Supporting information file for:

Chelate ring stacking interactions in the supramolecular assemblies of Zn(II) and Cd(II) coordination compounds: a combined experimental and theoretical study

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Table S1 Crystal data and structure refinement parameters for complexes **1-7**.

Crystal data	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Empirical formula	$C_{12}H_{10}Br_2ZnN_4O$	$C_{12}H_{10}Cl_2ZnN_4O$	$C_{24}H_{22}CdN_{10}O_9$	$C_{18}H_{14}Br_2CdN_4O$	$C_{18}H_{14}Cl_2ZnN_4O$	$C_{18}H_{14}Br_2ZnN_4O$	$C_{72}H_{52}I_6Zn_5N_{16}O_8$
Formula weight	451.43	362.51	706.91	574.55	438.60	527.52	2357.65
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic	Triclinic	Triclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	P-1	P-1	P-1	P-1	C2/c
a (Å)	7.6877 (14) Å	7.4184 (4)	9.2443 (18)	9.3470 (14)	9.0285 (6)	9.1458 (6)	29.7670 (12)
b (Å)	10.3625 (19)	10.1888 (6)	10.2822 (13)	11.4750 (12)	11.7143 (8)	11.7060 (9)	10.3466 (4)
c (Å)	18.182 (3)	18.1480 (13)	14.4976 (16)	18.590 (2)	17.5898 (11)	18.2478 (12)	25.8735 (10)
α (°)	90.00	90.00	82.264 (10)	78.554 (5)	82.781 (8)	80.629 (9)	90.00
β (°)	91.183 (2)	91.187 (4)	86.277 (13)	76.342 (6)	78.436 (5)	77.512 (8)	98.543 (2)
γ (°)	90.00	90.00	88.430 (13)	87.434 (4)	88.107 (8)	88.044 (9)	90.00
V (Å^3)	1448.1 (5)	1371.42 (15)	1362.4 (4)	1899.0 (4)	1808.1 (2)	1881.9 (2)	7880.3 (5)
Z / D_c (g cm^{-3})	4 / 2.071	4 / 1.756	2 / 1.723	4 / 2.010	4 / 1.611	4 / 1.862	4 / 1.987
Measured refls.	7344	2408	25804	28816	21321	18385	43440
Independent refls.	2540	2408	7336	9056	8108	8410	8113
S / R_{int}	1.08 / 0.031	1.05 / 0.001	1.02 / 0.101	1.04 / 0.040	0.95 / 0.033	0.83 / 0.047	1.02 / 0.073
R1/wR2	0.038/0.093	0.038/0.093	0.052/0.077	0.028/0.060	0.029/0.076	0.028/0.061	0.054/0.124
$\Delta\rho_{max}/\Delta\rho_{min}$ (eÅ^{-3})	1.00/-0.60	0.65/-0.38	0.54/-0.75	0.63/-0.65	0.47/-0.36	0.55/-0.40	2.06/-2.64

Table S2 Selected bond distances and angles for complexes **1**-**7** (Å, º)

