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Homochiral column structure of *rac*- and Λ-$[M^{III}(tn)_3]P_3O_9$ (M = Co, Cr; tn = 1,3-diaminopropane; P_3O_9 = cyclotriphosphate(3–)) produced by multiple hydrogen bonds†

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Table S1 Hydrogen bond distances and angles for *rac*-$[Co(tn)_3]P_3O_9 \cdot 7.3H_2O$

Co1 (N1–N6)

D–H···A	D···A/Å	D–H/Å	H···A/Å	∠D–H···A/°
N(1)–H(1)···O(5)	2.866(5)	0.920	2.029	151
N(1)–H(2)···O(4)*	2.874(4)	0.920	1.955	178
N(2)–H(9)···O(38)	2.855(4)	0.920	1.942	172
N(2)–H(10)···O(41)†	3.251(5)	0.920	2.524	136
N(3)–H(11)···O(5)	3.023(5)	0.920	2.268	139
N(3)–H(12)···O(50)†	3.102(5)	0.920	2.290	147
N(4)–H(19)···O(15)	2.904(4)	0.920	2.025	160
N(4)–H(20)···O(36)‡	2.950(5)	0.920	2.038	171
N(5)–H(21)···O(5)	2.798(4)	0.920	2.014	142
N(5)–H(22)···O(36)‡	2.893(5)	0.920	1.977	174
N(6)–H(29)···O(15)	3.216(4)	0.920	2.423	144
N(6)–H(29)···O(38)	2.987(5)	0.920	2.356	126
N(6)–H(30)···O(4)*	2.959(4)	0.920	2.049	170

Co2 (N7–N12)

D–H···A	D···A/Å	D–H/Å	H···A/Å	∠D–H···A/°
N(7)–H(31)···O(14)	2.868(4)	0.920	2.022	152
N(7)–H(32)···O(22)§	2.964(4)	0.920	2.059	168
N(8)–H(39)···O(48)	2.901(4)	0.920	1.989	171
N(8)–H(40)···O(47)	2.923(5)	0.920	2.100	148
N(9)–H(41)···O(14)	3.157(4)	0.920	2.308	153
N(9)–H(42)···O(43)	2.962(5)	0.920	2.228	136
N(10)–H(49)···O(24)	2.918(5)	0.920	2.023	164
N(10)–H(50)···O(32)□	3.031(5)	0.920	2.197	150
N(11)–H(51)···O(14)	2.846(4)	0.920	1.942	167
N(11)–H(52)···O(46)¶	2.884(5)	0.920	2.012	158
N(12)–H(59)···O(24)	3.049(4)	0.920	2.158	163
N(12)–H(59)···O(48)	3.038(5)	0.920	2.574	112
N(12)–H(60)···O(22)§	2.994(4)	0.920	2.108	162

Table S1 (continued) Hydrogen bond distances and angles for *rac*-$[Co(tn)_3]P_3O_9 \cdot 7.3H_2O$

Co1 (N13–N18)

D–H···A	D···A/Å	D–H/Å	H···A/Å	∠D–H···A/°
N(13)–H(61)···O(23)	2.817(4)	0.920	1.921	164
N(13)–H(62)···O(13)§	2.911(4)	0.920	2.003	169
N(14)–H(69)···O(35)	2.916(4)	0.920	2.011	168
N(14)–H(70)···O(34)	3.037(5)	0.920	2.243	144
N(15)–H(71)···O(27)	2.846(5)	0.920	1.942	167
N(15)–H(72)···O(25)	3.034(4)	0.920	2.335	133
N(16)–H(79)···O(6)**	2.854(4)	0.920	2.036	147
N(16)–H(80)···O(33)□	2.964(5)	0.920	2.097	157
N(17)–H(81)···O(23)	2.850(4)	0.920	1.944	168
N(17)–H(82)···O(27)	3.039(4)	0.920	2.358	131
N(17)–H(82)···O(33)□	3.051(5)	0.920	2.261	144
N(18)–H(89)···O(6)**	3.014(4)	0.920	2.151	156
N(18)–H(89)···O(35)	3.024(5)	0.920	2.545	113
N(18)–H(90)···O(13)§	3.059(4)	0.920	2.192	157

Symmetry operators; *: –x –y –z; †: x–1 1/2–y –1/2+z; ‡: x–1 y z–1; §: 2–x –y 1–z; □: x+1 y z; ¶: x 1/2–y –1/2+z; **: x+2 y z+1.

