Supplementary Material (ESI) for CrystEngComm

Structural diversity of complexes between Cu(II) or Ni(II) and endocyclic oxygen- or nitrogen-containing ligands: Synthesis, X-ray structure determinations and circular dichroism spectra

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Electronic Supplementary Information

Crystallography

{[(Cu(H$_2$L^1)(L^5)(OH$_2$)]·[Cu(L^1)$_2$]}·3H$_2$O (1)

Table S1. Hydrogen Bond Geometry

D	H	A	D-H(Å)	H-A(Å)	D-A(Å)	DHA (º)
O(1)	H(1O)	O(3W)^{i}	0.840(12)	1.614(13)	2.4376(15)	166.3(19)
O(4)	H(2O)	O(4W)^{iii}	0.832(19)	1.626(19)	2.4515(16)	172(2)
O(1W)	H(3O)	O(12)^{iii}	0.77(2)	1.88(2)	2.6524(15)	179(2)
O(1W)	H(4O)	O(2W)	0.81(2)	1.84(2)	2.6393(16)	166.5(19)
O(2W)	H(5O)	O(5)^{ii}	0.78(2)	1.93(2)	2.6987(16)	171.9(19)
O(2W)	H(6O)	O(8)^{i}	0.840(11)	2.118(7)	2.9201(17)	159.6(17)
O(3W)	H(7O)	O(8)	0.79(2)	1.79(2)	2.5697(16)	174(2)
O(3W)	H(8O)	O(6)^{ii}	0.78(2)	1.82(2)	2.5938(15)	172(2)
O(4W)	H(9O)	O(9)^{iv}	0.76(2)	1.89(2)	2.6309(16)	163(2)
O(4W)	H(10O)	O(7)	0.77(2)	1.94(2)	2.7064(16)	173(2)

Symmetry Operator
^{i} –x+1, -y, -z+1 ^{ii} -x, y, z ^{iii} –x+1, -y+1, -z+1 ^{iv} –x+2, y, z

[Cu$_2$(HL^1)$_2$(L^1)(L^6)]·5.5H$_2$O (2)

Table S2. Hydrogen Bond Geometry

D	H	A	D-H(Å)	H-A(Å)	D-A(Å)	DHA (º)
O(2)	H(2O)	O(21)^{iii}	0.84(3)	1.72(2)	2.555(3)	171(3)
O(10)	H(10O)	O(4W)^{iv}	0.84(3)	1.64(3)	2.449(3)	160(4)
O(16)	H(16O)	O(11)^{vii}	0.84(3)	1.71(2)	2.546(3)	173(4)
O(24)	H(24O)	O(2W)^{v}	0.84(3)	1.69(3)	2.529(3)	173(4)
O(1W)	H(1W)	O(9W)^{iii}	0.891(14)	1.834(11)	2.702(3)	164(4)
O(1W)	H(2W)	O(20)	0.89(3)	1.84(3)	2.703(3)	165(4)
O(2W)	H(3W)	O(12)^{viii}	0.89(3)	1.94(2)	2.818(3)	171(3)
O(2W)	H(4W)	O(3W)^{viii}	0.89(3)	1.81(3)	2.699(3)	175(3)
O(3W)	H(5W)	O(1W)^{ii}	0.89(3)	1.951(17)	2.769(3)	152(3)

