Supporting Information (SI)

Cadmium (II) supramolecular complexes constructed from phenylbenzoxazole-based ligand: self-assembly, structural features and nonlinear optical properties

Na Zhang[a], Dan Liu[a], Huihui Zhang[a], Jianhua Yu[a], Zhichao Wu[a], Qiyong Zhu[b,] *, Hongping Zhou[a,] *

[a]*College of Chemistry and Chemical Engineering, Anhui University and Key Labotatory of Functional Inorganic Materials Chemistry of Anhui Province, 230601, Hefei, P.R. China*
[b]*Department of Chemistry, Huainan Normal College, Huainan, 232001 P.R. China*

Corresponding author. Fax: +86-551-63861279; Tel: +86-551-63861279
E-mail: zhpzhp@263.net

Table S1: Selected bond lengths (Å) and angles (°) for complexes **1**-**4**

Table S2: Third-order NLO data for complexes **1** and **3**

Table S1: Selected bond lengths (Å) and angles (°) for complexes **1**-**4**

$C_{19}H_{15}Cd_2Cl_2N_3O$(1)					
Cd(1)-N(3)	2.296(2)	N(3)-Cd(1)-Cl(1)$^{\#1}$	159.40(6)	Cl(2)-Cd(1)-Cl(2)$^{\#2}$	85.90(3)
Cd(1)-Cl(1)$^{\#1}$	2.5260(9)	N(3)-Cd(1)-N(2)	71.12(8)	N(3)-Cd(1)-Cl(1)	90.42(6)
Cd(1)-N(2)	2.566(2)	Cl(1)$^{\#1}$-Cd(1)-N(2)	88.44(6)	Cl(1)$^{\#1}$-Cd(1)-Cl(1)	82.26(3)
Cd(1)-Cl(2)	2.5866(9)	N(3)-Cd(1)-Cl(2)	99.47(6)	N(2)-Cd(1)-Cl(1)	77.10(5)
Cd(1)-Cl(2)$^{\#2}$	2.6519(8)	Cl(1)$^{\#1}$-Cd(1)-Cl(2)	100.10(3)	Cl(2)-Cd(1)-Cl(1)	92.83(3)
Cd(1)-Cl(1)	2.7622(9)	N(2)-Cd(1)-Cl(2)	165.89(5)	Cl(2)$^{\#2}$-Cd(1)-Cl(1)	177.47(2)
Cd(1)$^{\#1}$- Cl(1)	2.5260(9)	N(3)-Cd(1)-Cl(2)$^{\#2}$	91.95(6)	Cd(1)$^{\#1}$-Cl(1)-Cd(1)	97.74(3)
Cd(1)$^{\#2}$ -Cl(2)	2.6519(8)	Cl(1)$^{\#1}$-Cd(1)-Cl(2)$^{\#2}$	95.81(3)	Cd(1)-Cl(2)-Cd(1)$^{\#2}$	94.10(3)
		N(2)-Cd(1)-Cl(2)$^{\#2}$	104.53(5)		
$C_{19}H_{15}Cd_2Br_2N_3O$ (2)					
Cd(1) -Br(1)	2.7080(5)	Cd(1)-Br(1)-Cd(1)$^{\#1}$	92.422(14)	Br(2)-Cd(1)-Br(1)$^{\#1}$	98.389(15)
Cd(1)$^{\#1}$-Br(1)	2.8255(5)	N(3)-Cd(1)-N(2)	71.22(9)	Br(1)-Cd(1)-Br(1)$^{\#1}$	87.578(14)
Cd(1)-N(3)	2.292(2)	N(3)-Cd(1)-Br(2)	160.03(6)	N(3)-Cd(1)-Br(2)$^{\#2}$	87.68(6)
Cd(1)-N(2)	2.567(3)	N(2)-Cd(1)-Br(2)	88.90(6)	N(2)-Cd(1)-Br(2)$^{\#2}$	79.44(6)
Cd(1)-Br(2)	2.6636(5)	N(3)-Cd(1)-Br(1)	100.08(6)	Br(2)-Cd(1)-Br(2)$^{\#2}$	86.796(15)
Cd(1)-Br(1)$^{\#1}$	2.8255(5)	N(2)-Cd(1)-Br(1)	168.85(6)	Br(1)-Cd(1)-Br(2)#2	93.509(14)
Cd(1)-Br(2)$^{\#2}$	2.9010(5)	Br(2)-Cd(1)-Br(1)	99.400(13)	Br(1)$^{\#1}$-Cd(1)-Br(2)$^{\#2}$	174.464(11)
Cd(1)$^{\#2}$-Br(2)	2.9010(5)	N(3)-Cd(1)-Br(1)$^{\#1}$	86.78(6)	Cd(1)-Br(2)-Cd(1)$^{\#2}$	93.203(15)
		N(3)-Cd(1)-Br(1)$^{\#1}$	98.64(6)		