Table S2 Hydrogen bond distances and angles for *rac*-$[Cr(tn)_3]P_3O_9 \cdot 7.5H_2O$

Cr1 (N1–N6)

D–H···A	D···A/Å	D–H/Å	H···A/Å	∠D–H···A/°
N(1)–H(1)···O(20)	2.896(4)	0.920	2.030	156
N(1)–H(2)···O(9)	2.892(3)	0.920	1.985	168
N(2)–H(9)···O(8)*	2.903(3)	0.920	1.995	169
N(2)–H(10)···O(6)†	3.067(3)	0.920	2.200	157
N(3)–H(11)···O(8)*	3.093(3)	0.920	2.249	152
N(3)–H(11)···O(9)*	3.257(4)	0.920	2.528	136
N(3)–H(12)···O(9)	2.824(3)	0.920	1.915	170
N(4)–H(19)···O(26)‡	2.943(3)	0.920	2.187	139
N(4)–H(20)···O(29)‡	2.938(4)	0.920	2.026	171
N(5)–H(21)···O(7)	2.928(3)	0.920	2.119	146
N(5)–H(22)···O(20)	3.027(2)	0.920	2.151	159
N(6)–H(29)···O(19)	3.013(3)	0.920	2.156	155
N(6)–H(30)···O(6)†	2.899(3)	0.920	2.062	151

Cr2 (N7–N12)

D–H···A	D···A/Å	D–H/Å	H···A/Å	∠D–H···A/°
N(7)–H(31)···O(32)§	2.960(3)	0.920	2.059	166
N(7)–H(32)···O(22)	3.235(5)	0.920	2.431	146
N(8)–H(39)···O(15)	2.800(3)	0.920	1.907	163
N(8)–H(40)···O(16)□	2.963(3)	0.920	2.045	175
N(9)–H(41)···O(14)¶	3.071(3)	0.920	2.298	141
N(9)–H(41)···O(32)§	3.007(2)	0.920	2.350	128
N(9)–H(42)···O(16)□	2.946(3)	0.920	2.035	170
N(10)–H(49)···O(15)	2.829(3)	0.920	2.136	131
N(10)–H(50)···O(27)	2.919(3)	0.920	2.004	172
N(11)–H(51)···O(14)¶	2.882(3)	0.920	1.996	161
N(11)–H(52)···O(27)	2.930(2)	0.920	2.013	174
N(12)–H(59)···O(17)	2.926(2)	0.920	2.028	165
N(12)–H(60)···O(13)	2.998(2)	0.920	2.243	139

Symmetry operators; *: 1–x –y 1–z; †: x–1 y z; ‡: x+1 y+1 z+1; §: 2–x 1–y –z; □: 1–x 1–y –z; ¶: x+1 y z.

Table S3 Relevant coordination bond lengths (Å) and angles (°) with their estimated standard deviations in parentheses for Λ-$[Co(tn)_3]P_3O_9 \cdot 2.5H_2O$

