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Supporting Information for the article

REGULATION OF π··· π STACKING INTERACTIONS BETWEEN TRIIMIDAZOLE LUMINOPHORES AND COMPREHENSIVE EMISSION QUENCHING BY COORDINATION TO Cu(II)

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Table S1. Selected bond lengths (Å) in coordination metal environment in **1-8.**

1			
Cu(1)-N(1)	2.213(6)	Cu(1)-O(3)	1.972(5)
Cu(1)-O(1)	1.960(5)	Cu(1)-O(4)	1.951(6)
Cu(1)-O(2)	1.952(4)		
O(1)-Cu(1)-N(1)	89.6(2)	O(4)-Cu(1)-O(1)	89.6(2)
O(2)-Cu(1)-N(1)	96.26(19)	O(4)-Cu(1)-N(1)	95.1(2)
O(2)-Cu(1)-O(4)	168.6(2)	O(3)-Cu(1)-O(1)	89.5(2)
O(2)-Cu(1)-O(3)	89.4(2)	O(3)-Cu(1)-N(1)	102.0(2)
O(2)-Cu(1)-O(1)	89.6(2)	O(4)-Cu(1)-O(3)	89.2(2)
2			
Cu(1)-O(1)	1.973(4)	Cu(1)-O(4)	1.968(4)
Cu(1)-O(2)	1.960(4)	Cu(1)-N(1)	2.240(4)
Cu(1)-O(3)	1.973(4)		
O(1)-Cu(1)-O(3)	168.7(1)	O(4)-Cu(1)-O(3)	89.4(2)
O(1)-Cu(1)-N(1)	99.6(2)	O(4)-Cu(1)-N(1)	89.7(2)
O(2)-Cu(1)-O(4)	168.2(2)	O(2)-Cu(1)-N(1)	101.9(2)
O(2)-Cu(1)-O(1)	91.1(2)	O(3)-Cu(1)-N(1)	91.7(2)
O(2)-Cu(1)-O(3)	88.0(2)	O(4)-Cu(1)-O(1)	89.2(2)
3			
Cu(1)-O(1A)	2.02(2)	Cu(4)-O(6B)	1.93(2)
Cu(1)-O(3A)	1.97(2)	Cu(4)-O(2B)	1.95(2)
Cu(1)-O(5A)	1.94(2)	Cu(4)-O(8B)	1.96(3)
Cu(1)-O(7A)	1.92(3)	Cu(4)-O(4B)	2.04(2)
Cu(1)-N(1B)[f]	2.19(2)	Cu(4)-N(3B)	2.19(2)
Cu(2)-O(6A)	1.94(2)	Cu(5)-O(3C)	1.952(14)
Cu(2)-O(8A)	1.95(2)	Cu(5)-O(7C)	1.958(14)
Cu(2)-O(4A)	1.99(2)	Cu(5)-O(5C)	1.958(14)
Cu(2)-O(2A)	2.05(2)	Cu(5)-O(1C)	1.97(2)

