

# Potassium tetracyanoaurate(III) monohydrate: a redetermination

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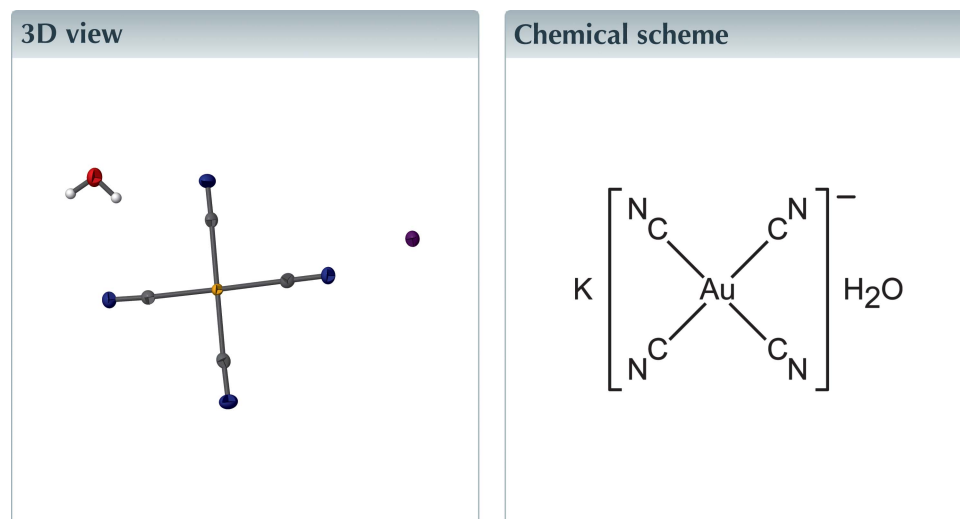
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Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

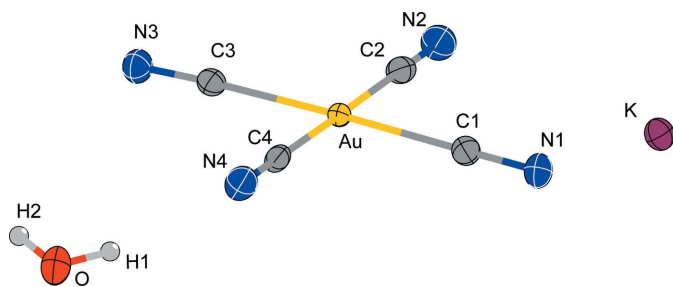
The structure of the title metal complex salt,  $\text{K}[\text{Au}(\text{CN})_4]\cdot\text{H}_2\text{O}$ , has been redetermined using X-ray diffraction data at 173 K in order to improve the precision. The previous determination was based on neutron diffraction data [Bertinotti & Bertinotti (1970). *Acta Cryst. B* **26**, 422–428]. The title compound crystallizes in the space group  $P2_12_12_1$  with one potassium cation, one  $[\text{Au}(\text{CN})_4]^-$  anion and one water molecule in the asymmetric unit. The  $\text{Au}^{\text{III}}$  atom lies on a general position and has an almost square-planar coordination sphere defined by four cyanide ligands. Interactions between the potassium cation and N atoms of the complex anion, as well as  $\text{O}—\text{H}\cdots\text{N}$  hydrogen bonds, lead to the formation of a three-dimensional framework structure.



## Structure description

Potassium tetracyanoaurate(III) monohydrate,  $\text{K}[\text{Au}(\text{CN})_4]\cdot\text{H}_2\text{O}$ , is one of the typical starting compounds for preparation of various tetracyanoaurate(III) salts. The crystal structure of  $\text{K}[\text{Au}(\text{CN})_4]\cdot\text{H}_2\text{O}$  has already been determined by neutron diffraction (Bertinotti & Bertinotti, 1970). However, because of the need for more precise structural data, we have redetermined the crystal structure using X-ray diffraction data at 173 K. The redetermination of the title salt confirms the previous model but shows an improvement with respect to the precision on bond lengths and angles, with respective standard uncertainties decreased to about one half to one third of those of the previous determination by neutron diffraction. In addition, in the current study all atoms were refined with anisotropic displacement parameters and the absolute structure was determined.

