Supplementary Material

New polynuclear compounds based on *N*-benzyliminodipropionic acid: Solution studies, synthesis and X-ray crystal structures

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1) Species Distribution Diagrams

Species distribution diagrams of the M(II)-bzlidp system, in 0.50 mol L⁻¹ Me₄NCl at 20.0 °C (total [M²⁺] = 5 mmol L⁻¹ and total [bzlidp] = 5 mmol L⁻¹). The fully deprotonated ligand is represented as L²⁻. **Figure S1)** M = Mn; **Figure S2)** M = Co; **Figure S3)** M = Zn; **Figure S4)** M = Cd; **Figure S5)** M = Pb.

Figure S1

Figure S2

Figure S3

Figure S4

Figure S5

2) Hydrogen bonds

Table S1. Bond distances (Å) and bond angles (°) of hydrogen bonds in compound **1**¹

D-H...A	D-H(Å)	H...A (Å)	D...A (Å)	D-H...A (°)
N1H1...O2	0.86(3)	2.24(2)	2.831(2)	126(2)
N1H1...O3	0.86(3)	2.28(3)	2.887(2)	128(2)
O1W-H1WA...O2 ^{#1}	0.86	1.86	2.623(2)	146
O1W-H1WB...O4 ^{#2}	0.86	1.93	2.674(2)	143
O3W-H3WA...O4W	0.87	1.88	2.561(3)	134
O3W-H3WB...O4 ^{#1}	0.86	1.77	2.550(2)	149
O4W-H4WA...O1 ^{#3}	0.85	1.91	2.753(3)	172
O4W-H4WB...O7	0.85	1.89	2.735(3)	174
O2W-H2WA...O6 ^{#4}	0.78(3)	2.16(3)	2.940(3)	171(3)
O2W-H2WB...O5 ^{#3}	0.80(4)	2.04(4)	2.826(3)	169(4)

¹ Symmetry transformation to generate equivalent atoms: #1 = 1-x, -y, 1-z; #2 = -x, -y, 1-z; #3 = 1-x, 1-y, 1-z; #4 = 2-x, 1-y, 1-z

Table S2. Bond distances (Å) and bond angles (°) of hydrogen bonds in compound **2**¹

D-H...A	D-H(Å)	H...A (Å)	D...A (Å)	D-H...A (°)
N1H1...O3	0.92(2)	1.99(2)	2.702(2)	133(2)
N1H1...O6i ^{#1}	0.92(2)	2.27(2)	2.992(2)	135(2)

¹ Symmetry transformation to generate equivalent atoms: #1 1/2-x, 1/2+y, 3/2-z

Table S3 Bond distances (Å) and bond angles (°) of hydrogen bonds in compound **3**¹

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	D-H...A (°)
O1WH1WA...O2 ^{#1}	0.83(3)	1.87(3)	2.6991(18)	174(2)
O1WH1WB...O3 ^{#2}	0.85(3)	1.98(3)	2.7963(17)	162(2)
O2WH2WB...O1 ^{#2}	0.85(2)	2.57(3)	2.9772(17)	111(2)
O2WH2WB...O2 ^{#2}	0.85(2)	1.82(2)	2.6464(19)	166(3)
O2WH2WA...O4 ^{#3}	0.81(3)	1.84(3)	2.6423(18)	169(2)

¹ Symmetry codes: #1 = x, 1+y, z; #2 = 2-x, 1-y, 1-z; #3 = 2-x, 1/2+y, 3/2-z.

3) Packing of compound 1

Figure S6. Unit cell of the structure of **1**. Thermal ellipsoids are shown at 50% probability. Hydrogen atoms are omitted for clarity. Color code: copper, orange; oxygen, red; nitrogen, blue; carbon, grey; sulfur, yellow; fluorine, green.