

Poly[μ_2 -aqua-bis[μ_4 -2-(1*H*-1,2,3-benzotriazol-1-yl)acetato]dipotassium]

Qiong Liu

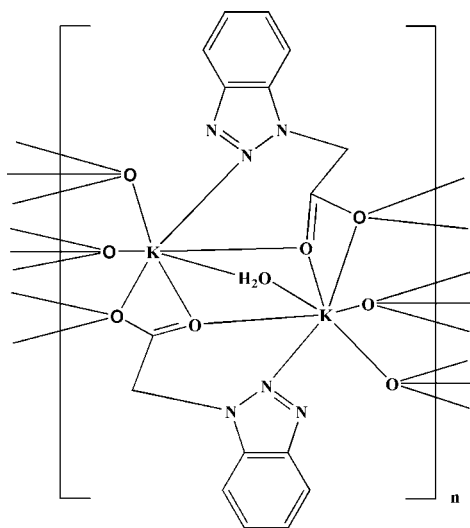
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.069; wR factor = 0.135; data-to-parameter ratio = 15.7.

In the title compound, $[\text{K}_2(\text{C}_8\text{H}_6\text{N}_3\text{O}_2)_2(\text{H}_2\text{O})]_n$, each K^+ ion is seven-coordinated by one O atom from a bridging water molecule, five carboxylate O atoms and one N atom from a benzotriazole group, forming a distorted mono-capped octahedral geometry. In the crystal, the carboxylate groups act as bridging ligands, forming a two-dimensional polymer parallel to (001). The aqua ligand, which lies on a twofold rotation axis, forms intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds within these layers.

Related literature

 For background and the synthesis, see: Hu *et al.* (2008).


Experimental

Crystal data

 $[\text{K}_2(\text{C}_8\text{H}_6\text{N}_3\text{O}_2)_2(\text{H}_2\text{O})]$
 $M_r = 448.53$

 Monoclinic, $C2$
 $a = 12.159$ (2) Å
 $b = 4.5893$ (9) Å
 $c = 17.666$ (4) Å
 $\beta = 104.98$ (3)°
 $V = 952.2$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.54$ mm⁻¹
 $T = 296$ K
 $0.30 \times 0.20 \times 0.12$ mm

Data collection

 Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.878$, $T_{\max} = 0.937$

 4827 measured reflections
 2140 independent reflections
 1508 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.053$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.069$
 $wR(F^2) = 0.135$
 $S = 1.05$
 2140 reflections
 136 parameters
 H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.46$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³
 Absolute structure: Flack (1983), 925 Friedel pairs
 Flack parameter: -0.02 (9)

Table 1

Selected bond lengths (Å).

K1—O2 ⁱ	2.718 (4)	K1—O1	2.872 (4)
K1—O3	2.760 (3)	K1—N2	2.934 (4)
K1—O2 ⁱⁱ	2.829 (3)	K1—O1 ⁱⁱ	3.287 (3)
K1—O2 ⁱⁱⁱ	2.835 (4)		

 Symmetry codes: (i) $x + \frac{1}{2}, y + \frac{1}{2}, z$; (ii) $-x + 1, y, -z + 1$; (iii) $x + \frac{1}{2}, y - \frac{1}{2}, z$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 ^{iv} ···O1 ^{iv}	0.87 (6)	1.87 (7)	2.729 (5)	167 (7)

 Symmetry code: (iv) $x, y - 1, z$.

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5422).

References

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 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 Hu, T. L., Du, W. P., Hu, B. W., Li, J. R., Bu, X. H. & Cao, R. (2008). *CrystEngComm*, **10**, 1037–1043.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supporting information

Acta Cryst. (2012). E68, m379 [https://doi.org/10.1107/S1600536812008963]

Poly[μ_2 -aqua-bis[μ_4 -2-(1*H*-1,2,3-benzotriazol-1-yl)acetato]dipotassium]**Qiong Liu****S1. Comment**

Organic ligands based on azole heterocycles or carboxylate groups which contain N and O donors have both good coordination ability and diverse coordination modes (Hu *et al.*, 2008). Therefore, the ligand 1*H*-benzotriazole-1-acetic acid was chosen to create coordination architectures. The synthesis of the ligand was the first step. But, when we synthesized the ligand according to the method of literature (see experimental section), the title complex (I) was obtained instead of the target ligand.

