Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic supplementary information

for

Homochiral tartrate-bridged dinuclear chromium(III) complex anion with resonance-assisted hydrogen bond for proton conduction

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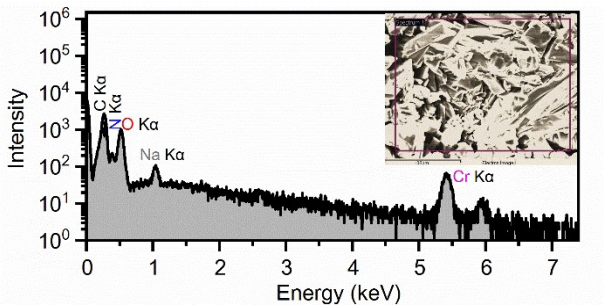

Figure S1. Energy dispersive X-ray spectrum for crystals of compound **1**.

EDX was performed on a field emission scanning electron microscope (model JSM-7000F) operated at 10 keV.

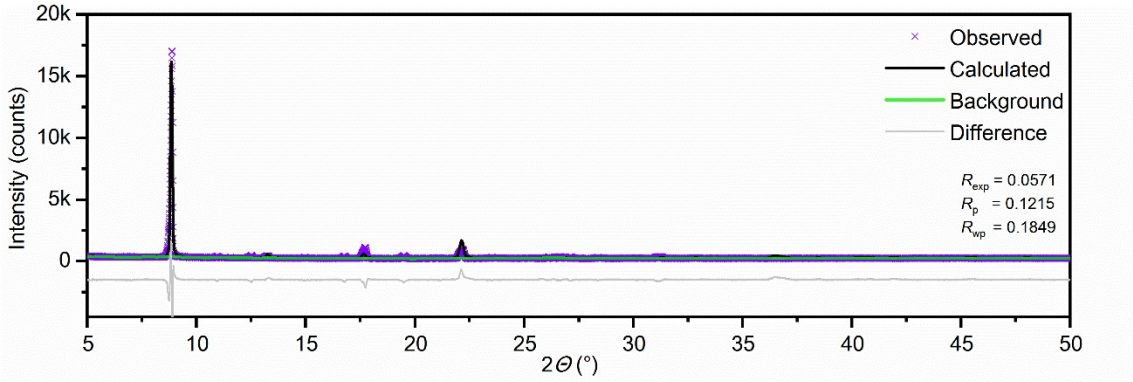

Figure S2. PXRD pattern and profile fitting results for $Na[Cr_2(bpy)_2(L\text{-tart})_2H]\cdot 9H_2O$ (**1**)

Table S1. Crystallographic data and structure refinement details for compound **1**

Temperature/K	100		200	
Crystal colour, habit	red, stick			
Empirical formula	$C_{28}H_{39}Cr_2N_4NaO_{21}$			
M_r/g mol^{-1}	894.62			
Crystal system	Monoclinic			
Space group	*P*2			
a/Å	21.0907(6)		19.9810(5)	
b/Å	8.6541(2)		8.7003(2)	
c/Å	22.8011(5)		22.9085(5)	
α/°	90		90	
β/°	110.661(3)		99.220(2)	
γ/°	90		90	
V/Å^3	3894.02(18)		3930.98(16)	
Z	2		2	
ρ_{calcd}/g cm^{-3}	1.526		1.512	
μ/mm^{-1}	5.481		5.430	
F(000)	1848		1848	
θ range/°	3.54–79.64		3.21–77.82	
Measured reflections	35728		29681	
Independent reflections	15014		11359	
Observed reflections	12819		10097	
No. of parameters, restraints	1034, 5	837, 2	1061, 3	835, 5
R_{int}	0.0807		0.0453	
R, w*R* [$I > 2\sigma(I)$]	0.0967, 0.2704	0.0572, 0.1501	0.0753, 0.2164	0.0653, 0.1870
R, w*R* [all data]	0.1080, 0.2857	0.0671, 0.1441	0.0840, 0.2244	0.0725, 0.1924
Goodness of fit	1.173	1.076	1.089	1.053
Flack parameter	0.006(5)	0.011(5)	0.006(9)	0.010(7)
$\Delta\rho$max, $\Delta\rho$min/e Å^{-3}	2.494, -1.006	0.544; -0.856	1.138, -0.718	1.518, -0.580
PLATON SQUEEZE details	-	Volume 1 = 1378 Å^3 Volume 2 = 7 Å^3 Electron count 1 = 492 Electron count 2 = 8 Probe radius = 1.2 Å	-	Volume 1 = 1398 Å^3 Volume 2 = 14 Å^3 Electron count 1 = 514 Electron count 2 = 8 Probe radius = 1.2 Å

Table S2. Geometric parameters of the aromatic stacking interactions in $Na[Cr_2(bpy)_2(L\text{-}tart)_2H]\cdot 9H_2O$ (**1**)