Cu(2)-N(1A)	2.13(3)	Cu(5)-O(1*w*)	2.11(2)
Cu(1)-Cu(2)	2.636(3)	Cu(6)-O(8C)	1.950(14)
Cu(3)-O(1B)	2.00(2)	Cu(6)-O(2C)	1.965(14)
Cu(3)-O(3B)	1.98(3)	Cu(6)-O(4C)	1.987(13)
Cu(3)-O(5B)	1.99(2)	Cu(6)-O(6C)	1.986(14)
Cu(3)-O(7B)	1.90(2)	Cu(6)-N(1C)	2.21(2)
Cu(3)-N(3A)	2.22(3)		
O(7A)-Cu(1)-O(5A)	89.0(12)	O(6B)-Cu(4)-O(2B)	170.1(10)
O(7A)-Cu(1)-O(3A)	166.3(10)	O(6B)-Cu(4)-O(8B)	91.7(11)
O(5A)-Cu(1)-O(3A)	89.0(11)	O(2B)-Cu(4)-O(8B)	88.8(11)
O(7A)-Cu(1)-O(1A)	89.5(11)	O(6B)-Cu(4)-O(4B)	89.1(11)
O(5A)-Cu(1)-O(1A)	174.3(10)	O(2B)-Cu(4)-O(4B)	87.8(10)
O(3A)-Cu(1)-O(1A)	91.2(10)	O(8B)-Cu(4)-O(4B)	164.3(10)
O(7A)-Cu(1)-N(1B)^{f}	96.9(11)	O(6B)-Cu(4)-N(3B)	96.5(10)
O(5A)-Cu(1)-N(1B)^{f}	89.6(9)	O(2B)-Cu(4)-N(3B)	93.2(10)
O(3A)-Cu(1)-N(1B)^{f}	96.6(9)	O(8B)-Cu(4)-N(3B)	99.5(10)
O(1A)-Cu(1)-N(1B)^{f}	96.0(9)	O(4B)-Cu(4)-N(3B)	96.0(10)
O(6A)-Cu(2)-O(8A)	91.0(11)	O(3C)-Cu(5)-O(7C)	168.6(14)
O(6A)-Cu(2)-O(4A)	84.4(11)	O(3C)-Cu(5)-O(5C)	93.5(13)
O(8A)-Cu(2)-O(4A)	169.1(10)	O(7C)-Cu(5)-O(5C)	87.4(13)
O(6A)-Cu(2)-O(2A)	162.7(10)	O(3C)-Cu(5)-O(1C)	92.3(14)
O(8A)-Cu(2)-O(2A)	87.2(10)	O(7C)-Cu(5)-O(1C)	85.2(15)
O(4A)-Cu(2)-O(2A)	94.3(10)	O(5C)-Cu(5)-O(1C)	169.9(14)
O(6A)-Cu(2)-N(1A)	100.1(10)	O(3C)-Cu(5)-O(1*w*)	93.6(10)
O(8A)-Cu(2)-N(1A)	92.9(10)	O(7C)-Cu(5)-O(1*w*)	97.4(11)
O(4A)-Cu(2)-N(1A)	97.7(11)	O(5C)-Cu(5)-O(1*w*)	101.5(10)
O(2A)-Cu(2)-N(1A)	97.2(10)	O(1C)-Cu(5)-O(1*w*)	86.3(10)
O(7B)-Cu(3)-O(3B)	171.1(10)	O(8C)-Cu(6)-O(2C)	87.7(13)
O(7B)-Cu(3)-O(5B)	91.7(11)	O(8C)-Cu(6)-O(4C)	168.8(13)
O(3B)-Cu(3)-O(5B)	91.3(11)	O(2C)-Cu(6)-O(4C)	87.8(12)
O(7B)-Cu(3)-O(1B)	85.4(11)	O(8C)-Cu(6)-O(6C)	89.2(12)
O(3B)-Cu(3)-O(1B)	89.8(11)	O(2C)-Cu(6)-O(6C)	167.6(13)
O(5B)-Cu(3)-O(1B)	166.5(10)	O(4C)-Cu(6)-O(6C)	93.0(13)
O(7B)-Cu(3)-N(3A)	93.6(11)	O(8C)-Cu(6)-N(1C)	93.6(11)
O(3B)-Cu(3)-N(3A)	94.5(11)	O(2C)-Cu(6)-N(1C)	98.5(10)
O(5B)-Cu(3)-N(3A)	93.0(10)	O(4C)-Cu(6)-N(1C)	97.3(11)
O(1B)-Cu(3)-N(3A)	100.3(10)	O(6C)-Cu(6)-N(1C)	93.7(10)
4			
Cu(1)-N(1)	2.010(2)	Cu(1)-O(1)	1.929(2)
N(1)-Cu(1)-O(1)	90.28(9)	N(1)-Cu(1)-O(1)^{c}	89.72(9)
5			
Cu(1)-N(1)	2.000(4)	Cu(1)-N(7)	2.002(4)
Cu(1)-O(1)	2.40(3)		
N(1)-Cu(1)-N(7)	90.4(2)	N(7)^{b} -Cu(1)-O(1)	83.6(7)
N(7)-Cu(1)-O(1)	96.4(7)	N(1)-Cu(1)-O(1)	96.0(8)
N(1)-Cu(1)-O(1)^{b}	84.0(8)		
6			
Cu(1)-N(1)	2.060(3)	Cu(1)-N(7)	2.016(3)
Cu(1)-O(1)	2.425(2)		
N(1)-Cu(1)-N(7)	90.54(11)	N(1)-Cu(1)-O(1)^{a}	94.36(10)

N(7)-Cu(1)-O(1)	93.37(10)	N(1)-Cu(1)-O(1)	85.64(10)
N(7)[a]-Cu(1)-O(1)	86.63(10)		
7			
Cu(1)-N(1)	2.001(3)	Cu(1)-O(1*w*)	2.026(3)
Cu(1)-O(1)	2.330(3)		
N(1)-Cu(1)-O(1)	88.33(13)	N(1)-Cu(1)-O(1*w*)[d]	86.69(14)
N(1)-Cu(1)-O(1)[d]	91.67(13)	O(1*w*)-Cu(1)-O(1)[d]	87.87(12)
N(1)-Cu(1)-O(1*w*)	93.31(14)	O(1*w*)-Cu(1)-O(1)	92.13(12)
8			
Cu(1)-O(1)	1.957(5)	Cu(1)-N(1)	2.002(6)
Cu(1)-O(4)	1.979(5)	Cu(1)-N(7)	1.980(6)
O(1)-Cu(1)-O(4)	87.1(2)	O(1)-Cu(1)-N(1)	164.1(2)
O(1)-Cu(1)-N(7)	91.8(2)	O(4)-Cu(1)-N(1)	90.1(2)
O(4)-Cu(1)-N(7)	172.56(2)	N(7)-Cu(1)-N(1)	92.9(2)

Symmetry transformations used to generate equivalent atoms: [a] -*x*, 1-*y*, -*z*; [b] 1-*x*, -*y*, 1-*z*; [c] 2-*x*, 1-*y*, -*z*; [d] 1-*x*, -*y*, -*z*; [e] 1-*x*, 1-*y*, -*z*; [f] *x*+1, *y*+1, *z;*

Table S2. Geometric parameters of hydrogen bonds [distances (Å) and angles(°)] for **2-4**, **6-8**.

