Supplementary Information (SI) for Dalton Transactions.

One-pot Method in Water to Synthesize a New Cyanurate $K(H_2C_3N_3O_3)\cdot H_2O$ with Large Birefringence

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Supporting Information

Table S1. A few representative compounds with synthetic methods and birefringence containing $(HC_3N_3O_3)^{2-}$ and $(H_2C_3N_3O_3)^{-}$ anionic groups and alkali metals.

Alkali metal	Compound	
Li	$Li_2(HC_3N_3O_3)\cdot 2H_2O$[1]	Vapor liquid diffusion in an acetone-water solution: 2LiOH : $H_3C_3N_3O_3$ in DI H_2O. Stir the solution until transparent and then put beaker in acetone.
		Space group: *$P2_1/c$* a=3.41420 b=16.97400 c=11.17600 α=90.0000 β=90.9200 γ=90.0000
		0.345 @ 532 nm
Na	$Na_2(HC_3N_3O_3)\cdot H_2O$[2]	2.71NaOH (590 mg) : $H_3C_3N_3O_3$ (702.5 mg) in 20 mL DI H_2O. Stir and heat at the boiling point. $Na_3(C_3N_3O_3)$ was formed in the concentrated 5mL solution and was removed by hot vacuum filtration. The rest sample was dispersed in 2mL DI H_2O and stir for 30 min, vacuum filtered and dried in the air.
		Space group: $P\bar{1}$ a=3.51660 b=7.83000 c=11.39660 α=86.4400 β=85.5350 γ=85.0720
		N/A
	$Na(H_2C_3N_3O_3)\cdot H_2O$[2]	$NaOH\cdot 10H_2O$ (286.2 mg) : $H_3C_3N_3O_3$ (129.1 mg) in 10 mL DI H_2O. Stir and heat at the boiling point. The product was removed by hot vacuum filtration in the concentrated 5mL solution.
		Space group: $P\bar{1}$ a=3.59720 b=9.12590 c=9.23440 α=91.1370 β=99.1420 γ=91.5540
		N/A
K	$K_2(HC_3N_3O_3)$[3]	Slow evaporation method in aqueous solution: 3KOH : $H_3C_3N_3O_3$ in DI H_2O. Stir the solution until transparent and then heat it up to the boiling point until water was evaporated.
		Space group: *Cmcm* a=13.09700 b=6.62650 c=6.88360 α=90.0000 β=90.0000 γ=90.0000
		0.35 @ 800 nm
	$K(H_2C_3N_3O_3)\cdot H_2O$ (this work)	**Method I**: Slow evaporation method in aqueous solution: $3K_2CO_3$: $2H_3C_3N_3O_3$ in DI H_2O. The product was obtained after 7 days at 50 °C.
		Method II: Slow evaporation method in aqueous solution: 2KOH : $H_3C_3N_3O_3$ in DI H_2O. Stir the solution and the product was obtained after 7 days at 50 °C.
		Space group: *C2/m* a=11.02680 b=16.36860 c=7.19580 α=90.0000 β=103.7650 γ=90.0000
		0.5@ 546.1 nm

Rb	$Rb_2(HC_3N_3O_3)$[1]	Vapor liquid diffusion in an acetone-water solution: $3RbOH : H_3C_3N_3O_3$ in DI H_2O. Stir the solution until transparent and then put beaker in acetone.
		Space group: *Cmcm* a=13.42900 b=6.69500 c=7.25900 α=90.0000 β=90.0000 γ=90.0000
		0.4 @ 532 nm
	$Rb(H_2C_3N_3O_3)\cdot H_2O$[4]	Rb_2CO_3(115.5 mg) : $2H_3C_3N_3O_3$ (129.1 mg) in 40 mL DI H_2O. Stir and heat the solution at 80 °C until it becomes clear. Then the solution was poured into a petri dish and slowly evaporated overnight at 30 °C. The product is thick rhombohedral plates.
		$Rb(H_2C_3N_3O_3)\cdot H_2O$-I Space group: $P2_1/c$ a=7.34510 b=12.25100 c=17.14100 α=90.0000 β=91.8830 γ=90.0000
		N/A
Cs	$Cs(H_2C_3N_3O_3)\cdot 0.5H_2O$[4]	Cs_2CO_3(162.9 mg) : $2H_3C_3N_3O_3$ (129.1 mg) in 40 mL DI H_2O. Stir and heat the solution at 80 °C until it becomes clear. Then the solution was poured into a petri dish and was slowly evaporated overnight at 30 °C. The product is hygroscopic and is thin tetragonal plates.
		Space group:$P2_1/m$ a=10.90460 b=16.10660 c=11.70270 α=90.0000 β=100.8980 γ=90.0000
		N/A

