Electronic Supplementary Information

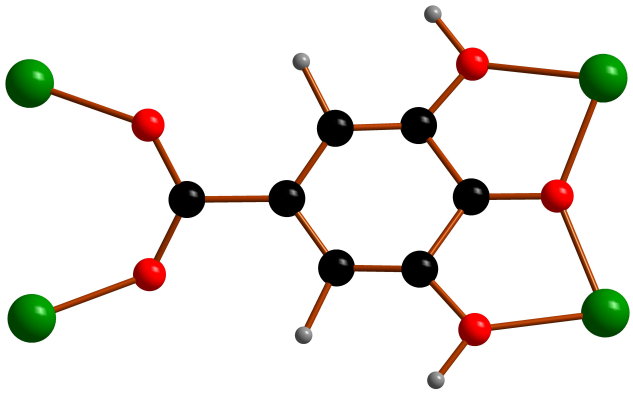

Fig. S1 Illustration of the coordination environment and positions of the hydrogen atom around one gallate ligand in Ni gallate, as determined by neutron powder diffraction at 50 K. The green, red, black and grey spheres are the Ni, oxygen, carbon and hydrogen atoms, respectively.

Table S1 Crystal structure of Ni gallate in $P3_121$ at 100 K, as determined using synchrotron X-ray diffraction. Positions of the hydrogen atoms are not included in the published structure due to insufficient precision in their locations. Displacement parameters of atoms of the same type are constrained to be equal.

Atom	Wyckoff Position	x	y	z	B (Å^2)
Ni	6*c*	0.03614(7)	0.98297(7)	0.08296(5)	0.267(8)
O1	3*b*	0	0.8746(5)	1/6	0.67(3)
O2	6*c*	0.1043(6)	0.7857(5)	0.0652(2)	0.67(3)
O3	6*c*	-0.0370(6)	0.1568(5)	0.11491(20)	0.67(3)
O6	3*a*	0.8982(5)	0	1/3	0.67(3)
O7	6*c*	0.3031(5)	0.1762(6)	0.1000(2)	0.67(3)
O8	6*c*	-0.2140(5)	0.8135(5)	0.05193(20)	0.67(3)
C1	3*b*	0	0.7221(8)	1/6	0.43(3)
C2	6*c*	0.0486(9)	0.6646(7)	0.1140(3)	0.43(3)
C3	3*b*	0	0.2370(8)	1/6	0.43(3)
C4	3*b*	0	0.4055(8)	1/6	0.43(3)
C5	6*c*	0.0491(8)	0.5092(8)	0.1135(3)	0.43(3)
C6	3*a*	0.7520(8)	0	1/3	0.43(3)
C7	6*c*	0.3606(8)	0.2984(7)	0.0525(3)	0.43(3)
C8	3*a*	0.2655(8)	0	1/3	0.43(3)
C9	3*a*	0.4371(8)	0	1/3	0.43(3)
C10	6*c*	-0.4833(7)	0.4547(7)	0.0537(3)	0.43(3)
O9	6*c*	0.6791(6)	0.1331(7)	0.0472(3)	1.92(7)
O10	6*c*	0.5343(6)	0.8114(7)	0.1238(3)	1.92(7)
a = 8.81154(1) c = 21.19947(1)					
R_p = 7.9 % R_{wp} = 11.0 χ^2 = 7.0					

Table S2 Crystal structure of Co gallate in $P3_121$ at 100 K, as determined using synchrotron X-ray diffraction. Positions of the hydrogen atoms are not included in the published structure due to insufficient precision in their locations. Displacement parameters of atoms of the same type are constrained to be equal.

Atom	Wyckoff Position	x	y	z	B (Å^2)
Co	6*c*	0.02184(12)	0.98429(14)	0.08289(9)	0.274(16)
O1	3*b*	0	0.8750(7)	1/6	0.34(4)
O2	6*c*	0.0847(9)	0.7778(8)	0.0625(3)	0.34(4)
O3	6*c*	-0.0452(9)	0.1596(8)	0.1156(3)	0.34(4)
O6	3*a*	0.8978(6)	0	1/3	0.34(4)
O7	6*c*	0.3007(7)	0.1826(8)	0.1002(3)	0.34(4)
O8	6*c*	-0.2256(7)	0.8121(8)	0.0515(3)	0.34(4)
C1	3*b*	0	0.7237(11)	1/6	0.26(5)
C2	6*c*	0.0404(13)	0.6660(10)	0.1118(4)	0.26(5)
C3	3*b*	0	0.2441(12)	1/6	0.26(5)
C4	3*b*	0	0.4148(11)	1/6	0.26(5)
C5	6*c*	0.0359(12)	0.5056(10)	0.1121(4)	0.26(5)
C6	3*a*	0.7496(11)	0	1/3	0.26(5)
C7	6*c*	0.3574(12)	0.2953(10)	0.0541(4)	0.26(5)
C8	3*a*	0.2717(12)	0	1/3	0.26(5)
C9	3*a*	0.4399(11)	0	1/3	0.26(5)
C10	6*c*	-0.4870(12)	0.4604(10)	0.0537(4)	0.26(5)
O9	6*c*	0.6771(9)	0.1314(9)	0.0471(4)	1.94(11)
O10	6*c*	0.5269(10)	0.8121(9)	0.1239(5)	1.94(11)
		a = 8.91594(1) c = 21.25397(1)			
		R_p = 4.0 % R_{wp} = 5.1 χ^2 = 1.9			

