

# Poly[diaqua( $\mu_2$ -3-carboxypyrazine-2-carboxylato)( $\mu_2$ -pyrazine-2,3-dicarboxylic acid)potassium(I)]

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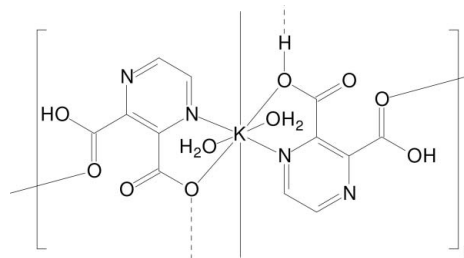
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Key indicators: single-crystal X-ray study;  $T = 303$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.029;  $wR$  factor = 0.089; data-to-parameter ratio = 11.6.

The structural unit of the title compound,  $[\text{K}(\text{C}_6\text{H}_3\text{N}_2\text{O}_4)(\text{C}_6\text{H}_4\text{N}_2\text{O}_4)(\text{H}_2\text{O})_2]_n$ , consists of one potassium cation, one hydrogen pyrazine-2,3-dicarboxylate anion, one pyrazine-2,3-dicarboxylic acid molecule and two water molecules; this is twice the asymmetric unit, since the potassium cation lies on an inversion centre. Each anion or acid molecule is linked to two potassium cations, while the potassium cation has contacts to four symmetry-equivalent organic ligands, with two different coordination modes towards this cation. In addition, each potassium cation is coordinated by two water O atoms, raising the coordination number to eight. One of the carboxyl groups of the acid retains its H atom, which forms a hydrogen bond to a coordinated water molecule. The other carboxyl group is deprotonated in half of the ligands and protonated in the other half, taking part in a strong  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bond disordered over an inversion centre. The stabilization of the crystal structure is further assisted by  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds in which water acts as the donor.

## Related literature

For related literature, see: Clegg & Liddle (2004); Cuesta *et al.* (2003); Ptasiewicz-Bak & Leciejewicz (1997*a,b*); Starosta & Leciejewicz (2005); Takusagawa & Shimada (1973); Tombul *et al.* (2006, 2007). Richard *et al.* (1973). Nepveu *et al.* (1993).



## Experimental

### Crystal data

$[\text{K}(\text{C}_6\text{H}_3\text{N}_2\text{O}_4)(\text{C}_6\text{H}_4\text{N}_2\text{O}_4)(\text{H}_2\text{O})_2]$   
 $M_r = 410.35$   
 Triclinic,  $P\bar{1}$   
 $a = 7.4171$  (11) Å  
 $b = 8.0252$  (12) Å  
 $c = 8.1153$  (13) Å  
 $\alpha = 68.39$  (2)°  
 $\beta = 81.18$  (1)°  
 $\gamma = 64.24$  (2)°  
 $V = 404.43$  (13) Å<sup>3</sup>  
 $Z = 1$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.40$  mm<sup>-1</sup>  
 $T = 303$  (2) K  
 $0.40 \times 0.36 \times 0.14$  mm

### Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector  
 Absorption correction: numerical [using a multifaceted crystal model based on expressions derived by Clark & Reid (1995)]  
 $T_{\min} = 0.858$ ,  $T_{\max} = 0.947$   
 4541 measured reflections  
 1639 independent reflections  
 1357 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.017$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$   
 $wR(F^2) = 0.089$   
 $S = 0.82$   
 1639 reflections  
 141 parameters  
 3 restraints  
 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.30$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.24$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

N1—K1	2.8655 (15)	K1—O3 <sup>i</sup>	2.8771 (15)
O1—K1	2.8995 (12)	K1—O1 <sup>i</sup>	2.8995 (12)
O3—K1	2.8771 (15)	K1—O2 <sup>ii</sup>	3.0897 (13)
K1—N1 <sup>i</sup>	2.8655 (15)	K1—O2 <sup>iii</sup>	3.0897 (13)