The title complex (I) is a polymeric potassium(I) complex of which the asymmetric is shown in Fig. 1. The environment of the K^I ion is a distorted mono-capped octahedral geometry. Each K^I ion is coordinated by one O atom from a water molecule, five carboxylate O atoms and one N atom from the ligands. The polymeric structure is a two-dimensional layer parallel to (001) (see, Fig .2).

S2. Experimental

Reagents and solvents were of commercially available quality. The title compound was synthesized according to the method of Hu *et al.* 2008. To a bromoacetonitrile solution of 1*H*-Benzotriazole (11.9 g), potassium hydroxide (6.8 g), anhydrous K_2CO_3 (13.8 g) and TEBA (benzyltriethylammoniumchloride, 99%, 0.15 g) were added. The mixture was stirred at room temperature for 30 min. After cooling to 283 K, 8.4 ml (0.075 mol) ethyl bromoacetate was added dropwise with further stirring. After standing at room temperature overnight the mixture was filtered and the filtrate was distilled under diminished pressure to obtain a yellow liquid. 100 ml water was added to the yellow liquid and the mixture was left to stand for 12 h at a condition of circumfluence. Single crystals suitable for X-ray diffraction were obtained after removing the solvent and recrystallizing in water and methanol solution (30 mL, 5: 1, v/v) at room temperature. Yield: 20%.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions ($C-H = 0.93-0.97 \text{ \AA}$) and were included in the refinement in the riding model approximation, with $U_{iso}(H)$ set to $1.2U_{eq}(C)$. The unique water H atom was located in a difference Fourier map, and were refined freely.

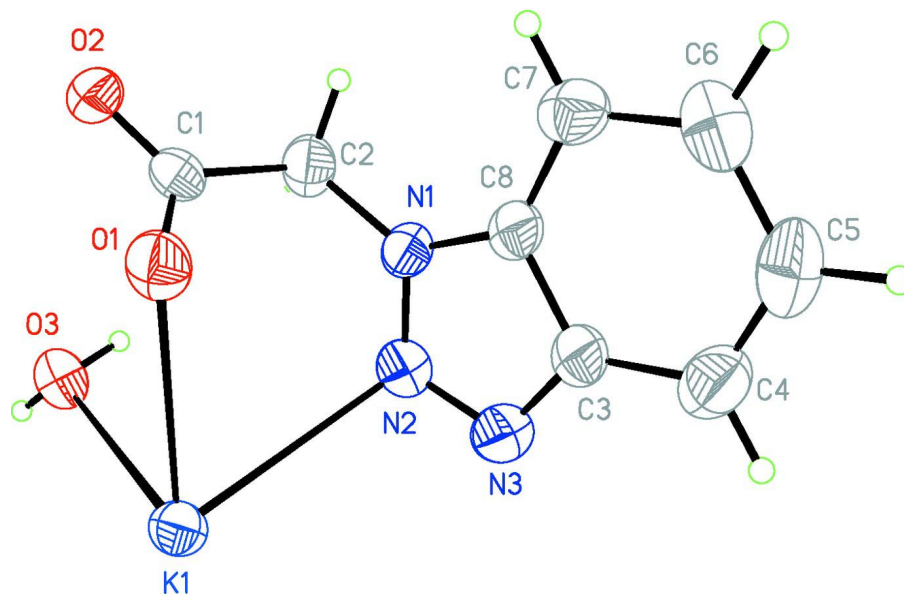


Figure 1

The asymmetric unit of the title complex showing 40% probability displacement ellipsoids for non-hydrogen atoms.