	Bond length / Å		
Co(1)–N(1)	1.977(2)	Co(1)–N(4)	1.998(2)
Co(1)–N(2)	1.9850(19)	Co(1)–N(5)	1.9882(18)
Co(1)–N(3)	2.0090(18)	Co(1)–N(6)	1.9760(18)
Co(2)–N(7)	1.984(2)	Co(2)–N(10)	1.9784(19)
Co(2)–N(8)	1.979(2)	Co(2)–N(11)	1.993(2)
Co(2)–N(9)	1.9842(19)	Co(2)–N(12)	1.9891(19)
	$Co–N_{av}$	1.987 Å	
	Bond angle / °		
N(1)–Co(1)–N(2)	93.56(8)	N(7)–Co(2)–N(8)	94.06(9)
N(3)–Co(1)–N(4)	88.76(8)	N(9)–Co(2)–N(10)	93.93(8)
N(5)–Co(1)–N(6)	94.43(7)	N(11)–Co(2)–N(12)	89.83(8)

Table S4 Hydrogen bond distances and angles for Λ-$[Co(tn)_3]P_3O_9 \cdot 2.5H_2O$

Co1 (N1–N6)

D–H···A	D···A/Å	D–H/Å	H···A/Å	∠D–H···A/°
N(1)–H(1)···O(9)	2.776(2)	0.950	1.851	164
N(1)–H(2)···O(20)	2.924(2)	0.950	2.121	141
N(2)–H(9)···O(4)*	2.821(2)	0.950	1.878	172
N(2)–H(10)···O(15)	2.920(2)	0.950	1.970	178
N(3)–H(11)···O(9)	2.981(2)	0.950	2.176	142
N(3)–H(12)···O(15)	2.910(2)	0.950	1.968	171
N(4)–H(19)···O(4)*	2.870(2)	0.950	2.118	135
N(4)–H(20)···O(17)†	2.886(2)	0.950	1.938	175
N(5)–H(21)···O(7)	2.942(2)	0.950	2.043	157
N(5)–H(22)···O(17)†	2.847(2)	0.950	1.915	166
N(6)–H(29)···O(6)*	2.986(2)	0.950	2.145	147
N(6)–H(30)···O(23)	3.003(3)	0.950	2.171	146

Co2 (N7–N12)

D–H···A	D···A/Å	D–H/Å	H···A/Å	∠D–H···A/°
N(7)–H(31)···O(16)‡	2.793(2)	0.950	2.021	137
N(7)–H(32)···O(5)	3.193(2)	0.950	2.407	140
N(8)–H(39)···O(13)	2.937(2)	0.950	2.035	158
N(8)–H(40)···O(21)§	2.962(2)	0.950	2.129	146
N(9)–H(41)···O(14)‡	3.087(2)	0.950	2.321	137
N(9)–H(42)···O(18)‡	2.819(3)	0.950	1.947	152
N(10)–H(49)···O(13)	2.858(2)	0.950	1.939	162
N(10)–H(50)···O(8)	2.806(2)	0.950	1.873	167
N(11)–H(51)···O(16)‡	2.948(2)	0.950	2.131	143
N(11)–H(52)···O(8)	3.002(2)	0.950	2.080	163
N(12)–H(59)···O(10)	3.261(2)	0.950	2.447	144
N(12)–H(59)···O(13)	3.031(2)	0.950	2.253	139
N(12)–H(60)···O(5)	2.898(2)	0.950	1.973	164

Table S4 Hydrogen bond distances and angles for Λ-$[Co(tn)_3]P_3O_9 \cdot 2.5H_2O$ (continued)

O_{H2O}

D–H···A	D···A/Å	D–H/Å	H···A/Å	∠D–H···A/°
O(19)–H(61)···O(5)	2.904(2)	0.857	2.057	170
O(19)–H(62)···O(15)	2.904(2)	0.931	2.035	155
O(20)–H(63)···O(6)[¶]	2.788(2)	0.831	1.960	175
O(20)–H(64)···O(21)	2.898(2)	0.942	1.967	169
O(21)–H(65)···O(14)**	2.761(2)	0.829	1.936	173
O(21)–H(66)···O(22)	2.808(2)	0.869	1.949	170
O(22)–H(67)···O(7)[¶]	2.761(2)	0.920	1.852	169
O(22)–H(68)···O(18)[††]	2.740(2)	0.876	1.868	172
O(23)–H(69)···O(22)	2.835(2)	0.766	2.080	169
O(23)–H(70)···O(8)*	2.805(2)	0.885	1.945	164