$C_{40}H_{38}Cd_2I_4N_6$ (3)					
I(1)-Cd(1)	2.7911(12)	Cd(1)-I(1)-Cd(1)$^{\#1}$	90.73(2)	I(2)-Cd(1)-I(1)	124.42(2)
I(1)-Cd(1)$^{\#1}$	3.0804(10)	N(3)-Cd(1)-N(2)	70.20(10)	N(3)-Cd(1)-I(1)$^{\#1}$	90.59(8)
Cd(1)-N(3)	2.316(3)	N(3)-Cd(1)-I(2)	123.15(8)	N(2)-Cd(1)-I(1)$^{\#1}$	159.86(7)
Cd(1)-N(2)	2.532(3)	N(2)-Cd(1)-I(2)	96.91(8)	I(2)-Cd(1)-I(1)$^{\#1}$	98.80(4)
Cd(1)-I(2)	2.7139(12)	N(3)-Cd(1)-I(1)	111.54(9)	I(1)-Cd(1)-I(1)$^{\#1}$	89.27(2)
Cd(1)-I(1)$^{\#1}$	3.0804(10)	N(2)-Cd(1)-I(1)	92.20(7)		
$C_{21}H_{15}CdN_5OS_2$ (4)					
Cd(1)-N(4)	2.300(2)	S(1)-Cd(1)$^{\#2}$	2.6434(8)	N(5)-Cd(1)-S(1)$^{\#1}$	96.34(6)
Cd(1)-N(3)	2.323(2)	N(4)-Cd(1)-N(3)	93.88(9)	N(2)-Cd(1)-S(1)$^{\#1}$	169.64(5)
Cd(1)-N(5)	2.357(3)	N(4)-Cd(1)-N(5)	171.47(8)	N(4)-Cd(1)-S(2)$^{\#2}$	91.20(8)
Cd(1)-N(2)	2.537(2)	N(3)-Cd(1)-N(5)	90.14(9)	N(3)-Cd(1)-S(2)$^{\#2}$	158.56(5)
Cd(1)-S(1)$^{\#1}$	2.6434(8)	N(4)-Cd(1)-N(2)	94.15(7)	N(5)-Cd(1)-S(2)$^{\#4}$	82.40(8)
Cd(1)-S(2)$^{\#2}$	2.6899(13)	N(3)-Cd(1)-N(2)	70.04(7)	N(2)-Cd(1)-S(2)$^{\#2}$	88.83(5)
S(2)-C(21)	1.647(3)	N(5)-Cd(1)-N(2)	80.14(7)	S(1)#1-Cd(1)-S(2)$^{\#2}$	100.42(3)
S(2)-Cd(1)$^{\#1}$	2.6899(13)	N(4)-Cd(1)-S(1)$^{\#1}$	90.35(6)	C(21)-S(2)-Cd(1)$^{\#1}$	91.11(9)
S(1)-C(20)	1.646(3)	N(3)-Cd(1)-S(1)$^{\#1}$	100.37(5)	C(20)-S(1)-Cd(1)$^{\#2}$	95.61(8)
[a]Symmetry transformations used to generate equivalent atoms: For1: #1 -x, -y+1, -z, #2: -x+1, -y+1, -z; #1 For2:-x+1,-y+2,-z, #2 -x,-y+2,-z;For3: #1 -x+1,-y+2,-z+1, For4 #1: x, -y+1/2, z+1/2, #2: x, -y+1/2, z-1/2					

Table S2: Third-order NLO data for complexes **1** and **3**

compound	Complex **1**	Complex **3**
β (cm GW^{-1})	0.16	0.13
σ (GW)	6415.55	5593.66
γ (m^2 W^{-1})	2.36×10^{-16}	3.03×10^{-16}
$\chi^{(3)}$ (esu)	5.93×10^{-14}	5.72×10^{-14}