Supporting Information

Rich structural chemistry in π-conjugated hydroisocyanurates: layered structures of $A_2B(H_2C_3N_3O_3)_4\cdot nH_2O$ (A=K, Rb, Cs; B=Mg, Ca; n = 4, 10) with high ultraviolet transparency and strong optical anisotropy

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Experimental procedures

Synthesis. All chemicals containing K_2CO_3, Rb_2CO_3, $Mg(OH)_2$, $Ca(OH)_2$, Cs_2CO_3 and $H_3C_3N_3O_3$ were used without further purification and their dissolution in deionized water took place in air.

Compounds **I**, **II** and **III** were synthesized by dissolving K_2CO_3/Rb_2CO_3 (0.25 mmol), $Mg(OH)_2$/$Ca(OH)_2$ (0.25 mmol) and $H_3C_3N_3O_3$ (1 mmol) in 40 mL of demineralized water in a clean beaker with stirring and heating using magnetic stirrer at the boiling point until the solution was concentrated to 25 mL. Then the beaker was put in the open air to cool down naturally. Colorless rod-like crystals with regular shapes were obtained after cooling down to room temperature.

Compound **IV** was obtained by dissolving Cs_2CO_3 (0.25 mmol), $Mg(OH)_2$ (0.25 mmol) and $H_3C_3N_3O_3$ (1 mmol) in 50 mL of demineralized water in a clean beaker with stirring and heating using magnetic stirrer at the boiling point until the solution was concentrated to 30 mL. Then the beaker was put in the open air to cool down naturally. Colorless rod-like crystals with regular shapes were obtained after cooling down to room temperature.

Powder X-ray diffraction. The powder X-ray diffraction (PXRD) data of the target samples were successfully collected on Bruker D8 Focus diffractometer equipped with Cu Kα radiation(λ=1.5418 Å) in the 2θ range of 5-70° at room temperature.

UV–vis–NIR diffuse reflectance spectrum. The UV-vis-NIR diffuse reflectance spectra were measured in the wavelength range from 200 nm to 1500 nm with $BaSO_4$ as a reference material by Cary 7000 UV-vis-NIR universal measurement spectrophotometer under an integrating sphere.

Infrared spectrum. Infrared (IR) spectroscopy was collected on a Varian Excalibur 3100 spectrometer in the 400 - 3700 cm^{-1} range. **I**, **II**, **III** and **IV** and KBr samples were mixed thoroughly with mass ratio about 1:100, respectively.

Raman spectrum. Room temperature Raman spectra of **I** - **IV** were measured using an InVia Raman spectrometer (Renishaw, Inc.) with exciting wavelength at 532 nm in the 100-2500 cm^{-1} range.

Elemental Analysis. Energy dispersive X-ray spectroscopy (EDX) elemental mapping images of **I** - **IV** were analyzed by field emission scanning electron microscopy (SEM, Hitachi S-4800) at an accelerating voltage of 10 kV.

Thermal analysis. Thermal gravimetric analysis (TGA) were carried out on NETZSCH STA 409 CD thermal analyzer at a temperature range of 50-650 °C and 50-600 °C for **III** and **IV** respectively with a heating rate of 10 K/min in nitrogen atmosphere.

Single crystal structure determination. The single-crystal X-ray diffraction data was gathered on a Rigaku AFC10 single-crystal diffractometer equipped with graphite-monochromatic Mo Kα radiation (λ= 0.71073 Å) and Saturn CCD detector at 293 K. The intensity data, data reduction and cell refinement were captured by the CrystalClear program. The crystal structures were settled by the direct method with grogram SHELXS-97 and further refined by full matrix least squares on F^2 by SHELXL-97 programs. The structure was confirmed by using the ADDSYM algorithm from the program PLATON with no higher symmetry discovered. The crystallographic data are given in Table S1 - 3.

Computational methods.

The first-principles calculations for four compounds were performed by density functional theory (DFT)[1] method implemented in CASTEP package,[2] which has been successfully applied on metal cyanurates.[3-5] The generalized gradient density approximation (GGA-PBEsol functional)[6] was adopted and the norm-conserving pseudopotentials[7] for all elements were utilized to model ion-electron interactions. K $3p^64s^1$, Rb $4p^65s^1$, Cs $5p^66s^1$, Mg $2p^63s^2$, Ca $3p^64s^2$, C $2s^22p^2$, N $2s^22p^3$, O $2s^22p^4$ and H $1s^1$ electrons were treated as the valence electrons, respectively. The kinetic energy cutoff of 770 eV and Monkhorst-Pack *k*-point meshes[8] (2×2×4 for **I**, **II**, **III**; 4×3×2 for **IV**) in the first Brillouin zone were chosen to ensure the calculated results accuracy.

