Optical and Photoelectronic Properties of a New Material: Optoelectronic Application

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Table SI-1. Selected bond distances (Å) and angles (°) in the molecular structure of [Zn^{II}(TFMPP)(4,4'-bipy)].2(4,4'-bipy).2H_2O (**I**).

Zinc(II) coordination polyhedron			
Zn-N1	2.0715(13)	N1-Zn-N2	87.36(5)
Zn-N2	2.0885(13)	N1-Zn-N3	100.99(4)
Zn-N3	2.1295(18)	N2-Zn-N3	99.95(4)
4-4'-bipyridine axial ligand			
N3-C25	1.3415(19)	C25-N3-Zn	121.28(10)
C25-C26	1.381(2)	C26-C25-N3	123.05(15)
C26-C27	1.391(2)	C27-C28-N3	121.35(11)
C27-C28	1.488(3)	C28-C29-N4	119.01(16)
C28-C29	1.390(2)	C29-C30-N4	124.41(17)
C29-C30	1.386(2)		
C30-N4			

Table SI-2. Selected hydrogen bonds and intermolecular C–H...Cg interactions of complex (**I**).

Complex	Symmetry of A	D[a]···A[b] (Å)	D–H···A (°)
O1-H1O1…N5	x,y,z	2.984(2)	148
O1– H2O1…N6	1-x,y,1/2-z	2.937(2)	167
C15– H15…F1	x,y,z	2.711(2)	101
C15– H15…F1	-x,1-y,-z	3.231(2)	141'
C26–H26…O1	1/2-x,1/2+y,1/2-z	3.163(2)	131
C20–H20…*Cg*1	1-x,1-y,-z	3.638(2)	159
C34–H34…*Cg*1	x,y,z	3.687(2)	138
C38–H38…*Cg*2	x,y,z	3.613(2)	142

[a] D = donor atom, [b] A = acceptor atom.
Cg1 is the centroid of the N1/C1-C4 five-member ring,
Cg2 is the centroid of the N2/C6-C9 five-member ring.

Table SI-3. π–π interactions (Å) for (**I**).

Cg(I)	*Cg(I)*	*Cg…Cg*		*α*	*Cg(I)_Prep*	*Cg(J)_Prep*
Cg(26)	*Cg*(27)^{i}	3.6771(11)	18.4	3.3988(8)	3.4890(8)	

Cg26 is the centroid of the N5-C31/C35 six-member ring.
Cg27 is the centroid of the N6-C36/C40 six-member ring.

Symmetry code: (i) 1-x,y,1/2-z