O(3W)	H(6W)	O(4)	0.89(3)	1.99(3)	2.867(3)	166(3)
O(4W)	H(7W)	O(6W)^{ix}	0.89(3)	1.72(3)	2.601(3)	169(4)
O(4W)	H(8W)	O(8W)^{x}	0.89(3)	1.80(3)	2.660(4)	163(4)
O(5W)	H(9W)	O(14)^{vi}	0.89(3)	2.06(2)	2.845(3)	146(4)
O(5W)	H(10W)	O(7)^{ii}	0.89(3)	2.266(17)	3.105(3)	157(4)
O(6W)	H(11W)	O(22)	0.89(3)	1.838(10)	2.708(3)	165(4)
O(6W)	H(12W)	O(14)	0.89(3)	1.93(2)	2.807(3)	167(4)
O(7W)	H(13W)	O(8)	0.89(3)	1.80(4)	2.678(4)	169(5)
O(7W)	H(14W)	O(8W)^{xi}	0.89(3)	2.03(3)	2.910(4)	170(5)
O(8W)	H(15W)	O(5W)	0.89(3)	1.916(16)	2.766(4)	159(4)
O(8W)	H(16W)	O(7W)^{i}	0.89(3)	1.853(10)	2.731(4)	168(4)
O(9W)	H(17W)	O(1W)^{xii}	0.89(3)	2.05(3)	2.879(3)	156(3)
O(9W)	H(18W)	O(10W)^{xiii}	0.89(3)	1.95(3)	2.799(4)	159(3)
O(10W)	H(19W)	O(19)^{ii}	0.89(3)	2.14(4)	3.008(3)	165(4)
O(10W)	H(20W)	O(4)	0.89(3)	2.00(2)	2.815(3)	151(4)
O(11W)	H(21W)	O(7W)^{xiv}	0.89(3)	1.99(5)	2.835(5)	159(6)
O(11W)	H(22W)	O(14)^{ix}	0.89(3)	2.34(5)	3.020(4)	133(5)
O(11W)	H(22W)	O(6W)^{ix}	0.89(3)	2.63(3)	3.463(4)	156(5)

Symmetry Operators

^{i} –x+1, y+1/2, -z+3/2 ^{ii} –x+1, -y+1, -z +1 ^{iii} x, -y+1/2, z-1/2 ^{iv} x, y-1, z ^{v} x, y+1, z
^{vi} x-1, y, z ^{vii} x, -y+3/2, z+1/2 ^{viii} x, -y+1/2, z+1/2 ^{ix} x, -y+3/2, z-1/2 ^{x} –x+1, -y+2, -z +1
^{xi} –x+1, -y+2, -z -1/2 ^{xii} –x+1, y-1/2, -z+3/2 ^{xiii} –x+1, -y, -z +1 ^{xiv} –x+2, -y+1, -z

{[Cu(HL^3)(L^3)$_{0.5}$(OH_2)]·1.75H_2O}$_n$ (3)

Table S3. Hydrogen Bond Geometry

D	H	A	D-H(Å)	H-A(Å)	D-A(Å)	DHA (º)
O(5)	H(1O)	O(10)^{iii}	0.839(19)	1.76(2)	2.5909(19)	172(3)
O(9)	H(2O)	O(12)	0.870(19)	1.968(9)	2.811(4)	163(3)
O(9)	H(3O)	O(4)^{vi}	0.870(13)	1.907(9)	2.7454(18)	161(3)
O(10)	H(4O)	O(4)	0.870(13)	1.949(6)	2.8079(17)	169(3)
O(10)	H(5O)	O(1)	0.868(16)	1.944(16)	2.8113(19)	179(3)
O(10)	H(5O)	O(3)	0.868(16)	2.56(2)	3.0021(19)	112(2)
O(11)	H(6O)	O(9)	0.804(13)	1.812(4)	2.682(4)	179(4)
O(11)	H(7O)	O(7)^{iv}	0.870(1)	2.446(2)	2.932(3)	115.88(11)
O(11)	H(7O)	O(7)^{v}	0.870(1)	2.446(2)	2.932(3)	115.88(11)
O(11)	H(7O)	O(8)^{iv}	0.870(1)	2.444(5)	3.314(5)	180.000(1)
O(11A)	H(6O1)	O(9)^{i}	0.870(1)	1.93(3)	2.771(6)	163(11)
O(11A)	H(6O1)	O(12)^{iii}	0.870(1)	2.63(11)	3.059(7)	112(9)
O(11A)	H(7O1)	O(7)^{v}	0.870(1)	2.525(4)	3.015(6)	116.4(4)
O(11A)	H(7O1)	O(8)^{iv}	0.870(1)	2.614(9)	3.322(7)	139.2(6)
O(12)	H(8O)	O(9)^{ii}	0.8698(10)	2.25(4)	2.993(4)	143(6)

O(12)	H(8O)	O(12)[ii]	0.8698(10)	2.50(6)	3.111(10)	128(6)
O(12)	H(9O)	O(10)[vi]	0.8698(10)	2.07(4)	2.838(4)	147(6)

Symmetry Operators

[i] -x, y, -z+1/2 [ii] -x, -y, -z+1 [iii] x, -y, z-1/2 [iv] -x+1/2, -y+1/2, -z+1 [v] x-1/2, -y+1/2, z-1/2 [vi] -x, y, -z+3/2

Specific details:

The O(11) and O(11A) water molecules are disordered over 3 positions with a total occupancy of 1. Their isotropic thermal parameter was refined identically.

