Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Novel Pharmaceutical Salts of Cephalexin with Organic Counterions: Structural Analysis and Properties

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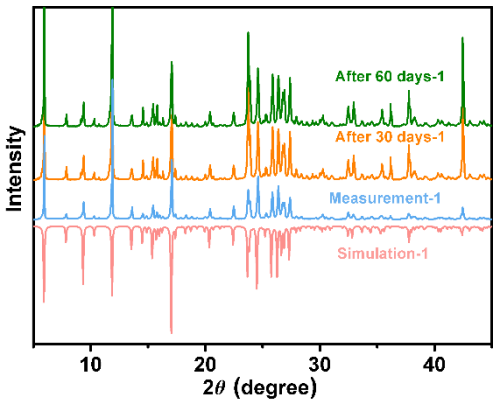

Fig. S1 The measured PXRD patterns of salt **1** match well with the simulated ones based on the corresponding crystal structure. And salt **1** show good physical stability when it was placed for 30 and 60 days under the conditions of ambient temperature and pressure.

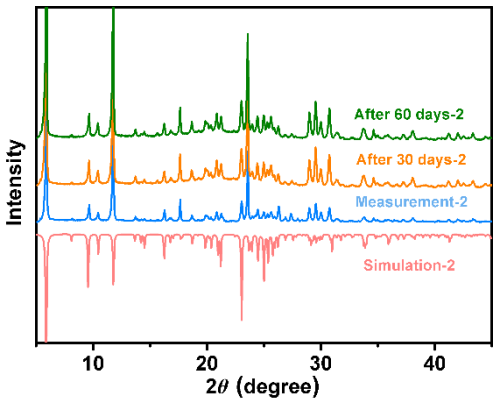

Fig. S2 The measured PXRD patterns of salt **2** at 293 K match well with the simulated ones based on the crystal structure collected at 150 K. And salt **2** show good physical stability when it was placed for 30 and 60 days under the conditions of ambient temperature and pressure.

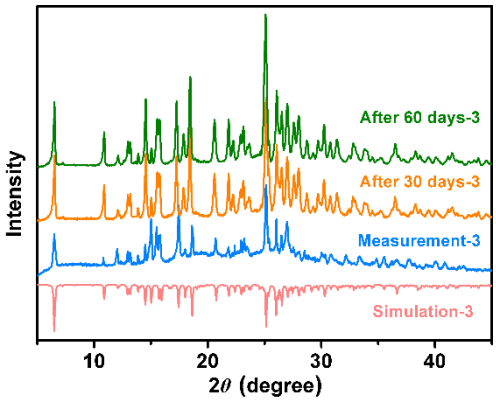

Fig. S3 The measured PXRD patterns of salt **3** at 293 K match well with the simulated ones based on the crystal structure collected at 150 K. And salt **3** show good physical stability when it was placed for 30 and 60 days under the conditions of ambient temperature and pressure.

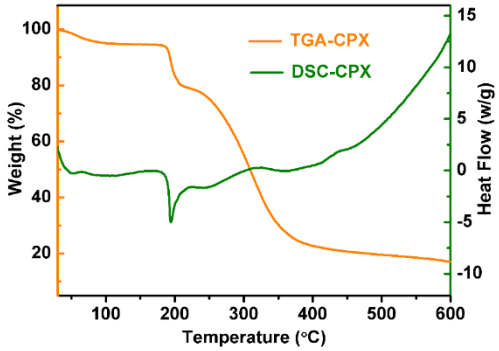

Fig. S4 TGA-DSC curve of CPX.

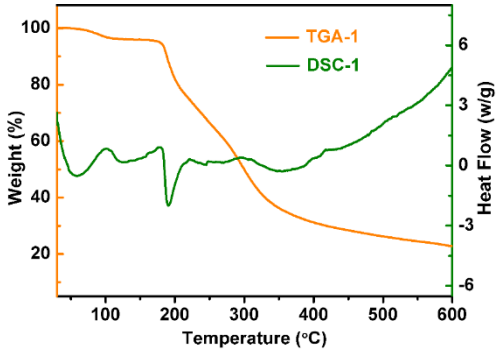

Fig. S5 TGA-DSC curve of salt **1**.