Complex **1**					
Zn1-O1	2.319(4)	Zn1-N1	2.144(4)	Zn1-N2	2.117(4)
Zn1-Br1	2.3716(8)	Zn1-Br2	2.3605(9)		
N2-Zn1-N1	75.04(16)	N1-Zn1-O1	145.73(14)	N2-Zn1-Br2	125.17(11)
N1-Zn1-Br2	102.32(11)	O1-Zn1-Br2	95.20(10)	N2-Zn1-Br1	116.84(11)
Complex **2**					
Zn1-O1	2.308(3)	Zn1-N1	2.153(3)	Zn1-N2	2.122(3)
Zn1-Cl1	2.2530(11)	Zn1-Cl2	2.2334(12)		
N2-Zn1-N1	74.63(12)	N2-Zn1-Cl2	124.45(10)	N1-Zn1-Cl2	102.17(10)
N1-Zn1-O1	145.74(11)	Cl2-Zn1-O1	94.71(8)	Cl1-Zn1-O1	94.94(8)
Complex **3**					
Cd1-O6	2.306(3)	Cd1-N7	2.358(3)	Cd1-N3	2.377(3)
Cd1-O1	2.398(2)	Cd1-N8	2.412(3)	Cd1-O7	2.454(3)
Cd1-O2	2.547(2)	Cd1-O8	2.570(3)		
O6-Cd1-N7	93.89(10)	O6-Cd1-N3	89.89(10)	N7-Cd1-N3	142.98(9)
O6-Cd1-O1	80.86(9)	N7-Cd1-O1	149.23(9)	N3-Cd1-O1	67.68(9)
O6-Cd1-N8	85.66(10)	N7-Cd1-N8	68.16(9)	N3-Cd1-N8	148.85(9)
Complex **4**					
Br1-Cd1	2.5547(4)	Br2-Cd1	2.5035(5)	Br3-Cd2	2.5526(4)
Br4-Cd2	2.5288(4)	Cd1-N2	2.343(2)	Cd1-N1	2.344(2)
Cd1-O1	2.4614(19)	Cd2-N5	2.334(2)	Cd2-N6	2.371(2)
Cd2-O2	2.437(2)				
N2-Cd1-N1	68.57(8)	N2-Cd1-O1	66.69(7)	N1-Cd1-O1	134.03(8)
N5-Cd2-N6	67.58(8)	N5-Cd2-O2	133.14(7)	N6-Cd2-O2	67.21(7)
Complex **5**					
O1-Zn1	2.4010(16)	O2-Zn2	2.3262(14)	Cl1-Zn1	2.2252(6)
Cl2-Zn1	2.1926(5)	Cl3-Zn2	2.2410(7)	Cl4-Zn2	2.2066(5)
N1-Zn1	2.1405(17)	N2-Zn1	2.1237(15)	N5-Zn2	2.1310(16)
N6-Zn2	2.1395(15)				
N2-Zn1-N1	75.08(6)	N2-Zn1-Cl2	136.20(5)	N1-Zn1-Cl2	104.72(5)
N5-Zn2-N6	73.87(6)	N5-Zn2-Cl4	102.13(4)	N6-Zn2-Cl4	139.62(5)
Complex **6**					
Zn1-N2	2.121(2)	Zn1-N1	2.144(2)	Zn1-Br2	2.3374(5)
Zn1-Br1	2.3752(6)	Zn1-O1	2.412(2)	Zn2-N5	2.135(2)