The components of the title salt are displayed in Fig. 1. The asymmetric unit comprises one potassium cation, one  $[\text{Au}(\text{CN})_4]^-$  anion and one water molecule. The  $\text{Au}^{\text{III}}$  atom of

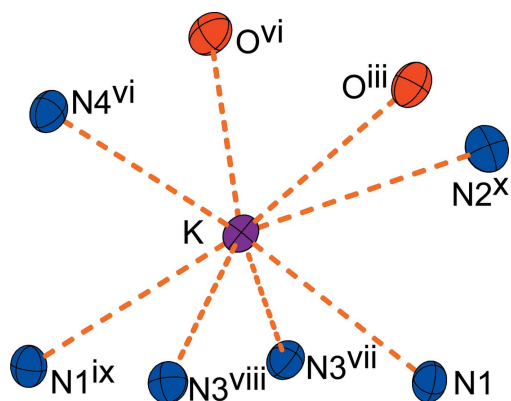


**Figure 1**

The asymmetric unit of the title salt, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level for non-H atoms.

the  $[\text{Au}(\text{CN})_4]^-$  anion is coordinated by four C atoms of four cyanido ligands in an almost square-planar configuration. The r.m.s. deviation of the least-squares plane formed by atoms Au, C1, C2, C3, C4, N1, N2, N3 and N4 is 0.0265 Å. The Au–C [1.998 (4)–2.007 (4) Å] and  $\text{C}\equiv\text{N}$  [1.138 (5)–1.146 (5) Å] bond lengths,  $\text{C–Au–C}_{\text{trans}}$  [178.63 (18), 179.39 (17)°],  $\text{C–Au–C}_{\text{cis}}$  [89.22 (16)–90.75 (17)°] and  $\text{Au–C–N}$  [177.3 (4)–179.7 (4)°] bond angles are consistent with values reported by Geisheimer *et al.* (2011) for the  $[\text{Au}(\text{CN})_4]^-$  anion in related compounds:  $[\text{N}(\text{C}_4\text{H}_9)_4][\text{Au}(\text{CN})_4]$  [Au–C = 1.992 (3)–2.002 (3) Å,  $\text{C}\equiv\text{N}$  = 1.139 (5)–1.148 (5) Å,  $\text{C–Au–C}_{\text{trans}}$  = 178.03 (12), 179.25 (13)°,  $\text{C–Au–C}_{\text{cis}}$  = 89.44 (13)–90.49 (14)°,  $\text{Au–C–N}$  = 177.0 (3)–178.4 (3)°];  $[\text{As}(\text{C}_6\text{H}_5)_4][\text{Au}(\text{CN})_4]$  [Au–C = 1.985 (2)–1.996 (2) Å,  $\text{C}\equiv\text{N}$  = 1.140 (3)–1.150 (3) Å,  $\text{C–Au–C}_{\text{trans}}$  = 179.35 (9), 179.74 (9)°,  $\text{C–Au–C}_{\text{cis}}$  = 89.41 (10)–90.75 (9)°,  $\text{Au–C–N}$  = 177.8 (2)–179.7 (3)°];  $[\text{N}(\text{P}(\text{C}_6\text{H}_5)_3)_2][\text{Au}(\text{CN})_4]$  [Au–C = 1.987 (6)–1.997 (5) Å,  $\text{C}\equiv\text{N}$  = 1.118 (5)–1.132 (6) Å,  $\text{C–Au–C}_{\text{trans}}$  = 179.10 (19), 179.47 (18)°,  $\text{C–Au–C}_{\text{cis}}$  = 88.85 (18)–91.00 (19)°,  $\text{Au–C–N}$  = 177.7 (6)–179.4 (6)°].

In the crystal, the potassium cation exhibits a coordination number of eight and is surrounded by six N atoms of the cyanido ligands [ $\text{K}\cdots\text{N}$  = 2.891 (4)–3.431 (4) Å] and two O



**Figure 2**

The environment of the  $\text{K}^+$  cation, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Orange dashed lines represent short contacts between the potassium ion and surrounding atoms. [Symmetry codes: (iii)  $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (vi)  $-x + \frac{1}{2}, -y + 1, z + \frac{1}{2}$ ; (vii)  $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$ ; (viii)  $-x + \frac{3}{2}, -y + 1, z + \frac{1}{2}$ ; (ix)  $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$ ; (x)  $x - 1, y, z$ .]

