BuN][CoCr(ox)_3]$	–	–	5	e
p-rad$[CoCr(ox)_3]\cdot H_2O$	–	10.0	13.8	f
m-rad$[CoCr(ox)_3]\cdot H_2O$	–	11.0	11.3	f
$(mhs)[CoCr(ox)_3]\cdot 0.5MeOH$	–	10.0	10	g
$[Co(MeOH)_2]_3[Cr(ox)_3]_2\cdot 6MeOH$	–	4.96	–	h
$\{[Co(H_2O)_2]_3[Cr(ox)_3]_2(18\text{-}crown\text{-}6)_2\}_\infty$	–	–	7.4	i
$[K(18\text{-}crown\text{-}6)]_3[Co_3(H_2O)_4\{Cr(ox)_3\}_3]$	–	2.2	6	j
$\{NBu_4[CoCr(ox)_3]\}_\infty$	–	15.1	10	k
$DAZOP[CoCr(ox)_3]$	–	–	13	l
$\{[Co(H_2O)_2]_3[Cr(ox)_3]_2(18\text{-}crown\text{-}6)_2\}$	–	22.6	7.6	m
$\{NH(prol)_3\}[CoCr(ox)_3]$	–	–	10	n
1-D compounds				
$[Cr_2Co(ox)_6][DAMS]_4[DAMBA]_2\cdot 2H_2O$	> 0	–	–	o
$(C2)_4[Co_2(H_2O)_3ClCr_2(ox)_6]Cl\cdot 2H_2O\cdot 2C_2H_6O$> 0	1.915	–	–	p
$[C_{12}H_{24}O_6K]_{1/2}[(C_{12}H_{24}O_6)(FC_6H_4NH_3)]_{1/2}[Co(H_2O)_2Cr(ox)_3]$	> 0	13.3	5.6	q
Trinuclear compounds				
$(TTF)_4\{Co(H_2O)_2[Cr(ox)_3]_2\}\cdot nH_2O$	>0	–	–	r
$(Bpyph)_2\{Co(H_2O)_2[Cr(ox)_3]_2\}\cdot 12.5H_2O$	2.3	–	–	s
$\{[Cr(bpy)(ox)_2]_2Co(Me_2bpy)\}\cdot 2H_2O$	1.215	–	–	t
$\{[Cr(phen)(ox)_2]_2Co(Me_2bpy)\}\cdot 2H_2O$	1.17	–	–	t
$(Tdbenz)_2(TsO)_2[Co(H_2O)_2\{(m\text{-}ox)Cr(ox)_2\}_2]\cdot 6H_2O\cdot 2MeOH$	1.815	–	–	u
$(C)_4[CoCr_2(ox)_6(H_2O)_2]\cdot 3.25H_2O$	1.35	–	–	v
Dinuclear compounds				
$[Cr(bpy)(ox)_2Co(Me_2phen)(H_2O)_2][Cr(bpy)(ox)_2]\cdot 4H_2O$	2.16	–		w
{[Cr(bpy)(ox)2]2Co(Me2phen)}	1.81	–		x
[Cr(salen)(ox)Co(taea)](BPh)4	1.3	–		y
[CrL(ox)2CoL'(H2O)2]+	1.1	–		z
This work				
Compound 1	–	+2.77	–	this work
Compound 3	–	+5.65	–	this work

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