Table S2. Refined atomic coordinates and isotropic displacement parameters for $K(H_2C_3N_3O_3)\cdot H_2O$.

Atoms	Wyckoff	*x*	*y*	*z*	Occupancy	U_{eq} (Å^2)
K001	*4i*	0.92440(5)	0.5000	0.25492(8)	1	0.03090(17)
K002	*4i*	0.58053(6)	0.5000	0.25766(9)	1	0.03472(18)
O003	*8j*	0.30310(11)	0.13506(7)	- 0.18914(19)	1	0.0311(3)
O004	*4h*	0.5000	0.60415(11)	0.5000	1	0.0346(4)
O005	*4i*	0.6955(2)	0.5000	-0.0348(4)	1	0.0386(5)
O006	*4g*	0.5000	0.37313(11)	0	1	0.0369(5)
O007	*4i*	0.8060(2)	0.5000	0.5507(4)	1	0.0375(5)
O008	*8j*	0.69384(12)	0.84276(8)	0.6990(2)	1	0.0348(3)
N009	*4h*	0.5000	0.85047(12)	0.5000	1	0.0263(4)
N00A	*4g*	0.5000	0.12690(12)	0	1	0.0249(4)
N00B	*8j*	0.40074(14)	0.25363(9)	-0.0955(2)	1	0.0262(3)
N00C	*8j*	0.59829(14)	0.72391(10)	0.5957(2)	1	0.0283(3)
C00D	*8j*	0.39972(16)	0.16978(10)	-0.0960(2)	1	0.0231(4)
C00E	*4h*	0.5000	0.67876(15)	0.5000	1	0.0249(5)
C00F	*4g*	0.5000	0.29919(14)	0	1	0.0250(5)
C00G	*8j*	0.59953(16)	0.80846(10)	0.5998(2)	1	0.0247(4)
H00B	*8j*	0.3382(18)	0.2837(13)	-0.153(3)	1	0.029(5)
H00C	*8j*	0.661(2)	0.6960(15)	0.659(3)	1	0.043(7)
H005	*8j*	0.718(2)	0.5330(14)	-0.079(3)	1	0.043(8)
H007	*8j*	0.7976(19)	0.5327(13)	0.608(3)	1	0.031(6)

Table S3. Selected bond lengths (Å) for $K(H_2C_3N_3O_3)\cdot H_2O$.

Bond		Distances (Å)	Bond		Distances (Å)
K001	O005	2.866(3)	O003	C00D	1.252(2)
	O007	2.749(3)	O004	C00E	1.221(3)
	O007	2.969(3)	O006	C00F	1.210(3)
	O008	2.9394(13)	O008	C00G	1.246(2)
	O008	2.9394(13)	N009	C00G	1.3483(19)
	N009	3.0160(17)		C00G	1.3484(19)
	N009	3.0160(17)	N00A	C00D	1.3523(19)
	N00A	3.0170(14)		C00D	1.3523(19)
	N00A	3.0170(14)	N00B	C00D	1.373(2)
K002	O004	2.7336(12)		C00F	1.3669(19)
	O004	2.7336(12)	N00C	C00E	1.356(2)
	O005	3.084(3)		C00G	1.384(2)
	O005	2.703(3)			
	O006	2.7848(14)			
	O006	2.7848(14)			
	O007	2.852(3)			

Table S4. The birefringence of cyanurates and hydroisocyanurates.