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

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O3—H3A $\cdots$ O4 <sup>iv</sup>	0.85 (2)	1.899 (10)	2.7334 (17)	167 (2)
O3—H3B $\cdots$ N2 <sup>ii</sup>	0.848 (9)	2.035 (10)	2.8701 (19)	168 (2)
O5—H5 $\cdots$ O3 <sup>v</sup>	0.86 (3)	1.76 (3)	2.5994 (17)	168 (2)
O1—H1 $\cdots$ O1 <sup>iv</sup>	0.80 (4)	1.68 (4)	2.480 (2)	171 (5)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *Mercury* (Macrae *et al.*, 2006);

software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2158).

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## supporting information

*Acta Cryst.* (2008). E64, m246–m247 [https://doi.org/10.1107/S1600536807066202]

## Poly[*diaqua*( $\mu_2$ -3-carboxypyrazine-2-carboxylato)( $\mu_2$ -pyrazine-2,3-dicarboxylic acid)potassium(I)]

Mustafa Tombul, Kutalmis Güven and Ingrid Svoboda

### S1. Comment

Pyrazine-2,3-dicarboxylic acid (Takusagawa & Shimada, 1973) and its dianion (Richard *et al.*, 1973; Nepveu *et al.*, 1993) have been reported to be well suited for the construction of multidimensional frameworks (nD, n = 1–3), owing to the presence of two adjacent carboxylate groups (O donor atoms) as substituents on the N-heterocyclic pyrazine ring (N donor atoms). In recent years, a variety of metal-organic compound of pyrazine-2,3-dicarboxylic acid have been characterized crystallographically due to growing interest in supramolecular chemistry. These include the calcium (Ptasiewicz-Bak- & Leciejewicz, 1997a; Starosta & Leciejewicz, 2005), magnesium (Ptasiewicz-Bak- H. & Leciejewicz, 1997b), sodium (Tombul *et al.*, 2006) and caesium (Tombul *et al.*, 2007) complexes. We present here the synthesis and crystal structure of the hydrated potassium complex, (I), formed with pyrazine-2,3-dicarboxylic acid.

The structural unit of the title compound, (I), contains one potassium cation, one hydrogen pyrazine-2,3-dicarboxylate anion, one pyrazine-2,3-dicarboxylic acid molecule and two water molecules; this is twice the asymmetric unit, as the potassium ion lies on an inversion centre. Pyrazine-2,3-dicarboxylic acid is, on average, only half deprotonated at one of the carboxylate groups (O1) and together with the symmetry-related oxygen atom (O1<sup>v</sup>) which is also half deprotonated, completes the charge balance of the cation. In the crystal structure, the anion or acid molecule is linked to two potassium cations, while the K<sup>+</sup> cation is surrounded by four organic ligands, two of which are coordinated by utilizing both N and O atoms and the other two are coordinated solely by O atoms. In addition, each potassium cation is coordinated by two water molecules, achieving a coordination number of eight. The primary coordination comprises six oxygen atoms, together with two nitrogen atoms. The planes of the carboxylic/carboxylate groups (O4/C5/O1) and (O2/C6/O5) form dihedral angles with the ring plane of 54.33 (14) and 53.75 (14)°, respectively. The K—O distances are in the range 2.877 (2) Å to 3.089 (2) Å, in accordance with the corresponding values reported for other potassium complexes (Clegg & Liddle, 2004; Cuesta *et al.*, 2003).

In the crystal structure, an asymmetric strong hydrogen bond occurs, linking carboxylate O atoms (Table 2). Atom H1 is involved in this bond and maintains the charge balance within the structure. The ordered carboxyl group forms a hydrogen bond in which water serves as acceptor. The water molecules are involved in normal, slightly bent, hydrogen bonds with hydrogen pyrazine-2,3-dicarboxylate (Table 2); the acceptors are carboxylate O atoms and N atoms of the aromatic ring.

