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Supplementary Material

Effect of co-crystal formers on the supramolecular patterns and luminescent properties of co-crystals comprising Fenbufen and diverse *N*-heterocycles

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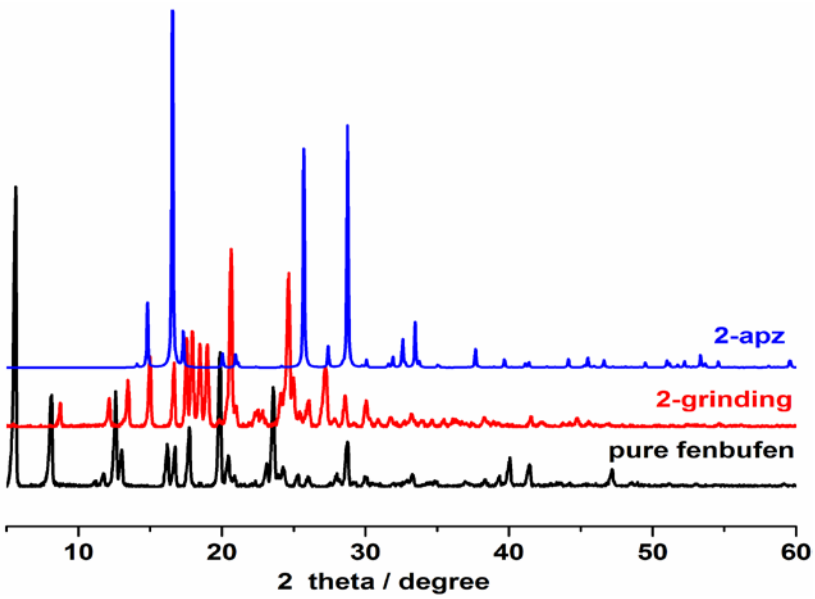

Fig. S1 Comparison of the PXRD patterns among the pure Fbf, 2-apz and new phase obtained from grinding method.

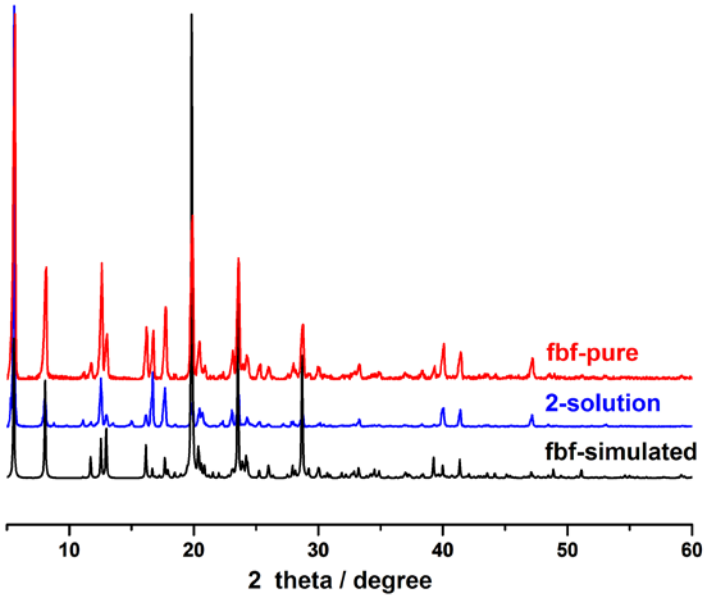

Fig. S2 Comparison of the PXRD patterns among the pure Fbf and precipitates from the solution for preparing compound **2**, as well as the simulated PXRD pattern from crystal structure of Fbf.

