Supplementary Materials

Table S1. Crystallographic data and refinement parameters for potassium mefenamate–water (1/3).

Crystal data	
Chemical formula	$\{K(C_{15}H_{14}NO_2)(H_2O)_3\}$
M_r	333.42
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	80(2)
a (Å)	11.837(3)
b (Å)	35.406(9)
c (Å)	7.697(3)
α (°)	
β (°)	91.53(3)
γ (°)	
V (Å ^{3})	3224.7(17)
Z	8
Radiation type	Mo $K\alpha$
Crystal size (mm)	0.43 × 0.22 × 0.07
Data collection	
Diffractometer	Xcalibur Ruby-CCD κ-geometry diffractometer
No. of measured, independent and observed [I >2σ(I)] reflections	25361, 8639, 7053
R_{int}	0.025
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.098, 1.05
No. of parameters	447
No. of restraints	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\varrho_{max}$, $\Delta\varrho_{min}$ (e Å^{-3})	0.40, -0.25

Table S2. Bond lengths in potassium mefenamate–water (1/3).

Bonds in the chain formed with K1 ion		Bonds in the chain formed with K2 ion	
Bond	**Bond length [Å]**	**Bond**	**Bond length [Å]**
K1–O2W	2.7509(14)	K2–O4W	2.7782(14)
K1–O3W	2.7265(13)	K2–O6W	2.7139(13)
K1–O1A	2.7938(12)	K2–O1B	2.8163(12)
K1–O1W^{vi}	2.7988(12)	K2–O4W^{vi}	2.7856(15)
K1–O2W^{vi}	2.8256(14)	K2–O6W^{ii}	2.8250(12)
K1–O3W^{ii}	3.0639(13)	K2–O5W^{vi}	2.8431(12)
K1–O1W	3.3033(15)	K2–O5W	3.2332(15)
K1···K1^{ii}	4.0263(14)	K2···K2^{ii}	3.9858(15)
K1···K1^{vi}	4.0262(14)	K2···K2^{vi}	3.9858(15)
O1A–C1A	1.2736(16)	O1B–C1B	1.2657(15)
O21A–C1A	1.275(18)		
O2A–C1A	1.264(2)	O2B–C1B	1.2702(16)
C1A–C2A	1.5106(19)	C1B–C2B	1.5090(18)
C2A–C3A	1.4184(18)	C2B–C3B	1.4210(18)
C2A–C7A	1.4003(19)	C2B–C7B	1.4010(18)
N1A–C3A	1.3986(17)	N1B–C3B	1.3955(17)
N1A–C8A	1.4281(16)	N1B–C8B	1.4301(16)
C3A–C4A	1.4062(19)	C3A–C4A	1.4070(18)
C4A–C5A	1.3873(19)	C4B–C5B	1.3838(19)
C5A–C6A	1.3969(19)	C5B–C6B	1.3988(19)
C6A–C7A	1.3862(19)	C6B–C7B	1.3876(19)

C8A–C9A	1.4022(19)	C8B–C9B	1.4012(19)
C8A–C13A	1.3989(17)	C8B–C13B	1.3988(18)
C9A–C10A	1.4094(18)	C9B–C10B	1.4104(18)
C9A–C14A	1.5127(18)	C9B–C14B	1.5083(18)
C10A–C11A	1.3938(19)	C10B–C11B	1.3954(19)
C10A–C17A	1.509(2)	C10B–C15B	1.508(2)
C11A–C12A	1.391(2)	C11B–C12B	1.388(2)
C12A–C13A	1.3892(19)	C12B–C13B	1.3885(19)

Symmetry codes: ii = x, -y+3/2, z-1/2; vi = x, -y+3/2, z+1/2.

Table S3. Selected angles for potassium mefenamate–water (1/3).

Angles in the chain formed with K1 ion		**Angles in the chain formed with K2 ion**	
	Angle [°]		**Angle [°]**
O3W–K1–O2W	161.64(3)	O6W–K2–O4W	160.94(4)
O3W–K1–O1A	70.75(4)	O6W–K2–O1B	73.25(4)
O2W–K1–O1A	112.66(4)	O4W–K2–O1B	117.99(4)
O3W–K1–O1W^{vi}	89.55(4)	O6W–K2–O5W^{vi}	85.71(4)
O2W–K1–O1W^{vi}	103.53(3)	O4W–K2–O5W^{vi}	102.75(4)
O1A–K1–O1W	50.87(3)	O1B–K2–O5W	52.33(3)
O1A–K1–O1W^{vi}	117.93(3)	O1B–K2–O5W^{vi}	111.08(3)
O3W–K1–O2W^{vi}	84.86(4)	O6W–K2–O4W^{vi}	78.59(4)
O2W–K1–O2W^{vi}	88.15(4)	O4W–K2–O4W^{vi}	87.53(4)
O3W–K1–O3W^{ii}	118.22(4)	O6W–K2–O6W^{vi}	121.79(4)
O1W–K1–O1W^{vi}	131.43(3)	O5W–K2–O5W^{vi}	136.35(3)