The scissors operator, set as the difference between the experimental and PBE bandgaps, was adopted in birefringence calculations. The specific IR and Raman vibrational modes were assigned by Vibrational Analysis module in CASTEP package based on linear response method.[9]

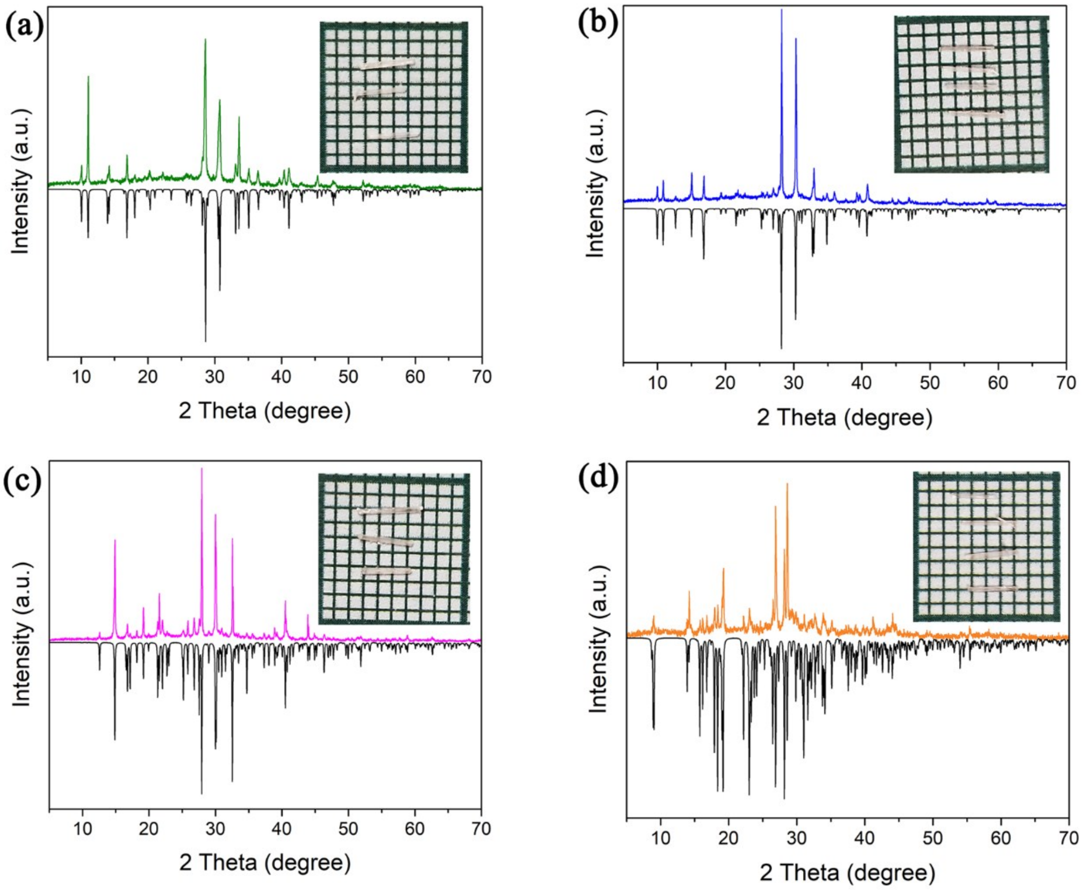

Figure S1. The calculated and experimental PXRD patterns for **I** - **IV**.