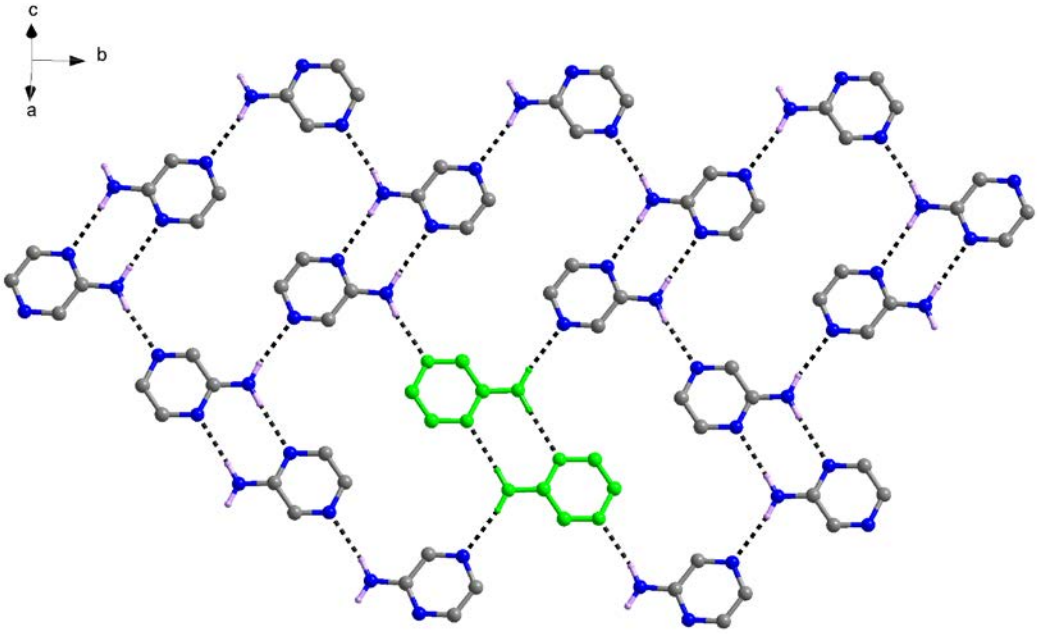

Fig. S3 Infinite rigid layer structure assemble from pure 2-apz with the dimer highlighted by green color.

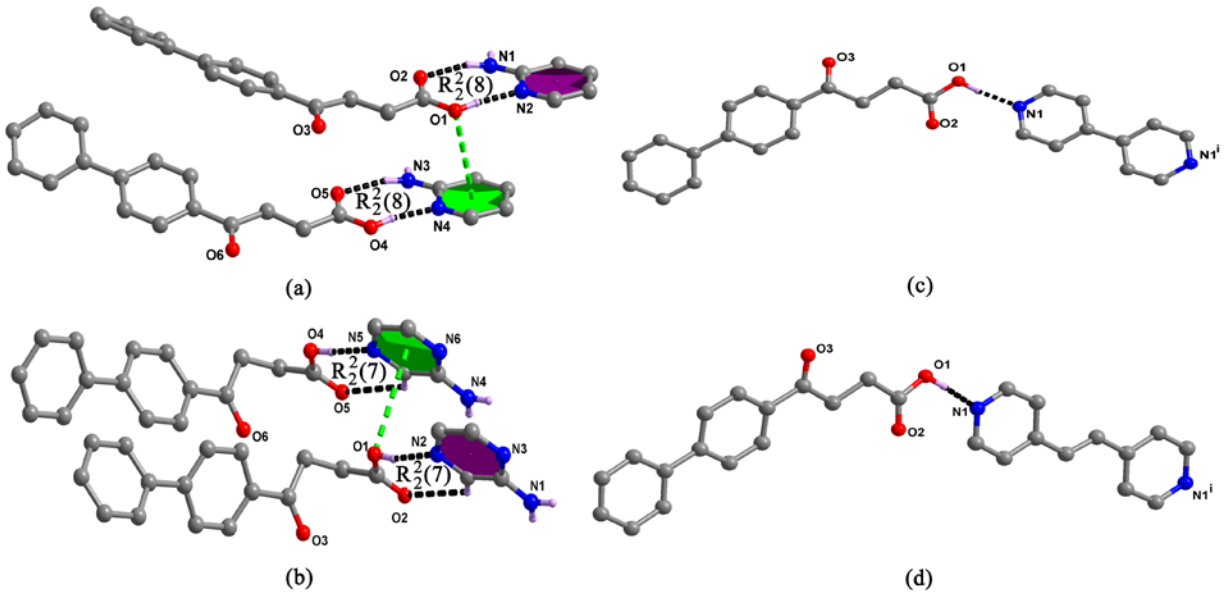

Fig. S4 Crystal structures of compounds **1** (a), **2** (b), **3** (c) and **4** (d).