### S2. Experimental

K<sub>2</sub>CO<sub>3</sub> (346 mg, 2.5 mmol) was carefully added to an aqueous solution (20 ml) of pyrazine-2,3-dicarboxylic acid (1680 mg, 10 mmol), until no further bubbles formed. The reaction mixture gave a colourless and clear solution which was stirred at 333 K for 2.5 h, until it solidified. The solid product was redissolved in water (10 ml) and allowed to stand for a week at room temperature, after which transparent fine crystals were harvested.

## S3. Refinement

The H atoms were all located in a difference map, but those attached to carbon atoms were repositioned geometrically and treated as riding, with C—H in the range 0.93–0.98 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . O-bound H atoms were refined freely.

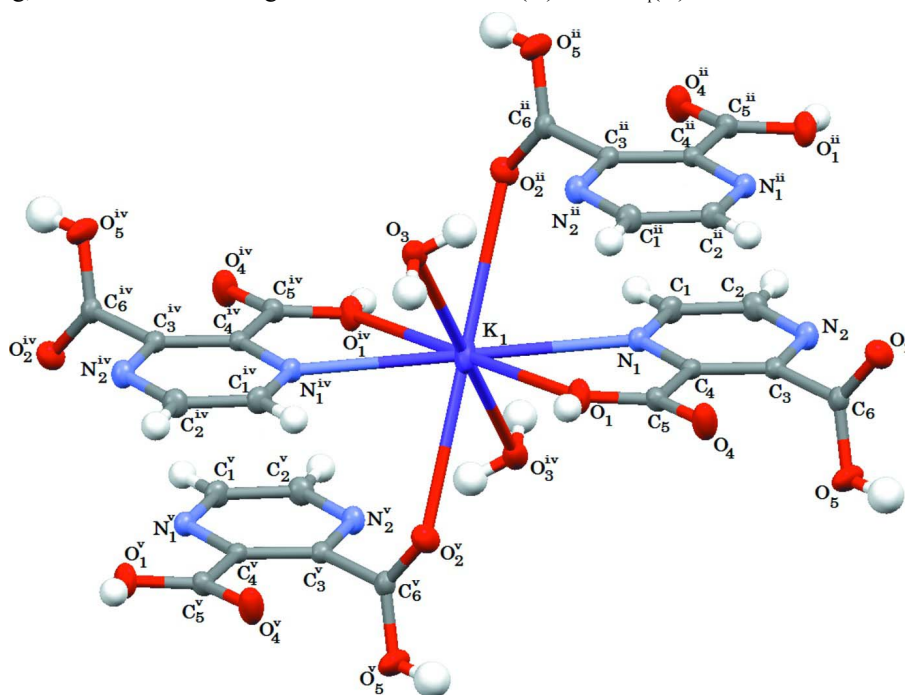


Figure 1

A segment of the structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry Codes: (ii)  $-x + 1, -y, -z + 1$ ; (iv)  $-x, -y + 1, -z + 1$ ; (v)  $x - 1, y + 1, z$ .]