#	Compounds	Space group	Band gap (eV)	Δn	Angle (°)	Ref.
				$(C_3N_3O_3)^{3-}$		
1	$Na_3(C_3N_3O_3)$	$R\bar{3}c$		0.395@800nm [d]	0	2,5,6
2	$Ca_3(C_3N_3O_3)_2$	$R3c$	5.63 [b]	0.372@589.3 nm [d]	0	7,8
3	α −$Sr_3(C_3N_3O_3)_2$	Cc	null	N/A	θ =1.*6715* γ = 25.39, 26.35	9
4	β−$Sr_3(C_3N_3O_3)_2$	$R3c$	5.57 [b]	0.374@589.3 nm [d]	0	8,10
5	$Ba_3(C_3N_3O_3)_2$ (I)	$R\bar{3}$	5.14(2) [a]	0.32@800 nm [d]	0	11
6	$Ba_3(C_3N_3O_3)_2$ (II)	$R\bar{3}c$	null	null	0	10,12
7	$Eu_3(C_3N_3O_3)_2$	$R3c$	null	null	0	10
8	LiSr(C3N3O3)	$C2/c$	null	null		13
9	$KLa_2(C_3N_3O_3)_2Cl$	$P6_3/m$	~ 5.0	0.316@1064 nm [d]		14
10	$Ba_2Mg(C_3N_3O_3)_2$	$R\bar{3}$	230 nm [a] (5.39)	0.351@800 nm [d]		15
11	$Ba_2Ca(C_3N_3O_3)_2$	R	225 nm [a] (5.51)	0.345@800 nm [d]		15
12	$Ba_2Sr(C_3N_3O_3)_2$	$R\bar{3}$	225 nm [a] (5.51)	0.35@800 nm [d]		16
13	$Ba_2Pb(C_3N_3O_3)_2$	$R\bar{3}$	264 nm [a] (4.70)	0.31@800 nm [d]		16
14	$K_4Cu_3(C_3N_3O_3)_2Cl$	$P\bar{3}m1$	351 nm [a] (3.53)	0.249@800 nm [d]		17
15	$K_4Cu_3(C_3N_3O_3)_2Br$	$P\bar{3}m1$	364 nm [a] (3.41)	0.244@800 nm [d]		17
16	$K_6Cd_3(C_3N_3O_3)_4$	$I\bar{4}3d$	5.23 [a]	null		18
17	$Zn_5(OH)_4(C_3N_3O_3)_2$	$P2_1/n$	4.98 [a]	0.318@400 nm [d]		19
18	$MgZn_4(OH)_4(C_3N_3O_3)_2$	$P2_1/n$	5.00 [a]	0.316@400 nm [d]		19
				$(HC_3N_3O_3)^{2-}$		
19	$Ca(HC_3N_3O_3)\cdot 3.5H_2O$	$P2_1/c$	null	null	θ= 7.86 γ= 28.61	4
20	$Sr(HC_3N_3O_3)$	$P2_1/c$	4.93 [a]	0.184@800 nm [d]	θ= 49.37 γ= 0	20