Symmetry operators; *: x–1 y z; †: 1–x 1/2+y 1/2–z; ‡: x+1 y z; §: 3/2–x –y 1/2–z; □: 2–x 1/2+y 1/2–z; ¶: x–1/2 1/2–y 1–z; **: 1–x –1/2+y 1/2–z; ††: 1/2–x –y 1/2+z.

Table S5 Relevant coordination bond lengths (Å) and angles (°) with their estimated standard deviations in parentheses for Λ-$[Cr(tn)_3]P_3O_9 \cdot 2.5H_2O$

	Bond length / Å		
Cr(1)–N(1)	2.0752(16)	Cr(1)–N(4)	2.0990(17)
Cr(1)–N(2)	2.0793(17)	Cr(1)–N(5)	2.0832(16)
Cr(1)–N(3)	2.1066(18)	Cr(1)–N(6)	2.0839(17)
Cr(2)–N(7)	2.089(2)	Cr(2)–N(10)	2.0712(16)
Cr(2)–N(8)	2.0846(17)	Cr(2)–N(11)	2.0965(18)
Cr(2)–N(9)	2.0994(19)	Cr(2)–N(12)	2.0905(18)
	$Cr–N_{av}$	2.088 Å	

	Bond angle / °		
N(1)–Cr(1)–N(2)	92.06(6)	N(7)–Cr(2)–N(8)	89.84(7)
N(3)–Cr(1)–N(4)	86.86(7)	N(9)–Cr(2)–N(10)	90.92(7)
N(5)–Cr(1)–N(6)	92.78(6)	N(11)–Cr(2)–N(12)	86.97(7)

Table S6 Hydrogen bond distances and angles for Λ-$[Cr(tn)_3]P_3O_9 \cdot 2.5H_2O$

Cr1 (N1–N6)

D–H···A	D···A/Å	D–H/Å	H···A/Å	∠D–H···A/°
N(1)–H(1)···O(9)	2.775(2)	0.950	1.843	166
N(1)–H(2)···O(20)	2.925(2)	0.950	2.101	144
N(2)–H(9)···O(4)*	2.838(2)	0.950	1.901	168
N(2)–H(10)···O(15)	2.936(2)	0.950	1.986	177
N(3)–H(11)···O(9)	3.014(2)	0.950	2.202	143
N(3)–H(12)···O(15)	2.9115(19)	0.950	1.969	172
N(4)–H(19)···O(4)*	2.878(2)	0.950	2.124	135
N(4)–H(20)···O(17)†	2.891(2)	0.950	1.946	173
N(5)–H(21)···O(7)	2.923(2)	0.950	2.019	158
N(5)–H(22)···O(17)†	2.866(2)	0.950	1.933	167
N(6)–H(29)···O(6)*	2.933(2)	0.950	2.079	149
N(6)–H(30)···O(23)	2.972(2)	0.950	2.125	148

Cr2 (N7–N12)

D–H···A	D···A/Å	D–H/Å	H···A/Å	∠D–H···A/°
N(7)–H(31)···O(18)‡	3.122(2)	0.950	2.186	168
N(7)–H(32)···O(16)‡	2.778(2)	0.950	2.228	116
N(8)–H(39)···O(13)	2.926(2)	0.950	2.058	151
N(8)–H(40)···O(21)§	2.937(2)	0.950	2.069	151
N(9)–H(41)···O(14)‡	3.007(2)	0.950	2.198	142
N(9)–H(42)···O(18)‡	2.843(2)	0.950	1.943	157
N(10)–H(49)···O(13)	2.848(2)	0.950	1.936	160
N(10)–H(50)···O(8)□	2.8057(19)	0.950	1.866	170
N(11)–H(51)···O(16)‡	2.912(2)	0.950	2.135	138
N(11)–H(52)···O(8)□	3.086(2)	0.950	2.176	160
N(12)–H(59)···O(10)	3.319(2)	0.950	2.477	148
N(12)–H(59)···O(13)	3.117(2)	0.950	2.381	134
N(12)–H(60)···O(5)	2.8822(18)	0.950	1.969	161