**Table 1**

Hydrogen-bond geometry (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
$\text{O--H2}\cdots\text{N1}^{\text{i}}$	0.84	2.32	3.157 (5)	178
$\text{O--H1}\cdots\text{N2}^{\text{ii}}$	0.84	2.27	2.952 (5)	139

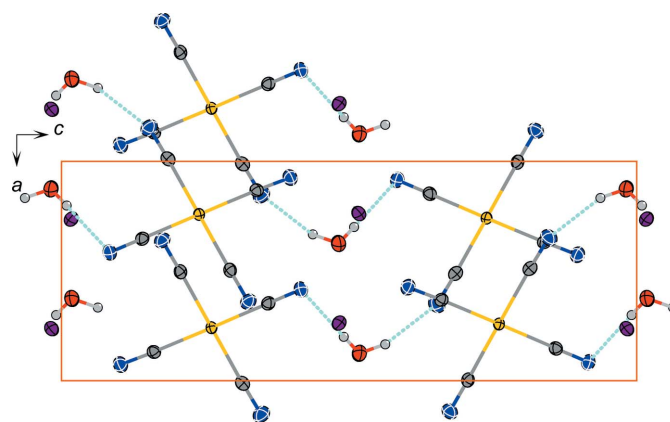
Symmetry codes: (i)  $-x + \frac{3}{2}, -y + 1, z - \frac{1}{2}$ ; (ii)  $-x + 2, y - \frac{1}{2}, -z + \frac{1}{2}$ .

**Table 2**

Experimental details.

Crystal data	$\text{K}[\text{Au}(\text{CN})_4]\cdot\text{H}_2\text{O}$
Chemical formula	358.16
$M_r$	Orthorhombic, $P2_12_12_1$
Crystal system, space group	173
Temperature (K)	6.6460 (7), 7.0733 (8), 17.4356 (19)
$a, b, c$ (Å)	819.63 (15)
$V$ (Å <sup>3</sup> )	4
$Z$	Mo $K\alpha$
Radiation type	18.40
$\mu$ (mm <sup>-1</sup> )	Crystal size (mm)
Crystal size (mm)	0.30 × 0.30 × 0.20
Data collection	
Diffractometer	Rigaku R-Axis RAPID imaging-plate
Absorption correction	Multi-scan ( <i>ABSCOR</i> ; Higashi, 1995)
$T_{\text{min}}, T_{\text{max}}$	0.437, 1.000
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	17391, 2828, 2666
$R_{\text{int}}$	0.045
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.745
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.015, 0.034, 1.03
No. of reflections	2828
No. of parameters	101
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	1.44, -1.09
Absolute structure	Flack $x$ determined using 1076 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	-0.006 (6)

Computer programs: *RAPID-AUTO* (Rigaku, 2006), *SHELXT* (Sheldrick, 2015a), *DIAMOND* (Brandenburg, 2017) and *SHELXL2014* (Sheldrick, 2015b) and *pubCIF* (Westrip, 2010).



**Figure 3**

The crystal packing of the title salt, viewed along the  $b$  axis. Light-blue dashed lines represent the hydrogen bonds. Orange solid lines indicate the unit cell.

atoms of water molecules [ $K \cdots O = 2.804(3), 2.886(3) \text{ \AA}$ ] (Fig. 2). Two  $O-H \cdots N$  hydrogen bonds between the water molecule of crystallization and the  $[Au(CN)_4]^-$  anion further stabilize the crystal packing of the title salt (Fig. 3, Table 1).

### Synthesis and crystallization

To an aqueous solution of  $H[AuCl_4] \cdot 4H_2O$  (2.007 g) neutralized by an aqueous solution of KOH was added an aqueous solution of KCN (1.286 g) at room temperature under stirring. The colour of the solution also changed immediately from yellow to colourless just after the addition. Slow evaporation of the solution gave colourless platelet single crystals.