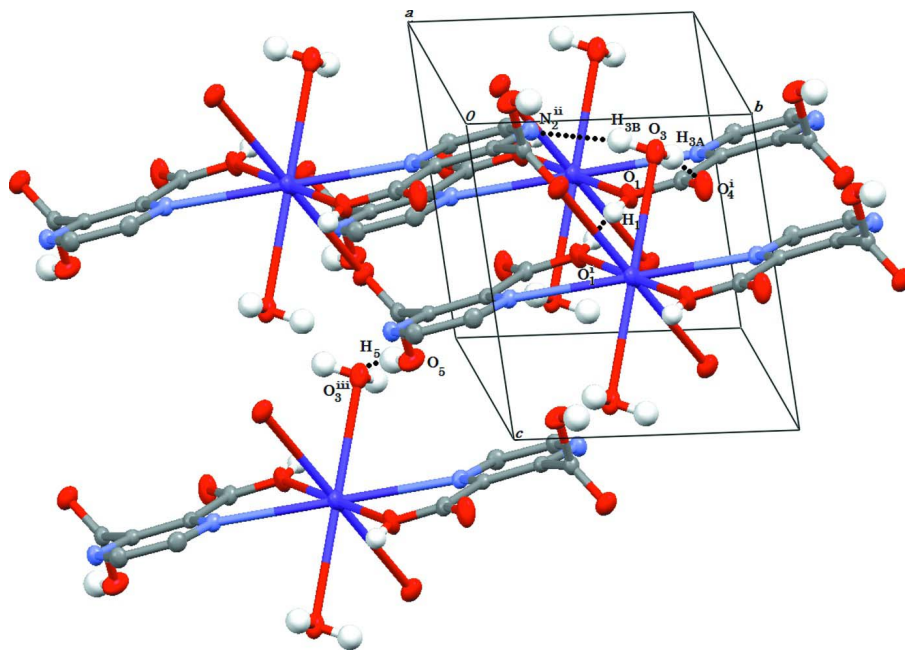


Figure 2

A packing diagram for (I). Dashed lines indicate hydrogen bonds. (H1A and H2 are omitted for clarity). [Symmetry Codes: (i)  $-x + 1, -y + 1, -z + 1$ ; (ii)  $-x + 1, -y, -z + 1$ ; (iii)  $x + 1, y - 1, z + 1$ .]

### Poly[ $\text{diaqua}(\mu_2\text{-3-carboxypyrazine-2-carboxylato})(\mu_2\text{-pyrazine-2,3-dicarboxylic acid})\text{potassium(I)}$ ]

#### Crystal data

$[\text{K}(\text{C}_6\text{H}_3\text{N}_2\text{O}_4)(\text{C}_6\text{H}_4\text{N}_2\text{O}_4)(\text{H}_2\text{O})_2]$

$M_r = 410.35$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 7.4171$  (11) Å

$b = 8.0252$  (12) Å

$c = 8.1153$  (13) Å

$\alpha = 68.39$  (2)°

$\beta = 81.18$  (1)°

$\gamma = 64.24$  (2)°

$V = 404.43$  (13) Å<sup>3</sup>

$Z = 1$

$F(000) = 210$

$D_x = 1.685$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2574 reflections

$\theta = 2.7\text{--}27.5^\circ$

$\mu = 0.40$  mm<sup>-1</sup>

$T = 303$  K

Prism, colorless

$0.40 \times 0.36 \times 0.14$  mm

#### Data collection

Oxford Diffraction Xcalibur

diffractometer with Sapphire CCD detector

Radiation source: Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: 8.4012 pixels mm<sup>-1</sup>

$\omega$  and  $\varphi$  scans

Absorption correction: numerical

[using a multifaceted crystal model based on expressions derived by Clark & Reid (1995)]

$T_{\min} = 0.858, T_{\max} = 0.947$

4541 measured reflections

1639 independent reflections

1357 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$

$\theta_{\max} = 26.4^\circ, \theta_{\min} = 2.7^\circ$

$h = -9 \rightarrow 9$

$k = -9 \rightarrow 9$

$l = -10 \rightarrow 10$

Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.089$

$S = 0.82$

1639 reflections

141 parameters

3 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

$w = 1/[\sigma^2(F_o^2) + (0.0664P)^2 + 0.1925P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.30 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$

Extinction correction: *SHELXL*,

$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.043 (8)

