Monunuclear or coordination polymer complexes? Both are possible for 3,6,9-trioxaundecanedioic acid.

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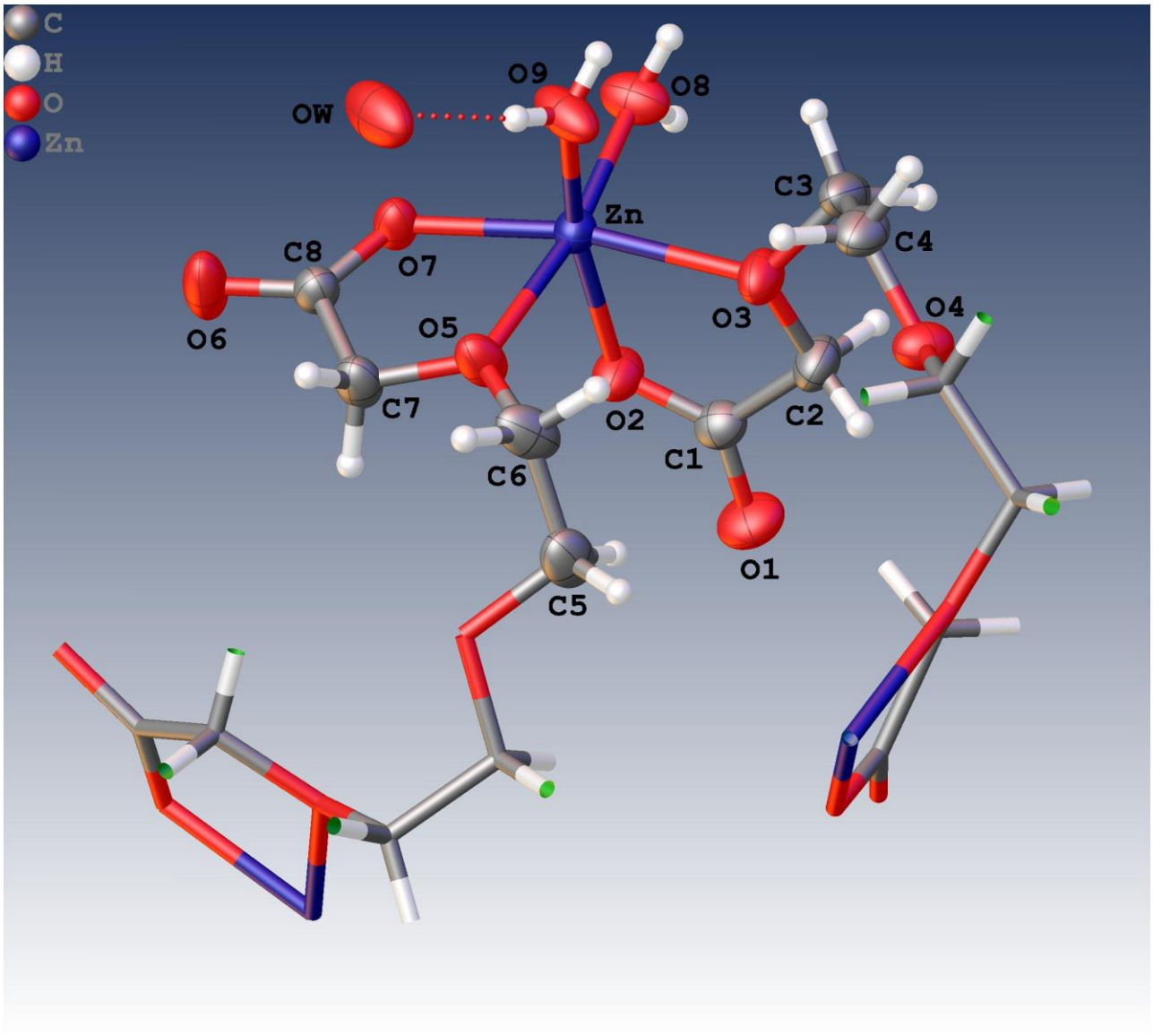


Figure S1. Ortep view of one asymmetric unit of the two isomorphous Zn(II) and Co(II) polymeric crystals. Displacement ellipsoids are drawn at 50% probability level while hydrogen size is arbitrary.