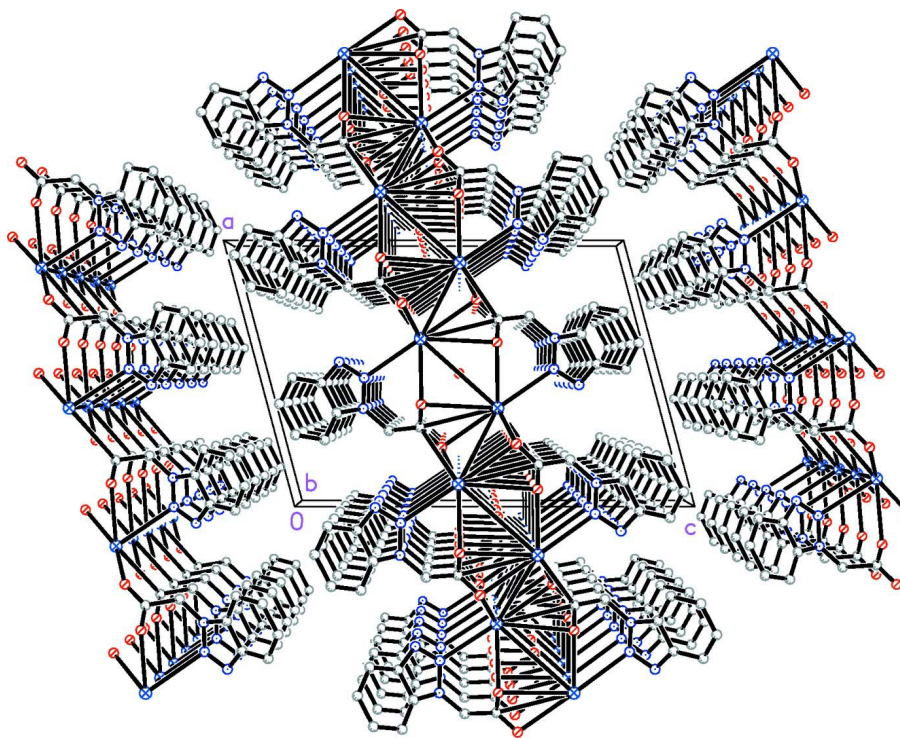


Figure 2

A packing diagram of the title compound, viewed along the *b* axis, showing the two-dimensional layered structure.

Poly[μ_2 -aqua-bis[μ_4 -2-(1*H*-1,2,3-benzotriazol-1-yl)acetato]dipotassium]

Crystal data

[K₂(C₈H₆N₃O₂)₂(H₂O)] $M_r = 448.53$ Monoclinic, *C*2Hall symbol: *C* 2y $a = 12.159$ (2) Å $b = 4.5893$ (9) Å $c = 17.666$ (4) Å $\beta = 104.98$ (3)° $V = 952.2$ (3) Å³ $Z = 2$ $F(000) = 460$ $D_x = 1.564$ Mg m⁻³Mo *K* α radiation, $\lambda = 0.71073$ Å

Cell parameters from 4308 reflections

 $\theta = 3.4$ – 27.6 ° $\mu = 0.54$ mm⁻¹ $T = 296$ K

Prism, colorless

 $0.3 \times 0.2 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.878$, $T_{\max} = 0.937$

4827 measured reflections

2140 independent reflections

1508 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.053$ $\theta_{\max} = 27.5$ °, $\theta_{\min} = 3.4$ ° $h = -15$ → 15 $k = -5$ → 5 $l = -22$ → 22

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.069$ $wR(F^2) = 0.135$ $S = 1.05$

2140 reflections

136 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier

map

Hydrogen site location: inferred from

neighbouring sites

H atoms treated by a mixture of independent

and constrained refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0551P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.46$ e Å⁻³ $\Delta\rho_{\min} = -0.24$ e Å⁻³

Absolute structure: Flack (1983), 925 Friedel

pairs

Absolute structure parameter: -0.02 (9)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
K1	0.62160 (7)	0.3984 (3)	0.43153 (5)	0.0478 (3)
O1	0.3919 (3)	0.6125 (7)	0.39356 (19)	0.0563 (9)
O2	0.2403 (2)	0.3829 (10)	0.41277 (15)	0.0495 (7)

