Electronic Supplementary Material (ESI) for Dalton Transactions.
This journal is © The Royal Society of Chemistry 2021

Supporting Information

$Zn(H_2C_3N_3O_3)_2 \cdot 3H_2O$: the first single-$d^{10}$ transition metal based ultraviolet hydroisocyanurate crystal with large birefringence

Dandan Wang, [a] Xinyuan Zhang, [*, a] Fei Liang, [*, b] Zhanggui Hu [a] and Yicheng Wu [a]

[a] Tianjin Key Laboratory of Functional Crystal Materials, Institute of Functional Crystals, School of Materials Science and Engineering, Tianjin University of Technology, Tianjin 300384, China.

[b] State Key Laboratory of Crystal Materials and Institute of Crystal Materials, Shandong University, Jinan 250100, China.

Contents.

1. Supplementary Tables.

Table S1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) of **ZHCY**.

Atom	x	y	z	$U_{(eq)}$[a]
Zn1	4998.6(6)	831.5(4)	7573.3(3)	30.22(13)
O1	6416(4)	3405(3)	6374(2)	39.3(6)
O2	6673(4)	3297(2)	10267(2)	35.4(5)
O3	8775(4)	8028(2)	9608(2)	40.7(6)
O4	1370(4)	2660(2)	3657(2)	39.0(6)
O5	1020(4)	2675(3)	7480(2)	39.8(6)
O6	3710(4)	7320(2)	6842(2)	38.9(6)
O7	3200(5)	130(3)	5723(2)	51.2(7)
O8	2957(5)	-75(4)	8410(3)	60.6(8)
O9	7617(5)	138(3)	7778(3)	54.8(7)
C1	6812(5)	4076(3)	7498(3)	26.3(6)
C2	6929(5)	4019(3)	9523(3)	26.2(6)
C3	8133(5)	6585(3)	9215(3)	29.0(6)
C4	1619(5)	3340(3)	4766(3)	28.5(6)
C5	1406(5)	3347(3)	6723(3)	29.0(6)
C6	2901(5)	5881(3)	6437(3)	26.7(6)
N1	6378(4)	3247(3)	8275(2)	25.0(5)
N2	7783(5)	5665(3)	9952(3)	29.6(6)
N3	7709(4)	5715(3)	7995(3)	29.4(6)
N4	1031(5)	2536(3)	5514(2)	36.6(7)
N5	2284(4)	4995(3)	7151(3)	28.5(6)
N6	2537(4)	4984(3)	5241(2)	27.4(5)

[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 **ZHCY**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn1	31.9(2)	23.13(19)	30.4(2)	5.78(14)	10.15(15)	5.48(14)
O1	58.9(15)	25.6(11)	21.7(11)	4.8(9)	14.1(11)	-0.2(10)
O2	55.7(14)	25.0(11)	23.2(11)	9.3(9)	15.7(10)	8.1(10)
O3	60.4(15)	19.8(11)	33.9(13)	5.4(9)	15.3(11)	6.7(10)
O4	63.7(15)	22.7(11)	26.9(12)	4.6(9)	22.8(11)	5.7(10)
O5	59.8(15)	26.2(11)	29.3(12)	10.3(10)	21.5(11)	1.8(11)
O6	58.6(15)	15(1)	35.7(13)	3.3(9)	20.7(11)	2.1(10)
O7	58.8(17)	29.1(13)	41.7(15)	9.9(11)	-2.8(13)	2.5(12)
O8	64.5(19)	48.1(17)	63(2)	6.0(15)	35.3(16)	9.0(15)
O9	49.8(16)	38.5(15)	68(2)	10.0(14)	17.2(14)	13.2(13)
C1	26.5(14)	24.6(14)	23.3(15)	7.4(12)	6.8(12)	4.5(11)
C2	30.6(15)	21.1(14)	25.2(15)	5.7(11)	9.7(12)	8.9(12)
C3	33.2(15)	24.2(15)	26.5(15)	7.4(12)	8.2(13)	9.0(12)
C4	38.8(16)	20.3(14)	24.6(15)	6.6(12)	12.6(13)	7.1(12)
C5	36.9(16)	22.2(14)	25.6(15)	7.2(12)	13.3(13)	5.4(12)
C6	30.8(15)	24.4(14)	24.1(15)	7.0(12)	10.8(12)	8.5(12)
N1	32.4(13)	18.6(11)	19.0(12)	4.6(9)	7.6(10)	4.7(10)
N2	46.0(16)	20.8(12)	18.4(13)	4(1)	11.5(12)	8.4(11)
N3	40.5(15)	19.8(12)	25.5(14)	9.4(11)	12.6(12)	4.5(11)
N4	61.4(18)	18.2(12)	26.5(14)	5.5(10)	22.1(13)	3.4(12)
N5	40.8(15)	18.8(12)	22.2(13)	3.6(10)	14.9(11)	3.6(10)
N6	39.7(14)	17.9(12)	25.6(13)	8.6(10)	17.3(11)	4.7(10)

Table S3. Selected bond lengths [Å] of **ZHCY**.

Bond	Length/Å
Zn1-N1	2.030
Zn1-O7	2.006
Zn1-O9	2.013
Zn1-O8	2.028
C1-O1	1.229
C2-O2	1.233
C3-O3	1.211
C4-N4	1.240
C5-O5	1.239
C6-O6	1.209
C1-N1	1.360
C1-N3	1.377
C2-N1	1.356
C2-N2	1.380
C3-N2	1.365
C3-N3	1.366

Table S4. Hydrogen bond lengths [Å] of **ZHCY**.