Table S6 Hydrogen bond distances and angles for Λ-$[Cr(tn)_3]P_3O_9 \cdot 2.5H_2O$ (continued)

O_{H2O}

D–H···A	D···A/Å	D–H/Å	H···A/Å	∠D–H···A/°
O(19)–H(61)···O(5)	2.925(2)	0.910	2.111	149
O(19)–H(62)···O(15)	2.884(2)	1.004	1.890	170
O(20)–H(63)···O(6)¶	2.796(2)	0.921	1.883	171
O(20)–H(64)···O(21)	2.8928(19)	0.857	2.051	167
O(21)–H(65)···O(14)**	2.7628(19)	0.980	1.788	173
O(21)–H(66)···O(22)	2.785(2)	0.918	1.895	163
O(22)–H(67)···O(7)¶	2.745(2)	0.873	1.877	173
O(22)–H(68)···O(18)††	2.771(2)	0.919	1.856	173
O(23)–H(69)···O(22)	2.865(2)	0.892	1.977	174
O(23)–H(70)···O(8)*	2.794(2)	0.982	1.833	165

Symmetry operators; *: x–1 y z; †: 1–x 1/2+y 1/2–z; ‡: x+1 y z; §: 3/2–x –y 1/2–z; □: 2–x 1/2+y 1/2–z; ¶: x–1/2 1/2–y 1–z; **: 1–x –1/2+y 1/2–z; ††: 1/2–x –y 1/2+z.

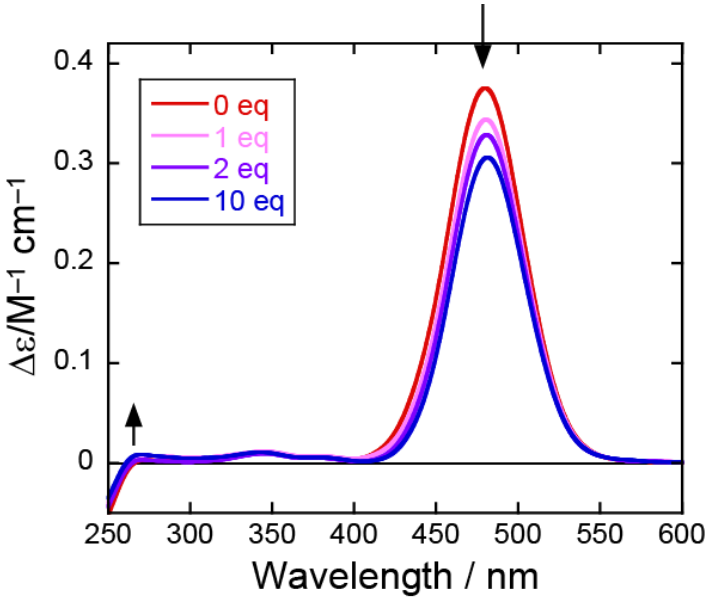

Fig. S1 CD spectral changes of Λ-**[**$Cr(tn)_3]Br_3$ (2.5 mM) as a function of $Na_3P_3O_9$ concentration (0–25 mM).