D-H···A	*d*(H···A), Å	*d*(D···A), Å	∠DHA, °	Symmetry operation for acceptor
2				
C(7)-H(7)···O(1)	2.37	3.234(7)	154.1	*x*, *y*, *z*
C(14)-H(14)···N(3)	2.24	3.021(8)	141.6	*x*, *y*, *z*
C(13)-H(13)···N2	2.57	3.490(9)	170.2	*x*-1, *y*-1, *z*
3				
O(1*w*)-H(1*w*1)···N(2C)	2.01(2)	2.84(2)	152(4)	*x*-1, *y*-1, *z*
O(2*w*)-H(1*w*2)···N(3C)	1.98	2.95(2)	162.6	*x*, *y*, *z*
O(2*w*)-H(2*w*2)···O(3A)	2.01	2.89(2)	146.8	*x*, *y*-1, *z*
O(3*w*)-H(1*w*3)···O(8A)	2.06	2.94(3)	147.6	*x*, *y*, *z*
O(3*w*)-H(2*w*3)···O(1C)	2.01	2.95(5)	159.3	*x*, *y*+1, *z*-1
C(13A)-H(13B)···O(7A)	2.64	3.31(4)	128.0	*x*-1, *y*, *z*
C(15A)-H(15A)···O(2C)	2.60	3.53(5)	165.2	*x*, *y*+1, *z*-1
C(17A)-H(17B)···O(4A)	2.53	3.40(5)	150.8	*x*+1, *y*, *z*
C(11C)-H(11H)···O(3*w*)	2.44	3.25(6)	142.0	*x*, *y*-1, *z*+1
C(1A)-H(1A)···O(7C)	2.59	3.43(4)	150.7	*x*, *y*+1, *z*-1
C(6A)-H(6A)···N(2B)	2.42	3.35(4)	172.9	*x*-1, *y*, *z*-1
C(9A)-H(9A)···O(1B)	2.50	3.11(4)	122.7	*x*, *y*, *z*
C(3B)-H(3B)···O(4C)	2.47	3.34(4)	156.2	*x*-1, *y*, *z*
C(6B)-H(6B)···N(2A)	2.47	3.39(4)	172.0	*x*+1, *y*, *z*+1
C(9B)-H(9B)···O(6B)	2.19	2.90(4)	132.4	*x*, *y*, *z*
C(4C)-H(4C)···O(3*w*)	2.54	3.30(4)	140.2	*x*+1, *y*, *z*+1
C(7C)-H(7C)···O(6B)	2.62	3.29(4)	129.4	*x*+1, *y*, *z*
C(9C)-H(9C)···O(6C)	2.43	2.97(3)	116.5	*x*, *y*, *z*
C(9C)-H(9C)···O(2*w*)	2.48	3.28(2)	144.9	*x*, *y*, *z*
4				
C(1)-H(1)···O(2)	2.42	3.259(4)	150.2	-*x*+1, -*y*+1, -*z*
C(3)-H(3)···O(2)	2.45	3.281(4)	148.1	-*x*+1, -*y*+1, -*z*
C(4)-H(4)···N(2)	2.66	3.424(4)	139.8	-*x*, -*y*, -*z*+1

C(7)-H(7)···O(1)	2.32	3.192(3)	156.3	-*x*+2, -*y*+1, -*z*+1
6				
C(3)-H(3)···N(8)	2.45	3.315(5)	155.3	-*x*+1, -*y*+1, -*z*+1
C(6)-H(6)···O(1)	2.45	3.375(5)	173.3	*x*, -*y*+3/2, *z*+1/2
C(10)-H(10)···O(2)	2.30	3.137(5)	149.2	*x*, *y*, *z*
C(15)-H(15)···N(9)	2.54	3.415(5)	157.5	*x*, *y*, *z*+1
C(16)-H(16)···O(2)	2.30	3.227(5)	172.2	*x*, *y*, *z*+1
C(3)-H(3)···N(8)	2.45	3.315(5)	155.3	-*x*+1, -*y*+1, -*z*+1
7				
O(2*w*)-H(2*w*2)···N(2)	2.11	2.906(5)	155.1	*x*+1/2, -*y*+1/2, *z*+1/2
O(2*w*)-H(1*w*2)···N(3)	2.01	2.837(5)	163.1	*x*, *y*, *z*
O(1*w*)-H(1*w*1)···O(2*w*)	1.80(2)	2.667(4)	175(3)	*x*, *y*, *z*-1
O(1*w*)-H(2*w*1)···N(8)	2.55	3.317(5)	146.2	*x*, *y*, *z*
O(1*w*)-H(2*w*1)···O(2)	1.83	2.703(5)	173.5	*x*, *y*, *z*
C(1)-H(1)···O(1)	2.58	3.120(6)	117.7	-*x*+1, -*y*, -*z*
C(2)-H(2)···O(1)	2.48	3.285(5)	145.2	*x*-1, *y*, *z*
C(4)-H(4)···N(4)	2.51	3.036(6)	115.8	*x*, *y*, *z*
C(5)-H(5)···O(1)	2.58	3.079(5)	114.2	*x*, *y*, *z*
C(7)-H(7)···O(3)	2.53	3.431(6)	164.0	*x*-1, *y*, *z*
C(9)-H(9)···O(3)	2.40	3.285(6)	158.2	*x*-3/2, -*y*+1/2, *z*+1/2
C(10)-H(10)···O(2)	2.53	3.324(6)	143.2	*x*-1, *y*, *z*+1
C(13)-H(13)···N(4)	2.66	3.462(5)	144.5	-*x*+1, -y, -z+1
8				
C(1)-H(1)···O(5)	2.23	3.142(8)	166.4	*x*-1, *y*, *z*
C(2)-H(2)···N(3)	2.35	3.243(9)	159.6	-*x*, -*y*+1, -*z*
C(4)-H(4)···O(5)	2.62	3.494(10)	157.6	-*x*+1, -*y*+1, -*z*
C(5)-H(5)···N(2)	2.42	3.327(8)	164.6	-*x*+2, -*y*+2, -*z*
C(7)-H(7)···O(6)	2.20	3.119(9)	172.1	*x*+1, *y*+1, *z*
C(11)-H(11)···O(6)	2.58	3.445(9)	154.8	*x*+1, *y*+1, *z*
C(14)-H(14)···O(1)	2.65	3.264(9)	124.3	-*x*+1, -*y*+2, -*z*+1