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. In the final refinements, five reflections, (0 1 23), (0 3 23), (1 0 24), ( $\bar{1}$  6 20) and (1 6 20), were omitted due to poor agreements between observed and calculated intensities. The maximum and minimum electron

density peaks are located 0.75 and 0.75  $\text{\AA}$ , respectively, from the Au atom.

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## full crystallographic data

*IUCrData* (2017). 2, x170382 [https://doi.org/10.1107/S2414314617003820]

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## Potassium tetracyanidoaurate(III) monohydrate

*Crystal data*

$\text{K}[\text{Au}(\text{CN})_4] \cdot \text{H}_2\text{O}$

$M_r = 358.16$

Orthorhombic,  $P2_12_12_1$

$a = 6.6460$  (7) Å

$b = 7.0733$  (8) Å

$c = 17.4356$  (19) Å

$V = 819.63$  (15) Å<sup>3</sup>

$Z = 4$

$F(000) = 640$

$D_x = 2.902$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71075$  Å

Cell parameters from 8740 reflections

$\theta = 3.1$ – $31.9^\circ$

$\mu = 18.40$  mm<sup>-1</sup>

$T = 173$  K

Platelet, colorless

$0.30 \times 0.30 \times 0.20$  mm

*Data collection*

Rigaku R-AXIS RAPID imaging-plate diffractometer

Radiation source: X-ray sealed tube

Graphite monochromator

Detector resolution: 10.00 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.437$ ,  $T_{\max} = 1.000$

17391 measured reflections

2828 independent reflections

2666 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

$\theta_{\max} = 32.0^\circ$ ,  $\theta_{\min} = 3.1^\circ$

$h = -9 \rightarrow 9$

$k = -10 \rightarrow 10$

$l = -25 \rightarrow 23$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.015$

$wR(F^2) = 0.034$

$S = 1.03$

2828 reflections

101 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-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0069P)^2]$

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

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

$\Delta\rho_{\max} = 1.44$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -1.09$  e Å<sup>-3</sup>

Extinction correction: SHELXL2014

(Sheldrick, 2015*b*),

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

Extinction coefficient: 0.0093 (3)

Absolute structure: Flack  $x$  determined using

1076 quotients  $[(I^+) - (I^-)] / [(I^+) + (I^-)]$  (Parsons *et al.*, 2013)

Absolute structure parameter:  $-0.006$  (6)

*Special details*

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

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (\* indicates atom used to define plane)

- 2.5906 (0.0057) x + 6.3743 (0.0030) y + 3.3049 (0.0146) z = 2.5384 (0.0067)

\* 0.0043 (0.0013) Au \* -0.0216 (0.0038) C1 \* 0.0054 (0.0039) C2 \* -0.0097 (0.0037) C3 \* 0.0245 (0.0037) C4 \* -0.0325 (0.0030) N1 \* 0.0402 (0.0031) N2 \* -0.0400 (0.0030) N3 \* 0.0293 (0.0030) N4