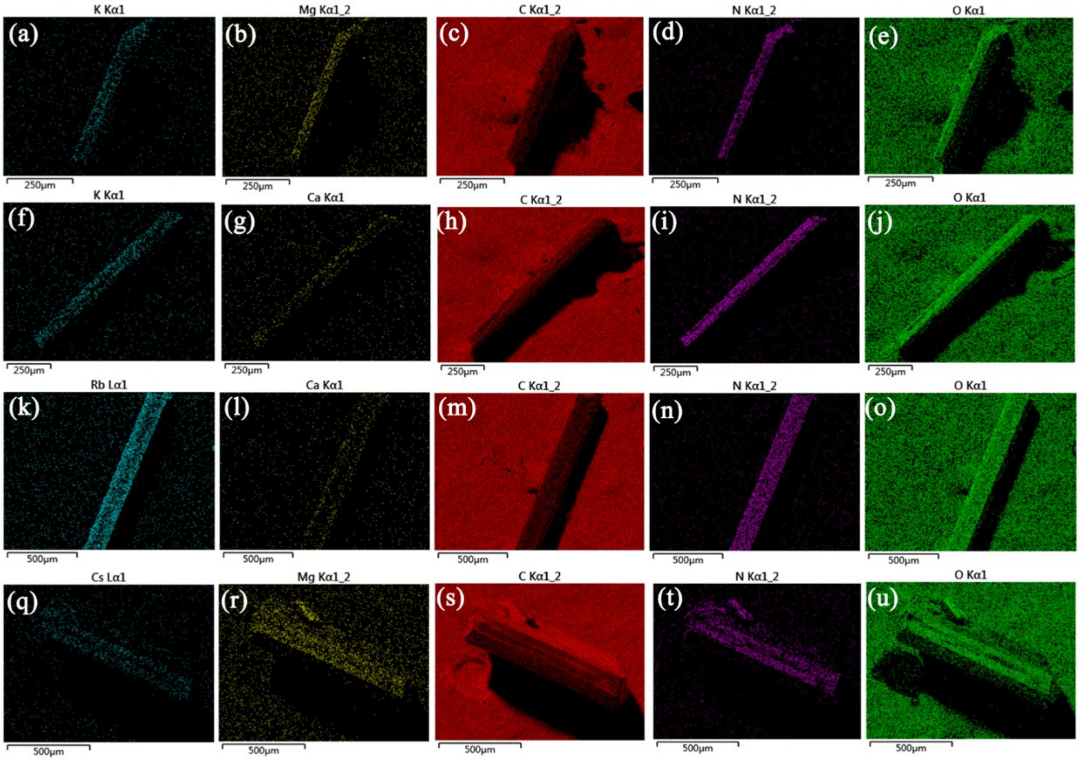

Figure S2. (a)-(e) EDX elemental mapping images of K, Mg, C, N and O; (f)-(j) EDX elemental mapping images of K, Ca, C, N and O; (k)-(o) EDX elemental mapping images of Rb, Ca, C, N and O; (q)-(u) EDX elemental mapping images of Cs, Mg, C, N and O.

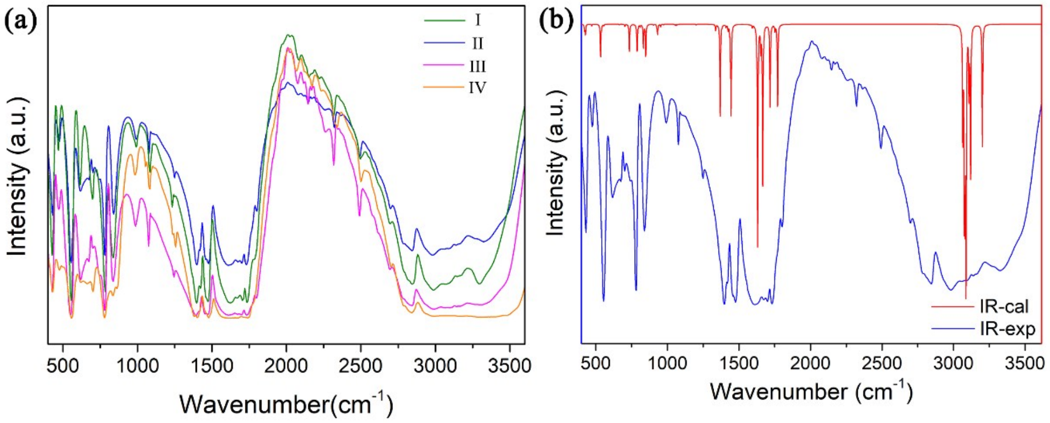

Figure S3. (a) The IR spectra for **I** – **IV**. (b) The experimental and theoretical IR spectra of **I**.

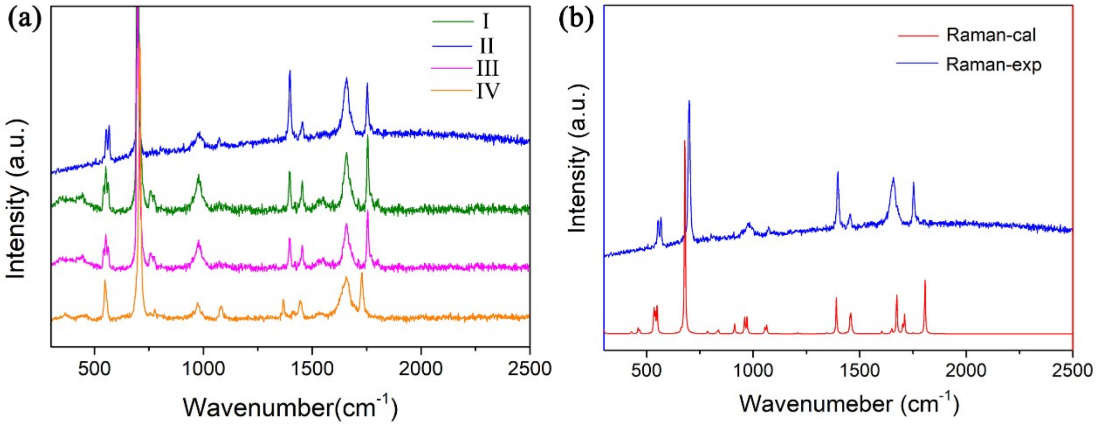

Figure S4. (a) The Raman spectra for **I**, **II**, **III** and **IV**, respectively. (b) The experimental and theoretical Raman spectra of I.