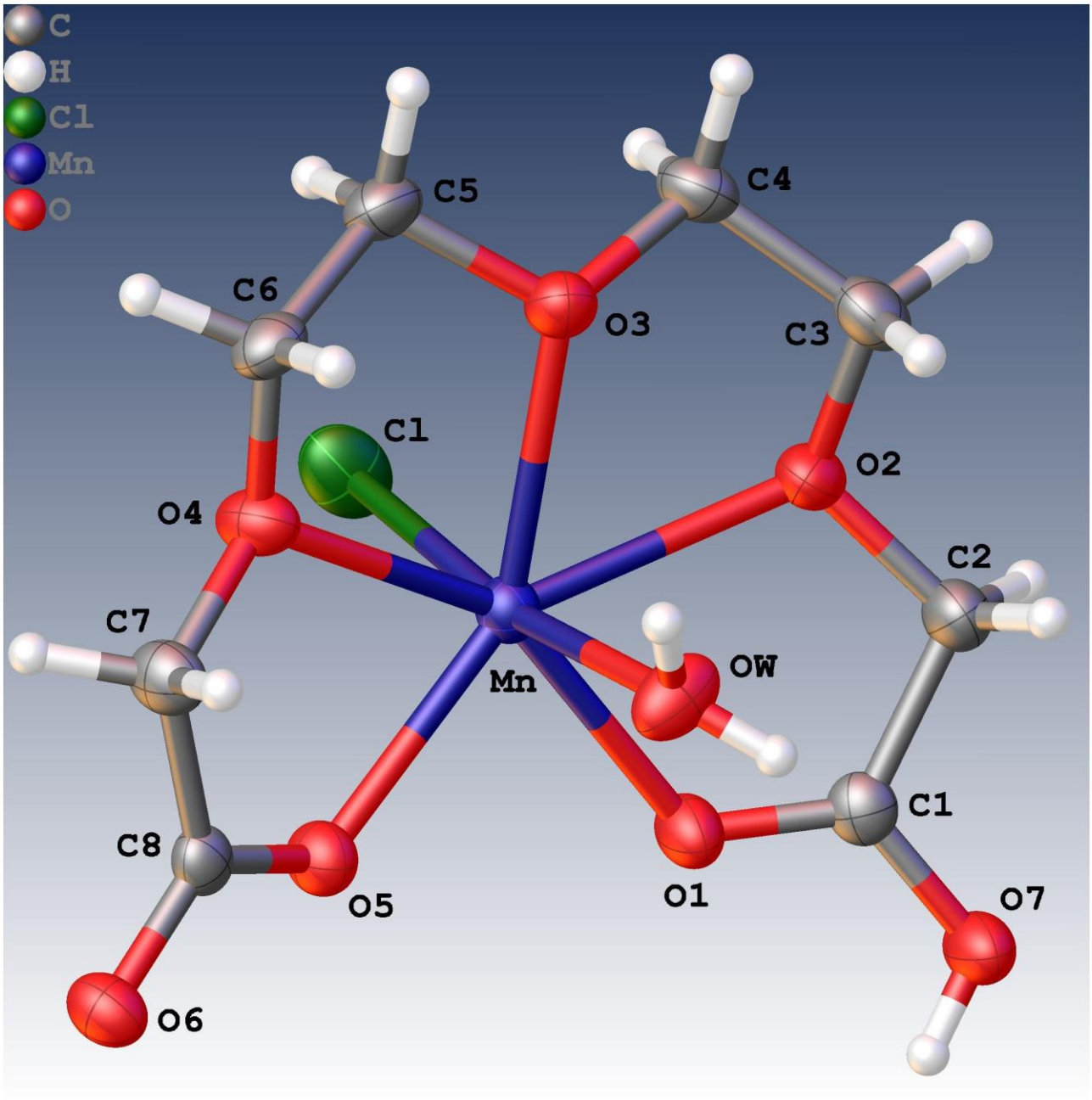


Figure S2. View of the Mn(II) complex with the protonated ligand. Displacement ellipsoids are drawn at 50% probability level while hydrogen size is arbitrary.

Table S1. Selected distances [Å] and angles [°] for Zn and Co complexes *(1st and 2nd values, respectively)*.