Rms deviation of fitted atoms = 0.0265

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Au	0.75839 (2)	0.57191 (2)	0.26080 (2)	0.01211 (5)
C1	0.6473 (6)	0.4715 (7)	0.3595 (2)	0.0172 (9)
C2	1.0114 (6)	0.6470 (7)	0.3147 (2)	0.0177 (8)
C3	0.8687 (6)	0.6664 (6)	0.1607 (2)	0.0163 (8)
C4	0.5035 (6)	0.4994 (6)	0.2069 (2)	0.0165 (8)
N1	0.5844 (5)	0.4150 (6)	0.4160 (2)	0.0214 (8)
N2	1.1526 (6)	0.6928 (7)	0.3475 (2)	0.0255 (9)
N3	0.9262 (6)	0.7151 (6)	0.1027 (2)	0.0220 (8)
N4	0.3604 (5)	0.4584 (6)	0.1752 (2)	0.0228 (8)
K	0.23731 (16)	0.46003 (12)	0.51708 (4)	0.02024 (17)
O	0.6252 (5)	0.3372 (5)	0.01812 (17)	0.0252 (7)
H1	0.6663	0.3529	0.0632	0.038*
H2	0.7007	0.4050	-0.0090	0.038*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Au	0.01349 (7)	0.01157 (7)	0.01126 (8)	-0.00070 (7)	0.00035 (6)	-0.00005 (4)
C1	0.0172 (18)	0.018 (2)	0.017 (2)	0.0028 (16)	-0.0013 (15)	-0.0003 (16)
C2	0.0190 (19)	0.015 (2)	0.0191 (19)	0.0003 (17)	0.0032 (16)	0.0007 (17)
C3	0.0159 (18)	0.016 (2)	0.0173 (19)	0.0017 (16)	0.0008 (15)	-0.0012 (16)
C4	0.0193 (19)	0.015 (2)	0.0151 (19)	0.0006 (16)	0.0010 (15)	0.0038 (16)
N1	0.0222 (17)	0.025 (2)	0.0169 (18)	0.0003 (18)	0.0017 (13)	0.0020 (16)
N2	0.0248 (19)	0.026 (2)	0.0257 (19)	-0.0061 (17)	-0.0049 (16)	-0.0004 (18)
N3	0.0233 (18)	0.024 (2)	0.0189 (18)	-0.0015 (17)	0.0023 (14)	0.0012 (17)
N4	0.0215 (17)	0.024 (2)	0.0228 (19)	-0.0051 (16)	-0.0039 (14)	0.0029 (16)
K	0.0197 (4)	0.0224 (4)	0.0186 (4)	0.0006 (5)	0.0028 (4)	-0.0012 (3)
O	0.0252 (15)	0.031 (2)	0.0194 (15)	0.0023 (13)	0.0014 (12)	0.0035 (14)

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

Au—C2	1.998 (4)	K—O <sup>vi</sup>	2.804 (3)
Au—C1	2.002 (4)	K—O <sup>iii</sup>	2.886 (4)
Au—C4	2.003 (4)	K—N4 <sup>vi</sup>	2.891 (4)
Au—C3	2.007 (4)	K—N3 <sup>vii</sup>	2.923 (4)