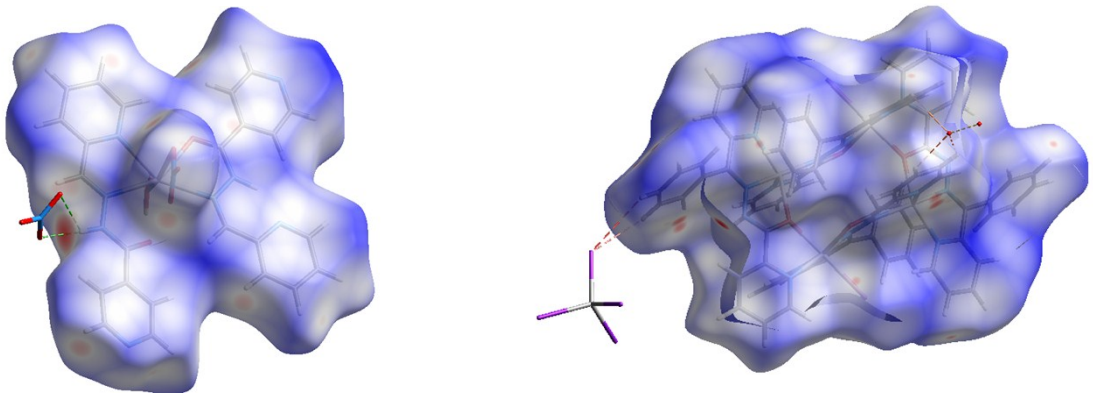
Zn2-N6	2.153(2)	Zn2-O2	2.3249(19)	Zn2-Br4	2.3566(5)
Zn2-Br3	2.3803(5)				
N2-Zn1-N1	74.92(8)	N2-Zn1-Br2	138.59(7)	N1-Zn1-Br2	104.53(7)
N5-Zn2-N6	73.57(8)	N5-Zn2-O2	142.01(8)	N6-Zn2-O2	70.98(8)
Complex **7**					
I1-Zn1	2.7928(9)	I2-Zn3	2.6288(11)	I3-Zn3	2.6087(10)
Zn1N4	2.116(6)	Zn1-O2	2.121(5)	Zn1-N6	2.147(5)
Zn1-N5	2.174(6)	Zn1-O1	2.182(4)	Zn2-N7^{i}	2.044(5)
Zn2-N2	2.047(6)	Zn2-N8^{i}	2.052(6)	Zn2-N1	2.146(6)
Zn2-O1	2.235(4)				
N4-Zn1-O2	119.1(2)	N4-Zn1-N6	166.8(2)	O2-Zn1-N6	73.84(19)
N2-Zn2-N1	76.0(2)	N1-Zn2-O1	149.3(2)	I3-Zn3-I2	109.29(2)

Symmetry codes: (i) −x−1/2, −y+7/2, −z for **7**.

Table S3. Summary of the various contact contributions (in %) in Hirshfeld surface area for all analyzed structures.

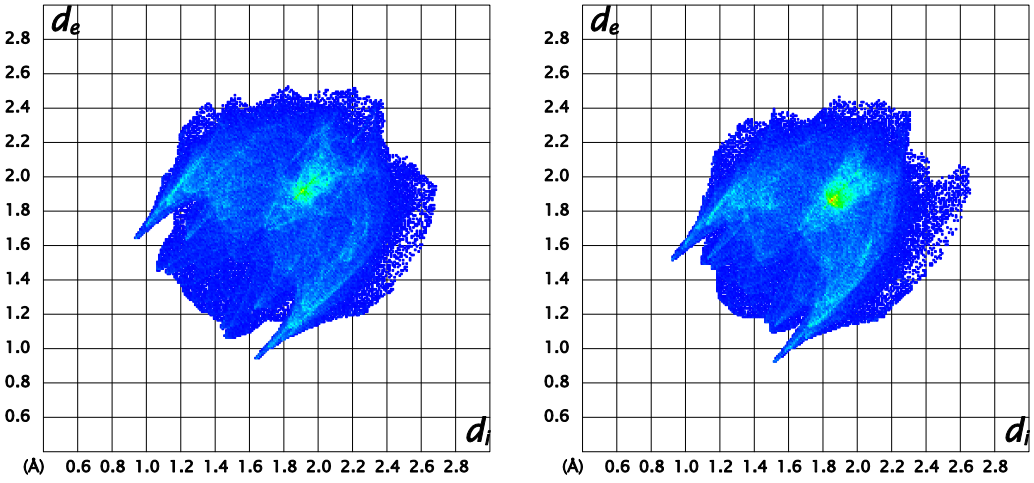
Contact type /Structure	**1**	**2**	**3**	**4**		**5**		**6**		**7**
				Mol. A	Mol. B	Mol. A	Mol. B	Mol. A	Mol. B	
H···H	22.5	23.5	24.1	28.3	31.9	31.0	33.0	30.1	33.0	41.1
O···H/H···O	6.7	6.5	31.7	5.2	5.2	5.1	5.3	5.2	5.2	10.3
C···H/H···C	7.7	7.2	13.8	20.4	16.5	20.1	17.1	20.2	16.4	19.1
C···C	9.4	10.4	11.0	3.1	4.9	3.9	6.2	3.4	5.7	4.6
N···C/C···N	4.1	4.2	1.8	2.9	3.1	2.8	2.7	2.7	2.9	1.1
N···H/H···N	8.4	8.5	15.8	4.3	3.8	5.4	4.9	4.7	4.3	3.8
O···N/N···O	0.3	0.4	1.2	1.0	0.5	1.1	0.6	1.1	0.5	0.0
N···N	2.1	2.2	0.6	0.6	1.0	0.4	0.8	0.5	0.8	0.0
R···H/H···R	35.9	35.2	-	29.2	28.2	27.6	27.2	28.7	28.0	17.9
R···C/C···R	1.3	0.5	-	1.6	2.4	0.5	0.2	1.1	1.6	0.7