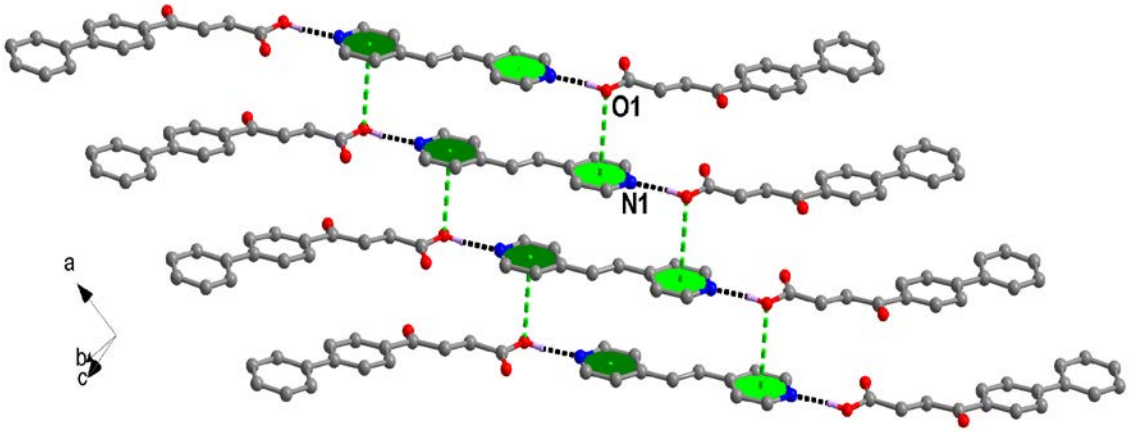

Fig. S5 Tape structure in compound **4** extended by hydrogen bonding and lone pair···π interactions.