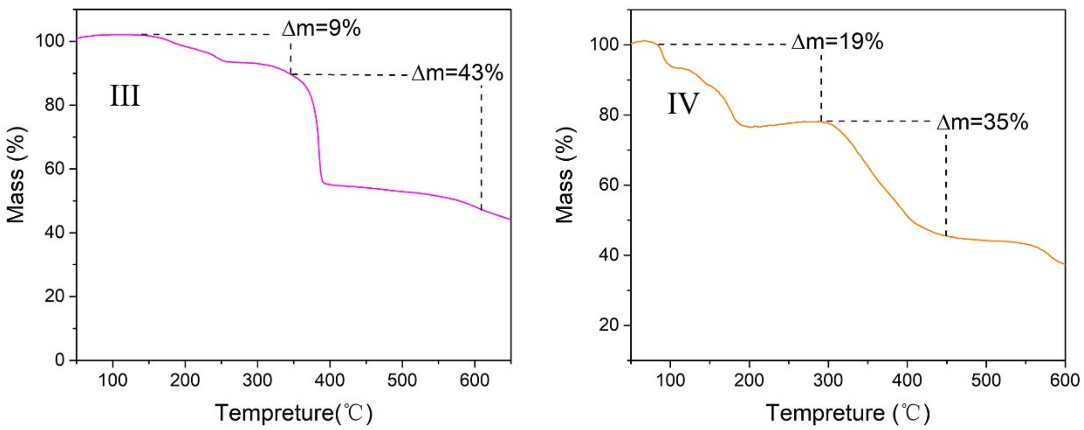

Figure S5. The TG curves for **III** and **IV**.

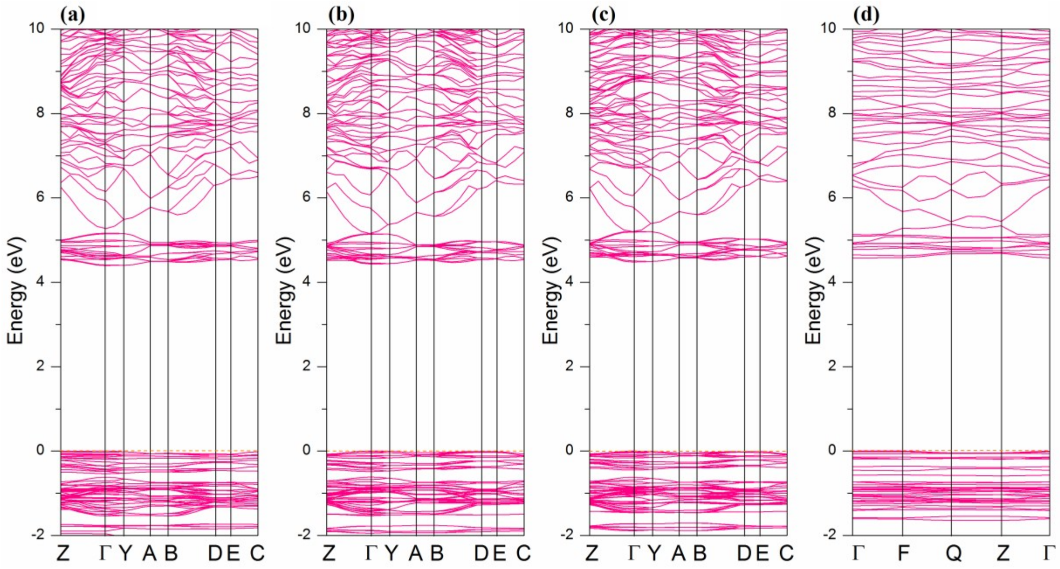

Figure S6. The band structures of I - IV.

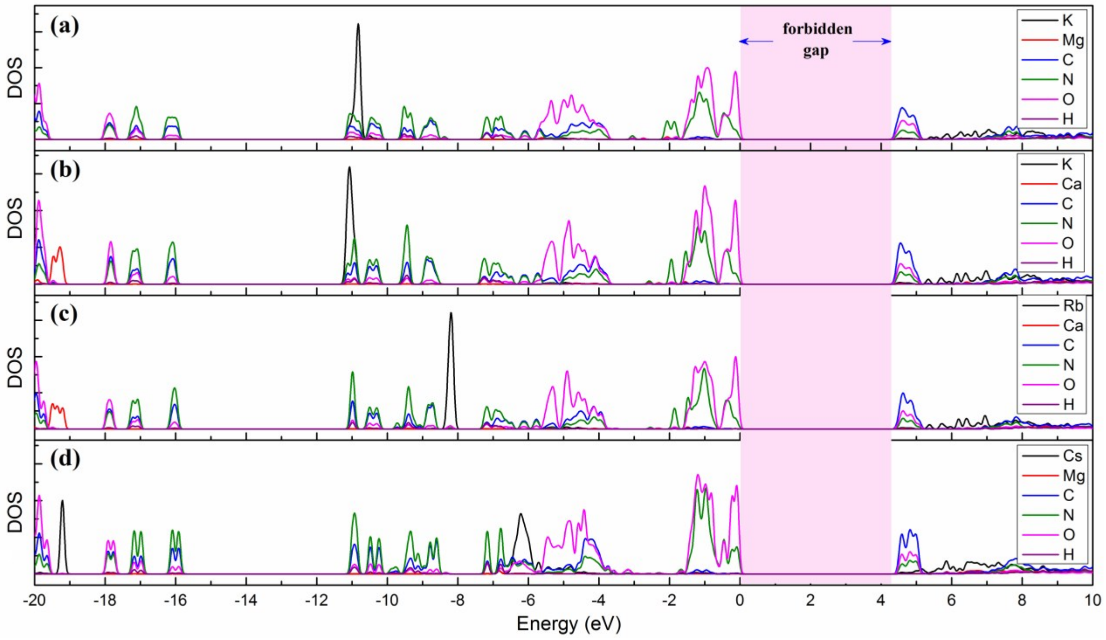

Figure S7. The density of states of I - IV.