Hydrogen Bond	Length/Å
N2-H2···O5	2.02
N3-H3···O4	2.027
N5-H5···O2	2.036
N6-H6···O1	2.01

Table S5. Selected bond angles (°) of **ZHCY**.

Angle	(°)
C1-N1-C2	120.4
C2-N2-C3	125.0
C1-N3-C3	124.5
C4-N4-C5	119.4
C5-N5-C6	124.1
C4-N6-C6	124.3
N1-C1-N3	118.4
N1-C2-N2	117.9
N2-C3-N3	113.3
N4-C4-N6	121.7
N4-C5-N5	119.4
N5-C6-N6	113.5

2. Supplementary Figures.

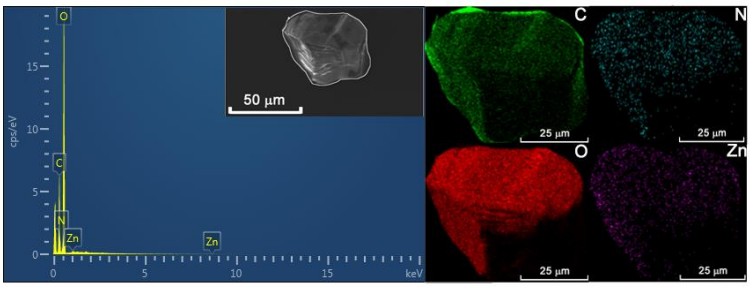

Figure S1. EDS analysis of **ZHCY**.

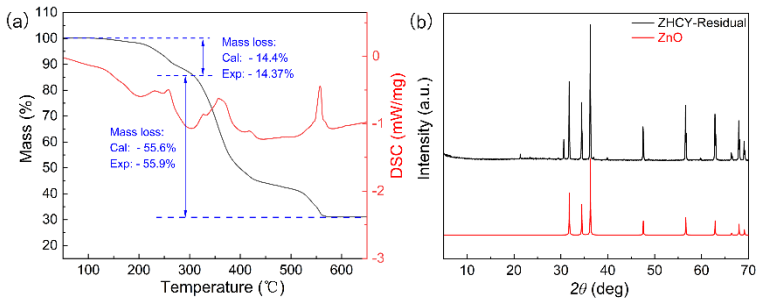

Figure S2. The TG and DSC curves (a) and PXRD patterns for the residual (b) of **ZHCY**.

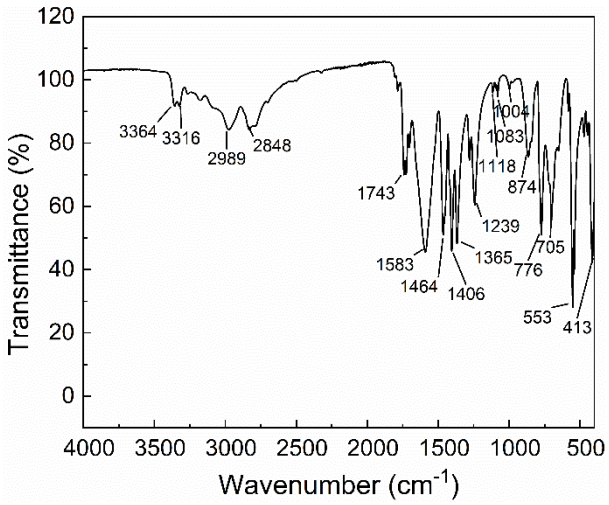

Figure S3. The IR spectrum of **ZHCY**.

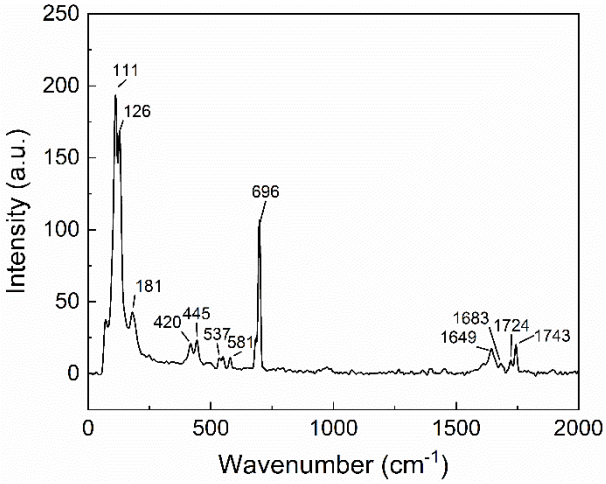

Figure S4. The Raman spectrum of **ZHCY**.

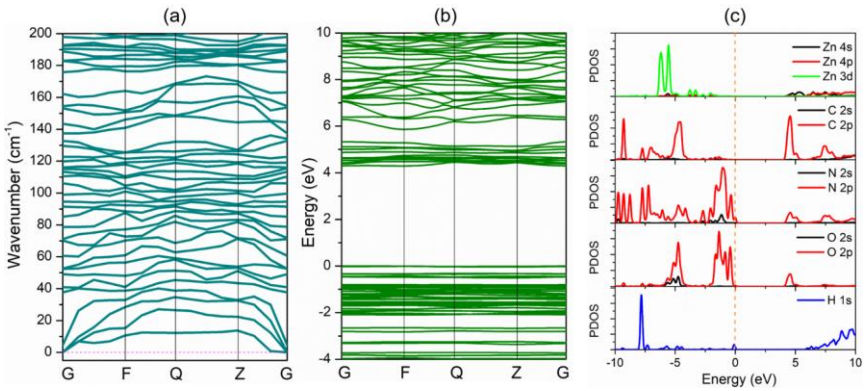

Figure S5. Band calculations of **ZHCY**. (a) phonon dispersion spectrum, (b) band structure, (c) partial density of states.