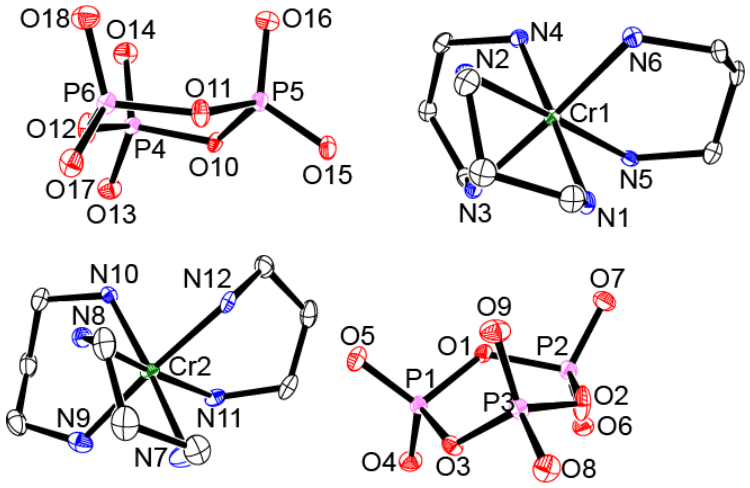

Fig. S2 ORTEP view of Λ-$[Cr(tn)_3]P_3O_9 \cdot 2.5H_2O$ with selected atom numbering schemes. Water molecules and hydrogen atoms are omitted for clarity.

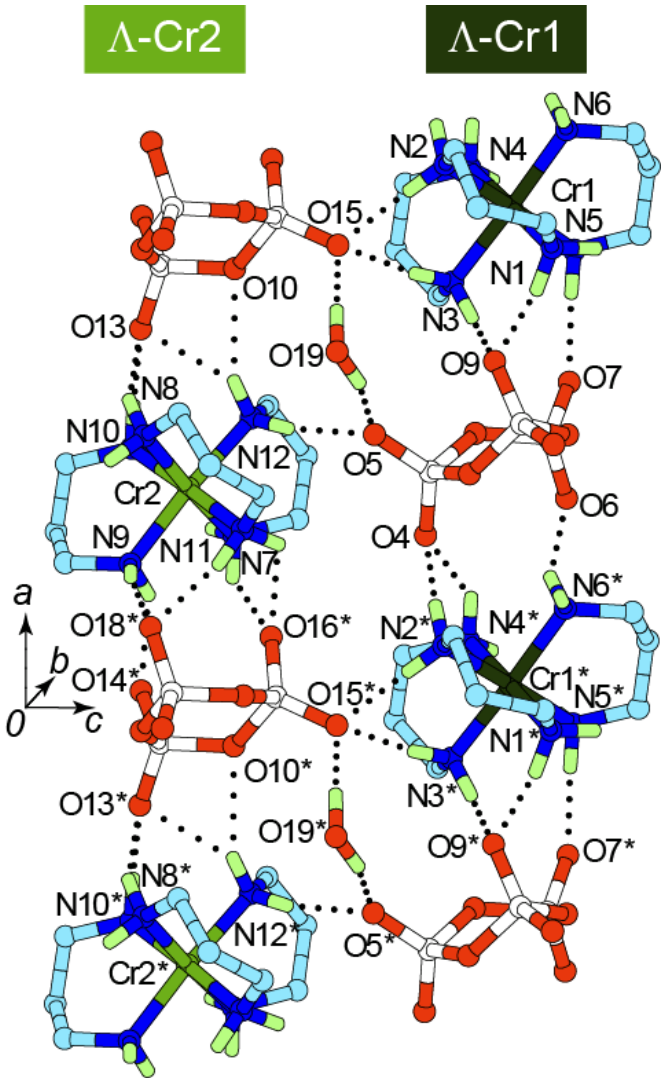

Fig. S3 Homochiral column-pair structure of Λ-$[Cr(tn)_3]P_3O_9{\cdot}2.5H_2O$, which was constructed by multiple hydrogen bonds between the alternately stacked $[Cr(tn)_3]^{3+}$ cations and $P_3O_9^{3-}$ anions, and the neighboring columns are further linked by hydrogen bonds. Symmetry operator *: *x*–1, *y*, *z*.