Electronic Supplementary Material for CrystEngComm

Supplementary Information

Zinc(II) and cobalt(II) complexes of (3-carboxymethoxy-naphthalen-2-yloxy)-acetic acid : a structural study

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The X-ray single crystal data were collected at 296K with $Mo_{K\alpha}$ radiation (λ = 0.71073 Å) using a Bruker Nonius SMART CCD diffractometer equipped with graphite monochromator. The SMART software was used for data collection and also for indexing the reflections and determining the unit cell parameters; the collected data were integrated using SAINT software. The structures were solved by direct methods and refined by full-matrix least-squares calculations using SHELXTL software. All the non-H atoms were refined in the anisotropic approximation against F^2 of all reflections. The H-atoms, except those attached to N, O were placed at their calculated positions and refined in the isotropic approximation; those attached to heteroatoms (N, O) were located in the difference Fourier maps, and refined with isotropic displacement coefficients.

Crystal data and refinement parameters for the complexes **1-8**

Compound No.	**1**	**2**	**3**
Formulae	$C_{28}H_{22}Na_2O_{14}Zn$	$C_{26}H_{29}N_7O_7Zn$	$C_{148}H_{176}N_{20}O_{70}Zn_8$
Mol. wt.	693.81	616.93	3878.05
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	C2/c	$P2_1/c$	P-1
Temperature /K	296	296	296
Wavelength /Å	0.71073	0.71073	0.71073
a /Å	16.3719(6)	9.3548(3)	11.3948(5)
b /Å	22.7018(6)	18.3574(6)	17.2622(7)
c /Å	7.4514(2)	18.7369(6)	22.0932(9)
α/°	90.00	90.00	98.390(2)
β/°	94.705(2)	115.724(2)	90.784(2)
γ/°	90.00	90.00	98.487(2)
V/ $Å^3$	2760.14(15)	2898.80(16)	4249.4(3)
Z	4	4	1
Density/Mgm^{-3}	1.670	1.414	1.515
Abs. Coeff. /mm^{-1}	0.997	0.903	1.209
Abs. correction	None	None	None
F(000)	1416	1280	2004
Total no. of	20978	24225	42586

reflections			
Reflections, $I > 2\sigma(I)$	3376	4849	16377
Max. 2θ/°	28.35	25.00	26.00
Ranges (h, k, l)	-21 <= h <=21 -30 <= k <=30 -9 <= l <= 9	-10 <= h <=10 -21 <= k <=21 -20 <= l <= 21	-13 <= h <= 14 -20 <= k <= 21 -27 <= l <= 26
Complete to 2θ (%)	97.9	95.0	98.1
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/ Restraints/Parameters	3376 / 0 / 204	4849 / 0 / 380	16377 / 0/ 1133
Goof (F^2)	1.028	1.036	1.054
R indices [$I > 2\sigma(I)$]	0.0328	0.0442	0.0692
R indices (all data)	0.0438	0.0600	0.1093

Compound No.	**4**	**5**	**6**
Formulae	$C_{40}H_{42}N_4Na_2O_{18}Zn_2$	$C_{25}H_{28}N_2O_9Zn$	$C_{25}H_{28}CoN_2O_9$
Mol. wt.	1043.50	565.86	559.42
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	P-1	$P2_1/c$	P2(1)/c
Temperature /K	296	296	296
Wavelength /Å	0.71073	0.71073	0.71073
a /Å	8.6774(7)	10.727(2)	10.7482(5)
b /Å	11.7824(9)	17.456(4)	17.4273(8)
c /Å	12.3236(15)	16.435(3)	16.4072(6)
α/°	108.070(3)	90.00	90.00
β/°	94.205(3)	120.721(12)	120.690(2)
γ/°	109.158(2)	90.00	90.00
V/ $Å^3$	1109.77(18)	2645.6(9)	2642.8(2)
Z	1	4	4
Density/Mgm^{-3}	1.561	1.421	1.406
Abs. Coeff. /mm^{-1}	1.181	0.982	0.703
Abs. correction	None	None	None
F(000)	536	1176	1164
Total no. of reflections	12883	22153	26662
Reflections, $I > 2\sigma(I)$	5282	4737	6238
Max. 2θ/°	28.36	25.50	28.36
Ranges (h, k, l)	-11<= h <= 11 -15<= k <= 15 -16<= l <= 16	-10 <= h <= 12 -20 <= k <= 20 -19 <= l <= 19	-11 <= h <= 14 -22 <= k <= 22 -21 <= l <= 21
Complete to 2θ (%)	94.9	96.4	94.5
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/ Restraints/Parameters	5282 / 0 / 304	4737/ 0/ 343	6238/ 0 / 355
Goof (F^2)	1.038	1.051	1.056
R indices [$I > 2\sigma(I)$]	0.0397	0.0583	0.0464
R indices (all data)	0.0576	0.0757	0.0759