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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.2243 (2)	−0.0442 (2)	0.6857 (2)	0.0317 (4)	
H1A	0.0951	−0.0140	0.6552	0.038*	
C2	0.3500 (2)	−0.2386 (2)	0.7694 (2)	0.0335 (4)	
H2	0.3046	−0.3358	0.7905	0.040*	
C3	0.5925 (2)	−0.1443 (2)	0.78702 (18)	0.0249 (3)	
C4	0.4681 (2)	0.0507 (2)	0.69820 (18)	0.0236 (3)	
C5	0.5421 (2)	0.2104 (2)	0.6487 (2)	0.0289 (3)	
C6	0.8033 (2)	−0.2156 (2)	0.8493 (2)	0.0277 (3)	
N1	0.28268 (17)	0.10040 (18)	0.64756 (16)	0.0281 (3)	
N2	0.53451 (18)	−0.28984 (18)	0.82048 (17)	0.0310 (3)	
O1	0.41860 (17)	0.38402 (16)	0.56448 (17)	0.0394 (3)	
H1	0.476 (7)	0.455 (6)	0.533 (5)	0.039 (11)*	0.50
O2	0.94651 (16)	−0.29530 (18)	0.77161 (16)	0.0392 (3)	
O3	0.14687 (17)	0.66521 (18)	0.15762 (17)	0.0407 (3)	
H3A	0.195 (3)	0.727 (3)	0.190 (3)	0.057 (6)*	
H3B	0.245 (2)	0.563 (2)	0.149 (3)	0.057 (6)*	
O4	0.71570 (17)	0.16296 (17)	0.68558 (19)	0.0476 (4)	
O5	0.80518 (19)	−0.1943 (2)	1.00104 (17)	0.0504 (4)	
H5	0.925 (4)	−0.241 (4)	1.038 (3)	0.065 (7)*	
K1	0.0000	0.5000	0.5000	0.0471 (2)	

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0200 (7)	0.0376 (8)	0.0396 (8)	-0.0125 (6)	-0.0024 (6)	-0.0137 (7)
C2	0.0279 (8)	0.0336 (8)	0.0424 (9)	-0.0165 (6)	0.0010 (6)	-0.0120 (7)
C3	0.0220 (7)	0.0276 (7)	0.0250 (7)	-0.0091 (6)	-0.0002 (5)	-0.0101 (5)
C4	0.0213 (7)	0.0259 (7)	0.0239 (7)	-0.0076 (6)	-0.0016 (5)	-0.0107 (5)
C5	0.0255 (7)	0.0271 (7)	0.0356 (8)	-0.0088 (6)	-0.0030 (6)	-0.0134 (6)
C6	0.0236 (7)	0.0241 (7)	0.0329 (8)	-0.0082 (6)	-0.0042 (6)	-0.0075 (6)
N1	0.0210 (6)	0.0293 (6)	0.0322 (7)	-0.0067 (5)	-0.0031 (5)	-0.0116 (5)
N2	0.0253 (6)	0.0274 (6)	0.0377 (7)	-0.0107 (5)	-0.0017 (5)	-0.0079 (5)
O1	0.0301 (6)	0.0261 (6)	0.0558 (8)	-0.0121 (5)	-0.0066 (5)	-0.0039 (5)
O2	0.0221 (5)	0.0465 (7)	0.0535 (7)	-0.0108 (5)	0.0004 (5)	-0.0257 (6)
O3	0.0316 (6)	0.0372 (7)	0.0555 (8)	-0.0072 (5)	-0.0149 (5)	-0.0206 (6)
O4	0.0308 (6)	0.0333 (6)	0.0824 (10)	-0.0118 (5)	-0.0192 (6)	-0.0174 (6)
O5	0.0297 (6)	0.0743 (9)	0.0417 (7)	-0.0057 (6)	-0.0116 (5)	-0.0282 (6)
K1	0.0338 (3)	0.0339 (3)	0.0456 (3)	-0.0005 (2)	-0.0012 (2)	0.0006 (2)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

