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SUPPLEMENTARY MATERIAL TO

A new zinc(II) supramolecular square: synthesis, crystal structure, thermal behavior and luminescence

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TABLE S-I. Crystal data and structure refinement for **1**

Parameter	Value
Chemical formula	$C_{72}H_{56}N_{12}O_{18}Zn_4$
Formula weight	1638.77
Wavelength, Å	0.71073
Temperature, K	293(2)
Crystal system	Triclinic
Space group	*P*-1
a / Å	10.773(2)
b / Å	12.641(3)
c / Å	13.573(3)
α / °	107.44(3)
β / °	102.66(3)
γ / °	93.89(3)
V / Å^3	1702.8(6)
Z	1
D_{calc} / g cm^{-3}	1.598
μ / mm^{-1}	1.475
F(000)	836
($\theta_{min} - \theta_{max}$) / °	3.15–25.03
Diffraction measured fraction, θ_{max} / °	25.03
Refined difference density, max/min	0.450/–0.363
Reflection collected/unique (R_{int})	13258 / 5920 (0.0597)
Data/restraints/parameters	5920/6/494
Goodness-of-fit on F^2	1.045
R indices (all data)	$R_1 = 0.0472$, $wR_2 = 0.0919$
Final *R* indices ($I > 2\sigma(I)$)	$R_1 = 0.0863$, $wR_2 = 0.1076$

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TABLE S-II. Selected bond lengths (Å) and angles (°) for **1**; symmetry transformations used to generate equivalent atoms: A: –*x*+2, –*y*+1, –*z*+2

Bond	Value	Bond	Value
Bond length, Å			
Zn(1)–N(1)	2.125(3)	Zn(1)–N(2)	2.196(4)
Zn(2)–N(3)	2.192(3)	Zn(2) –N(4)	2.124(4)
Zn(2)–N(5)^{A}	2.023(4)	Zn(1)–N(6)	2.034(3)
Zn(1)–O(2)	2.009(3)	Zn(1)–O(3)	2.038(3)
Zn(2)–O(5)	2.057(3)	Zn(2)–O(6)	1.971(3)
Bond angle, °			
O(2)–Zn(1)–N(6)	99.99(13)	O(2)–Zn(1)–O(3)	89.18(12)
N(6)–Zn(1)–O(3)	95.62(13)	O(2)–Zn(1)–N(1)	110.16(13)
N(6)–Zn(1)–N(1)	149.54(15)	O(3)–Zn(1)–N(1)	89.16(12)
O(2)–Zn(1)–N(2)	92.84(14)	N(6)–Zn(1)–N(2)	98.16(14)
O(3)–Zn(1)–N(2)	165.50(11)	N(1)–Zn(1)–N(2)	76.66(13)
O(6)–Zn(2)–N(5)^{A}	136.09(14)	O(6)–Zn(2)–O(5)	88.94(12)
N(5)^{A}–Zn(2)–O(5)	92.79(14)	O(6)–Zn(2)–N(4)	113.64(15)
N(5)^{A}–Zn(2)–N(4)	110.12(15)	O(5)–Zn(2)–N(4)	92.33(14)
O(6)–Zn(2)–N(3)	89.50(12)	N(5)^{A}–Zn(2)–N(3)	96.66(13)
O(5)–Zn(2)–N(3)	167.89(14)	N(4)–Zn(2)–N(3)	77.31(13)