21	$Sr(HC_3N_3O_3)\cdot 2H_2O$	*Ima2*	216 nm [a] (5.74)	null	θ =3.21 γ =1.60	4
22	$Sr(HC_3N_3O_3)\cdot 2.5H_2O$	*Pnc2*	4.11 -4.52 [b]	0.341@800 nm [d]	θ =16.33 γ =8.17	20
23	$Sr(HC_3N_3O_3)\cdot 3H_2O$	$P2_1/c$	null	null	θ =4.62 γ =16.41, 11.84	4
24	$Li_2(HC_3N_3O_3)\cdot 2H_2O$	$P2_1/c$	5.05 [a]	0.345@532 nm [d]	θ =38.17; γ =19.71	1
25	$Na_2(HC_3N_3O_3)$	*Pnma*	~245 nm [a] (5.06)	null	θ =0 γ =3.86	2
26	$Na_2(HC_3N_3O_3)\cdot H_2O$	$P\bar{1}$	~245 nm [a] (5.06)	0.306 [d]	θ =0 γ =23.39	1,2
27	$K_2(HC_3N_3O_3)$	*Cmcm*	4.94 [a]	0.35@800 nm [d]	0	1,3
28	$Rb_2(HC_3N_3O_3)$	*Cmcm*	4.96 [a]	0.4@532 nm [d]	0	1
29	$LiRb(HC_3N_3O_3)\cdot 2H_2O$	$Pna2_1$	5.13 [a]	0.259 @ 532 nm [d]		1
30	$LiK(HC_3N_3O_3)\cdot 2H_2O$	$Pna2_1$	5.23 [a]	0.186@514 nm [c]		21
				0.280@ 532 nm [d]		1
31	$RbNa(HC_3N_3O_3)\cdot 2H_2O$	$Pna2_1$	5.10 [a]	0.194 [d]		22
32	$NaRb_{0.86}Cs_{0.14}(HC_3N_3O_3)\cdot 2H_2O$	$Pna2_1$	5.16 [a]	0.238@532 nm [d]		1
33	$Pb_2Cd(HC_3N_3O_3)_2(OH)_2$	*C2/c*	4.10 [a]	0.291@800 nm [d]		23
34	$Pb_3(HC_3N_3O_3)_2(OH)_2$	*C2/c*	3.95 [a]	0.342@800 nm [d]		23
35	$Li_2Zn_2(H_2Cya)_2(HCya)(OH)_2\cdot 2H_2O$	$I4_1/a$	5.21 [a]	0.174@1064 nm [d]		24
36	$BaZn_2(H_2Cya)_2(HCya)(OH)_2\cdot 2H_2O$	$I4_1/a$	3.72 [b]	0.191@1064 nm [d]		24
			$(H_2C_3N_3O_3)^-$			
37	$Li(H_2N_3C_3O_3)\cdot 1.75H_2O$	$P\bar{1}$	null	null	θ =0 γ=86.31, 89.55, 27.0	25
38	$Na(H_2C_3N_3O_3)\cdot H_2O$	$P\bar{1}$	~245 nm [a] (5.06)	0.39 [d]	θ =0 γ =17.28	1,2
*****	**$K(H_2C_3N_3O_3)(H_2O)$**	***C2/m***		**0.5@546.1 nm** [d]	**θ =0.16, 0.38 γ= 35.64**	**this work**
39	$Rb(H_2C_3N_3O_3)\cdot H_2O$ -I	$P2_1/c$	null	0.2 [d]	γ =42.93	1,4
40	$Rb(H_2C_3N_3O_3)\cdot H_2O$ -II	$P\bar{1}$	null			4
41	$Cs(H_2C_3N_3O_3)\cdot 0.5H_2O$	$P2_1/m$	~240 nm [a] (5.17)	0.39 [d]	18.38	1,4
42	$Sr(H_2C_3N_3O_3)\cdot 4H_2O$	$P2_1/c$	null	0.391 [d]	16.39	1,4