N1	0.3763 (3)	0.3467 (9)	0.2538 (2)	0.0481 (10)
N2	0.4845 (3)	0.2466 (10)	0.2740 (2)	0.0601 (12)
N3	0.5400 (3)	0.3627 (15)	0.2268 (2)	0.0670 (13)
C1	0.3119 (3)	0.4388 (11)	0.3754 (2)	0.0388 (11)
C2	0.2979 (4)	0.2654 (12)	0.2991 (3)	0.0541 (13)
H2A	0.3078	0.0599	0.3119	0.065*
H2B	0.2208	0.2920	0.2670	0.065*
C3	0.4673 (4)	0.5401 (12)	0.1754 (3)	0.0489 (12)
C4	0.4849 (5)	0.7071 (14)	0.1142 (3)	0.0687 (16)
H4A	0.5550	0.7097	0.1023	0.082*
C5	0.3952 (5)	0.8677 (19)	0.0721 (3)	0.0718 (16)
H5A	0.4048	0.9844	0.0313	0.086*
C6	0.2893 (5)	0.8601 (15)	0.0894 (3)	0.0667 (15)
H6A	0.2297	0.9691	0.0588	0.080*
C7	0.2702 (4)	0.6970 (12)	0.1501 (3)	0.0562 (13)
H7A	0.2001	0.6952	0.1620	0.067*
C8	0.3618 (4)	0.5360 (11)	0.1923 (3)	0.0442 (11)
O3	0.5000	0.0180 (11)	0.5000	0.0529 (13)
H3	0.465 (4)	-0.090 (18)	0.461 (3)	0.083 (17)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0443 (5)	0.0509 (5)	0.0467 (6)	-0.0037 (6)	0.0089 (4)	0.0024 (6)
O1	0.060 (2)	0.054 (2)	0.055 (2)	-0.0158 (18)	0.0148 (16)	-0.0082 (17)
O2	0.0438 (15)	0.0609 (18)	0.0465 (17)	0.003 (2)	0.0165 (12)	0.004 (2)
N1	0.044 (2)	0.062 (3)	0.041 (2)	-0.008 (2)	0.0158 (16)	-0.006 (2)
N2	0.052 (3)	0.081 (3)	0.046 (3)	0.001 (2)	0.0098 (19)	-0.003 (2)
N3	0.050 (2)	0.095 (4)	0.058 (3)	-0.005 (3)	0.017 (2)	-0.008 (3)
C1	0.039 (2)	0.035 (3)	0.038 (2)	0.004 (2)	0.0025 (17)	0.007 (2)
C2	0.057 (3)	0.062 (3)	0.045 (3)	-0.020 (2)	0.016 (2)	-0.007 (2)
C3	0.052 (3)	0.058 (3)	0.037 (3)	-0.010 (3)	0.013 (2)	-0.016 (2)
C4	0.064 (4)	0.085 (4)	0.063 (4)	-0.015 (3)	0.028 (3)	-0.013 (3)
C5	0.103 (4)	0.069 (4)	0.051 (3)	-0.011 (5)	0.032 (3)	-0.003 (4)
C6	0.087 (4)	0.060 (4)	0.050 (3)	0.007 (4)	0.012 (3)	0.002 (3)
C7	0.052 (3)	0.061 (3)	0.057 (3)	0.004 (3)	0.016 (2)	-0.016 (3)
C8	0.045 (3)	0.052 (3)	0.037 (3)	-0.007 (2)	0.013 (2)	-0.017 (2)
O3	0.065 (3)	0.042 (3)	0.048 (3)	0.000	0.008 (3)	0.000

Geometric parameters (Å, °)

K1—O2 ⁱ	2.718 (4)	C1—C2	1.536 (6)
K1—O3	2.760 (3)	C1—K1 ⁱⁱ	3.301 (4)
K1—O2 ⁱⁱ	2.829 (3)	C1—K1 ^v	3.461 (5)
K1—O2 ⁱⁱⁱ	2.835 (4)	C2—H2A	0.9700
K1—O1	2.872 (4)	C2—H2B	0.9700
K1—N2	2.934 (4)	C3—C4	1.386 (7)
K1—O1 ⁱⁱ	3.287 (3)	C3—C8	1.389 (6)