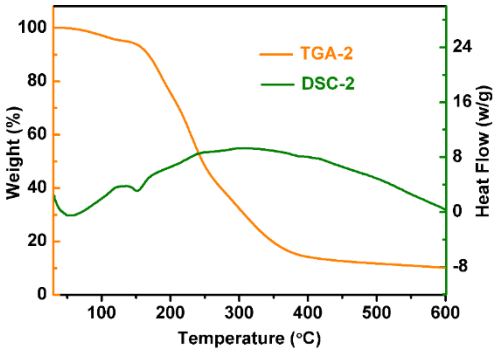

Fig. S6 TGA-DSC curve of salt **2**.

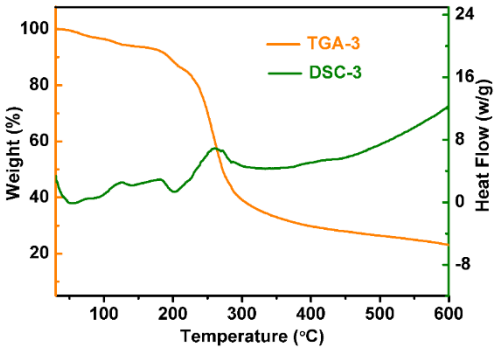

Fig. S7 TGA-DSC curve of salt **3**.