43	$Zn(H_2C_3N_3O_3)_2\cdot 3H_2O$	$P\bar{1}$	5.24 [a]	0.283@ 800 nm [d]	θ =6.20 γ =23.69, 21.33	[26]
44	$LiRb(H_2C_3N_3O_3)_2\cdot 2H_2O$	$P2_1/m$	5.16 [a]	0.256 [d]	34.63	[1,27]
45	$LiCs(H_2C_3N_3O_3)_2\cdot 2H_2O$	$P2_1/m$	5.12 [a]	0.24 [d]	34.69	[1,27]
46	$Mg(H_2C_3N_3O_3)_2\cdot 8H_2O$	$P\bar{1}$	5.15 [a]	0.293@800 nm [d]	θ =1.42 γ =6.18	[20,25]
47	$Mg(H_2C_3N_3O_3)_2\cdot 6H_2O$	$P\bar{1}$	5.21 [a]	0.093@800 nm [d]	θ =1.87 γ =49.44, 55.08, 77.79	[20]
48	$Ca(H_2C_3N_3O_3)_2\cdot 3H_2O$	$P\bar{1}$	5.14 [a]	0.245@800 nm [d]	θ =2.94 γ =37.44	[20]
49	α−$Sr(H_2C_3N_3O_3)_2\cdot 2H_2O$	$P\bar{1}$	5.12 [a]	0.379@800 nm [d]	θ =21.99 γ =45.88, 32.09	[20]
50	β−$Sr(H_2C_3N_3O_3)_2\cdot 2H_2O$	$P2_1/c$	4.11 -4.52 [b]	0.257@800 nm [d]	θ =21.38 γ =9.59,11.80	[20]
51	$Ba(H_2C_3N_3O_3)_2\cdot 2H_2O$	$P\bar{1}$	5.13 [a]	0.271@800 nm [d]	θ =7.97 γ =44.37	[20]
52	$RbNH_4(H_2C_3N_3O_3)_2\cdot 2H_2O$	*Pnma*	5.24 [a]	0.40 @ 1064 nm [d]	θ =0 γ =14.12	[28]
53	$Li_2Ca(H_2C_3N_3O_3)_4\cdot 6H_2O$	*Cmcm*	5.21 [a]	**0.407@800 nm** [d]		[29]
54	$Na_2Ba(H_2C_3N_3O_3)_4\cdot 6H_2O$	*C2/c*	5.10 [a]	0.394@800 nm [d]		[29]
55	$K_2Mg(H_2C_3N_3O_3)_4\cdot 4H_2O$	*C2/m*	5.38 [a]	0.376@800 nm [d]		[30]
56	$K_2Ca(H_2C_3N_3O_3)_4\cdot 4H_2O$	*C2/m*	5.32 [a]	0.371@800 nm [d]		[30]
57	$K_2Zn(H_2C_3N_3O_3)_4\cdot 4H_2O$	*C2/m*	5.23 [a]	0.305@800 nm [d]		[31]
58	$K_2Cd(H_2C_3N_3O_3)_4\cdot 4H_2O$	*C2/m*	5.15 [a]	0.251@800 nm [d]		[31]
59	$Rb_2Ca(H_2C_3N_3O_3)_4\cdot 4(H_2O)$	*C2/m*	5.37 [a]	0.362 at 800 nm [d]		[30]
60	$Cs_2Mg(H_2C_3N_3O_3)_4\cdot 10H_2O$	$P\bar{1}$	5.30 [a]	0.391 [d]		[1,30]
61	$Cs_2Zn(H_2C_3N_3O_3)_4\cdot 4H_2O$	*C2/m*	4.40 [b]	0.264@800 nm [d]		[31]
62	$Rb_3Na(H_2C_3N_3O_3)_4\cdot 3H_2O$	$Pmn2_1$	5.30 [a]	0.389@532 nm [d]		[1]
63	$Cs_3Na(H_2C_3N_3O_3)_4\cdot 3H_2O$	$Pmn2_1$	5.46 [a]	0.29 @514 nm [d]		[32]
				0.365@532 nm [d]		[1]
64	$K_2Pb(H_2C_3N_3O_3)_4\cdot 4H_2O$	*Cm*	3.90 [a]	0.325@532 nm [d]		[33]
65	$K_3Pb(H_2C_3N_3O_3)_5\cdot 6H_2O$	*C2/m*	4.55 [a]	0.193@532 nm [d]		[33]
66	$Pb(H_2C_3N_3O_3)(OH)$	$P\bar{1}$	3.96 [a]	0.203@1064 nm [d]		[34]