O1—C1	1.234 (5)	C4—C5	1.366 (8)
O1—K1 ⁱⁱ	3.287 (3)	C4—H4A	0.9300
O2—C1	1.248 (4)	C5—C6	1.399 (6)
O2—K1 ^{iv}	2.718 (4)	C5—H5A	0.9300
O2—K1 ⁱⁱ	2.829 (3)	C6—C7	1.376 (7)
O2—K1 ^v	2.835 (4)	C6—H6A	0.9300
N1—N2	1.351 (5)	C7—C8	1.383 (7)
N1—C8	1.367 (6)	C7—H7A	0.9300
N1—C2	1.444 (5)	O3—K1 ⁱⁱ	2.760 (3)
N2—N3	1.314 (6)	O3—H3	0.87 (6)
N3—C3	1.362 (7)		
O2 ⁱ —K1—O3	158.80 (10)	O2 ⁱ —K1—H3	171.8 (13)
O2 ⁱ —K1—O2 ⁱⁱ	86.48 (10)	O3—K1—H3	16.0 (9)
O3—K1—O2 ⁱⁱ	78.97 (8)	O2 ⁱⁱ —K1—H3	93.3 (9)
O2 ⁱ —K1—O2 ⁱⁱⁱ	111.47 (9)	O2 ⁱⁱⁱ —K1—H3	76.6 (13)
O3—K1—O2 ⁱⁱⁱ	82.54 (10)	O1—K1—H3	71.3 (12)
O2 ⁱⁱ —K1—O2 ⁱⁱⁱ	84.30 (10)	N2—K1—H3	76.2 (9)
O2 ⁱ —K1—O1	101.92 (10)	O1 ⁱⁱ —K1—H3	82.9 (10)
O3—K1—O1	73.74 (9)	C1 ⁱⁱ —K1—H3	82.2 (9)
O2 ⁱⁱ —K1—O1	122.19 (10)	C1 ⁱⁱⁱ —K1—H3	95.4 (13)
O2 ⁱⁱⁱ —K1—O1	138.77 (10)	K1 ^{vi} —K1—H3	135.8 (9)
O2 ⁱ —K1—N2	105.55 (11)	K1 ^{vii} —K1—H3	84.5 (11)
O3—K1—N2	91.61 (10)	K1 ⁱⁱ —K1—H3	49.8 (12)
O2 ⁱⁱ —K1—N2	164.82 (13)	C1—O1—K1	119.5 (3)
O2 ⁱⁱⁱ —K1—N2	82.69 (10)	C1—O1—K1 ⁱⁱ	79.9 (3)
O1—K1—N2	65.15 (10)	K1—O1—K1 ⁱⁱ	87.70 (10)
O2 ⁱ —K1—O1 ⁱⁱ	91.55 (9)	C1—O2—K1 ^{iv}	134.2 (4)
O3—K1—O1 ⁱⁱ	67.34 (9)	C1—O2—K1 ⁱⁱ	100.9 (2)
O2 ⁱⁱ —K1—O1 ⁱⁱ	41.81 (9)	K1 ^{iv} —O2—K1 ⁱⁱ	95.88 (10)
O2 ⁱⁱⁱ —K1—O1 ⁱⁱ	120.67 (8)	C1—O2—K1 ^v	109.7 (3)
O1—K1—O1 ⁱⁱ	80.53 (11)	K1 ^{iv} —O2—K1 ^v	111.47 (8)
N2—K1—O1 ⁱⁱ	143.94 (10)	K1 ⁱⁱ —O2—K1 ^v	93.30 (11)
O2 ⁱ —K1—C1 ⁱⁱ	94.83 (10)	N2—N1—C8	110.1 (3)
O3—K1—C1 ⁱⁱ	66.33 (9)	N2—N1—C2	120.2 (4)
O2 ⁱⁱ —K1—C1 ⁱⁱ	21.80 (8)	C8—N1—C2	129.6 (4)
O2 ⁱⁱⁱ —K1—C1 ⁱⁱ	99.89 (11)	N3—N2—N1	108.6 (4)
O1—K1—C1 ⁱⁱ	100.70 (11)	N3—N2—K1	104.3 (3)
N2—K1—C1 ⁱⁱ	157.01 (12)	N1—N2—K1	116.5 (3)
O1 ⁱⁱ —K1—C1 ⁱⁱ	21.59 (9)	N2—N3—C3	108.3 (4)
O2 ⁱ —K1—C1 ⁱⁱⁱ	92.76 (12)	O1—C1—O2	127.2 (4)
O3—K1—C1 ⁱⁱⁱ	102.35 (12)	O1—C1—C2	117.7 (4)
O2 ⁱⁱ —K1—C1 ⁱⁱⁱ	89.46 (10)	O2—C1—C2	115.0 (4)
O2 ⁱⁱⁱ —K1—C1 ⁱⁱⁱ	19.86 (9)	O1—C1—K1 ⁱⁱ	78.5 (2)
O1—K1—C1 ⁱⁱⁱ	145.45 (10)	O2—C1—K1 ⁱⁱ	57.28 (19)
N2—K1—C1 ⁱⁱⁱ	80.89 (11)	C2—C1—K1 ⁱⁱ	145.0 (3)
O1 ⁱⁱ —K1—C1 ⁱⁱⁱ	130.64 (9)	O1—C1—K1 ^v	94.1 (3)
C1 ⁱⁱ —K1—C1 ⁱⁱⁱ	109.10 (11)	O2—C1—K1 ^v	50.5 (3)