Table S3 Crystal structure of Co gallate in $P3_121$ at 300 K, as determined using synchrotron X-ray diffraction. Positions of the hydrogen atoms are not included in the published structure due to insufficient precision in their locations. Displacement parameters of atoms of the same type are constrained to be equal.

Atom	Wyckoff Position	x	y	z	B (Å^2)
Co	3*b*	0	0.97329(8)	1/6	0.803(17)
O1	3*a*	0.8896(3)	0.8896(3)	0.2055(4)	1.16(5)
O2	6*c*	0.7945(4)	0.6994(4)	0.2055(4)	1.16(5)
O3	6*c*	0.1731(4)	0.2175(4)	0.1029(2)	1.16(5)
C1	3*a*	0.7393(7)	0.7393(7)	0	1.30(6)
C2	6*c*	0.6811(6)	0.6331(8)	0.1054(5)	1.30(6)
C3	3*a*	0.2548(8)	0.2548(8)	0	1.30(6)
C4	3*a*	0.4272(6)	0.4272(6)	0	1.30(6)
C5	6*c*	0.5275(7)	0.4792(6)	0.1072(4)	1.30(6)
O4	6*c*	0.8188(7)	0.2959(6)	0.0803(5)	5.98(16)
		a = 8.91960(1) c = 10.67049(1)			
		R_p = 4.0 % R_{wp} = 5.2 χ^2 = 2.0			

Table S4 Crystal structure of Fe gallate in $P3_121$ at 100 K, as determined using synchrotron X-ray diffraction. Positions of the hydrogen atoms are not included in the published structure due to insufficient precision in their locations. Displacement parameters of atoms of the same type are constrained to be equal.

Atom	Wyckoff Position	x	y	z	B (Å^2)
Fe	3*b*	0	0.94289(11)	1/6	0.257(16)
O1	3*a*	0.8914(4)	0.8914(4)	0	0.32(4)
O2	6*c*	0.8062(5)	0.6877(4)	0.1990(3)	0.32(4)
O3	6*c*	0.1675(4)	0.1908(4)	0.1017(2)	0.32(4)
C1	3*a*	0.7285(9)	0.7285(9)	0	1.03(6)
C2	6*c*	0.6793(8)	0.6108(8)	0.1090(5)	1.03(6)
C3	3*a*	0.2442(9)	0.2442(9)	0	1.03(6)
C4	3*a*	0.4196(8)	0.4196(8)	0	1.03(6)
C5	6*c*	0.5046(10)	0.4516(10)	0.1116(4)	1.03(6)
O4a	6*c*	0.1332(13)	0.4560(13)	0.2462(8)	1.12(14)
O4b	6*c*	0.2743(20)	0.5160(14)	0.3068(11)	1.12(14)
O4c	6*c*	0.4486(16)	0.5815(14)	0.4390(10)	1.12(14)
		a = 8.67104(1) c = 10.87257(1)			
		R_p = 5.8 % R_{wp} = 7.5 χ^2 = 2.6			

Table S5 Crystal structure of Ni gallate in $P3_121$ at 50 K, as determined using neutron diffraction. All displacement parameters of atoms in the framework and those in the water molecules are constrained to be equal. Hydrogen atoms of the same type are constrained to have the same occupancy.