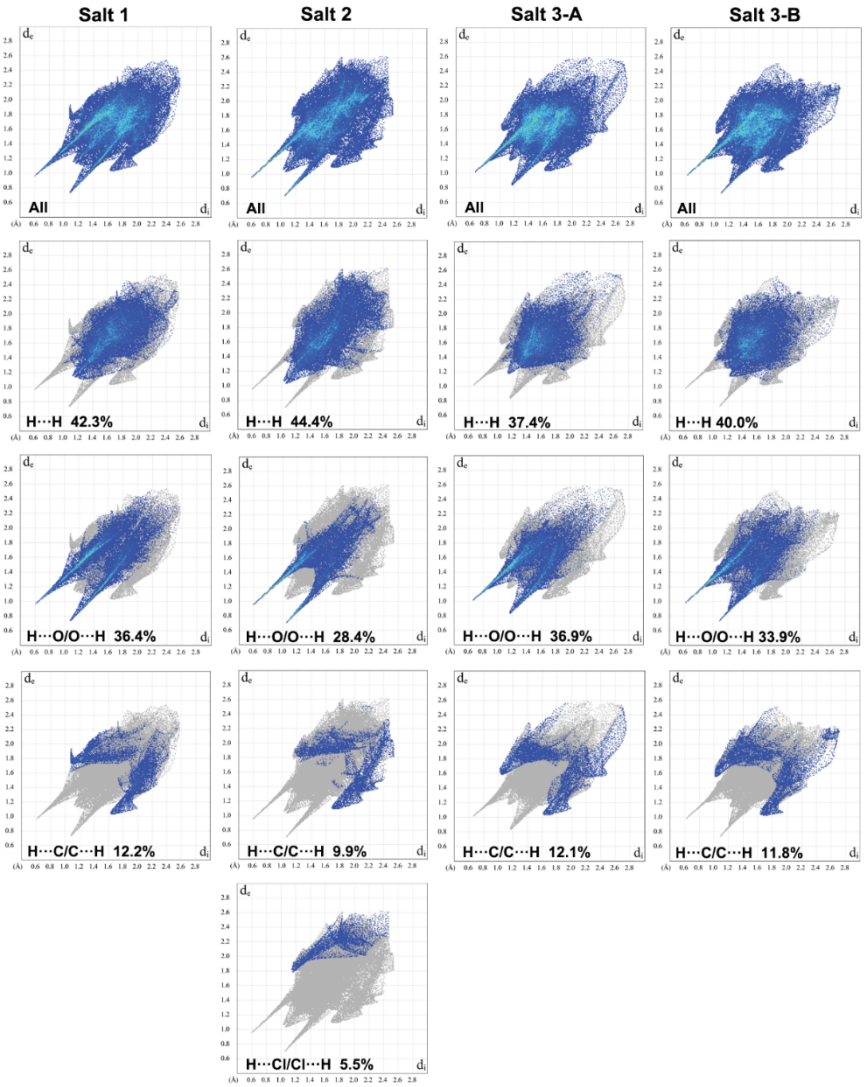

Fig. S8 2D fingerprint plots according to the d_{norm} value about different intermolecular contacts of CPX cations in salts **1**–**3**. Two CPX cations in the asymmetric unit of salt **3** were investigated individually and recorded as salt **3**-A and salt **3**-B, respectively.

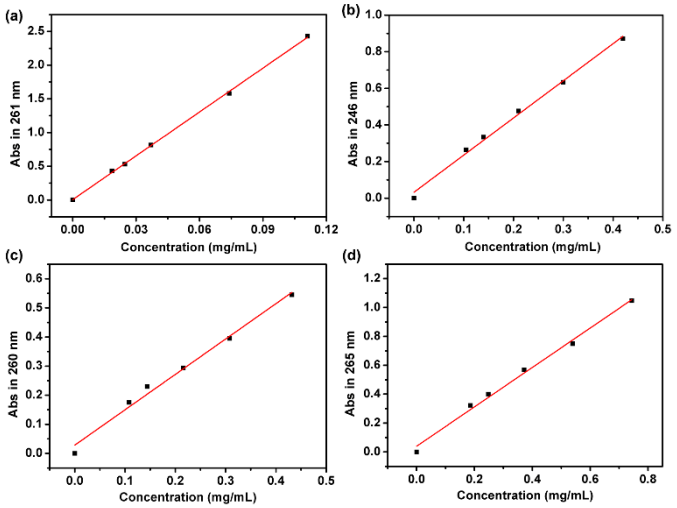

Fig. S9 Absorption calibration curves of (a) CPX, (b) salt **1**, (c) salt **2** and (d) salt **3**.

Table S1 Hydrogen bond distances [Å] and angles [°] in salts **1**

Compound	D–H···A [Å]	D–H [Å]	H···A [Å]	D···A [Å]	D–H···A [°]
CPX·DHBA·H_2O	O1–H1···O9^{i}	0.82	1.74	2.564(4)	179.3
(Salt **1**)	O7–H7···O5^{-}	0.82	1.80	2.518(4)	145.3
	O8–H8···O6^{-}	0.82	1.84	2.558(4)	145.3
	O9–H9A···O5^{-}	0.94	1.85	2.664(4)	143.0
	O9–H9B···O3^{ii}	0.86	2.07	2.904(4)	162.2
	N1^{+}–H1A···O6^{-iii}	0.89	1.81	2.671(4)	162.8
	N1^{+}–H1B···O2^{iv}	0.89	1.93	2.708(4)	144.8
	N1^{+}–H1C···O1^{v}	0.89	2.30	3.068(4)	145.2

Symmetry codes: (i): x+1, y, z; (ii): -x+1, y-1/2, -z+1; (iii): -x, y+1/2, -z+1; (iv): -x+1, y+1/2, -z+1; (v): x-1, y, z

Table S2 Hydrogen bond distances [Å] and angles [°] in salts **2**

Compound	D–H···A [Å]	D–H [Å]	H···A [Å]	D···A [Å]	D–H···A [°]
CPX·CSA·	O2–H2···O8	0.84	1.70	2.527(4)	168.7
1.5H_2O (Salt **2**)	O5–H5···O6^{-}	0.84	1.76	2.511(4)	147.9
	O8–H8A···O4^{i}	0.91	1.89	2.724(4)	151.0
	O8–H8B···O6^{-ii}	0.94	1.75	2.686(4)	173.6
	O9–H9A···O7^{-}	0.79	1.97	2.753(4)	176.2
	N2–H2A···O7^{-iii}	0.88	1.93	2.809(4)	177.2
	N3^{+}–H3A···O1^{iv}	0.91	1.98	2.852(4)	159.8
	N3^{+}–H3B···O5^{v}	0.91	1.92	2.803(4)	163.4
	N3^{+}–H3C···O3^{v}	0.91	1.89	2.794(4)	175.1