67	$Pb(H_2C_3N_3O_3)F$	$P\bar{1}$	4.96 [a]	0.079@1064 nm [d]	[34]
68	$Ba_3(H_2Cya)_2(HCya)_2{\cdot}4H_2O$	$P\bar{1}$	null	null	[4]
			($H_3C_3N_3O_3$)		
69	$LiCl(H_3C_3N_3O_3)$	*R3m*	5.76 [a]	0.28@800 nm [d]	[5,35]
70	$NaCl(H_3C_3N_3O_3)$	$P6_3/mmc$	null	null	[5]
71	$NaBr(H_3C_3N_3O_3)$	$P6_3/mmc$	5.44 [a]	0.297@800 nm [d]	[6]
72	$KBr(H_3C_3N_3O_3)_3$	*Pnma*	5.33 [a]	0.273@800 nm [d]	[36]
73	$RbCl(H_3C_3N_3O_3)_2$	*P21/m*	5.45 [a]	0.071@800 nm [d]	[37]
74	$RbBr(H_3C_3N_3O_3)_2$	*P21/m*	5.42 [a]	0.075@800 nm [d]	[37]
75	$RbBr(H_3C_3N_3O_3)$	*Pbcm*	5.39 [a]	0.138@800 nm [d]	[6]
76	$RbI(H_3C_3N_3O_3)$	*Pnma*	4.99 [a]	0.227@800 nm [d]	[6]
77	$CsBr(H_3C_3N_3O_3)$	*Pbcm*	5.36 [a]	0.137@800 nm [d]	[6]
78	$CsCl(H_3C_3N_3O_3)_2$	$P2_1/m$	5.43 [a]	0.105@800 nm [d]	[37]
79	$K(H_3C_3N_3O_3)(NO_3)$	$P2_1/c$	4.8 [a]	0.268@800 nm [d]	[38]
80	$Rb(H_3C_3N_3O_3)(NO_3)$	$P2_1/c$	4.98 [a]	0.243@800 nm [d]	[38]
81	$Rb_3(H_2Cya)_3(H_3Cya){\cdot}4H_2O$		240 nm [a] (5.17)	null	[4]

[a] cut-off edge [b] calculated [c] experimental [d] theoretical

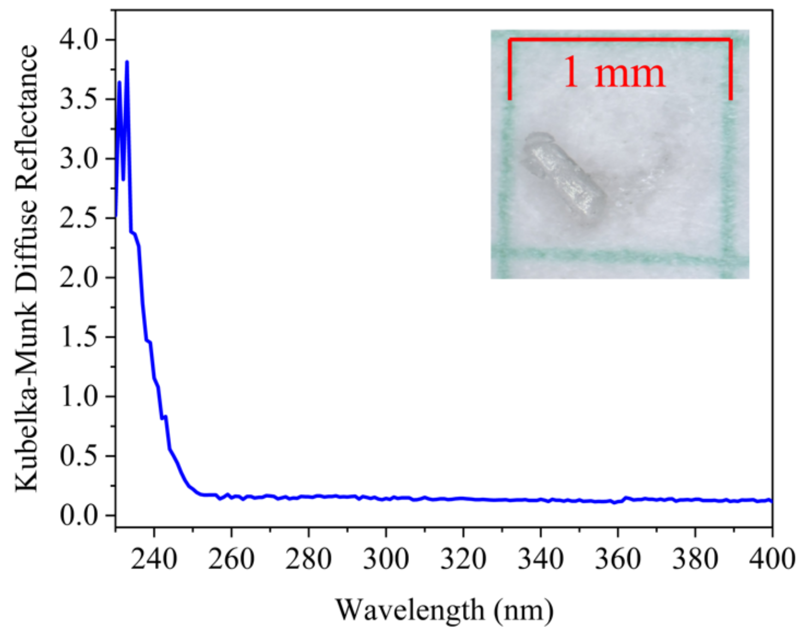

Figure S1. Kubelka-Munk Diffuse reflectance solid-state UV–Vis spectra of $K(H_2C_3N_3O_3)\cdot H_2O$. The insert is the optical photos of selected $K(H_2C_3N_3O_3)\cdot H_2O$ crystals. The unit of Y axis is R%.

