Supplementary Information

An alkali-metal isocyanurate $Cs_3(H_2C_3N_3O_3)_3(H_3C_3N_3O_3)\cdot 3H_2O$: synthesis and characterization

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1. Supplementary Tables.

Table S1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) of **$Cs_3(H_2C_3N_3O_3)_3(H_3C_3N_3O_3)\cdot 3H_2O$**.

Atom	x	y	z	$U_{(eq)}$[a]
Cs1	2068.9(3)	7920.1(3)	1421.7(3)	34.97(9)
Cs2	6103.3(3)	1847.2(3)	1739.3(3)	40.36(9)
Cs3	12085.4(3)	7236.1(3)	4586.1(3)	41.13(9)
O9	9134(3)	7621(3)	3841(3)	33.2(7)
O10	8344(3)	577(3)	3668(3)	39.7(8)
O6	9263(3)	8316(3)	1214(3)	37.0(8)
O3	2772(3)	1083(3)	1412(3)	37.1(8)
N3	2565(4)	3140(4)	1294(3)	28.5(9)
N9	6965(4)	7715(4)	3703(3)	27.6(8)
N5	7435(4)	6353(3)	1277(3)	28.5(8)
C5	6049(4)	5737(4)	1255(3)	25.3(9)
C2	-278(5)	1919(4)	1048(3)	26.8(9)
C12	11642(5)	3102(4)	3716(3)	25.6(9)
Cs1	2068.9(3)	7920.1(3)	1421.7(3)	34.97(9)
Cs2	6103.3(3)	1847.2(3)	1739.3(3)	40.36(9)

[a] $U_{(eq)}$ is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Anisotropic displacement parameters ($Å^2×10^3$) of **$Cs_3(H_2C_3N_3O_3)_3(H_3C_3N_3O_3)·3H_2O$**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cs1	29.55(16)	28.38(15)	53.2(2)	13.88(13)	16.29(14)	15.67(12)
Cs2	36.54(18)	34.22(16)	56.0(2)	12.94(14)	20.20(16)	17.09(14)
Cs3	37.23(18)	35.90(17)	54.5(2)	12.59(15)	18.89(16)	16.83(14)
O5	27.1(17)	21.5(15)	61(2)	19.9(15)	18.6(16)	9.2(13)
O2	19.0(16)	29.2(16)	61(2)	14.3(16)	15.1(16)	8.5(13)
O7	32.8(19)	26.9(17)	81(3)	18.5(17)	26.6(19)	18.2(15)
O4	25.7(17)	34.9(18)	71(3)	24.4(17)	22.8(18)	18.5(15)
N2	24(2)	18.2(18)	43(2)	12.5(17)	14.1(18)	6.9(16)
N6	24(2)	19.6(18)	51(3)	15,3(18)	18.0(19)	9.9(16)
N12	20.0(19)	22.8(18)	42(2)	13.7(16)	16.2(18)	7.9(16)
C5	24(2)	25(2)	29(2)	8.4(18)	11.1(19)	8.7(18)
C2	25(2)	24(2)	35(3)	9.4(19)	13(2)	12.6(19)
C12	25(2)	24(2)	32(2)	10.1(18)	14(2)	10.3(18)

Table S3. Selected bond lengths [Å] of $Cs_3(H_2C_3N_3O_3)_3(H_3C_3N_3O_3)\cdot 3H_2O$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cs1	Cs3[1]	4.4595(6)	Cs1	O2[4]	3.390(3)
O2	Cs1[4]	3.390(3)	Cs1	O7	3.632(4)
O2	Cs2[1]	3.098(3)	Cs1	O4	3.145(3)
O2	C2	1.243(5)	Cs1	C2[4]	3.486(4)
O4	C4	1.221(5)	Cs2	Cs1[5]	4.5650(6)
N6	C6	1.380(5)	Cs2	O8	3.575(3)
N5	C6	1.349(5)	N10	C10	1.344(5)
N1	C1	1.341(5)	N4	C5	1.378(5)

[1]-1+X,+Y,+Z; [2]+X,1+Y,+Z; [3]-1+X,1+Y,+Z; [4]-X,1-Y,-Z; [5]+X,-1+Y,+Z; [6]2-X,1-Y,1-Z; [7]1+X, +Y,+Z; [8]1-X,1-Y,-Z; [9]1+X,-1+Y,+Z

Table S4. Selected bond angles (°) of $Cs_3(H_2C_3N_3O_3)_3(H_3C_3N_3O_3)\cdot 3H_2O$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O6[1]	Cs1	O3[2]	72.63(8)	O12	Cs3	O9	121.38(8)
O12	Cs3	O8[6]	61.74(8)	O6[1]	Cs1	O7	133.83(8)
O12	Cs3	O11[2]	133.50(8)	O6[1]	Cs1	O4	150.71(8)
O12	Cs3	O7[8]	67.65(7)	O6[1]	Cs1	O15[2]	114.65(9)
O12	Cs3	N10[6]	122.41(7)	O3[2]	Cs1	N1[4]	92.44(8)
O6[1]	Cs1	N1[4]	64.99(9)	O3[2]	Cs1	O4	85.21(7)
O3[2]	Cs1	Cs3[1]	111.24(6)	O11[2]	Cs3	O8[6]	131.31(7)

