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Supplementary Information

Time Controlled Structural/Packing Transformation and Tunable Luminescence of Cd(II)-Chloride-triBZ-ntb Coordination Assemblies: An Experimental and Theoretical Exploration

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Table S1 Selected bond lengths and angles for the complexes.

Complex Cd5

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N3	Cd2	2.232(7)	N19	Cd1	2.248(6)
N6	Cd2	2.234(7)	N20	Cd1	2.653(7)
N13	Cd1	2.230(6)	N16	Cd1	2.247(7)
Cl4	Cd1	2.413(2)			

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N3	Cd2	N6	97.2(3)	N19	Cd1	N20	69.7(2)
N3	Cd2	N10	72.0(2)	N19	Cd1	Cl4	110.18(18)
N3	Cd2	N9	101.4(2)	N16	Cd1	N19	105.7(2)
N3	Cd2	Cl8	113.2(2)	N16	Cd1	N20	69.6(2)
N6	Cd2	N10	71.8(2)	N16	Cd1	Cl4	107.0(2)
N6	Cd2	N9	129.5(3)	N13	Cd1	N19	98.2(2)

N6	Cd2	Cl8	109.34(19)	N13	Cd1	N20	70.2(2)
N9	Cd2	N10	70.2(2)	N13	Cd1	N16	121.3(2)
N9	Cd2	Cl8	105.57(18)	N13	Cd1	Cl4	113.39(19)
Cl8	Cd2	N10	174.19(17)	Cl4	Cd1	N20	176.29(16)
Cl5	Cd3	Cl9	99.75(9)	Cl7	Cd3	Cl5	115.46(9)
Cl6	Cd3	Cl5	110.75(8)	Cl7	Cd3	Cl6	109.25(8)
Cl6	Cd3	Cl9	107.62(9)	Cl7	Cd3	Cl9	113.52(10

Complex Cd10

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
N3	Cd1	2.298(2)	N9	Cd1	2.262(2)
N6	Cd1	2.564(2)	N10	Cd1	2.604(2)

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N3	Cd1	N6	98.29(7)	N9	Cd1	N6	74.89(8)
N3	Cd1	N10	68.56(7)	N9	Cd1	N10	72.26(8)
N3	Cd1	Cl1	106.25(6)	N9	Cd1	Cl1	114.14(7)
N3	Cd1	Cl2	85.67(6)	N9	Cd1	Cl2	89.26(6)
N6	Cd1	N10	65.70(6)	N10	Cd1	Cl2	98.16(4)
N6	Cd1	Cl2	159.98(6)	Cl1	Cd1	N6	93.44(5)
N9	Cd1	N3	139.27(9)	Cl1	Cd1	N10	156.54(5)

Complex Cd20

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
N13	Cd2	2.243(6)	N6	Cd1	2.244(7)
N16	Cd2	2.256(7)	N9	Cd1	2.226(6)
N19	Cd2	2.238(7)	N10	Cd1	2.598(6)
N20	Cd2	2.616(6)	Cl1	Cd1	2.411(3)
Cl2	Cd2	2.399(2)	Cl3	Cd3	2.455(2)
C1	C2	1.462(16)	Cl4	Cd3	2.415(3)

C1	N1	1.127(15)	Cl5	Cd3	2.469(2)
N3	Cd1	2.257(6)	Cl6	Cd3	2.468(2)