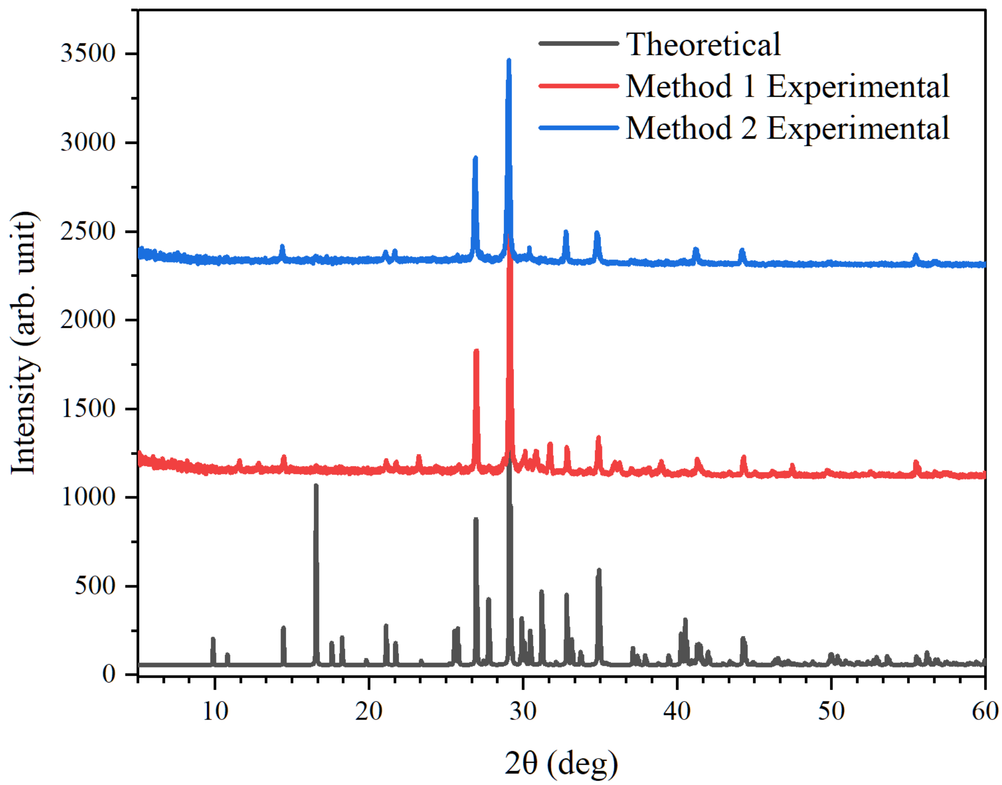

Figure S2. Room temperature powder X-ray diffraction of $K(H_2C_3N_3O_3)\cdot H_2O$.

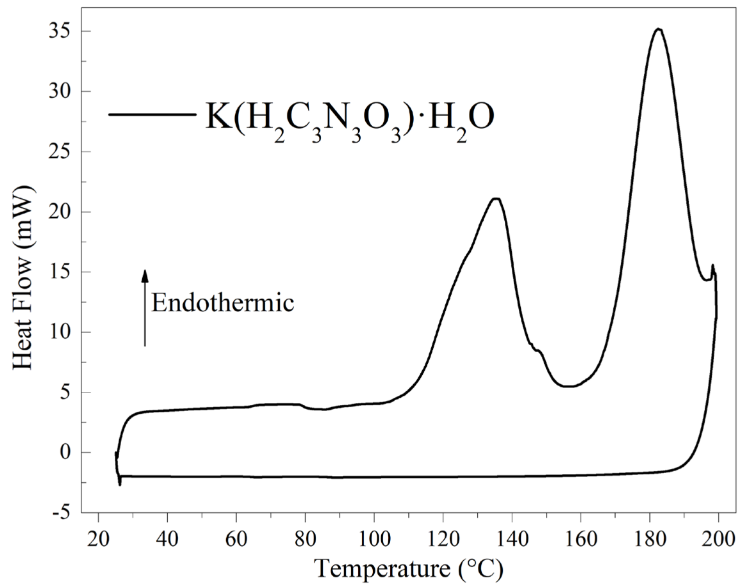

Figure S3. DSC results of $K(H_2C_3N_3O_3)\cdot H_2O$.