O2A–C1A–O1A	123.31(13)	O1B–C1B–O2B	122.83(12)
O2A–C1A–C2A	118.84(13)	O2B–C1B–C2B	118.74(11)
O1A–C1A–C2A	117.84(12)	O1B–C1B–C2B	118.41(11)
N1A–C3A–C4A	121.86(12)	N1B–C3B–C4B	121.13(12)
N1A–C3A–C2A	118.95(12)	N1B–C3B–C2B	119.61(12)
C3A–N1A–C8A	124.29(11)	C3B–N1B–C8B	124.66(11)

Symmetry codes: ii = x, -y+3/2, z-1/2; vi = x, -y+3/2, z+1/2.

Table S4. Geometry of the hydrogen bonds in potassium mefenamate–water (1/3).

D–H···*A*	**D–H [Å]**	**H···*A* [Å]**	**D···*A* [Å]**	**D–H···*A* [Å]**
N1A–H1NA···O2A	0.914(17)	1.836(17)	2.6072(18)	140.5(14)
N1A–H1NA···O21A	0.914(17)	1.95(3)	2.648(18)	131.6(16)
N1B–H1NB···O2B	0.902(17)	1.915(17)	2.6158(16)	133.1(14)
O1W–H1W1···N1B^{i}	0.870(19)	2.144(19)	2.9958(17)	166.2(16)
O2W–H2W1···O2B^{i}	0.874(18)	2.077(18)	2.9487(16)	174.6(17)
O2W–H2W2···O1B^{ii}	0.88(2)	2.03(2)	2.8813(15)	162.7(17)
O3W–H3W2···O1W^{iii}	0.848(19)	1.950(19)	2.7737(18)	163.8(17)
O4W–H4W1···O1A^{iv}	0.87(2)	1.94(2)	2.7992(16)	169.0(17)
O4W–H4W2···O3W^{v}	0.828(19)	2.10(2)	2.8916(16)	160.2(17)
O5W–H5W2···N1A^{v}	0.867(19)	2.15(2)	2.9944(17)	165.4(16)
O6W–H6W1···O5W^{iii}	0.874(18)	1.984(18)	2.8137(18)	158.3(16)

Symmetry codes: i = x, y, z-1; ii = x, -y+3/2, z-1/2; iii = x, y, z+1; iv = x+1, -y+3/2, z+1/2; v = x+1, y, z.

Table S5. Selected QTAIM parameters (in a.u.) for the coordination polymers of potassium mefenamate–water (1/3).

		Bond length [Å]	**ϱ(r)**	**∇²(r)**	**ε(r)**	**V(r)**	**G(r)**	**H(r)**	**d [Å]**	**δ(A,B)**	**%δ(A,B) %K**
Binding to K1	K1 – O1W^{vi}	2.7988	0.0142	0.0613	0.1319	-0.0118	0.0135	0.0018	0.0013	0.0764	0.2111
	K2 – O3W^{ii}	3.0640	0.0063	0.0304	0.0596	-0.0048	0.0062	0.0014	0.0047	0.0400	0.1106
	K1 – O3W	2.7265	0.0165	0.0713	0.0857	-0.0138	0.0158	0.0020	0.0055	0.0977	0.2010
	K1 – O2W^{vi}	2.8259	0.0141	0.0582	0.0779	-0.0116	0.0131	0.0015	0.0010	0.0766	0.2116
	K1 – O1A	2.7937	0.0148	0.0612	0.0502	-0.0121	0.0137	0.0016	0.0035	0.1049	0.2898
	K1 – O1W	3.3031	0.0048	0.0213	0.7547	-0.0031	0.0042	0.0011	0.0024		
	K1 – O2W	2.7512	0.0161	0.0694	0.0876	-0.0137	0.0155	0.0018	0.0006	0.0939	0.2594
	K1 – C6B	3.3992	0.0057	0.0190	1.2683	-0.0029	0.0038	0.0009	0.2335		

	q(A)	**λ(A)**	**%λ(A)**
K1	0.9108	17.8318	98.5770
O1A	-1.2508	8.3327	90.0762
O2W	-1.2193	8.4901	92.0896
O3W	-1.2877	8.5698	92.2699
O2W	-1.2913	8.5278	91.7827
O2W^{vi}	-1.219	8.4745	91.9241
O3W^{ii}	-1.3265	8.4165	92.3660