Table S1. Crystal data and structure refinements for **I-IV.**

Molecule	**I**	**II**	**III**	**IV**
Formula weight	686.88	702.65	795.39	982.59
Temperature/K	293(2)	293(2)	293(2)	293(2)
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	*C*2/m	*C*2/m	*C*2/m	$P\bar{1}$
a/Å	11.7623(7)	10.6818(3)	10.7222(8)	6.7827(2)
b/Å	15.9722(9)	16.2953(4)	16.4782(10)	11.4995(3)
c/Å	6.9802(4)	7.0758(2)	7.1339(5)	11.8268(3)
α/°	90.00	90.00	90.00	113.871(3)
β/°	116.867 (6)	99.574(3)	99.950(7)	102.466(2)
γ/°	90.00	90.00	90.00	102.313(2)
Volume/Å^3	1169.72(12)	1214.48(6)	1241.48(15)	775.58(4)
Z	2	2	2	2
ρ_{calc} g/cm^3	1.950	1.921	2.128	2.104
μ/mm^{-1}	0.542	6.279	4.252	2.480
F(000)	700.0	716.0	788.0	482.0
Goof on F^2	1.056	1.14	1.091	1.076
Final R indexes	R_1 = 0.0414,	R_1 = 0.0546,	R_1 = 0.0344,	R_1 = 0.0212,
[I>=2σ (I)]	wR_2 = 0.1073	wR_2 = 0.1482	wR_2 = 0.0894	wR_2 = 0.0532
Final R indexes	R_1 = 0.0441,	R_1 = 0.0595,	R_1 = 0.0380,	R_1 = 0.0236,
[all data]	wR_2 = 0.1106	wR_2 = 0.1732	wR_2 = 0.0910	wR_2 = 0.0543

$^aR_1=\sum||F_O|-|F_C||/\sum|F_O|$ and $wR_2=\left[\sum\left[w\left(F_O^2-F_C^2\right)^2\right]/\sum\left[w\left(F_O^2\right)^2\right]\right]^{\frac{1}{2}}$ for $F_O^2>2\sigma\left(F_C^2\right)$

Table S2. Fractional atomic coordinates, equivalent isotropic displacement parameters (Å^2) and bond valence sums (BVS) for **I-IV**.

I

Atom	*x*	*y*	*z*	Ueq	BVS
K1	0.14366(5)	0.5000	0.86569(9)	0.0276(2)	1.105
Mg1	0.5000	0.5000	1.0000	0.0160(3)	2.019
O1	0.5000	0.10722(10)	1.0000	0.0278(4)	-1.879
O2	0.59080(16)	0.5000	0.7978(3)	0.0218(4)	-1.967
O3	0.67303(16)	0.5000	1.2864(3)	0.0223(4)	-1.960
O5	0.29957(10)	0.35173(7)	0.9713(2)	0.0209(3)	-1.848
O4	0.0000	0.39332(11)	0.5000	0.0286(4)	-1.784
O6	0.19564(10)	0.14781(7)	0.5111(2)	0.0219(3)	-1.478
N1	0.5000	0.36050(11)	1.0000	0.0144(4)	-3.047
N2	0.0000	0.14074(12)	0.5000	0.0167(4)	-2.749
N3	0.40005(12)	0.23039(8)	0.9882(2)	0.0174 (3)	-2.579
N4	0.09928(12)	0.27025(8)	0.5076(2)	0.0183(3)	-2.580
C1	0.39699(13)	0.31710(10)	0.9858(2)	0.0139(3)	4.110
C2	0.10047(14)	0.18374(10)	0.5060(2)	0.0150(3)	4.117
C3	0.5000	0.18349(14)	1.0000	0.0164(5)	4.233
C4	0.0000	0.31711(14)	0.5000	0.0171(5)	4.216

II

Atom	x	y	z	Ueq	BVS
K1	0.13712(8)	0.5000	0.77959(10)	0.0389(3)	0.684
Ca1	0.5000	0.5000	1.0000	0.0361(4)	2.271
O1	0.5000	0.10436(14)	1.0000	0.0347(6)	-1.791
O2	0.6906(3)	0.5000	0.8661(4)	0.0367(6)	-2.230
O3	0.6066(3)	0.5000	1.3251(4)	0.0409(7)	-2.224
O5	0.30171(15)	0.34603(10)	0.8273(2)	0.0301(5)	-1.485
O4	0.0000	0.38943(15)	0.5000	0.0347(6)	-1.555