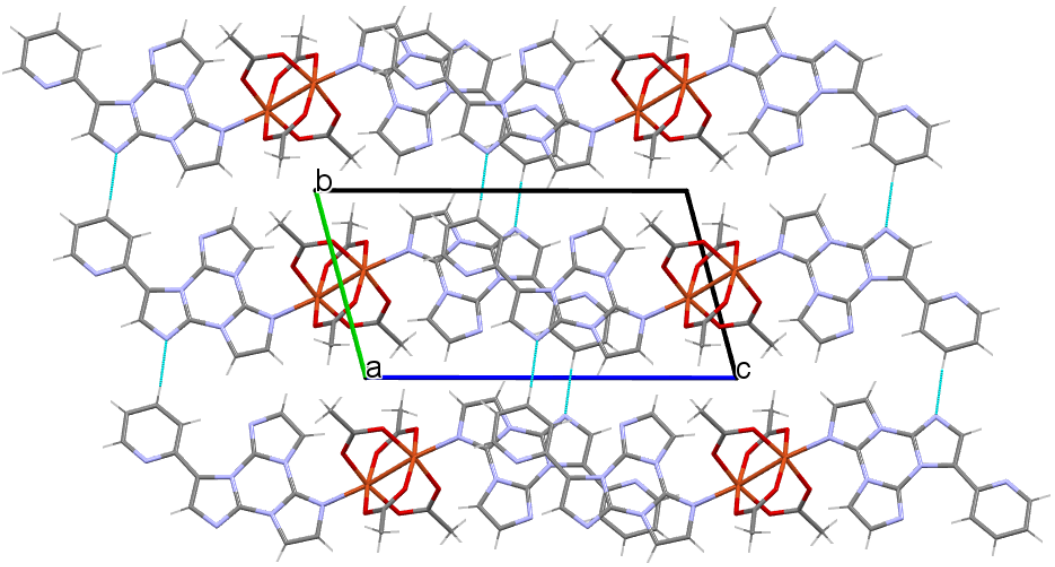


Figure S1. Fragments of two H-bonded chains in **2** with indication of CH…N hydrogen bonds.

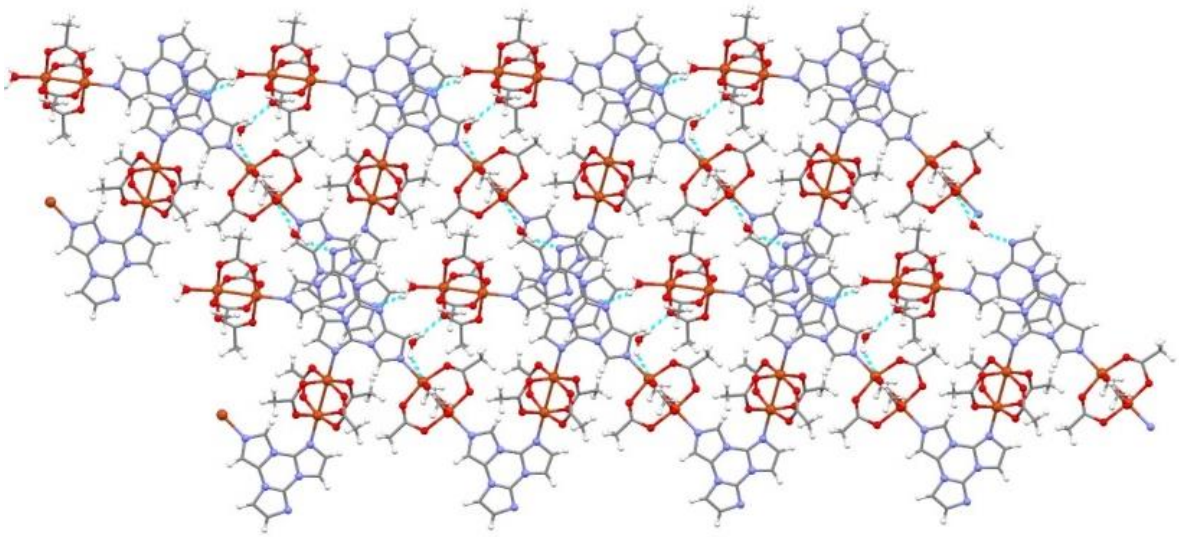


Figure S2. Fragment of supramolecular layer in **3**.