M–O2	2.016(1)	2.022(1)	M–O3	2.179(1)	2.168(1)
M–O5	2.225(1)	2.170(1)	M–O7	2.041(1)	2.047(1)
M–O8	2.037(1)	2.066(1)	M–O9	2.004(1)	2.004(1)
O2–M–O3	76.83(4)	76.65(4)	O2–M–O5	88.50(5)	87.94(5)
O2–M–O7	95.16(4)	95.36(5)	O2–M–O8	96.27(5)	96.09(5)
O3–M–O5	96.29(4)	99.58(5)	O7–M–O3	168.77(4)	171.19(4)
O7–M–O5	75.42(4)	76.15(4)	O8–M–O3	92.51(5)	89.26(5)
O8–M–O5	170.76(5)	170.94(5)	O8–M–O7	96.22(5)	95.35(5)
O9–M–O2	162.82(6)	163.47(6)	O9–M–O3	88.32(5)	89.62(5)
O9–M–O5	84.55(5)	85.28(5)	O9–M–O7	98.25(5)	97.62(6)
O9–M–O8	92.92(5)	92.86(6)			

D–H···A [Å]	d(D–H) [Å]		d(H···A) [Å]		d(D···A) [Å]		<(DHA) [°]	
O8–H8A···O1$^{\#1}$	0.79(2)	0.81(3)	1.96(2)	1.95(3)	2.732(2)	2.738(2)	164(2)	164(3)
O8–H8B···O6$^{\#2}$	0.83(2)	0.84(3)	1.89(2)	1.89(3)	2.712(2)	2.726(2)	175(2)	179(2)
O9–H9A···O7$^{\#2}$	0.74(2)	0.76(3)	1.98(3)	1.97(3)	2.721(2)	2.724(2)	175(3)	173(2)
O9–H9B···OW	0.71(2)	0.72(2)	1.92(2)	1.92(2)	2.631(2)	2.638(2)	174(3)	176(2)

Symmetry transformations used to generate equivalent atoms:
#1: -X, -Y, 2-Z; #2: 0.5-X, 0.5+Y, 1.5-Z;

Table S2. Selected lengths [Å] and angles [°] for Mn TODD complex**.**

Mn–Cl	2.450(1)	Mn–OW	2.219(2)	Mn–O1	2.217(2)
Mn–O2	2.404(1)	Mn–O3	2.339(2)	Mn–O4	2.286(2)
Mn–O5	2.177(1)				

O1–Mn–Cl	99.65(5)	O2–Mn–Cl	90.08(4)
O3–Mn–Cl	92.70(4)	O4–Mn–Cl	91.62(4)
O5–Mn–Cl	99.39(5)	O1–Mn–OW	83.20(7)
O2–Mn–OW	84.35(6)	O3–Mn–OW	80.43(6)
O4–Mn–OW	89.03(6)	O5–Mn–OW	88.01(6)
Cl–Mn–OW	172.34(5)	O1–Mn–O2	68.33(6)
O2–Mn–O3	69.41(6)	O3–Mn–O4	68.67(5)
O4–Mn–O5	70.49(6)	O5–Mn–O1	81.99(6)

C2–C1	1.497(3)	O1–C1	1.216(2)	O7–C1	1.296(3)
C7–C8	1.507(3)	O5–C8	1.239(2)	O6–C8	1.272(2)

O1–C1–C2	121.8(2)	O7–C1–C2	114.6(2)	O1–C1–O7	123.6(2)
O5–C8–C7	119.4(2)	O6–C8–C7	117.4(2)	O5–C8–O6	123.2(2)

O2–C2–C1–O1	−4.1(3)	O3–C4–C3–O2	60.8(2)
O3–C5–C6–O4	−54.4(2)	O5–C8–C7–O4	11.8(3)

D–H···A [Å]	d(D–H) [Å]	d(H···A) [Å]	d(D···A) [Å]	<(DHA) [°]
OW–HWB···O6$^{\#1}$	0.85(4)	1.89(5)	2.737(3)	170(3)
O7–H7···O6$^{\#2}$	0.82(4)	1.69(4)	2.512(2)	179(4)

Symmetry transformations used to generate equivalent atoms:

#1: 1-X, 2-Y, 0.5+Z; …….#2: 1-X, 2-Y, -0.5+Z

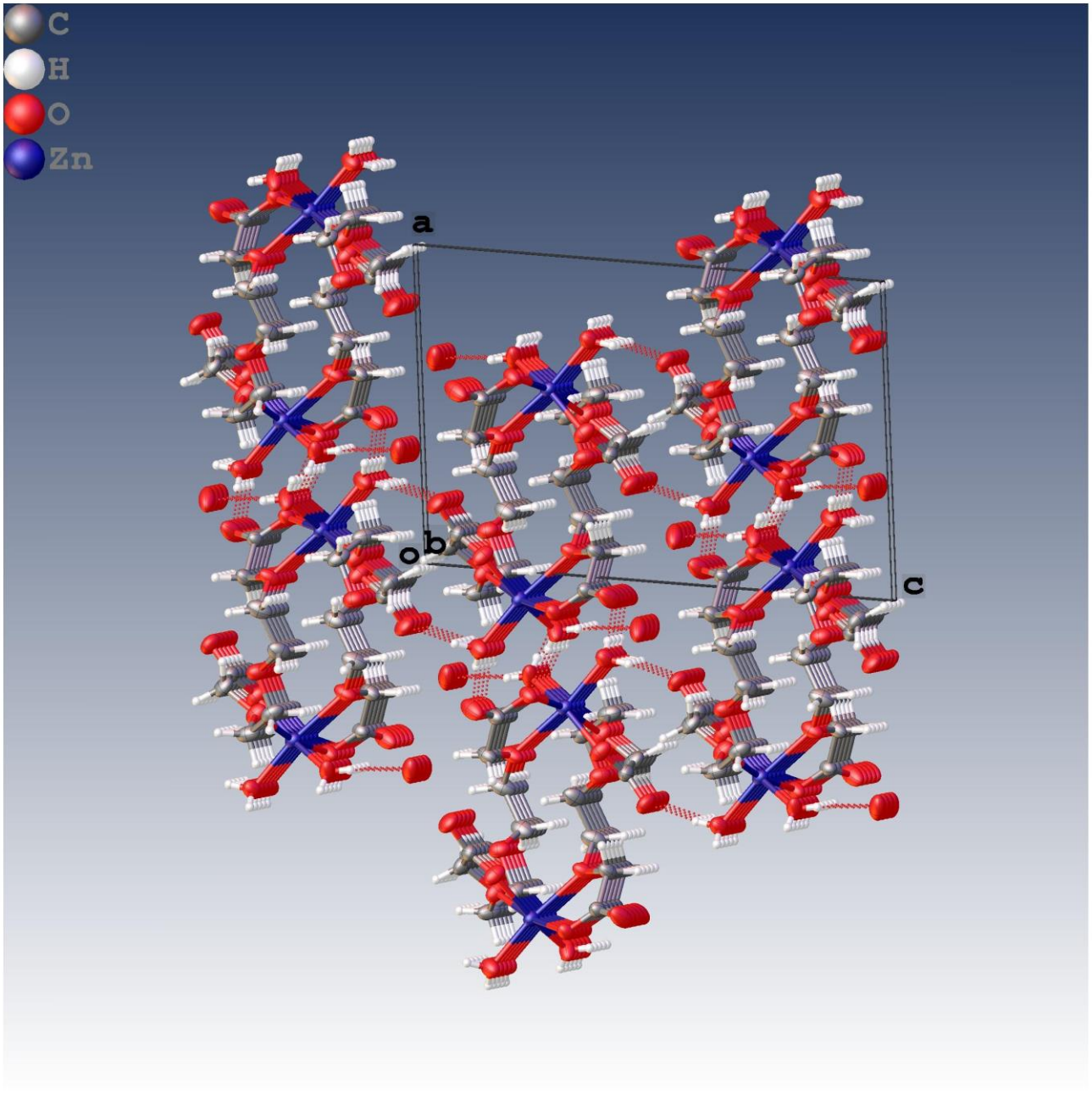


Figure S3. Zn and Co crystal packing showing the helix column parallel to b-axis and interconnected by the hydrogen bond involving the crystallization waters. Atoms are drawn at 50% probability level while hydrogen size is arbitrary.