O6	0.19636(15)	0.14871(9)	0.6797(2)	0.0291(5)	-1.471
N1	0.5000	0.35209(15)	0.0000	0.0233(6)	-3.241
N2	0.0000	0.14156(15)	0.5000	0.0232(6)	-2.885
N3	0.40067(17)	0.22532(11)	0.9090(2)	0.0244(5)	-2.592
N4	0.09915(17)	0.26851(11)	0.5916(2)	0.0240 (5)	-2.591
C1	0.39811(19)	0.31027(13)	0.9102 (3)	0.0216(5)	4.119
C2	0.10029(19)	0.18386(13)	0.5924(3)	0.0210(5)	4.130
C3	0.5000	0.18018(19)	0.0000	0.0231(6)	4.183
C4	0.0000	0.31424(18)	0.5000	0.0223(6)	4.188

III

Atom	*x*	*y*	*z*	Ueq	BVS
Rb1	0.13602(3)	0.5000	0.77450(5)	0.03095(18)	1.160
Ca1	0.5000	0.5000	0.0000	0.0291(3)	2.343
O1	0.5000	0.10791(15)	0.0000	0.0300(6)	-1.883
O2	0.6855(3)	0.5000	0.8610(4)	0.0329(6)	-1.715
O3	0.6023(3)	0.5000	0.3246(4)	0.0338(7)	-2.740
O5	0.30266(17)	0.34568(12)	0.8251(3)	0.0274(4)	-1.737
O4	0.0000	0.38471(16)	0.5000	0.0322(7)	-1.925
O6	0.19568(17)	0.14761(11)	0.6811(3)	0.0269(4)	-1.555
N1	0.5000	0.35202(17)	1.0000	0.0200(6)	-3.165
N2	0.0000	0.14052(18)	0.5000	0.0203(6)	-2.869
N3	0.40109(19)	0.22703(13)	0.9089(3)	0.0213(5)	-2.605
N4	0.0988(2)	0.26578(13)	0.5914(3)	0.0219(5)	-2.669
C1	0.3978(2)	0.31073(16)	0.9092(3)	0.0196(5)	4.151
C2	0.1003(2)	0.18198(16)	0.5926(3)	0.0186(5)	4.145
C3	0.5000	0.1821(2)	0.0000	0.0199(7)	4.230
C4	0.0000	0.3109(2)	0.5000	0.0204(7)	4.244

IV

Atom	*x*	*y*	*z*	Ueq	BVS

Cs1	0.33094(3)	0.554220(15)	0.169879(15)	0.03378(7)	-1.165
Mg1	0.5000	0.5000	0.5000	0.0211(2)	-2.198
C1	0.8555(4)	1.1921(2)	0.5533(2)	0.0242(5)	4.151
C2	0.8487(4)	1.1887(2)	0.3543(2)	0.0234(5)	4.147
C3	0.7325(4)	0.9764(2)	0.3582(2)	0.0271(5)	4.245
C4	0.2595(4)	1.0221(2)	0.2424(2)	0.0253(5)	4.152
C5	0.1600(4)	0.8072 (2)	0.0486 (2)	0.0258 (5)	4.263
C6	0.2618(4)	1.0207(2)	0.0465(2)	0.0269(5)	4.135
N1	0.7766(3)	1.05338(19)	0.48899(19)	0.0276(4)	-2.641
N2	0.7680(3)	1.04940(19)	0.29286(18)	0.0261(4)	-2.574
N3	0.8948(3)	1.25927(19)	0.48500(18)	0.0258(4)	-2.758
N4	0.2953(3)	1.09073(19)	0.17619(18)	0.0269(4)	-2.791
N5	0.1900(3)	0.88270(19)	0.17823(18)	0.0272 (4)	-2.600
N6	0.1941(3)	0.88115(19)	−0.01418(19)	0.0285(4)	-2.631
O1	0.6693(4)	0.85366(17)	0.30487(18)	0.0446(5)	-1.647
O2	0.6381(5)	0.6896(2)	0.0447(3)	0.0660(8)	-2.344
O3	0.8909(3)	1.25250(17)	0.67335(16)	0.0336(4)	-1.537
O4	0.1968(3)	0.49785(18)	0.41625(19)	0.0330(4)	-2.266
O5	0.2911(3)	1.07930(17)	0.36271(16)	0.0348(4)	-1.543
O6	0.4907(3)	0.37004(18)	0.31499(18)	0.0324(4)	-2.855
O7	0.8803(3)	1.24519(17)	0.28670(16)	0.0322(4)	-1.545
O8	0.3647(3)	0.33963(16)	0.52836(17)	0.0277(4)	-2.788
O9	0.1077(3)	0.68405(17)	−0.00441(17)	0.0343(4)	-1.602
O10	0.2896(4)	1.07699(18)	−0.02145(17)	0.0426(5)	-1.555
O11	0.7702(4)	0.4925(2)	0.2170(2)	0.0450(5)	-2.394

Table S3. Select bond lengths (Å) and angles (degree) for **I** - **IV**.