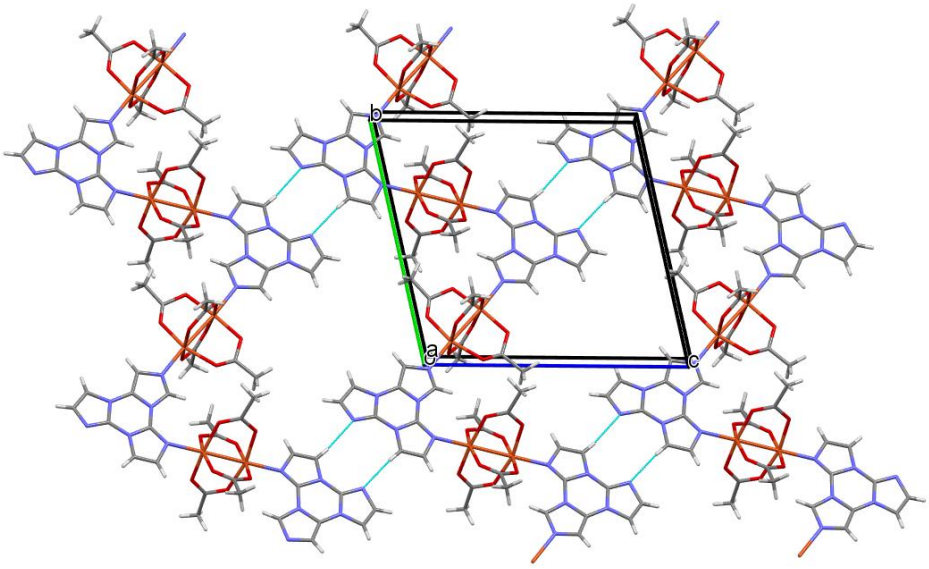


Figure S3. Association of coordination chains in the H-bonded layer in **3**.

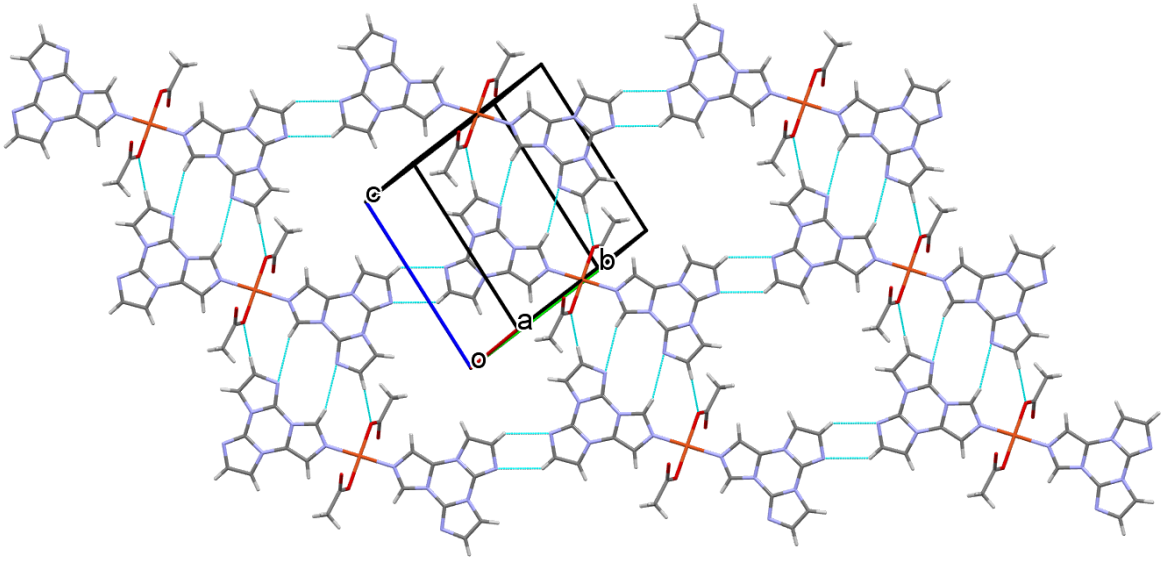


Figure S4. Association of complexes **4** in H-bonded layer.

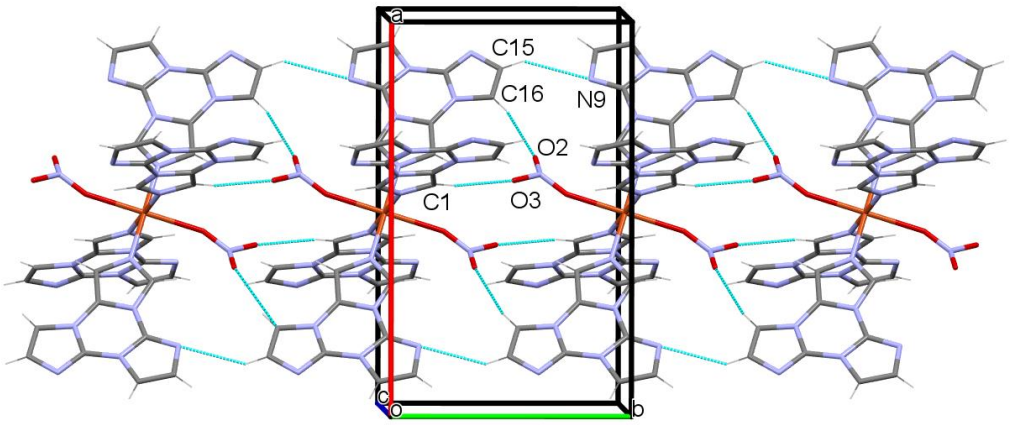


Figure S5. Association of mononuclear complexes in H-bonded chain in **5**.