O2 ⁱ —K1—K1 ^{vi}	43.10 (5)	C2—C1—K1 ^v	129.5 (3)
O3—K1—K1 ^{vi}	120.37 (5)	K1 ⁱⁱ —C1—K1 ^v	75.00 (9)
O2 ⁱⁱ —K1—K1 ^{vi}	43.41 (9)	N1—C2—C1	114.4 (4)
O2 ⁱⁱⁱ —K1—K1 ^{vi}	101.65 (7)	N1—C2—H2A	108.7
O1—K1—K1 ^{vi}	119.37 (7)	C1—C2—H2A	108.7
N2—K1—K1 ^{vi}	147.99 (10)	N1—C2—H2B	108.7
O1 ⁱⁱ —K1—K1 ^{vi}	59.71 (6)	C1—C2—H2B	108.7
C1 ⁱⁱ —K1—K1 ^{vi}	54.26 (8)	H2A—C2—H2B	107.6
C1 ⁱⁱⁱ —K1—K1 ^{vi}	92.65 (8)	N3—C3—C4	130.2 (5)
O2 ⁱ —K1—K1 ^{vii}	100.47 (7)	N3—C3—C8	108.9 (4)
O3—K1—K1 ^{vii}	78.52 (5)	C4—C3—C8	120.8 (5)
O2 ⁱⁱ —K1—K1 ^{vii}	41.03 (8)	C5—C4—C3	117.4 (5)
O2 ⁱⁱⁱ —K1—K1 ^{vii}	43.29 (5)	C5—C4—H4A	121.3
O1—K1—K1 ^{vii}	150.66 (8)	C3—C4—H4A	121.3
N2—K1—K1 ^{vii}	125.69 (9)	C4—C5—C6	121.2 (6)
O1 ⁱⁱ —K1—K1 ^{vii}	80.15 (7)	C4—C5—H5A	119.4
C1 ⁱⁱ —K1—K1 ^{vii}	58.57 (9)	C6—C5—H5A	119.4
C1 ⁱⁱⁱ —K1—K1 ^{vii}	50.74 (7)	C7—C6—C5	122.3 (6)
K1 ^{vi} —K1—K1 ^{vii}	67.72 (3)	C7—C6—H6A	118.9
O2 ⁱ —K1—K1 ⁱⁱ	122.38 (7)	C5—C6—H6A	118.9
O3—K1—K1 ⁱⁱ	39.22 (9)	C6—C7—C8	115.9 (5)
O2 ⁱⁱ —K1—K1 ⁱⁱ	76.91 (6)	C6—C7—H7A	122.1
O2 ⁱⁱⁱ —K1—K1 ⁱⁱ	120.90 (6)	C8—C7—H7A	122.1
O1—K1—K1 ⁱⁱ	50.16 (7)	N1—C8—C7	133.5 (4)
N2—K1—K1 ⁱⁱ	103.29 (9)	N1—C8—C3	104.0 (4)