I			
K1—O3^{i}	2.8007 (18)	N2—C2^{ix}	1.3510 (18)
K1—O1^{ii}	2.8459 (11)	N2—C2	1.3510 (18)
K1—O1^{iii}	2.8459 (11)	N3—C3	1.3648 (18)
K1—O5^{iv}	2.8796 (12)	N3—C1	1.385 (2)
K1—O5	2.8796 (12)	N4—C4	1.3679 (18)
K1—O4	2.8939 (11)	N4—C2	1.382 (2)
K1—O4^{v}	2.8939 (11)	C1—N1—C1^{viii}	118.71 (19)
K1—O2^{i}	2.9393 (18)	C2^{ix}—N2—C2	118.89 (19)
Mg1—O3	2.1117 (18)	C3—N3—C1	124.50 (14)
Mg1—O3^{i}	2.1117 (18)	C4—N4—C2	123.94 (14)
Mg1—O2	2.1203 (17)	O5—C1—N1	122.74 (15)
Mg1—O2^{i}	2.1203 (17)	O5—C1—N3	117.84 (13)
Mg1—N1^{i}	2.2281 (18)	N1—C1—N3	119.43 (13)
Mg1—N1	2.2281 (18)	O6—C2—N2	121.97 (16)
O1—C3	1.218 (3)	O6—C2—N4	118.25 (14)
O5—C1	1.2347 (19)	N2—C2—N4	119.78 (14)
O4—C4	1.217 (3)	O1—C3—N3^{viii}	123.29 (10)
O5—C1	1.2347 (19)	O1—C3—N3	123.29 (10)
O4—C4	1.217 (3)	N3^{viii}—C3—N3	113.4 (2)
O6—C2	1.2440 (19)	O4—C4—N4	123.18 (10)
N1—C1	1.3601 (17)	O4—C4—N4^{ix}	123.18 (10)
N1—C1^{viii}	1.3601 (17)	N4—C4—N4^{ix}	113.6 (2)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2; (ii) *x*−1/2, *y*+1/2, *z*; (iii) −*x*+1/2, −*y*+1/2,

$-z+2$; (iv) $x, -y+1, z$; (v) $-x, -y+1, -z+1$; (vi) $-x, -y+1, -z+2$; (vii) $x+1/2, y-1/2, z$; (viii) $-x+1, y, -z+2$; (ix) $-x, y, -z+1$.

II			
K1—O2^{i}	2.853 (3)	O6—C2	1.246 (3)
K1—O1^{ii}	2.8688 (15)	N1—C1^{x}	1.350 (2)
K1—O1^{iii}	2.8688 (15)	N1—C1^{xi}	1.350 (2)
K1—O4	2.8881 (16)	N2—C2	1.348 (2)
K1—O4^{iv}	2.8881 (16)	N2—C2^{xii}	1.348 (2)
K1—O3^{i}	2.952 (3)	N3—C3^{vii}	1.362 (2)
K1—O5^{v}	3.0500 (16)	N3—C1	1.385 (3)
K1—O5	3.0500 (16)	N4—C4	1.367 (2)
Ca1—O2^{i}	2.384 (3)	N4—C2	1.379 (3)
Ca1—O2	2.384 (3)	O1^{x}—C3—N3^{xi}	122.70 (13)
Ca1—O3^{i}	2.391 (3)	O1^{x}—C3—N3^{x}	122.70 (13)
Ca1—O3	2.391 (3)	N3^{xi}—C3—N3^{x}	114.6 (3)
Ca1—N1^{vii}	2.410 (2)	O4—C4—N4^{xii}	123.04 (13)
Ca1—N1^{viii}	2.410 (2)	O4—C4—N4	123.04 (13)
O1—C3^{vii}	1.235 (4)	N4^{xii}—C4—N4	113.9 (3)
O5—C1	1.242 (3)	N2—C2—N4	120.23 (18)
O4—C4	1.225 (4)	C1^{x}—N1—C1^{xi}	119.4 (3)
C1^{x}—N1—Ca1^{x}	120.31 (13)	O5—C1—N1^{vii}	121.7 (2)
C1^{xi}—N1—Ca1^{x}	120.31 (13)	O5—C1—N3	118.80 (19)
C2—N2—C2^{xii}	118.5 (3)	N1^{vii}—C1—N3	119.49 (19)
C3^{vii}—N3—C1	123.50 (19)	O6—C2—N2	121.9 (2)
C4—N4—C2	123.55 (19)	O6—C2—N4	117.89 (18)