{[Cu(L^4)(L^7)]ClO$_4$}$_n$ (4)

Table S4. Hydrogen Bond Geometry

D	H	A	D-H(Å)	H-A(Å)	D-A(Å)	DHA (º)
N(2)	H(1N)	O(7)[i]	0.88(3)	2.24(3)	3.117(4)	175(3)

Symmetry Operators

[i] x, -y+1/2, z-1/2

[Cu(L^2)(OH$_2$)$_4$)]$_n$ (5)

Specific details:

Although the crystals employed in this study appearing (at least visually) to be of good habit and free from imperfections, they proved not to be single and a two component twin, which was resolved using CELL_NOW [Bruker-Nonius (2007), CELL_NOW. Bruker AXS Inc. Madison, Wisconsin, USA], TWINABS [G. M. Sheldrick, *TWINABS: Empirical Absorption and Correction Software, University of Göttingen, Germany*, 1999-2007] and SAINT [Bruker-Nonius, SAINT v.7 Bruker AXS Inc. Madison, Wisconsin, USA, 2007].

Table S5. Hydrogen Bond Geometry

D	H	A	D-H(Å)	H-A(Å)	D-A(Å)	DHA (º)
O(7)	H(2O)	O(1)[i]	0.84(2)	1.91(2)	2.748(2)	176(3)
O(7)	H(1O)	O(3)[i]	0.84(2)	2.60(3)	3.004(2)	111(2)

O(7)	H(1O)	O(5)^{i}	0.84(2)	1.88(2)	2.716(2)	178(3)
O(7)	H(1O)	O(3)^{i}	0.84(2)	2.60(3)	3.004(2)	111(2)
O(8)	H(4O)	O(2)^{iv}	0.84(2))	2.38(3)	2.825(3)	114(3)
O(8)	H(3O)	O(4)^{ii}	0.84(2)	2.021(18)	2.787(3)	151(3)
O(9)	H(6O)	O(8)	0.84(2)	1.84(2)	2.669(2)	172(3)
O(9)	H(5O)	O(5)^{iii}	0.84(2)	1.78(2)	2.613(2)	172(3)
O(10)	H(8O)	O(4)^{ii}	0.84(2)	1.86(2)	2.699(2)	171(3)
O(10)	H(7O)	O(6)^{v}	0.84(2)	1.84(3)	2.674(2)	174(3)

Symmetry Operators

^{i} -x, -y+1, -z ^{ii}x, y+1, z ^{iii} x+1, y, z ^{iv} –x+1, -y+1, -z ^{iv} –x-1, -y+1, -z+1

[Ni(HL^{2})$_2$(OH$_2$)$_4$)] (6)

Table S6. Hydrogen Bond Geometry

D	H	A	D-H(Å)	H-A(Å)	D-A(Å)	DHA (º)
O(7)	H(2O)	O(4)^{i}	0.74(3)	2.12(3)	2.7808(19)	149(3)
O(7)	H(3O)	O(2)^{iii}	0.80(3)	1.89(3)	2.687(2)	173(2)
O(8)	H(4O)	O(2)^{iv}	0.79(2)	2.00(3)	2.6939(19)	146(2)
O(8)	H(5O)	O(7)^{i}	0.86(3)	1.95(3)	2.7943(19)	168(2)
O(5)	H(1O)	O(6)^{ii}	0.87(3)	1.84(3)	2.703(2)	171(2)

Symmetry Operator

^{i} –x+1, -y, -z+1 ^{ii} x+1, y-1, z ^{iii} –x, -y+1, -z+1 ^{iv} –x, -y, -z+1