Atom	Wyckoff Position	x	y	z	B (Å^2)	Fractional Occupancy
Ni	6*c*	0.0415(12)	0.9861(16)	0.0839(7)	0.50(6)	1
O1	3*b*	0	0.8739(19)	1/6	0.50(6)	1
O2	6*c*	0.090(3)	0.784(2)	0.0697(9)	0.50(6)	1
D2	6*c*	0.132(2)	0.770(2)	0.0234(10)	0.50(6)	0.833(17)
O3	6*c*	-0.035(2)	0.147(2)	0.1158(8)	0.50(6)	1
O6	3*a*	0.9041(20)	0	1/3	0.50(6)	1
O7	6*c*	0.303(3)	0.180(2)	0.0931(9)	0.50(6)	1
D7	6*c*	0.392(2)	0.228(2)	0.1286(10)	0.50(6)	0.833(17)
O8	6*c*	-0.199(2)	0.815(2)	0.0548(7)	0.50(6)	1
C1	3*b*	0	0.7265(17)	1/6	0.50(6)	1
C2	6*c*	0.046(2)	0.6618(17)	0.1131(6)	0.50(6)	1
C3	3*b*	0	0.2342(18)	1/6	0.50(6)	1
C4	3*b*	0	0.4025(17)	1/6	0.50(6)	1
C5	6*c*	0.053(2)	0.5056(18)	0.1113(6)	0.50(6)	1
D5	6*c*	0.106(3)	0.484(3)	0.0716(10)	0.50(6)	0.796(14)
C6	3*a*	0.7543(16)	0	1/3	0.50(6)	1
C7	6*c*	0.3748(17)	0.2982(15)	0.0501(6)	0.50(6)	1

C8	3*a*	0.2585(17)	0	1/3	0.50(6)	1
C9	3*a*	0.4328(16)	0	1/3	0.50(6)	1
C10	6*c*	-0.4987(16)	0.4620(16)	0.0497(6)	0.50(6)	1
D10	6*c*	-0.416(3)	0.496(3)	0.0971(10)	0.50(6)	0.796(14)
O9	6*c*	0.692(2)	0.130(2)	0.0432(10)	0.8(3)	1
D9A	6*c*	0.601(3)	0.058(3)	0.0734(11)	0.8(3)	0.658(11)
D9B	6*c*	0.797(3)	0.159(3)	0.0738(12)	0.8(3)	0.658(11)
O10	6*c*	0.5343(6)	0.8114(7)	0.1238(3)	0.8(3)	1
D10A	6*c*	0.454(3)	0.720(4)	0.1266(10)	0.8(3)	0.658(11)
D10B	6*c*	0.508(3)	0.839(3)	0.1147(12)	0.8(3)	0.658(11)
		a = 8.80722(1) c = 21.19003(1)				
		R_p = 3.1 % R_{wp} = 3.9 χ^2 = 3.5				

Table S6 Crystal structure of Co gallate in $P3_121$ at 75 K, as determined using neutron diffraction. All displacement parameters of atoms in the framework and those in the water molecules are constrained to be equal. Hydrogen atoms of the same type are constrained to have the same occupancy.

Atom	Wyckoff Position	x	y	z	B (Å^2)	Fractional Occupancy
Co	6*c*	0.0219	0.9843	0.0829	0.37(9)	1
O1	3*b*	0	0.885(2)	1/6	0.37(9)	1
O2	6*c*	0.088(3)	0.768(2)	0.0636(9)	0.37(9)	1
D2	6*c*	0.107(3)	0.748(2)	0.0143(10)	0.37(9)	0.86(2)
O3	6*c*	-0.049(3)	0.163(3)	0.1098(8)	0.37(9)	1
O6	3*a*	0.907(2)	0	1/3	0.37(9)	1
O7	6*c*	0.289(3)	0.172(2)	0.0852(9)	0.37(9)	1
D7	6*c*	0.370(2)	0.240(3)	0.1219(11)	0.37(9)	0.86(2)
O8	6*c*	-0.237(3)	0.815(3)	0.0489(8)	0.37(9)	1

C1	3*b*	0	0.7302(18)	1/6	0.37(9)	1
C2	6*c*	0.051(3)	0.676(2)	0.1144(6)	0.37(9)	1
C3	3*b*	0	0.231(2)	1/6	0.37(9)	1
C4	3*b*	0	0.4035(17)	1/6	0.37(9)	1
C5	6*c*	0.036(3)	0.508(2)	0.1157(7)	0.37(9)	1
H5	6*c*	0.168(4)	0.567(4)	0.0933(16)	0.37(9)	1
C6	3*a*	0.7541(17)	0	1/3	0.37(9)	1
C7	6*c*	0.362(2)	0.3147(18)	0.0522(7)	0.37(9)	1
C8	3*a*	0.2810(18)	0	1/3	0.37(9)	1
C9	3*a*	0.4563(19)	0	1/3	0.37(9)	1
C10	6*c*	-0.489(2)	0.4785(20)	0.0567(7)	0.37(9)	1
H10	6*c*	-0.387(4)	0.531(5)	0.0785(17)	0.37(9)	1
O9	6*c*	0.687(4)	0.161(3)	0.0473(16)	5.5(4)	1
D9A	6*c*	0.597(3)	0.019(4)	0.0619(11)	5.5(4)	1.01(3)
D9B	6*c*	0.803(4)	0.216(4)	0.0760(12)	5.5(4)	1.01(3)
O10	6*c*	0.498(4)	0.844(3)	0.1180(17)	5.5(4)	1
D10A	6*c*	0.601(4)	0.807(4)	0.1111(16)	5.5(4)	1.01(3)
D10B	6*c*	0.427(4)	0.716(3)	0.1342(14)	5.5(4)	1.01(3)
		$a = 8.92274(1)$	$c = 21.25786(1)$			
		$R_p = 3.1$ %	$R_{wp} = 3.8$	$\chi^2 = 4.0$		