		Bond length [Å]	**ϱ(r)**	**∇²(r)**	**ε(r)**	**V(r)**	**G(r)**	**H(r)**	**BPL - GBL_I**	**δ(A,B)**	**%δ(A,B) %K**
Binding to K2	K2 – O1B	2.8162	0.0141	0.0580	0.0446	-0.0114	0.0130	0.0015	0.0034	0.0987	0.273
	K2 – O5W^{vi}	2.8432	0.0124	0.0543	0.1251	-0.0101	0.0118	0.0017	0.0022	0.0663	0.1833
	K2 – O4W	2.7785	0.0154	0.0654	0.0761	-0.0129	0.0146	0.0017	0.0003	0.0894	0.2472
	K2 – O6W	2.7138	0.0163	0.0728	0.1026	-0.0137	0.0160	0.0022	0.0056	0.0947	0.2618

	K2 – O4W^{vi}	2.7862	0.0150	0.0635	0.0869	-0.0125	0.0142	0.0017	0.0021	0.0799	0.2207
	K2 – O5W	3.2330	0.0056	0.0241	0.2585	-0.0038	0.0049	0.0011	0.0035		
	K2 – C6A	3.5152	0.0045	0.0149	1.2019	-0.0022	0.0030	0.0008	0.2703		
	K2 – O6W^{ii}	2.8251	0.0136	0.0582	0.0832	-0.0113	0.0129	0.0016	0.0020	0.0663	0.1833

	q(A)	**λ(A)**	**%λ(A)**
K2	0.9111	17.8268	98.5509
O1B	-1.2554	8.3337	90.0422
O4W	-1.2233	8.4942	90.0954
O6W	-1.2784	8.5412	92.0543
O4W^{iv}	-1.2224	8.4819	91.9711
O5W^{iv}	-1.2919	8.5398	91.9057
O6W^{ii}	-1.3868	8.5888	92.1858
C6A	-1.2169	8.2368	89.3657
O5W	1.5617	2.7819	62.6791

K1 [7]		**Bond length [Å]**	**ϱ(r)**	**∇²(r)**	**ε(r)**	**V(r)**	**G(r)**	**H(r)**	**BPL - GBL_I**	**δ(A,B)**	**%δ(A,B) %K**
	K1 – C7^{v}	3.2877	0.0071	0.0263	5.2196	-0.0040	0.0053	0.0013	0.1935	0.026	0.0717
	K1 – O1^{ix}	2.8702	0.0125	0.0520	0.0483	-0.0093	0.0112	0.0019	0.0006	0.0712	0.1965
	K1 – O2	2.8842	0.0131	0.0523	0.2397	-0.0098	0.0114	0.0017	0.0007	0.073	0.2015
	K1 – O3	2.7982	0.0143	0.0640	0.0854	-0.0111	0.0135	0.0025	0.0019	0.08	0.2207
	K1 – O3^{x}	2.7688	0.0161	0.0691	0.0580	-0.0125	0.0149	0.0024	0.0003	0.09	0.2484
	K1 – O1	2.6983	0.0194	0.0823	0.0364	-0.0157	0.0181	0.0024	0.0005	0.1069	0.2951

	q(A)	**λ(A)**	**%λ(A)**
K1	0.8868	17.8198	98.3802
O1	-1.2803	8.2989	89.4253
O2	-1.2414	8.3125	89.9480
O1^{ix}	-1.2668	8.2788	89.3377

O3	-1.2599	8.4931	91.7196
O3^{x}	-1.2549	8.4876	91.7088
C7	0.1311	3.7967	64.6915

d [Å]—the difference between the length of the bond path and the distance between the atoms linked by this bond.

Symmetry codes: ii= x, -y+3/2, z-1/2; v = x+1, y, z; vi = x, -y+3/2, z+1/2; viii = x+1, y, z+1; ix = 2-x, 1-y, 1-z; x = 3-x, 1-y, 1-z