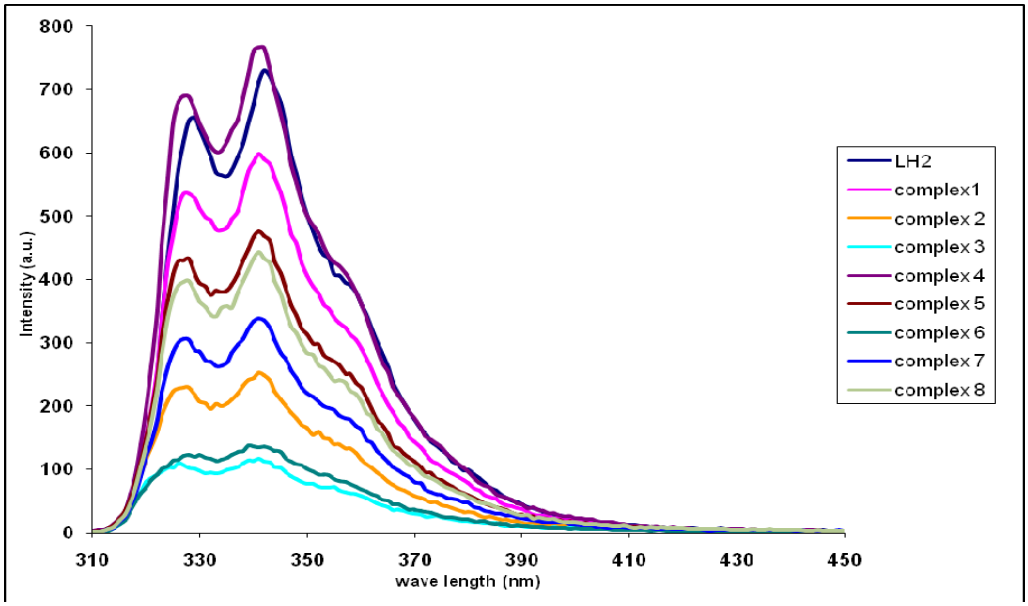
Compound No.	**7**	**8**
Formulae	$C_{38}H_{32}N_4O_9Zn$	$C_{34}H_{38}N_4O_{12}Zn$
Mol. wt.	754.05	760.05
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	P-1
Temperature /K	296	296
Wavelength /Å	0.71073	0.71073
a /Å	11.4686(7)	10.8004 (1)
b /Å	18.0561(11)	11.7121(2)
c /Å	17.4989(10)	15.6378(2)
α/°	90.00	102.683 (1)
β/°	103.013(3)	106.283 (1)
γ/°	90.00	101.937 (1)
V/ $Å^3$	3530.6(4)	1774.72(4)
Z	4	2
Density/Mgm^{-3}	1.419	1.422
Abs. Coeff. /mm^{-1}	0.758	0.760
Abs. correction	None	None
F(000)	1560	792
Total no. of reflections	32573	26316
Reflections, $I > 2\sigma(I)$	6187	8670
Max. 2θ/°	25.00	28.33
Ranges (h, k, l)	-13 <= h <= 13 -21 <= k <= 21 -20 <= l <= 20	-14 <= h <= 14 -15 <= k <= 15 -19 <= l <= 20
Complete to 2θ (%)	99.3	97.9
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/ Restraints/Parameters	6187/ 0 /423	8670 / 0 / 476
Goof (F^2)	1.155	1.025
R indices [$I > 2\sigma(I)$]	0.0911	0.0570
R indices (all data)	0.1300	0.0919