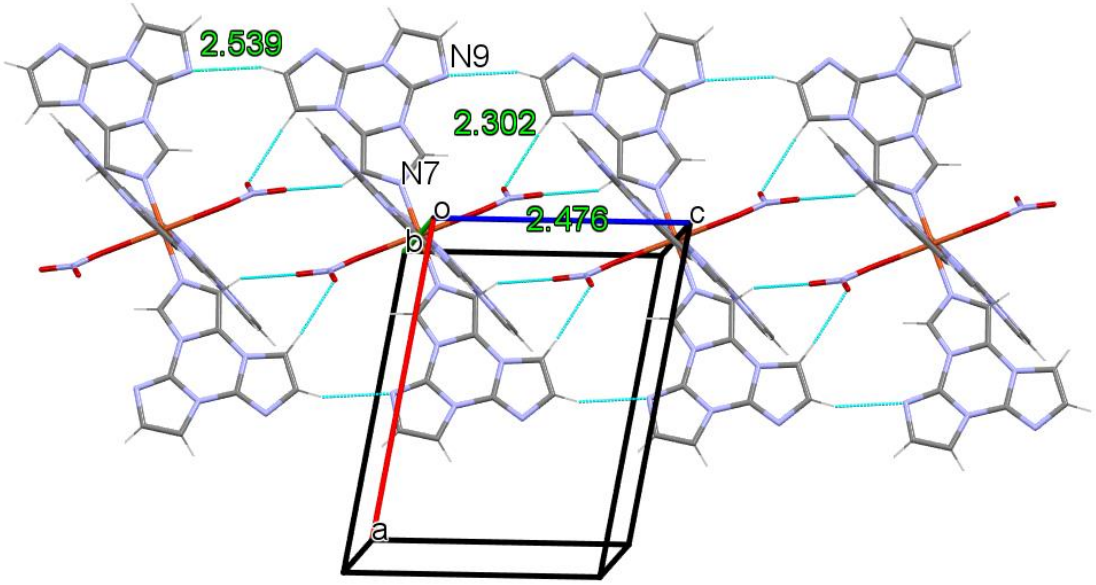


Figure S6. Association of mononuclear complexes in H-bonded chain in **6**.

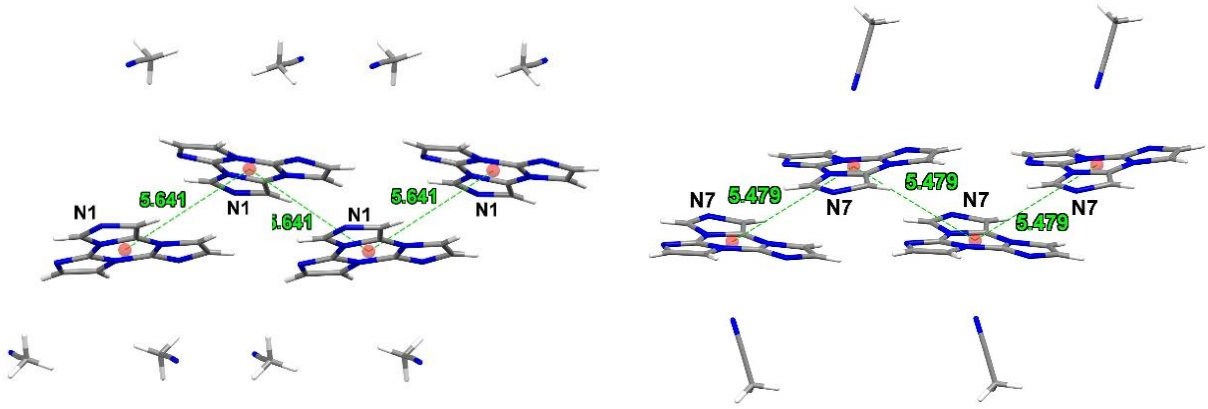


Figure S7. Walls of L_2 luminophores in **5** surrounded by acetonitrile solvent with indication of $Cg(L_2)\ldots Cg(L_2)$ separations.