[1]-1+X,+Y,+Z; [2]+X,1+Y,+Z; [3]-1+X,1+Y,+Z; [4]-X,1-Y,-Z; [5]+X,-1+Y,+Z; [6]2-X,1-Y,1-Z; [7]1+X, +Y,+Z; [8]1-X,1-Y,-Z; [9]1+X,-1+Y,+Z

Table S5. Birefringence properties of some isocyanurate compounds.

Compound	Δn	Ref
$K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$	0.181 @ 1064 nm	S1
$Li_2Zn_2(H_2C_3N_3O_3)_2(HC_3N_3O_3)(OH)_2 \cdot 2H_2O$	0.174 @ 1064 nm	S2
$BaZn_2(H_2C_3N_3O_3)_2(HC_3N_3O_3)(OH)_2 \cdot 2H_2O$	0.191 @ 1064 nm	S2
$Mg(H_2C_3N_3O_3)_2 \cdot 6H_2O$	0.093 @ 800 nm	S3
$RbLi(HC_3N_3O_3) \cdot 2H_2O$	0.180 @ 514.6 nm	S4
$SrHC_3N_3O_3$	0.184 @ 800 nm	S3
$RbNa(HC_3N_3O_3) \cdot 2H_2O$	0.194 @ 589.6 nm	S5
$KLi(HC_3N_3O_3) \cdot 2H_2O$	0.186 @ 514 nm	S6

2. Supplementary Figures.

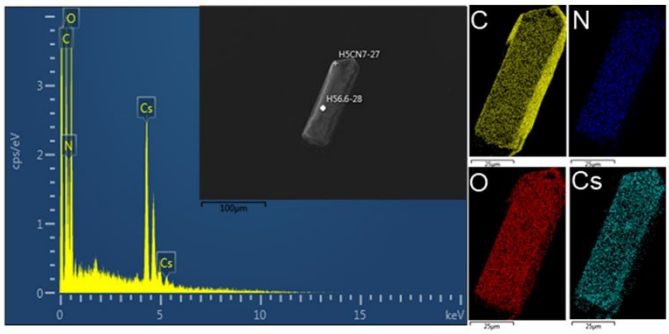

Figure S1. EDS analysis of $Cs_3(H_2C_3N_3O_3)_3(H_3C_3N_3O_3)\cdot 3H_2O$.

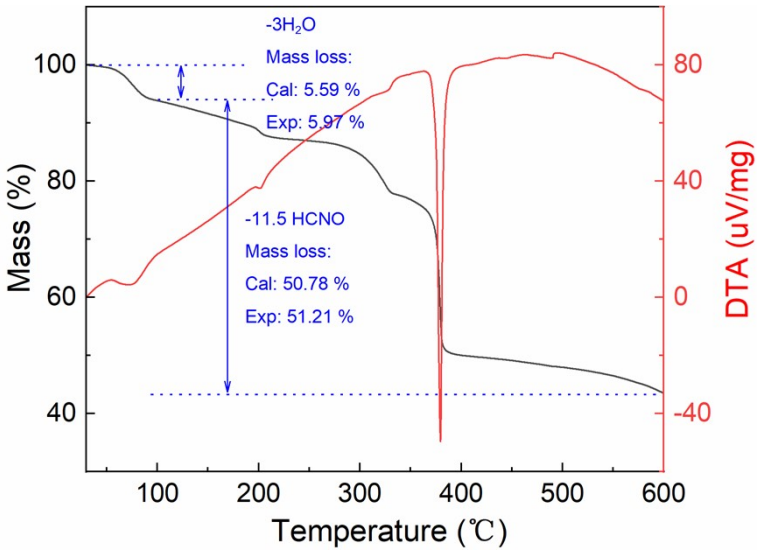

Figure S2. The TG and DTA curves (a) and PXRD patterns for the residual (b) of $Cs_3(H_2C_3N_3O_3)_3(H_3C_3N_3O_3)\cdot 3H_2O$.

