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Supporting information for article:

Cu(II) and Zn(II) β-diketonate coordination polymers based on pyrimidin-2-amine, pyrazine and 1,2-bis(4-pyridyl)ethane

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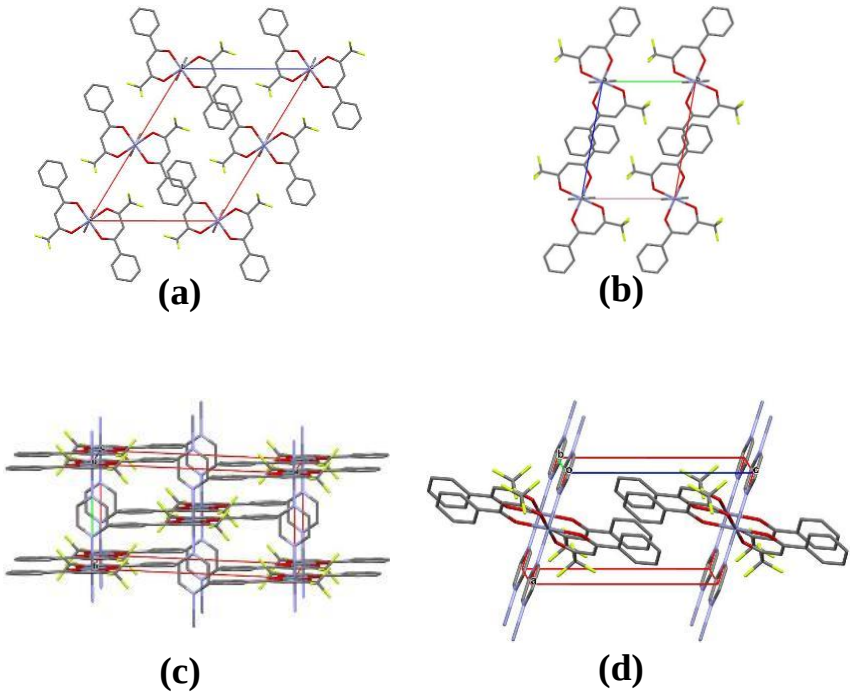

Figure S1 Packing diagrams along the chain of (a) **4a** and (b) **4b**; Unit cell contents of (c) **4a** and (d) **4b**; Hydrogen atoms are omitted for clarity.

Table S1 Selected hydrogen-bond parameters for **1**–**5** [Å and °]

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
(1)				
N3—H3A···O1	0.86	2.32	3.100 (3)	151.2
N3—H3B···O3	0.86	2.54	3.226 (3)	137.2
C10—H10···O2	0.93	2.41	2.727 (4)	100
C22—H22···O1^{i}	0.93	2.53	3.140 (3)	123
C24—H24···O3^{ii}	0.93	2.56	3.185 (4)	125
C3—H3···F1	0.93	2.37	2.735 (4)	103
C13—H13···F4	0.93	2.35	2.725 (4)	104
C7—H7···*Cg*5^{iii}	0.93	2.97	3.811 (4)	151
(2)				
N2—H2B···O1^{iv}	0.86	2.10	2.8878 (14)	152.0
N2—H2A···O1	0.86	2.10	2.8878 (14)	152.0
C10—H10···O2	0.93	2.40	2.719 (4)	100
C12—H12···O1^{v}	0.93	2.53	3.039 (3)	114
C3—H3···F1A	0.93	2.37	2.735 (12)	103
(3)				
C3—H3···F1	0.93	2.34	2.708 (8)	103
(4a)				
C3—H3···F1A	0.93	2.33	2.724 (11)	105
C10—H10···O2	0.93	2.36	2.685 (7)	100
(4b)				
C3—H3···F1	0.95	2.33	2.719 (4)	104
C7—H7···*Cg*3^{vi}	0.95	2.99	3.792 (3)	143
(5)				
C3—H3···F3	0.93	2.36	2.741 (3)	104
C10—H10···O2	0.93	2.37	2.700 (4)	101
C7—H7··· *Cg*3^{vii}	0.93	2.37	2.700 (4)	101

Symmetry code(s): (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+2, −*y*, −*z*; (iii) −*x*+1, −*y*–1, −*z*+1; (iv) −*x*+3/2, *y*, −*z*+1/2; (v) −*x*+1, −*y*+1, −*z*; (vi) *x*, *y*, *z*+1; (vii) *x*, *y*+1, *z*. *Cg*3 are N1/C11–C12/ N1'/C11'–C12' (4b) and N1/C11–C15 (5) ring centroids and *Cg*5 is N1/C21/N2/C24–C22 (1) ring centroid.

Table S2 Geometrical parameters for π–π interactions in **1**–**5** (Å, º)

*Cg*I···*Cg*J	*Cg*I···*Cg*J	*α*	*β*	*Cg*I-Perp (offset distance)	Ring slippage	Symmetry transformation for acceptors
1						
*Cg*6···*Cg*6	3.8187(18)	0	20.04	3.5874(13)	1.309	–*x* + 1, –*y* – 1, –*z* + 1
*Cg*7···*Cg*7	4.142(2)	0	29.46	–3.6061(17)	2.037	–*x* + 2, –*y* – 1, –*z*
2						
*Cg*4···*Cg*4	3.8665(19)	15	16.19	3.7131(13)	1.078	–*x* + ½, *y*, –*z* + ½
3						
*Cg*3···*Cg*3	4.135(14)	0	17.09	3.952(11)	1.215	–*x* + ½, –*y* + ½, –*z* + 1
4a						
*Cg*3···*Cg*3	4.080(2)	0	27.65	3.6136(1)	1.893	–*x* + ½, *y* – ½, –*z* + 1
4b						
*Cg*4···*Cg*4	3.878(3)	0	22.84	–3.574(2)	1.505	–*x*, –*y* + 1, –*z* + 1
5						
*Cg*4···*Cg*4	3.8925(17)	0	25.16	–3.5233(13)	1.655	–*x* – 1, –*y* + 1, –*z* + 1

CgI···CgJ, *α*, *β* and CgI-Perp are, respectively, the centroid-to-centroid distance between rings I and J (Å), the inter-ring dihedral angle (°), slip angle (°), and the perpendicular distance of CgI from ring J (Å). Ring slippage is in Å. For **1**: *Cg*6 and *Cg*7 are C5–C10 and C15–C20 ring centroids, respectively. For **2**, **4b** and **5**: *Cg*4 is C5–C10 ring centroid. For **3** and **4a**: *Cg*3 is C5–C10 ring centroid.