Table S7 Crystal structure of Co gallate in $P3_121$ at 293 K, as determined using neutron diffraction. Displacement parameters of the carbon atoms, hydrogen atoms and all atoms in the water molecule are constrained to be equal. The displacement parameters of the oxygen atoms and cobalt are also constrained to be equal.

Atom	Wyckoff Position	x	y	z	B (Å^2)	Fractional Occupancy
Co	3*b*	0	0.9733	1/6	1.40(12)	1
O1	3*a*	0.8786(15)	0.8786(15)	0	1.40(12)	1

O2	6*c*	0.7978(14)	0.7056(13)	0.2049(11)	1.40(12)	1
D2	6*c*	0.759(2)	0.6275(18)	0.2834(15)	2.9(3)	0.81(3)
O3	6*c*	0.1779(13)	0.2155(15)	0.1076(11)	1.40(12)	1
C1	3*a*	0.7414(13)	0.7414(13)	0	1.73(9)	1
C2	6*c*	0.6827(12)	0.6302(11)	0.1085(9)	1.73(9)	1
C3	3*a*	0.2669(14)	0.2669(14)	0	1.73(9)	1
C4	3*a*	0.4302(14)	0.4302(14)	0	1.73(9)	1
C5	6*c*	0.5151(11)	0.4923(13)	0.1135(8)	1.73(9)	1
H5	6*c*	0.461(3)	0.408(3)	0.178(2)	2.9(3)	1
O4	6*c*	0.733(3)	0.266(3)	0.087(2)	7.9(4)	1
D3	6*c*	0.816(2)	0.220(3)	0.136(2)	7.9(4)	0.98(3)
D4	6*c*	0.869(2)	0.373(3)	0.1107(19)	7.9(4)	0.98(3)
		a = 8.92226(1) c = 10.67993(1)				
		R_p = 3.0 % R_{wp} = 3.8 χ^2 = 3.2				

Table S8 Crystal structure of Fe gallate in $P3_121$ at 50 K, as determined using synchrotron X-ray diffraction. Displacement parameters of atoms of the same type are constrained to be equal.

Atom	Wyckoff Position	x	y	z	B (Å^2)	Fractional Occupancy
Fe	3*b*	0	0.9412(13)	1/6	0.63(19)	1
O1	3*a*	0.9000(13)	0.9000(13)	0	0.19(15)	1
O2	6*c*	0.8031(14)	0.6886(14)	0.1963(9)	0.19(15)	1
D2	6*c*	0.762(3)	0.601(3)	0.306(2)	2.5(4)	0.54(2)
O3	6*c*	0.1689(16)	0.1932(14)	0.1032(9)	0.19(15)	1
C1	3*a*	0.7460(13)	0.7460(13)	0	1.24(11)	1
C2	6*c*	0.6796(12)	0.6298(13)	0.1056(9)	1.24(11)	1
C3	3*a*	0.2448(16)	0.2448(16)	0	1.24(11)	1
C4	3*a*	0.4207(14)	0.4207(14)	0	1.24(11)	1
C5	6*c*	0.5255(14)	0.4659(12)	0.1054(9)	1.24(11)	1

D5	6*c*	0.488(2)	0.3747(16)	0.1891(12)	2.5(4)	0.91(3)
O4	6*c*	0.839(5)	0.290(5)	0.093(5)	18.6(8)	1
D3	6*c*	0.938(5)	0.409(4)	0.130(4)	18.6(8)	1
D4	6*c*	0.688(4)	0.237(6)	0.017(3)	18.6(8)	1
		a = 8.67104(1) c = 10.87257(1)				
		R_p = 5.8 % R_{wp} = 7.5 χ^2 = 2.6				