C1—N1	1.143 (5)	K—N3 <sup>viii</sup>	2.961 (4)
C2—N2	1.146 (5)	K—N1 <sup>ix</sup>	3.071 (4)
C3—N3	1.135 (5)	K—N2 <sup>x</sup>	3.431 (4)
C4—N4	1.138 (5)	K—K <sup>i</sup>	4.4972 (12)
N1—K	2.920 (4)	K—K <sup>ix</sup>	4.4972 (12)
N1—K <sup>i</sup>	3.071 (4)	O—K <sup>v</sup>	2.804 (3)
N2—K <sup>ii</sup>	3.431 (4)	O—K <sup>vii</sup>	2.886 (3)
N3—K <sup>iii</sup>	2.923 (4)	O—H1	0.8400
N3—K <sup>iv</sup>	2.961 (4)	O—H2	0.8400
N4—K <sup>v</sup>	2.891 (4)		
C2—Au—C1	90.01 (16)	N4 <sup>vi</sup> —K—N1 <sup>ix</sup>	74.67 (11)
C2—Au—C4	179.39 (17)	N1—K—N1 <sup>ix</sup>	113.35 (8)
C1—Au—C4	90.03 (17)	N3 <sup>vii</sup> —K—N1 <sup>ix</sup>	68.68 (11)
C2—Au—C3	90.75 (17)	N3 <sup>viii</sup> —K—N1 <sup>ix</sup>	72.36 (10)
C1—Au—C3	178.63 (18)	O <sup>vi</sup> —K—N2 <sup>x</sup>	67.62 (9)
C4—Au—C3	89.22 (16)	O <sup>iii</sup> —K—N2 <sup>x</sup>	54.90 (9)
N1—C1—Au	179.7 (4)	N4 <sup>vi</sup> —K—N2 <sup>x</sup>	133.59 (12)
N2—C2—Au	177.7 (4)	N1—K—N2 <sup>x</sup>	70.24 (10)
N3—C3—Au	177.3 (4)	N3 <sup>vii</sup> —K—N2 <sup>x</sup>	66.90 (11)
N4—C4—Au	178.9 (4)	N3 <sup>viii</sup> —K—N2 <sup>x</sup>	139.40 (10)
C1—N1—K	140.5 (3)	N1 <sup>ix</sup> —K—N2 <sup>x</sup>	133.45 (10)
C1—N1—K <sup>i</sup>	120.6 (3)	O <sup>vi</sup> —K—K <sup>i</sup>	166.83 (8)
K—N1—K <sup>i</sup>	97.27 (11)	O <sup>iii</sup> —K—K <sup>i</sup>	110.40 (7)
C2—N2—K <sup>ii</sup>	115.4 (3)	N4 <sup>vi</sup> —K—K <sup>i</sup>	115.09 (9)
C3—N3—K <sup>iii</sup>	133.8 (3)	N1—K—K <sup>i</sup>	42.63 (8)
C3—N3—K <sup>iv</sup>	125.2 (3)	N3 <sup>vii</sup> —K—K <sup>i</sup>	77.79 (8)
K <sup>iii</sup> —N3—K <sup>iv</sup>	99.69 (11)	N3 <sup>viii</sup> —K—K <sup>i</sup>	39.84 (7)
C4—N4—K <sup>v</sup>	126.9 (3)	N1 <sup>ix</sup> —K—K <sup>i</sup>	73.99 (8)
O <sup>vi</sup> —K—O <sup>iii</sup>	78.50 (5)	N2 <sup>x</sup> —K—K <sup>i</sup>	108.91 (7)
O <sup>vi</sup> —K—N4 <sup>vi</sup>	72.47 (10)	O <sup>vi</sup> —K—K <sup>ix</sup>	72.78 (7)
O <sup>iii</sup> —K—N4 <sup>vi</sup>	95.14 (11)	O <sup>iii</sup> —K—K <sup>ix</sup>	144.74 (7)
O <sup>vi</sup> —K—N1	137.61 (11)	N4 <sup>vi</sup> —K—K <sup>ix</sup>	95.29 (8)
O <sup>iii</sup> —K—N1	73.89 (11)	N1—K—K <sup>ix</sup>	115.57 (9)
N4 <sup>vi</sup> —K—N1	140.78 (11)	N3 <sup>vii</sup> —K—K <sup>ix</sup>	40.46 (8)
O <sup>vi</sup> —K—N3 <sup>vii</sup>	89.34 (10)	N3 <sup>viii</sup> —K—K <sup>ix</sup>	110.40 (9)
O <sup>iii</sup> —K—N3 <sup>vii</sup>	120.90 (10)	N1 <sup>ix</sup> —K—K <sup>ix</sup>	40.10 (7)
N4 <sup>vi</sup> —K—N3 <sup>vii</sup>	135.75 (11)	N2 <sup>x</sup> —K—K <sup>ix</sup>	94.69 (7)
N1—K—N3 <sup>vii</sup>	78.33 (10)	K <sup>i</sup> —K—K <sup>ix</sup>	95.28 (3)
O <sup>vi</sup> —K—N3 <sup>viii</sup>	149.29 (10)	K <sup>v</sup> —O—K <sup>vii</sup>	138.03 (13)
O <sup>iii</sup> —K—N3 <sup>viii</sup>	104.76 (11)	K <sup>v</sup> —O—H1	102.6
N4 <sup>vi</sup> —K—N3 <sup>viii</sup>	76.83 (10)	K <sup>vii</sup> —O—H1	102.6
N1—K—N3 <sup>viii</sup>	70.24 (11)	K <sup>v</sup> —O—H2	102.6
N3 <sup>vii</sup> —K—N3 <sup>viii</sup>	113.15 (8)	K <sup>vii</sup> —O—H2	102.6

O <sup>vi</sup> —K—N1 <sup>ix</sup>	98.92 (11)	H1—O—H2	105.0
O <sup>iii</sup> —K—N1 <sup>ix</sup>	169.76 (10)		

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

*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>
O—H2 $\cdots$ N1 <sup>iv</sup>	0.84	2.32	3.157 (5)	178
O—H1 $\cdots$ N2 <sup>xi</sup>	0.84	2.27	2.952 (5)	139

Symmetry codes: (iv)  $-x+3/2, -y+1, z-1/2$ ; (xi)  $-x+2, y-1/2, -z+1/2$ .