C1—N1	1.327 (2)	N1—K1	2.8655 (15)
C1—C2	1.383 (2)	O1—K1	2.8995 (12)
C1—H1A	0.9300	O1—H1	0.80 (4)
C2—N2	1.331 (2)	O3—K1	2.8771 (15)
C2—H2	0.9300	O3—H3A	0.85 (2)
C3—N2	1.3381 (19)	O3—H3B	0.848 (9)
C3—C4	1.392 (2)	O5—H5	0.86 (3)
C3—C6	1.5097 (19)	K1—N1 <sup>i</sup>	2.8655 (15)
C4—N1	1.3397 (18)	K1—O3 <sup>i</sup>	2.8771 (15)
C4—C5	1.507 (2)	K1—O1 <sup>i</sup>	2.8995 (12)
C5—O4	1.2248 (18)	K1—O2 <sup>ii</sup>	3.0897 (13)
C5—O1	1.2760 (19)	K1—O2 <sup>iii</sup>	3.0897 (13)
C6—O2	1.1983 (19)	K1—H3A	3.09 (2)
C6—O5	1.3073 (19)		
N1—C1—C2	121.91 (13)	N1 <sup>i</sup> —K1—O3	72.84 (4)
N1—C1—H1A	119.0	N1—K1—O3	107.16 (4)
C2—C1—H1A	119.0	O3 <sup>i</sup> —K1—O3	180.0
N2—C2—C1	121.64 (14)	N1 <sup>i</sup> —K1—O1 <sup>i</sup>	55.92 (4)
N2—C2—H2	119.2	N1—K1—O1 <sup>i</sup>	124.08 (4)
C1—C2—H2	119.2	O3 <sup>i</sup> —K1—O1 <sup>i</sup>	76.02 (4)
N2—C3—C4	121.58 (13)	O3—K1—O1 <sup>i</sup>	103.98 (4)
N2—C3—C6	113.19 (12)	N1 <sup>i</sup> —K1—O1	124.08 (4)
C4—C3—C6	125.20 (13)	N1—K1—O1	55.92 (4)
N1—C4—C3	121.03 (13)	O3 <sup>i</sup> —K1—O1	103.98 (4)
N1—C4—C5	118.15 (13)	O3—K1—O1	76.02 (4)
C3—C4—C5	120.76 (13)	O1 <sup>i</sup> —K1—O1	180.000 (1)
O4—C5—O1	125.67 (14)	N1 <sup>i</sup> —K1—O2 <sup>ii</sup>	107.44 (4)