Some bond distances (Å) and angles (º) in the complexes 1-8:

Complex	**Bond distances (Å) and angles (º)**
1	Zn1-O2, 1.97; Zn1-O5, 1.95; Na1-O1, 2.42;Na1-O1′, 2.45; Na1-O7, 2.37; Na1-O5, 2.38; <O2-Zn1-O5, 109.1; <O2-Zn1-O5′, 113.5; <O2-Zn1-O2′, 96.0; <O5-Zn1-O5′, 114.3; <O7-Na1-O1, 99.0; <O1- Na1-O1′, 81.4; <O7-Na1-O1′, 115.6.
2	Zn1-N1, 2.06; Zn1-N3, 2.02; Zn1-N5, 2.04; Zn1-O1, 2.20; Zn1-O6, 2.07; <N1-Zn1-N3, 106.7; <N1-Zn1-N5, 128.2; <N1-Zn1-O1, 82.0; <N1-Zn1-O6, 91.1; <N3-Zn1-N5, 124.8, <N3-Zn1-O1, 89.8; <N3-Zn1-O6, 99.8; <N5-Zn1-O1, 91.9; <N5-Zn1-O6, 86.1.
3	Zn1-N1, 2.16; Zn1-O1, 2.16; Zn1-O7, 2.04; Zn1-O13, 2.11; Zn1-O14, 2.12; Zn1-O15, 2.09; Zn2-N3, 2.06; Zn2-O5, 2.03; Zn2-O8, 2.14; Zn2-O11, 2.13; Zn2-O16, 1.99; Zn3-N5, 2.08; Zn3-O22, 2.02; Zn3-O24, 2.12; Zn3-O27, 2.11; Zn3-O32, 2.03; Zn4-N7, 2.14; Zn4-O17, 2.14; Zn4-O23,