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

III			
Rb1—O4	2.9298 (17)	N3—C3$^{\mathrm{vii}}$	1.363 (3)
Rb1—O4$^{\mathrm{i}}$	2.9298 (17)	N3—C1	1.380 (3)
Rb1—O1$^{\mathrm{ii}}$	2.9476 (16)	N4—C4	1.365 (3)
Rb1—O1$^{\mathrm{iii}}$	2.9476 (16)	N4—C2	1.381 (3)
Rb1—O2$^{\mathrm{iv}}$	2.951 (3)	C1—N1—C1$^{\mathrm{xii}}$	119.7 (3)
Rb1—O3$^{\mathrm{v}}$	3.010 (3)	C1—N1—Ca1$^{\mathrm{vii}}$	120.13 (15)
Rb1—O5$^{\mathrm{vi}}$	3.0929 (19)	C1$^{\mathrm{xii}}$—N1—Ca1$^{\mathrm{vii}}$	120.13 (15)
Rb1—O5	3.0929 (19)	C2$^{\mathrm{xiii}}$—N2—C2	119.0 (3)
Ca1—O2$^{\mathrm{v}}$	2.371 (3)	C3$^{\mathrm{vii}}$—N3—C1	124.1 (2)
Ca1—O2$^{\mathrm{ix}}$	2.371 (3)	C4—N4—C2	123.7 (2)
Ca1—O3$^{\mathrm{x}}$	2.385 (3)	O5—C1—N1	122.0 (3)
Ca1—O3	2.385 (3)	O5—C1—N3	119.0 (2)
Ca1—N1$^{\mathrm{v}}$	2.438 (3)	N1—C1—N3	119.0 (2)
Ca1—N1$^{\mathrm{ix}}$	2.438 (3)	O6—C2—N2	122.4 (3)
O1—C3	1.222 (5)	O6—C2—N4	117.8 (2)
O5—C1	1.234 (3)	N2—C2—N4	119.8 (2)
O4—C4	1.216 (5)	O1—C3—N3$^{\mathrm{xiv}}$	122.92 (15)
O6—C2	1.242 (3)	O1—C3—N3$^{\mathrm{ix}}$	122.92 (15)
N1—C1	1.355 (3)	N3$^{\mathrm{xiv}}$—C3—N3$^{\mathrm{ix}}$	114.2 (3)
N1—C1$^{\mathrm{xii}}$	1.355 (3)	O4—C4—N4	123.04 (16)
N2—C2$^{\mathrm{xiii}}$	1.347 (3)	O4—C4—N4$^{\mathrm{xiii}}$	123.04 (16)
N2—C2	1.347 (3)	N4—C4—N4$^{\mathrm{xiii}}$	113.9 (3)

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

IV			
Cs1—O2$^{\mathrm{i}}$	3.012 (2)	C6—N4	1.351 (3)
Cs1—O9$^{\mathrm{ii}}$	3.1396 (19)	C6—N6	1.383 (3)
Cs1—O3$^{\mathrm{iii}}$	3.1521 (18)	O3—C1—N3	121.7 (2)
Cs1—O11	3.193 (2)	O3—C1—N1	118.8 (2)
Cs1—O1	3.2048 (18)	N3—C1—N1	119.5 (2)
Cs1—O8$^{\mathrm{iv}}$	3.2723 (17)	O7—C2—N3	121.9 (2)
Cs1—O2	3.282 (2)	O7—C2—N2	118.4 (2)
Cs1—O9	3.2983 (18)	N3—C2—N2	119.66 (19)
Cs1—O6	3.4240 (19)	O1—C3—N1	122.6 (2)
Cs1—O4	3.487 (2)	O1—C3—N2	123.4 (2)
Mg1—O8$^{\mathrm{iv}}$	2.0658 (16)	N1—C3—N2	114.1 (2)
Mg1—O8	2.0658 (16)	O5—C4—N4	122.5 (2)
Mg1—O6$^{\mathrm{iv}}$	2.0687 (17)	O5—C4—N5	117.3 (2)
Mg1—O6	2.0687 (17)	N4—C4—N5	120.1 (2)
Mg1—O4$^{\mathrm{iv}}$	2.0711 (18)	O9—C5—N6	123.9 (2)
Mg1—O4	2.0711 (18)	O9—C5—N5	122.4 (2)
C1—O3	1.241 (3)	N6—C5—N5	113.8 (2)
C1—N3	1.353 (3)	O10—C6—N4	122.4 (2)
C1—N1	1.374 (3)	O10—C6—N6	118.0 (2)
C2—O7	1.242 (3)	N4—C6—N6	119.6 (2)
C2—N3	1.347 (3)	C3—N1—C1	124.12 (19)
C2—N2	1.380 (3)	C3—N2—C2	123.42 (19)
C3—O1	1.216 (3)	C2—N3—C1	119.17 (19)
C3—N1	1.358 (3)	C4—N4—C6	118.64 (19)
C3—N2	1.371 (3)	C5—N5—C4	123.68 (19)
C4—O5	1.247 (3)	C5—N6—C6	124.1 (2)

C4—N4	1.339 (3)	C3—N1—C1	124.12 (19)
C4—N5	1.381 (3)	C3—N2—C2	123.42 (19)
C5—O9	1.223 (3)	C2—N3—C1	119.17 (19)
C5—N6	1.353 (3)	C4—N4—C6	118.64 (19)
C5—N5	1.363 (3)	C5—N5—C4	123.68 (19)
C6—O10	1.239 (3)	C5—N6—C6	124.1 (2)

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

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