R = Cl, Br, I



(3) **(7)**

Fig. S1. Views of the Hirshfeld surfaces for **3** and **7** mapped with d_{norm}.



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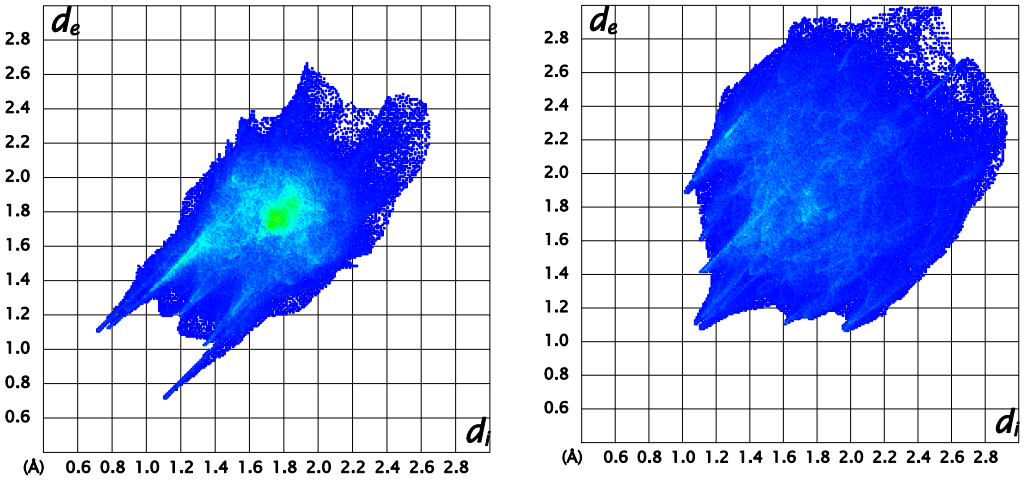
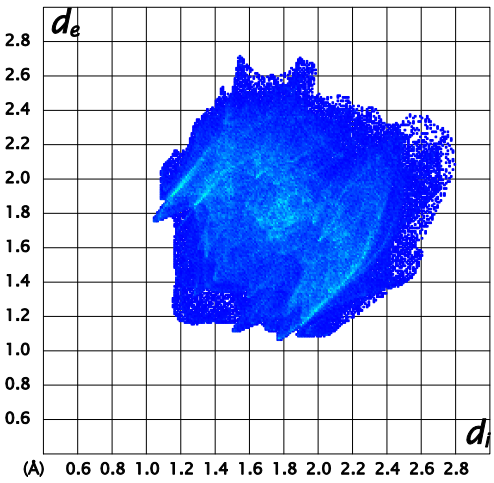