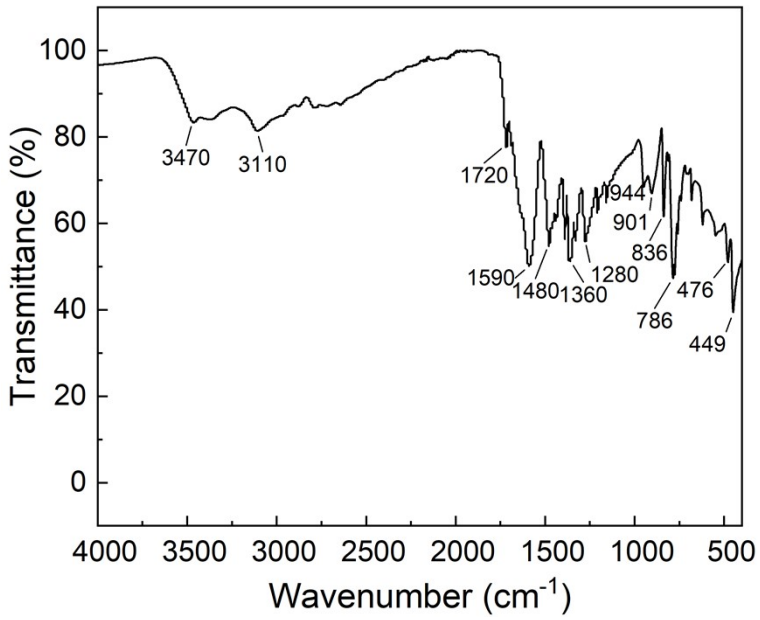

Figure S3. The IR spectrum of $Cs_3(H_2C_3N_3O_3)_3(H_3C_3N_3O_3)\cdot 3H_2O$.

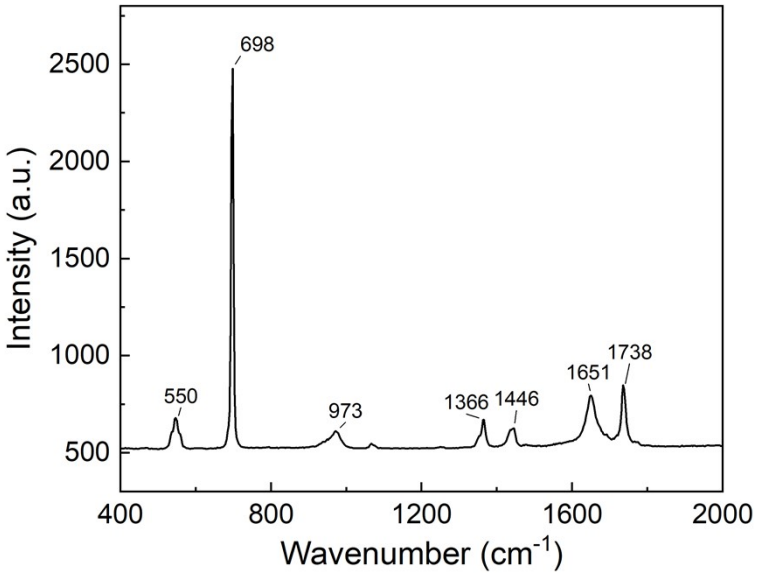

Figure S4. The Raman spectrum of $Cs_3(H_2C_3N_3O_3)_3(H_3C_3N_3O_3)\cdot 3H_2O$.

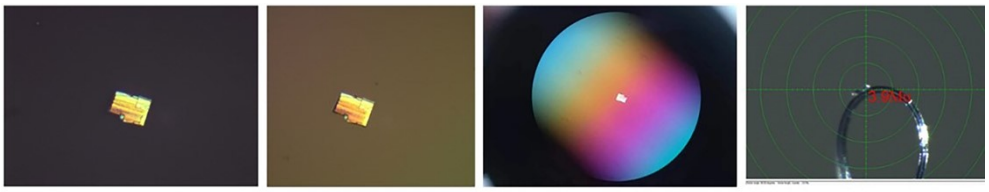

Figure S5. The measured birefringence of $Cs_3(H_2C_3N_3O_3)_3(H_3C_3N_3O_3)\cdot 3H_2O$.

References

S1. Y. Chen, C. L. Hu, Z. Fang and J. G. Mao, *Inorg. Chem. Front.*, 2021, **8**, 3547-3555.

S2. D. D. Wang, F. Liang, X. Y. Zhang, Z. G. Hu and Y. C. Wu, *Cryst. Growth Des*., 2021, **21**, 2348-2354.

S3. X. H. Meng, K. J. Kang, F. Liang, J. Tang, W. L. Yin, Z. S. Lin and M. J. Xia, *Inorg. Chem. Front*., 2020, **7**, 3674-3686.

S4. X. H. Meng, F. Liang, K. J. Kang, J. Tang, T. X. Zeng, Z. S. Lin and M. J. Xia, *Inorg. Chem*, 2019, **58**, 11289-11293.

S5. Y. X. Song, D. H. Lin, M. Luo, C. S. Lin, Q. L. Chen and N. Ye, *Inorg. Chem. Front*., 2020, **7**, 150-156.

S6. D. H. Lin, M. Luo, C. S. Lin, F. Xu and N. Ye, *J. Am. Chem. Soc*., 2019, **141**, 3390-3394.