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C80	N20	C96	110.7(6)	N3	Cd1	N10	69.9(2)
C80	N20	Cd2	108.1(4)	N3	Cd1	Cl1	110.97(19)
C96	N20	Cd2	103.9(5)	N6	Cd1	N3	109.3(2)
N13	Cd2	N16	112.9(2)	N6	Cd1	N10	69.9(2)
N13	Cd2	N20	69.3(2)	N6	Cd1	Cl1	110.0(2)
N13	Cd2	Cl2	106.00(17)	N9	Cd1	N3	108.3(2)
N16	Cd2	N20	69.6(2)	N9	Cd1	N6	109.2(2)
N16	Cd2	Cl2	109.43(19)	N9	Cd1	N10	70.1(2)
N19	Cd2	N13	112.5(2)	N9	Cd1	Cl1	109.03(18)
N19	Cd2	N16	100.5(2)	Cl1	Cd1	N10	179.00(15)
N19	Cd2	N20	70.5(2)	Cl3	Cd3	Cl5	106.04(8)
N19	Cd2	Cl2	115.66(19)	Cl3	Cd3	Cl6	108.10(8)
Cl2	Cd2	N20	173.67(16)	Cl4	Cd3	Cl3	115.24(9)
N1	C1	C2	171(3)	Cl4	Cd3	Cl5	106.94(9)
C3	C2	C1	117.3(16)	Cl4	Cd3	Cl6	110.43(11)
C7	C2	C1	121.1(17)	Cl6	Cd3	Cl5	109.93(10)