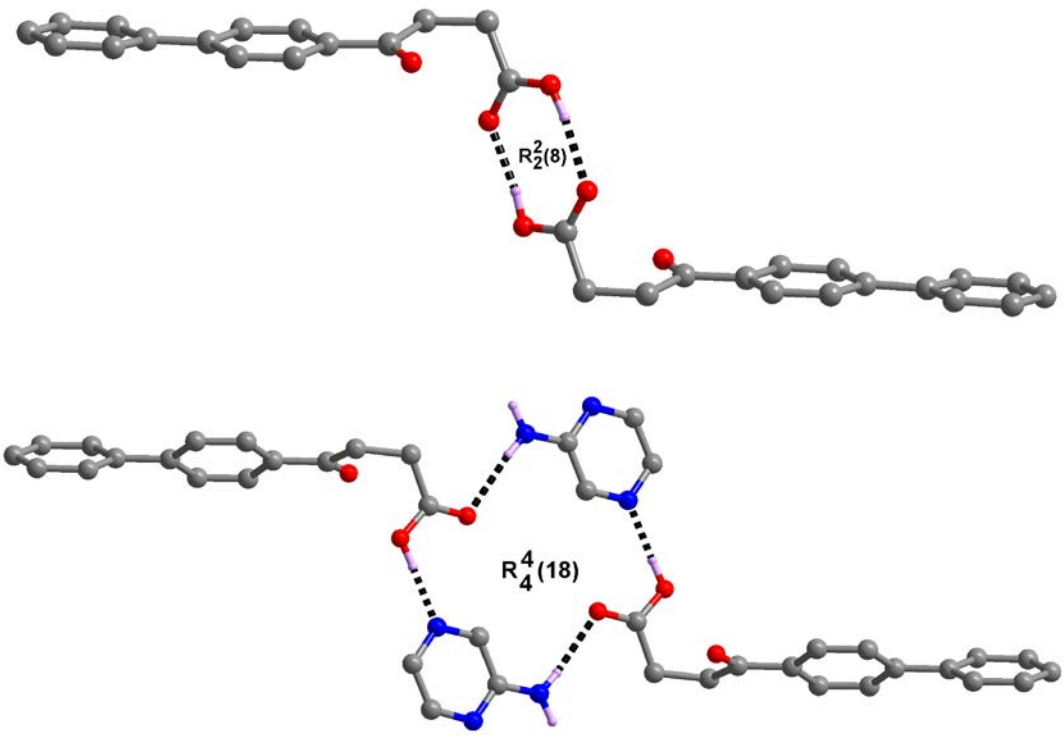

Fig. S6 Chair-shaped dimer in pure Fbf (top) and compound **2** (down) showing different hydrogen bonding rings.

Table S1 Summary of the C-H···O interactions in Fbf and compounds **1-4**

Compounds	C–H···O	d(C···O)	d(H···O)	∠(DHO)	Remarks
Fbf	C(3)-H(3A)···O(6)	3.412(5)	2.595(8)	141.9	P2-P2
	C(19)-H(19B)···O(3)	3.513(6)	2.636(6)	150.4	
1	C(13)-H(13B)···O(5)	3.375(2)	2.693	127.7	P2-P3
	C(12)-H(12B)···O(6)	3.432(3)	2.875	117.5	
2	C(11)-H(11B)···O(6)	3.390(8)	2.428	171.8	P2-P3
	C(27)-H(27B)···O(3)	3.446(1)	2.480	173.2	
3	-	-	-	-	-
4	C(9)-H(9A)···O(2)	3.323(1)	2.688	123.5	P1-P2

Table S2 Summary of the C-H···π interactions in compounds **1-4** and pure Fbf[a]

Compounds	C–H···Cg_n	d(C···Cg_n)	d(H···Cg_n)	∠(C-H-Cg_n)	Remarks
Fbf	C(7)-H(7A)···Cg_1	3.634(1)	2.972	129.5	P3-P4
	C(16)-H(16A)···Cg_1	3.733(6)	2.978	139.5	
	C(10)-H(10A)···Cg_2	3.745(1)	3.053	132.6	
	C(13)-H(13A)···Cg_2	3.704(7)	3.017	132.1	
	C(22)-H(22A)···Cg_3	3.529(5)	2.841	131.8	
	C(32)-H(32A)···Cg_3	3.733(3)	2.971	140.2	
	C(26)-H(26A)···Cg_4	3.730(4)	3.036	132.8	
	C(28)-H(28A)···Cg_4	3.755(9)	3.038	135.3	
1	C(38)-H(38A)···Cg_1	3.627(8)	2.890	137.3	P3-P4
	C(41)-H(41A)···Cg_1	3.652(6)	2.947	133.7	
2	C(14)-H(14A)···Cg_1	3.563(3)	3.131	110.4	P3-P4
	C(18)-H(18A)···Cg_1	3.553(8)	3.064	114.6	
	C(36)-H(36A)···Cg_2	3.525(2)	3.000	117.3	
	C(40)-H(40A)···Cg_2	3.539(7)	3.072	113.0	
3	C(8)-H(8A)···Cg_1	3.704(2)	2.880	143.5	P2-P3
4	-	-	-	-	-

[a] Cg_n (n=1, 2, 3 or 4) is used to distinguish different benzene rings.

Table S3 Different dihedral angles of Pn-P(n+1) (n=1, 2, 3) in Fbf and compounds **1-4**

Complexes	P1-P2	P2-P3	P3-P4
Fbf	79.3(3)	8.8(3)	5.0(4)
	80.1(3)	6.8(3)	2.6(4)
1	7.3(3)	9.5(3)	14.0(2)
	8.6(2)	17.9(2)	8.6(1)
2	81.6(2)	8.3(2)	40.3(2)
	86.0(2)	24.9(2)	36.5(2)
3	7.8(3)	4.8(3)	12.2(3)
4	11.8(6)	3.2(5)	7.8(5)