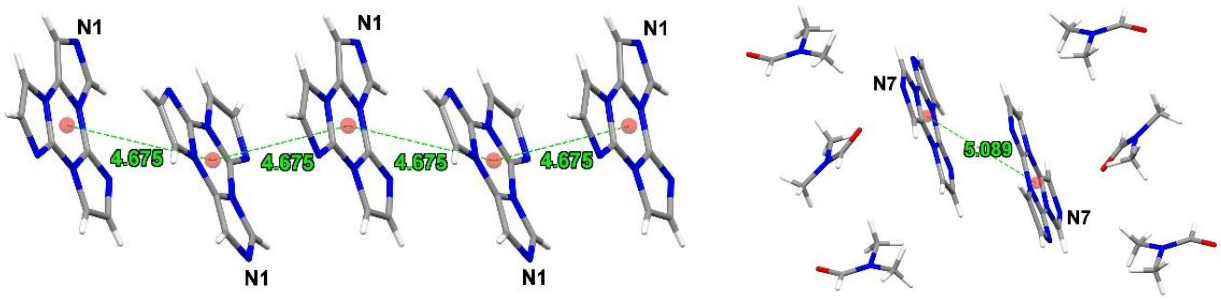


Figure S8. Complex **6**. View of infinite stacking of L_2 luminophores (defined by N1 atom) along the *c* axis with the interplanar angle of 8.53 °, and the stacking dimers (L_2 - defined by N7 atom) completely locked by dmf molecules.

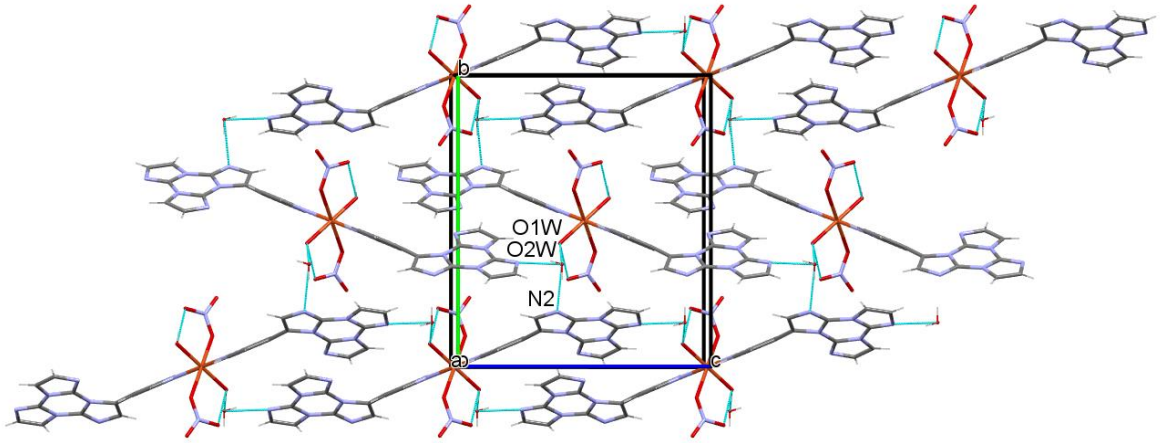


Figure S9. Representation of crystal structure **7**. View of three neighboring H-bonded double chains situated in T-shape mode and interconnected *via* bridging O2w water molecule in DDA mode.