	2.08; Zn4-O29, 2.08; Zn4-O30, 2.14; Zn4-O31, 2.16; <N1-Zn1-O1, 88.6; <N1-Zn1-O7, 86.2; <N1-Zn1-O13, 90.1; <N1-Zn1-O14, 90.6; <N1-Zn1-O15, 179.1; <O1-Zn1-O7, 88.3; <O1-Zn1-O13, 87.6; <O1-Zn1-O14, 176.4; <O1-Zn1-O15, 91.7; <N3-Zn2-O5, 103.7; <N3-Zn2-O8, 92.1; <N3-Zn2-O11, 89.2; <N3-Zn2-O16, 160.5; <O5-Zn2-O8, 87.9; <O5-Zn2-O11, 91.1; <O5-Zn2-O16, 95.7; <N5-Zn3-O22, 104.0; <N5-Zn3-O24, 92.2; <N5-Zn3-O27, 89.4; <N5-Zn3-O32, 160.6; <O22-Zn3-O24, 86.6; <O22-Zn3-O27, 89.8; <O22-Zn3-O32, 95.3; <N7-Zn4-O17, 90.1; <N7-Zn4-O23, 90.4; <N7-Zn4-O29, 175.8; <N7-Zn4-O30, 87.1; <N7-Zn4-O31, 88.0; <O17-Zn4-O23, 90.7; <O17-Zn4-O29, 91.9; <O17-Zn4-O30, 87.8; <O17-Zn4-O31, 175.0.
4	Zn1-N1, 2.05; Zn1-O1, 1.98; Zn1-O6, 1.94; Zn1-O7, 2.02; Zn1-O8, 2.41;Na1-O5, 2.42;Na1-O5′, 2.43; Na1-O9, 2.31; <N1-Zn1-O1, 105.2; <N1-Zn1-O6, 99.5; <N1-Zn1-O7, 97.7; <N1-Zn1-O8, 151.2; <O1-Zn1-O6, 108.5; <O1-Zn1-O7, 135.0; <O1-Zn1-O8, 89.3; <O6-Zn1-O7, 105.1; <O6-Zn1-O8, 99.3; <O7-Zn1-O8, 56.2; <O9-Na1-O5, 103.4; <O9-Na1-O5', 104.2; <O5-Na1-O5', 81.1.
5	Zn1-N1, 2.15; Zn1-N2, 2.15; Zn1-O1, 2.07; Zn1-O6, 2.07; Zn1-O7, 2.09;Zn1-O8, 2.18;<N1-Zn1-N2,87.6;<N1-Zn1-O1, 90.0; <N1-Zn1-O6, 92.7; <N1-Zn1-O8, 90.1; <N1-Zn1-O7, 177.4; <N2-Zn1-O1, 92.8; <N2-Zn1-O6, 88.3; <N2-Zn1-O7, 94.9; <N2-Zn1-O8, 175.3; <O1-Zn1-O8, 91.6; <O1-Zn1-O7, 88.8; <O1-Zn1-O6, 177.1; <O7-Zn1-O8, 86.6; <O7-Zn1-O6, 88.3.
6	Co1-N1, 2.14; Co1-N2, 2.15; Co1-O1, 2.08; Co1-O6, 2.07; Co1-O7, 2.08; Co1-O8, 2.17; <N1-Co1-N2, 87.6; <N1-Co1-O1, 90.0; <N1-Co1-O6, 92.7; <N1-Co1-O8, 90.9; <N1-Co1-O7, 177.3; <N2-Co1-O1, 92.9; <N2-Co1-O6, 88.2; <N2-Co1-O7, 94.9; <N2-Co1-O8, 175.7; <O1-Co1-O8, 91.1; <O1-Co1-O7, 88.8; <O1-Co1-O6, 177.0; <O7-Co1-O8, 86.8; <O7-Co1-O6, 88.4.
7	Zn1-N1, 2.14; Zn1-N2, 2.12; Zn1-N3, 2.14; Zn1-N4, 2.10; Zn1-O1, 2.30; Zn1-O2, 2.13; <N1-Zn1-N2, 78.4; <N1-Zn1-N3, 90.9; <N1-Zn1-N4, 102.0; <N1-Zn1-O1, 91.7; <N1-Zn1-O2, 150.8; <N2-Zn1-N4,101.0; <N2-Zn1-O2,95.4; <N2-Zn1-O1,89.7; <N2-Zn1-N3,169.1; <N3-Zn1-N4, 78.80; <N3-Zn1-O1,92.9; <N3-Zn1-O2, 95.0; <N4-Zn1-O1, 164.0; <N4-Zn1-O2, 107.2; <O1-Zn1-O2, 59.5.
8	Zn1-N1, 2.13; Zn1-N2, 2.11; Zn1-N3, 2.11; Zn1-N4, 2.12; Zn1-O1, 2.21; Zn1-O2, 2.27; <N1-Zn1-N2, 77.8; <N1-Zn1-N3, 98.9; <N1-Zn1-N4, 173.8; <N1-Zn1-O1, 91.4; <N1-Zn1-O2, 93.5; <N2-Zn1-N4, 99.2; <N2-Zn1-O2, 94.4; <N2-Zn1-O1, 150.3; <N2-Zn1-N3, 113.7; <N3-Zn1-N4, 77.1; <N3-Zn1-O1, 95.1; <N3-Zn1-O2, 151.0; <N4-Zn1-O1, 93.7; <N4-Zn1-O2, 92.1; <O1-Zn1-O2, 58.4.

Fluorescence emission of the ligand and complexes (10^{-3} M in dimethylsulphoxide):



For LH_2, Excitation wavelength = 290 nm, Emission wavelength = 330 and 343 nm.

For complexes, Excitation wavelength = 290 nm, Emission wavelength= 327 and 342 nm.