Symmetry codes: (i) x, y, z+1; (ii) x, y+1, z; (iii) -x+1, y, -z+1; (iv) x, y, z-1; (v) -x+1, y, -z

Table S3 Hydrogen bond distances [Å] and angles [°] in salts **3**

Compound	D–H···A [Å]	D–H [Å]	H···A [Å]	D···A [Å]	D–H···A [°]
CPX·SSA·	N2–H2A···O5	0.88	2.30	3.063(6)	144.4
4H_2O (Salt **3**)	N3^{+}–H3A···O24^{i}	0.91	1.98	2.858(6)	162.8
	N3^{+}–H3B···O23^{ii}	0.91	1.93	2.762(6)	151.6
	N3^{+}–H3B···O25^{ii}	0.91	2.59	3.046(6)	112.1
	N3^{+}–H3C···O2^{iii}	0.91	2.06	2.789(5)	135.9
	N5–H5D···O15	0.88	2.10	2.922(5)	154.4
	N6^{+}–H6A···O27^{iv}	0.91	1.91	2.797(6)	165.3
	N6^{+}–H6B···O28^{v}	0.91	1.95	2.857(6)	175.4
	N6^{+}–H6C···O12^{v}	0.91	2.18	2.851(5)	130.3
	N6^{+}–H6C···O22^{iv}	0.91	2.26	2.969(5)	134.7
	O1–H1···O26^{vi}	0.84	1.82	2.658(5)	174.5
	O5–H5···O6	0.84	1.84	2.572(5)	144.7
	O7–H7···O18	0.84	1.81	2.642(5)	172.3

O11–H11···O22^{vii}	0.84	1.78	2.618(5)	176.8
O15–H15A···O16	0.84	1.77	2.497(6)	144.3
O17–H17···O21	0.84	1.71	2.552(6)	177.4
O21–H21A···O14^{v}	0.82	1.99	2.808(6)	173.5
O21–H21B···O9	1.02	1.88	2.746(6)	141.0
O22–H22A···O8^{viii}	0.94	2.02	2.915(6)	160.5
O22–H22B···O9	1.01	1.78	2.770(6)	165.6
O23–H23A···O8	0.85	2.06	2.900(6)	170.0
O23–H23B···O28	1.07	2.04	2.902(6)	135.9
O24–H24A···O10	0.97	1.81	2.760(6)	168.2
O24–H24B···O25	0.70	2.17	2.861(6)	169.4
O25–H25A···O18^{ix}	0.79	2.15	2.939(5)	174.0
O25–H25B···O4^{ii}	0.89	2.12	2.868(5)	141.2
O26–H26A···O19^{x}	0.78	2.10	2.876(6)	177.5
O26–H26B···O20^{ix}	0.77	2.12	2.893(6)	178.5
O27–H27C···O20^{ix}	0.93	1.94	2.820(5)	155.4
O27–H27D···O24	0.79	1.95	2.738(5)	170.2
O28–H28D···O27	0.79	2.18	2.903(6)	152.3
O28–H28E···O19^{ix}	0.72	2.15	2.865(6)	167.0

Symmetry codes: (i) -x+1, y-1/2, -z+2; (ii) -x+1, y+1/2, -z+2; (iii) -x+2, y+1/2, -z+2; (iv) -x+1, y-1/2, -z+1; (v) -x+1, y+1/2, -z+1; (vi) x+1, y-1, z; (vii) x, y-1, z; (viii) x, y+1, z; (ix) x-1, y, z; (x) x-1, y+1, z