

SUPPORTING INFORMATION

Title: Modified Bipyridines: 5,5'-Diamino-2,2'-bipyridine Metal Complexes Assembled into Multidimensional Networks via Hydrogen Bonding and π – π Stacking Interactions

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Supporting information

Modified Bipyridines: 5,5'-Diamino-2,2'-bipyridine Metal Complexes Assembled into Multidimensional Networks via Hydrogen Bonds and π – π Stacking Interactions

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Details of the hydrogen bonding networks in the reported X-ray structures

Table 1. Hydrogen bonding interactions in [Ni(5)₃](SCN)₂ (**18**)

D-H...A	D-H [Å]	H...A [Å]	D...A [Å]	D-H...A [°]
N71-H712...S1	0.83(3)	2.71(3)	3.524(3)	169(2)
N72-H722...S2#1	0.87(3)	2.62(3)	3.480(3)	176(2)
N73-H731...S1#2	0.86(2)	2.51(2)	3.370(3)	172(2)
N74-H742...N2#3	0.83(3)	2.23(3)	3.055(4)	172(2)
N75-H752...N1#1	0.88(3)	2.09(3)	2.963(3)	168(3)
N76-H761...N2#4	0.86(3)	2.30(3)	3.146(4)	167(2)
N76-H762...S2#5	0.89(2)	2.80(2)	3.668(3)	164(2)

symmetry equivalent positions: #1 = x+1, y+1, z; #2 = -x+1, -y+1, -z+1; #3 = -x+2, -y+1, -z; #4 = -x+1, -y+1, -z; #5 = x, y+1, z

Table 3. Hydrogen bonding in [CuCl₂(5)] (20)

D-H...A	D-H [Å]	H...A [Å]	D...A [Å]	D-H...A [°]
N7-H71...Cl#1	0.685	2.799	3.422	152.54
N71-H72...Cl#2	0.755	2.858	3.541	151.75

symmetry equivalent positions: #1 = -x+0.5, y-0.5, -z+1.5; #2 = x-0.5, -y+0.5, z-0.5.

Table 4. Hydrogen bonding interactions in [Zn(5)₃](NO₃)₂ · 2 H₂O (22)

D-H...A	D-H [Å]	H...A [Å]	D...A [Å]	D-H...A [°]
N51-H51B...O91	0.880(4)	2.258(4)	3.048(6)	149.3(3)
N51-H51A...O91#15	0.879(4)	2.326(4)	3.051(5)	139.8(3)
N52-H52A...O91#4	0.880(5)	2.445(4)	3.038(6)	125.1(3)
N52-H52B...O5#4	0.881(5)	2.302(5)	3.061(7)	144.4(4)
N53-H53A...O2#6	0.882(4)	2.128(4)	2.923(5)	149.7(3)
N53-H53B...O4	0.879(5)	2.069(5)	2.889(7)	154.9(3)
N54-H54A...O1#7	0.881(4)	2.326(4)	3.148(6)	155.3(4)
N54-H54A...O2#7	0.881(4)	2.456(5)	3.217(6)	144.9(3)
N54-H54B...O2#9	0.879(5)	2.177(4)	3.029(6)	163.2(3)
N55-H55A...O6#15	0.880(4)	2.457(6)	3.114(7)	131.9(3)
N55-H55B...O1#15	0.878(4)	2.146(4)	3.004(5)	165.5(3)
N56-H56A...O6#14	0.880(4)	2.137(6)	3.010(7)	171.5(4)
O91-H911...O92	0.908(19)	1.881(19)	2.657(7)	142.1(19)
O91-H912...O5	0.89(2)	2.34(2)	2.901(6)	120.9(19)
O92-H921...O3	0.83(4)	2.31(5)	2.742(8)	113(3)
O92-H922...O4#12	0.82(3)	2.36(4)	2.892(8)	123(4)

symmetry equivalent positions: #4 = -y-0.25, -x+0.75, z-0.25; #6 = -x+1, -y+0.5, z; #7 = -y+0.25, x-0.25, z-0.25; #9 = -x+1, -y+1, -z; #12 = -y+1.25, x+0.25, -z+0.25; #14 = x, y+0.5, -z; #15 = y-0.25, -x+1.25, -z+0.25

Table 5. Hydrogen bonding in ¹_∞[Cd(μ-Cl)₂(5)] · 2 H₂O (25)

D-H...A	D-H [Å]	H...A [Å]	D...A [Å]	D-H...A [°]
N2-H21...O#2	0.999(7)	2.044(13)	2.993(18)	157.8(4)
N2-H22...O	0.999(7)	2.161(13)	2.978(18)	137.9(4)
O-H31...N2#4	1.002(7)	1.837(11)	2.835(17)	174.14(19)
O-H32...Cl	1.049(7)	2.266(13)	3.312(19)	174.7(2)

symmetry equivalent positions: #2 = -x+0.5, y+0.5, z; #4 = -x+0.5, -y+0.5, z+0.5; #6 = -x, -y, 1-z.