O1 ⁱⁱ —K1—K1 ⁱⁱ	42.14 (6)	C7—C8—C3	122.4 (5)
C1 ⁱⁱ —K1—K1 ⁱⁱ	55.66 (8)	K1—O3—K1 ⁱⁱ	101.56 (17)
C1 ⁱⁱⁱ —K1—K1 ⁱⁱ	140.67 (8)	K1—O3—H3	103 (4)
K1 ^{vi} —K1—K1 ⁱⁱ	101.41 (4)	K1 ⁱⁱ —O3—H3	120 (4)
K1 ^{vii} —K1—K1 ⁱⁱ	101.41 (4)		
O2 ⁱ —K1—O1—C1	160.5 (3)	K1 ⁱⁱ —O1—C1—O2	32.1 (5)
O3—K1—O1—C1	-40.9 (3)	K1—O1—C1—C2	-65.4 (4)
O2 ⁱⁱ —K1—O1—C1	-106.1 (3)	K1 ⁱⁱ —O1—C1—C2	-146.9 (4)
O2 ⁱⁱⁱ —K1—O1—C1	16.6 (4)	K1—O1—C1—K1 ⁱⁱ	81.5 (2)
N2—K1—O1—C1	58.8 (3)	K1—O1—C1—K1 ^v	155.27 (17)
O1 ⁱⁱ —K1—O1—C1	-109.9 (3)	K1 ⁱⁱ —O1—C1—K1 ^v	73.78 (9)
C1 ⁱⁱ —K1—O1—C1	-102.1 (3)	K1 ^{iv} —O2—C1—O1	-147.7 (4)
C1 ⁱⁱⁱ —K1—O1—C1	47.4 (4)	K1 ⁱⁱ —O2—C1—O1	-38.3 (5)
K1 ^{vi} —K1—O1—C1	-157.0 (3)	K1 ^v —O2—C1—O1	59.3 (5)
K1 ^{vii} —K1—O1—C1	-60.5 (4)	K1 ^{iv} —O2—C1—C2	31.3 (5)
K1 ⁱⁱ —K1—O1—C1	-77.0 (3)	K1 ⁱⁱ —O2—C1—C2	140.8 (3)
O2 ⁱ —K1—O1—K1 ⁱⁱ	-122.46 (8)	K1 ^v —O2—C1—C2	-121.7 (4)
O3—K1—O1—K1 ⁱⁱ	36.13 (8)	K1 ^{iv} —O2—C1—K1 ⁱⁱ	-109.5 (3)
O2 ⁱⁱ —K1—O1—K1 ⁱⁱ	-29.10 (15)	K1 ^v —O2—C1—K1 ⁱⁱ	97.5 (2)
O2 ⁱⁱⁱ —K1—O1—K1 ⁱⁱ	93.58 (13)	K1 ^{iv} —O2—C1—K1 ^v	153.0 (4)
N2—K1—O1—K1 ⁱⁱ	135.76 (13)	K1 ⁱⁱ —O2—C1—K1 ^v	-97.5 (2)
O1 ⁱⁱ —K1—O1—K1 ⁱⁱ	-32.88 (11)	N2—N1—C2—C1	79.5 (6)