O4—C5—C4	118.05 (13)	N1—K1—O2 <sup>ii</sup>	72.56 (4)
O1—C5—C4	116.21 (13)	O3 <sup>i</sup> —K1—O2 <sup>ii</sup>	116.00 (3)
O2—C6—O5	126.25 (14)	O3—K1—O2 <sup>ii</sup>	64.00 (3)
O2—C6—C3	121.86 (13)	O1 <sup>i</sup> —K1—O2 <sup>ii</sup>	81.35 (3)
O5—C6—C3	111.63 (13)	O1—K1—O2 <sup>ii</sup>	98.65 (4)
C1—N1—C4	117.01 (13)	N1 <sup>i</sup> —K1—O2 <sup>iii</sup>	72.56 (4)
C1—N1—K1	119.50 (9)	N1—K1—O2 <sup>iii</sup>	107.44 (4)
C4—N1—K1	123.12 (9)	O3 <sup>i</sup> —K1—O2 <sup>iii</sup>	64.00 (3)
C2—N2—C3	116.78 (13)	O3—K1—O2 <sup>iii</sup>	116.00 (3)
C5—O1—K1	125.42 (10)	O1 <sup>i</sup> —K1—O2 <sup>iii</sup>	98.65 (4)
C5—O1—H1	109 (3)	O1—K1—O2 <sup>iii</sup>	81.35 (4)
K1—O1—H1	126 (3)	O2 <sup>ii</sup> —K1—O2 <sup>iii</sup>	180.00 (2)
C6—O2—K1 <sup>iv</sup>	132.38 (10)	N1 <sup>i</sup> —K1—H3A	70.6 (3)
K1—O3—H3A	96.3 (15)	N1—K1—H3A	109.4 (3)
K1—O3—H3B	99.8 (15)	O3 <sup>i</sup> —K1—H3A	164.1 (2)
H3A—O3—H3B	106.6 (13)	O3—K1—H3A	15.9 (2)
C6—O5—H5	111.0 (16)	O1 <sup>i</sup> —K1—H3A	112.9 (3)
N1 <sup>i</sup> —K1—N1	180.0	O1—K1—H3A	67.1 (3)
N1 <sup>i</sup> —K1—O3 <sup>i</sup>	107.16 (4)	O2 <sup>ii</sup> —K1—H3A	79.1 (2)
N1—K1—O3 <sup>i</sup>	72.84 (4)	O2 <sup>iii</sup> —K1—H3A	100.9 (2)
N1—C1—C2—N2	1.9 (2)	O4—C5—O1—K1	-175.29 (12)
N2—C3—C4—N1	2.1 (2)	C4—C5—O1—K1	7.78 (19)
C6—C3—C4—N1	179.87 (13)	O5—C6—O2—K1 <sup>iv</sup>	154.68 (13)
N2—C3—C4—C5	-174.99 (13)	C3—C6—O2—K1 <sup>iv</sup>	-19.1 (2)
C6—C3—C4—C5	2.8 (2)	C1—N1—K1—O3 <sup>i</sup>	61.01 (11)
N1—C4—C5—O4	-175.63 (14)	C4—N1—K1—O3 <sup>i</sup>	-111.76 (11)
C3—C4—C5—O4	1.5 (2)	C1—N1—K1—O3	-118.99 (11)
N1—C4—C5—O1	1.5 (2)	C4—N1—K1—O3	68.24 (11)
C3—C4—C5—O1	178.67 (13)	C1—N1—K1—O1 <sup>i</sup>	1.94 (12)
N2—C3—C6—O2	74.92 (18)	C4—N1—K1—O1 <sup>i</sup>	-170.83 (10)
C4—C3—C6—O2	-103.06 (18)	C1—N1—K1—O1	-178.06 (12)
N2—C3—C6—O5	-99.65 (16)	C4—N1—K1—O1	9.17 (10)
C4—C3—C6—O5	82.37 (18)	C1—N1—K1—O2 <sup>ii</sup>	-64.29 (11)
C2—C1—N1—C4	-1.8 (2)	C4—N1—K1—O2 <sup>ii</sup>	122.94 (11)
C2—C1—N1—K1	-174.99 (12)	C1—N1—K1—O2 <sup>iii</sup>	115.71 (11)
C3—C4—N1—C1	-0.1 (2)	C4—N1—K1—O2 <sup>iii</sup>	-57.06 (11)
C5—C4—N1—C1	177.00 (12)	C5—O1—K1—N1 <sup>i</sup>	171.23 (11)
C3—C4—N1—K1	172.82 (10)	C5—O1—K1—N1	-8.77 (11)
C5—C4—N1—K1	-10.06 (17)	C5—O1—K1—O3 <sup>i</sup>	48.85 (13)
C1—C2—N2—C3	0.0 (2)	C5—O1—K1—O3	-131.15 (13)
C4—C3—N2—C2	-1.9 (2)	C5—O1—K1—O2 <sup>ii</sup>	-70.80 (13)
C6—C3—N2—C2	-179.99 (12)	C5—O1—K1—O2 <sup>iii</sup>	109.20 (13)

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



*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O3—H3A $\cdots$ O4 <sup>v</sup>	0.85 (2)	1.90 (1)	2.7334 (17)	167 (2)
O3—H3B $\cdots$ N2 <sup>ii</sup>	0.85 (1)	2.04 (1)	2.8701 (19)	168 (2)
O5—H5 $\cdots$ O3 <sup>vi</sup>	0.86 (3)	1.76 (3)	2.5994 (17)	168 (2)
O1—H1 $\cdots$ O1 <sup>v</sup>	0.80 (4)	1.68 (4)	2.480 (2)	171 (5)

Symmetry codes: (ii)  $-x+1, -y, -z+1$ ; (v)  $-x+1, -y+1, -z+1$ ; (vi)  $x+1, y-1, z+1$ .