Cg(*i*)···Cg(*j*)	Cg(*i*)···Cg(*j*)/Å[a]	*α*/°[b]	*β*/°[c]	Cg(*i*)···plane [Cg(*j*)]/Å[d]	Symmetry operator
(N1→C5)···(N5→C25)	4.029(7)	6.0(5)	28.4	3.437(4)	*x*, *y*, *z*
(N2→C10)···(N6→C30)	3.575(6)	1.5(5)	21.2	3.346(4)	*x*, –1 + *y*, *z*
(N3→C15)···(N8→C40)	3.603(8)	4.7(7)	20.4	3.445(6)	*x*, *y*, –1 + *z*
(N3→C15)···(N7→C35)	4.215(9)	7.1(8)	36.4	3.335(5)	*x*, –1 + *y*, –1 + *z*
(N4→C20)···(N8→C40)	3.760(8)	6.4(7)	23.7	3.468(5)	*x*, –1 + *y*, –1 + *z*

[a] Cg = centre of gravity of the aromatic ring. [b] *α* = angle between the planes of two aromatic rings. [c] *β* = angle between the Cg···Cg line and the normal to the plane of the first aromatic ring.

Table S3. Possible hydrogen–bonding geometry in $Na[Cr_2(bpy)_2(L\text{-tart})_2H]\cdot 9H_2O$ (**1**)

D···*A*	*D*···*A*/Å	D···A	*D*···*A*/Å
O25···O26	2.79(2)	O36 ···O28	3.07(3)
O25···O13	2.934(14)	O37 ···O42	2.88(3)
O26···O20	2.728(19)	O37···O39	2.94(3)
O26···O24	2.834(19)	O38···O14	2.822(13)
O27···O28	2.855(19)	O39···O36	2.73(4)
O27···O14	2.941(16)	O39···O11	2.88(2)
O28 ···O45	2.80(4)	O40···O48	2.45(8)
O28 ···O1	2.996(16)	O40···O26	3.23(8)
O29···O22	2.63(2)	O41···O47	2.24(4)
O29···O44	2.67(4)	O41···O3	2.649(16)
O30···O2	2.729(15)	O42 ···O12	2.80(2)
O30···O18	2.807(18)	O42 ···O30	3.45(3)
O31···O35	2.64(3)	O43···O48	2.36(6)
O31···O8	2.719(19)	O43···O48	3.12(6)
O32···O46	2.59(2)	O44···O24	2.73(4)
O32···O8	3.085(17)	O44···O20	3.15(3)
O33 ···O41	2.41(3)	O45···O39	2.98(4)
O33 ···O5	2.746(15)	O45···O30	3.03(4)
O34···O7	2.845(17)	O46···O46	2.09(3)
O34···O41	3.11(3)	O46···O10	2.639(18)
O35···O43	2.91(3)	O47 ···O10	2.44(3)
O35···O24	3.36(3)	O47 ···O3	2.59(3)
O36···O42	2.59(5)	O48···O24	3.04(6)

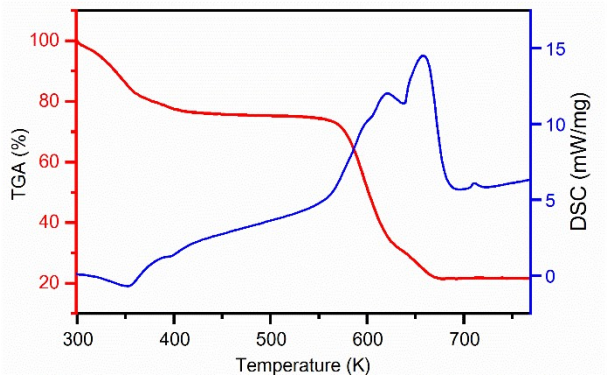

Figure S3. TGA and DSC curves for $Na[Cr_2(bpy)_2(L\text{-tart})_2H]\cdot 9H_2O$ (**1**)

TGA/DSC was measured under a synthetic air atmosphere at 10 K min^{-1} heating rate using a simultaneous thermal analyser Netzsch STA 449 F5 Jupiter.

Table S4. Thermoanalytical data for $Na[Cr_2(bpy)_2(L\text{-tart})_2H]\cdot 9H_2O$ (**1**)

ΔT (K)	*Mass loss* (%)			$T(DSC_{max})$ (K)
	exp.	*calc.*	*elimination*	
300–365	18.18	18.12	$9H_2O$	352 endo
540–625	bpy and $(L\text{-tart})_2H$ elimination is overlapped	34.92	2bpy	620 egzo
625–680		25.62	$(L\text{-tart})_2H$	657 egzo
residue	21.58	21.34	$Na_2O + Cr_2O_3$	710 egzo