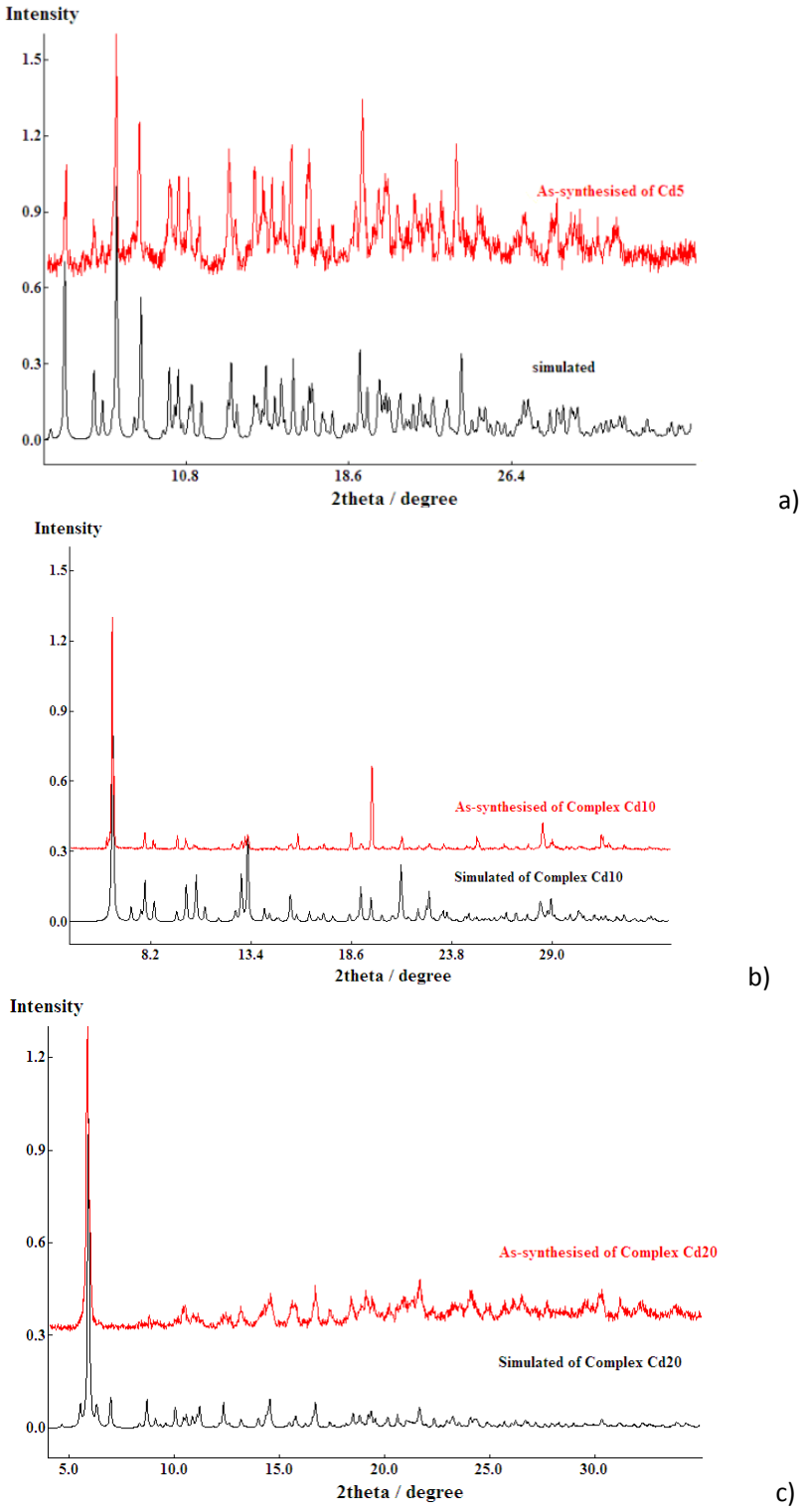


Fig. S1 PXRD patterns for complexes **Cd5** (a), **Cd10** (b) and **Cd20** (c).

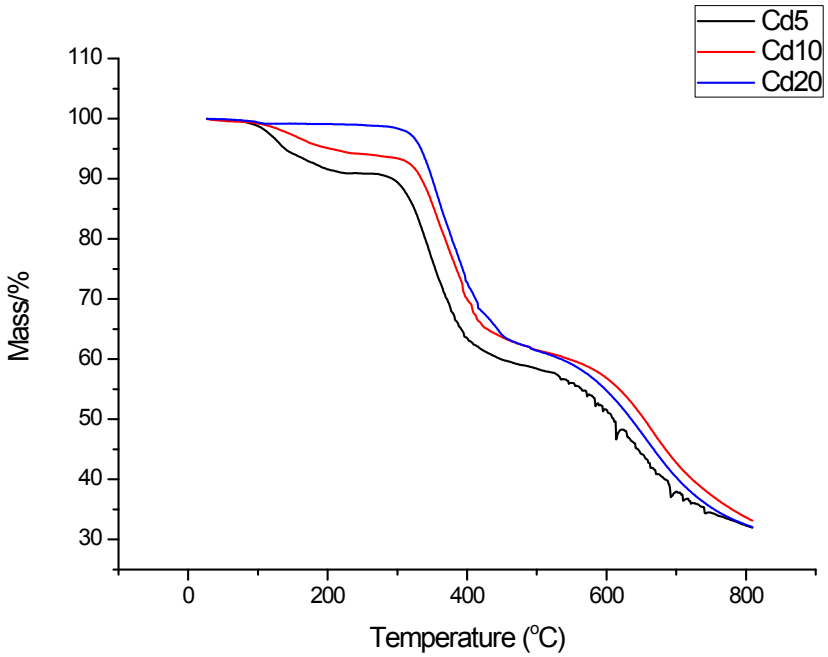
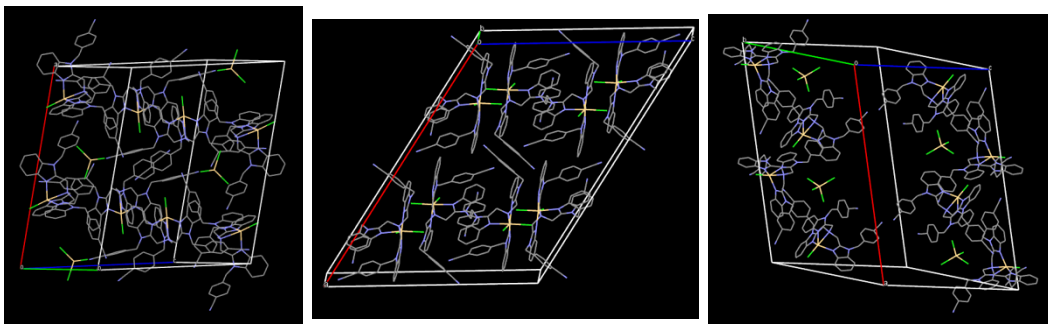


Fig. S2 TGA curves for complexes **Cd5**, **Cd10** and **Cd20**.



a) b)

c)

Fig. S3 The unit cell structures selected for complexes **Cd5, Cd10,** and **Cd20** (a-c) in MS theoretical study.