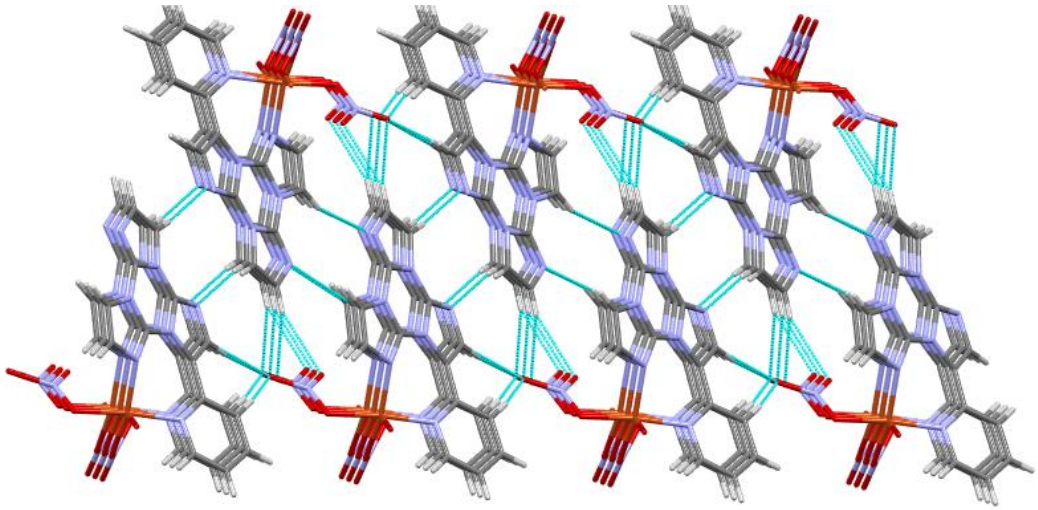
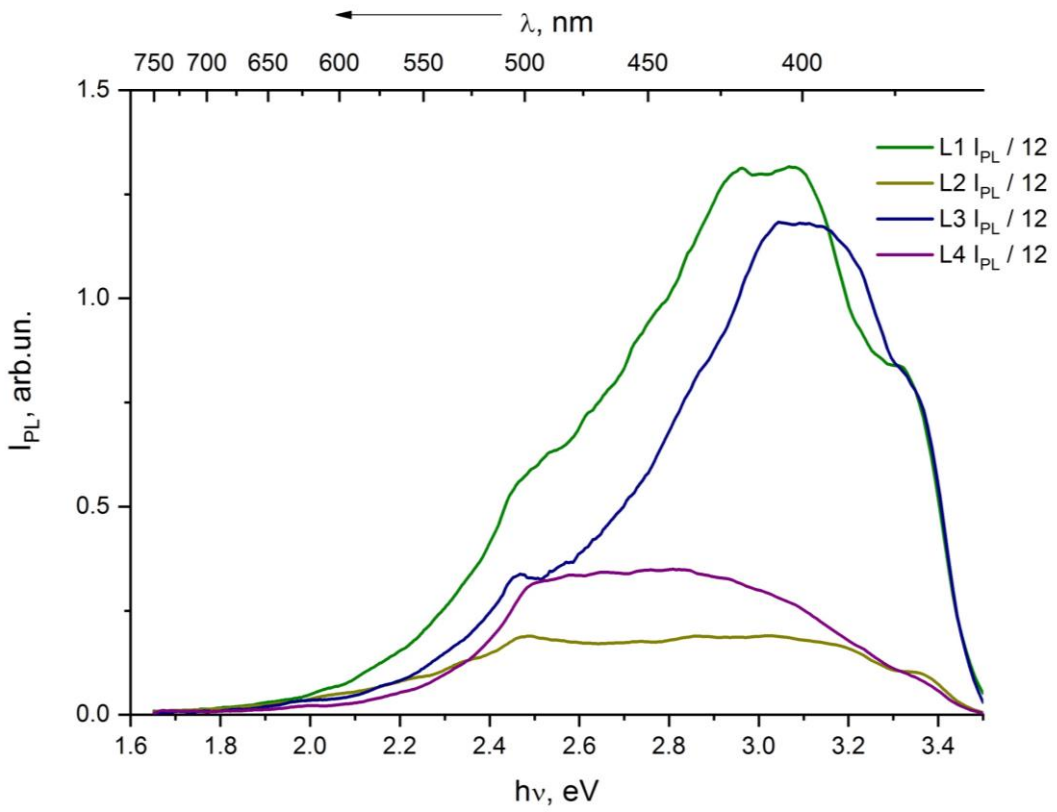
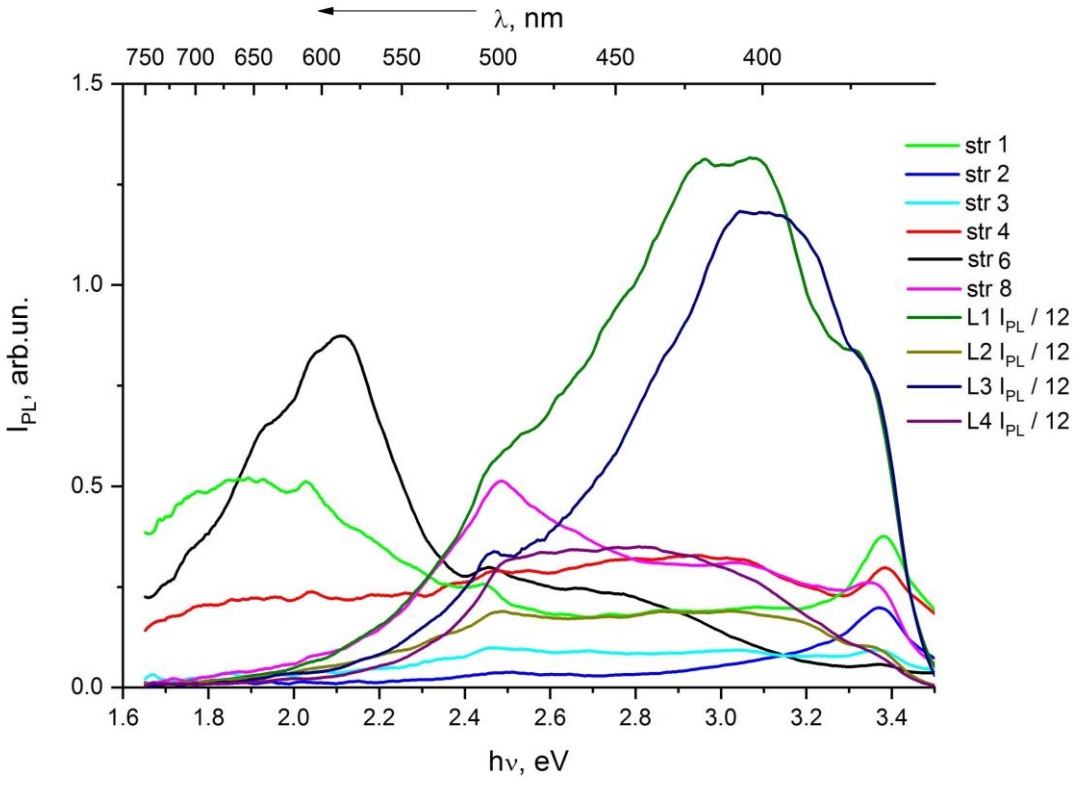


Figure S10. Interplay of weak intermolecular interactions in **8.**



(a)



(b)

Figure S11. Solid state emission spectra of (a) L_1-L_4 luminophores ; (b) L_1-L_4 luminophores and compounds **1-4, 6, 8**.