C1 ⁱⁱ —K1—O1—K1 ⁱⁱ	-25.14 (12)	C8—N1—C2—C1	-95.5 (5)
C1 ⁱⁱⁱ —K1—O1—K1 ⁱⁱ	124.37 (17)	O1—C1—C2—N1	-4.9 (6)
K1 ^{vi} —K1—O1—K1 ⁱⁱ	-79.99 (9)	O2—C1—C2—N1	175.9 (4)
K1 ^{vii} —K1—O1—K1 ⁱⁱ	16.52 (19)	K1 ⁱⁱ —C1—C2—N1	-116.0 (5)
C8—N1—N2—N3	-0.8 (6)	K1 ^v —C1—C2—N1	117.6 (4)
C2—N1—N2—N3	-176.7 (4)	N2—N3—C3—C4	-179.2 (5)
C8—N1—N2—K1	116.5 (3)	N2—N3—C3—C8	0.7 (6)
C2—N1—N2—K1	-59.4 (5)	N3—C3—C4—C5	-179.5 (6)
O2 ⁱ —K1—N2—N3	24.2 (4)	C8—C3—C4—C5	0.6 (7)
O3—K1—N2—N3	-168.4 (4)	C3—C4—C5—C6	-1.0 (9)
O2 ⁱⁱ —K1—N2—N3	-117.3 (5)	C4—C5—C6—C7	1.4 (10)
O2 ⁱⁱⁱ —K1—N2—N3	-86.1 (4)	C5—C6—C7—C8	-1.2 (8)
O1—K1—N2—N3	120.4 (4)	N2—N1—C8—C7	-179.7 (5)
O1 ⁱⁱ —K1—N2—N3	139.7 (3)	C2—N1—C8—C7	-4.3 (9)
C1 ⁱⁱ —K1—N2—N3	175.8 (4)	N2—N1—C8—C3	1.2 (5)
C1 ⁱⁱⁱ —K1—N2—N3	-66.1 (4)	C2—N1—C8—C3	176.6 (4)
K1 ^{vi} —K1—N2—N3	14.2 (5)	C6—C7—C8—N1	-178.2 (5)
K1 ^{vii} —K1—N2—N3	-91.4 (4)	C6—C7—C8—C3	0.7 (7)
K1 ⁱⁱ —K1—N2—N3	153.8 (4)	N3—C3—C8—N1	-1.1 (5)
O2 ⁱ —K1—N2—N1	-95.4 (3)	C4—C3—C8—N1	178.8 (5)
O3—K1—N2—N1	72.0 (3)	N3—C3—C8—C7	179.6 (5)
O2 ⁱⁱ —K1—N2—N1	123.1 (4)	C4—C3—C8—C7	-0.5 (7)
O2 ⁱⁱⁱ —K1—N2—N1	154.3 (4)	O2 ⁱ —K1—O3—K1 ⁱⁱ	35.2 (2)
O1—K1—N2—N1	0.8 (3)	O2 ⁱⁱ —K1—O3—K1 ⁱⁱ	82.75 (8)
O1 ⁱⁱ —K1—N2—N1	20.0 (5)	O2 ⁱⁱⁱ —K1—O3—K1 ⁱⁱ	168.36 (6)
C1 ⁱⁱ —K1—N2—N1	56.2 (5)	O1—K1—O3—K1 ⁱⁱ	-45.72 (7)
C1 ⁱⁱⁱ —K1—N2—N1	174.2 (4)	N2—K1—O3—K1 ⁱⁱ	-109.23 (9)
K1 ^{vi} —K1—N2—N1	-105.4 (3)	O1 ⁱⁱ —K1—O3—K1 ⁱⁱ	40.61 (7)
K1 ^{vii} —K1—N2—N1	149.0 (3)	C1 ⁱⁱ —K1—O3—K1 ⁱⁱ	64.09 (10)
K1 ⁱⁱ —K1—N2—N1	34.2 (3)	C1 ⁱⁱⁱ —K1—O3—K1 ⁱⁱ	169.75 (7)
N1—N2—N3—C3	0.0 (6)	K1 ^{vi} —K1—O3—K1 ⁱⁱ	69.19 (5)
K1—N2—N3—C3	-124.8 (4)	K1 ^{vii} —K1—O3—K1 ⁱⁱ	124.62 (4)
K1—O1—C1—O2	113.6 (5)		

Symmetry codes: (i) $x+1/2, y+1/2, z$; (ii) $-x+1, y, -z+1$; (iii) $x+1/2, y-1/2, z$; (iv) $x-1/2, y-1/2, z$; (v) $x-1/2, y+1/2, z$; (vi) $-x+3/2, y+1/2, -z+1$; (vii) $-x+3/2, y-1/2, -z+1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 \cdots O1 ^{viii}	0.87 (6)	1.87 (7)	2.729 (5)	167 (7)

Symmetry code: (viii) $x, y-1, z$.