(3) **(7)**



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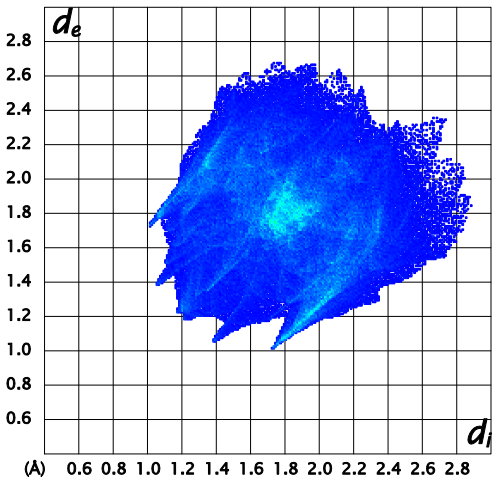
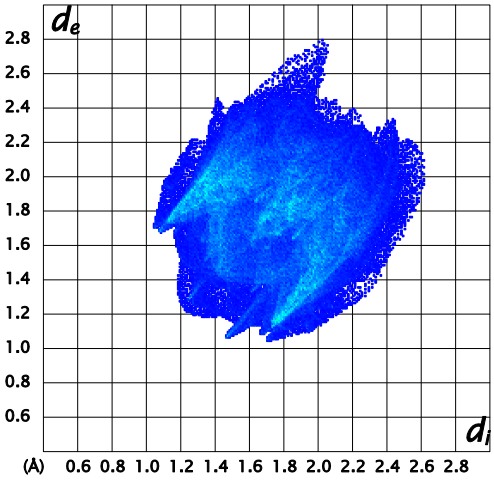
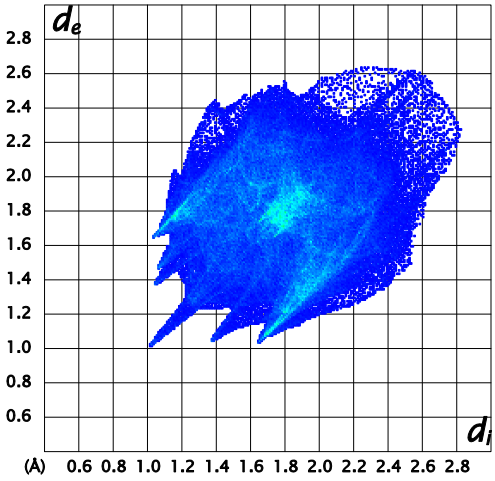


(4B)



(5A)



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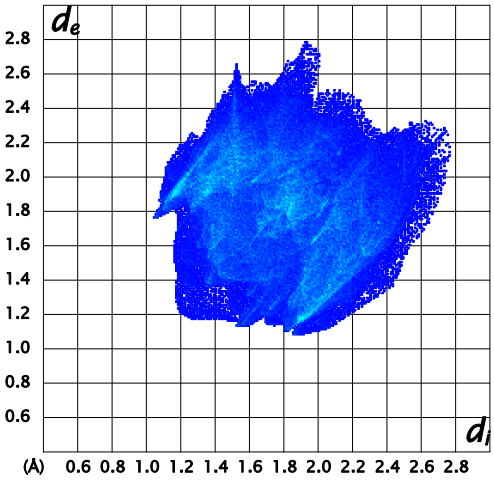

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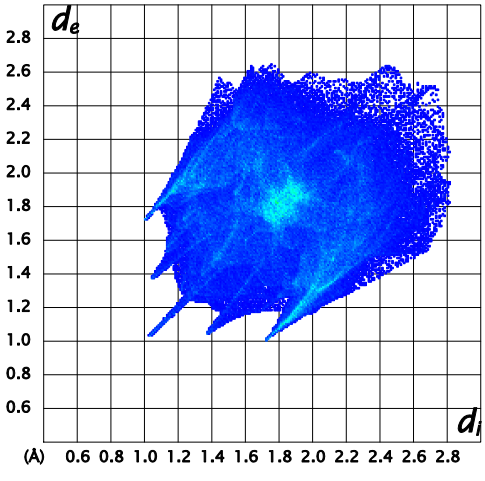

(6B)

Fig S2. Fingerprints of the compounds **1-7**.