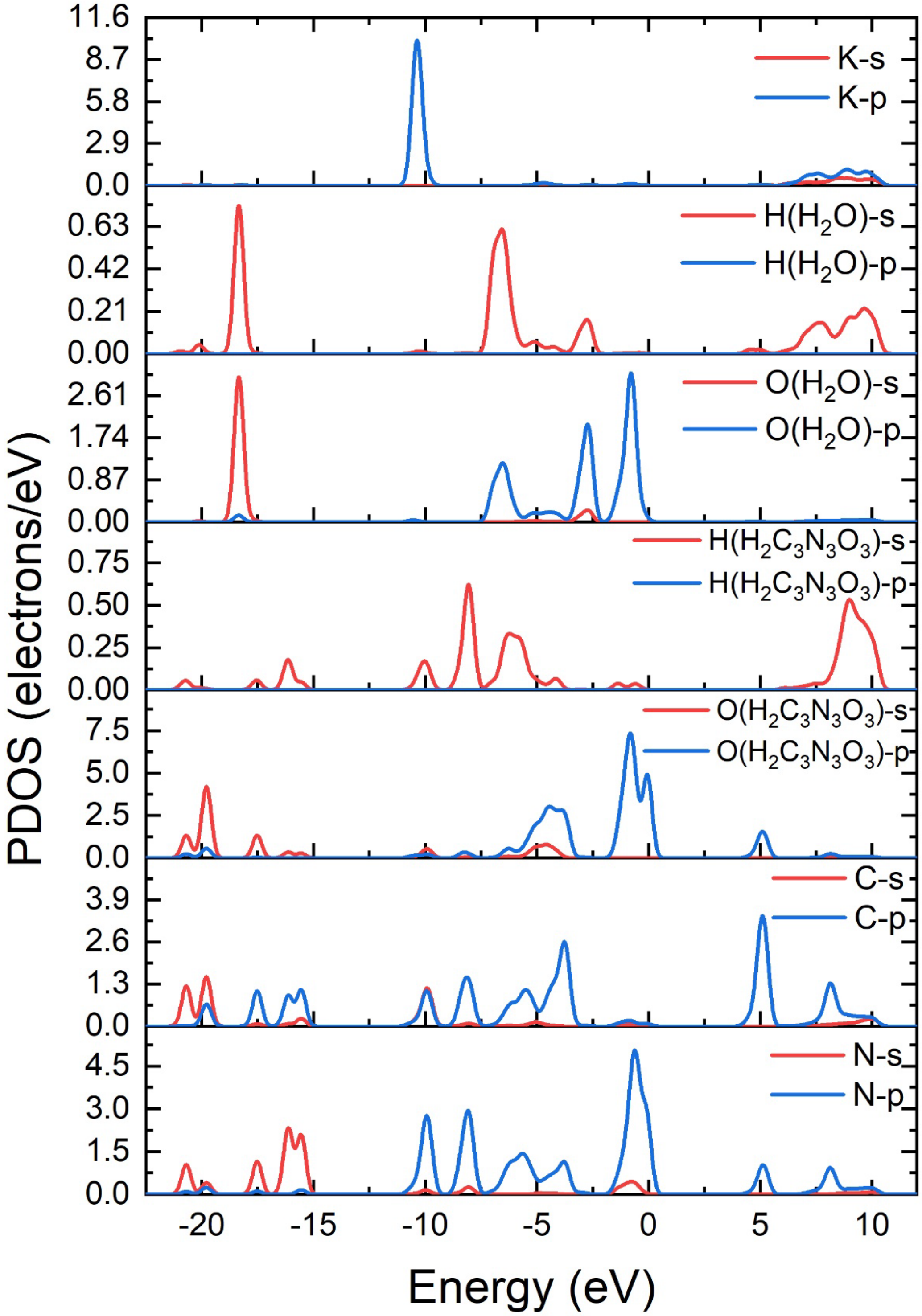

Figure S4. The partial density of states of $K(H_2C_3N_3O_3)\cdot H_2O$.

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