

## Potassium salt of salicylidene- $\beta$ -hydroxy-alanine

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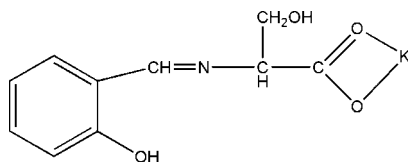
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Key indicators: single-crystal X-ray study;  $T = 291$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.024;  $wR$  factor = 0.068; data-to-parameter ratio = 11.6.

The title compound, poly[[ $\mu$ -3-hydroxy-2-(2-hydroxybenzylideneamino)propionato]potassium],  $[\text{K}(\text{C}_{10}\text{H}_{10}\text{NO}_4)]_n$ , is an effective material for preparing rare earth Eu complexes. It is composed of planar six-membered rings and planar five-membered rings formed by intramolecular O—H...N hydrogen bonding, which are oriented with respect to each other at a dihedral angle of  $3.56(4)^\circ$ . The  $\text{K}^+$  ion is surrounded by seven O atoms, five from three carboxylate groups and two from two hydroxyl groups. In the crystal structure, intermolecular O—H...O hydrogen bonds result in the formation of chains along the  $c$  axis.

### Related literature

For bond-length data, see: Allen *et al.* (1987). For related literature, see: Parekh & Patel (2005).



### Experimental

#### Crystal data

$[\text{K}(\text{C}_{10}\text{H}_{10}\text{NO}_4)]$

$M_r = 247.29$

Orthorhombic,  $Pca2_1$

$a = 7.9571(6)$  Å

$b = 17.7596(13)$  Å

$c = 7.7258(6)$  Å

$V = 1091.77(14)$  Å<sup>3</sup>

$Z = 4$

Mo  $K\alpha$  radiation

$\mu = 0.48$  mm<sup>-1</sup>

$T = 291(2)$  K

$0.16 \times 0.12 \times 0.10$  mm

#### Data collection

Bruker SMART 1K CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2000)

$T_{\text{min}} = 0.927$ ,  $T_{\text{max}} = 0.953$

5642 measured reflections  
1782 independent reflections

1689 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.068$

$S = 1.06$

1782 reflections

153 parameters

1 restraint

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.17$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.13$  e Å<sup>-3</sup>

Absolute structure: Flack (1983), 630 Friedel pairs

Flack parameter:  $-0.06(4)$

**Table 1**

Selected geometric parameters (Å, °).

K1—O1 <sup>i</sup>	2.6533 (14)	K1—Cl <sup>iii</sup>	3.0384 (19)
K1—O3 <sup>ii</sup>	2.7755 (16)	C1—O2	1.248 (2)
K1—O1	2.8215 (16)	C1—O1	1.248 (2)
K1—O2	2.8685 (17)	C2—N1	1.468 (2)
K1—O3 <sup>iii</sup>	2.9691 (16)	C3—O3	1.414 (3)
K1—O1 <sup>iii</sup>	2.9896 (15)	C4—N1	1.265 (2)
K1—O2 <sup>iii</sup>	2.9986 (17)	C6—O4	1.340 (3)
O1 <sup>i</sup> —K1—O3 <sup>ii</sup>	79.42 (5)	O3 <sup>iii</sup> —K1—O1 <sup>iii</sup>	75.97 (4)
O1 <sup>i</sup> —K1—O1	103.41 (4)	O1—K1—O1 <sup>iii</sup>	130.81 (4)
O3 <sup>ii</sup> —K1—O1	134.25 (4)	O2—K1—O1 <sup>iii</sup>	100.39 (4)
O1 <sup>i</sup> —K1—O2	135.38 (4)	O3 <sup>iii</sup> —K1—O1 <sup>iii</sup>	63.23 (4)
O3 <sup>ii</sup> —K1—O2	100.87 (5)	O1 <sup>i</sup> —K1—O2 <sup>iii</sup>	82.69 (4)
O1—K1—O2	45.55 (4)	O3 <sup>iii</sup> —K1—O2 <sup>iii</sup>	82.73 (5)
O1 <sup>i</sup> —K1—O3 <sup>iii</sup>	126.98 (5)	O1—K1—O2 <sup>iii</sup>	142.97 (4)
O3 <sup>ii</sup> —K1—O3 <sup>iii</sup>	138.77 (3)	O2—K1—O2 <sup>iii</sup>	141.92 (2)
O1—K1—O3 <sup>iii</sup>	75.63 (4)	O3 <sup>iii</sup> —K1—O2 <sup>iii</sup>	71.99 (4)
O2—K1—O3 <sup>iii</sup>	81.71 (4)	O1 <sup>iii</sup> —K1—O2 <sup>iii</sup>	43.17 (4)
O1 <sup>i</sup> —K1—O1 <sup>iii</sup>	122.26 (6)		

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

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3...O2 <sup>iv</sup>	0.80 (2)	1.89 (2)	2.634 (2)	156 (3)
O4—H4A...N1	0.86 (3)	1.84 (3)	2.625 (2)	151 (3)

Symmetry code: (iv)  $-x + \frac{5}{2}, y, z - \frac{1}{2}$ .

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2000); 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: HK2286).

### References

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**supplementary materials**

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## Potassium salt of salicylidene- $\beta$ -hydroxyalanine

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### Comment

The title compound, (I), is an effective material for preparing rare earth complexes (Parekh & Patel, 2005). We herein report its crystal structure.

In the molecule of (I) (Fig. 1), the bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). Intramolecular O—H $\cdots$ N hydrogen bonding (Table 2) results in the formation of planar five-membered ring A (O4/H4/N1/C4—C6). Ring B (C5—C10) is, of course, planar and the dihedral angle between planes A and B is 3.56 (4) $^\circ$ . On the other hand, the C2/C4—C10/N1/O4 unit is nearly planar, with an r.m.s. deviation of 0.0425 Å.

In the crystal structure, intermolecular O—H $\cdots$ O hydrogen bonds (Table 2 and Fig. 2) result in the formation of chains along the *c* axis.

### Experimental

The title compound was prepared by the literature method (Parekh & Patel, 2005). The resulting solid was recrystallized from ethanol-ether (1:1) mixture to give suitable crystals of (I) for X-ray analysis (yield; 65%).

### Refinement

H3 and H4A (for OH groups) were located in difference syntheses and refined isotropically [O3—H3 = 0.79 (3) Å,  $U_{\text{iso}}(\text{H}) = 0.053$  (8) Å<sup>2</sup> and O4—H4A = 0.85 (3) Å,  $U_{\text{iso}}(\text{H}) = 0.087$  (11) Å<sup>2</sup>]. The remaining H atoms were positioned geometrically, with C—H = 0.93, 0.98 and 0.97 Å for aromatic, methine and methylene H atoms, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

### Figures

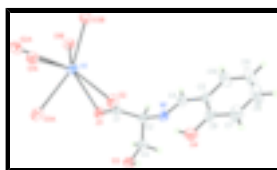


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry codes: (A)  $-x + 3/2, y, z + 1/2$ ; (B)  $x, y, z + 1$ ].

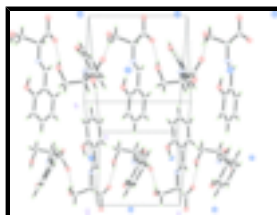


Fig. 2. A packing diagram for (I).

## poly[[ $\mu$ -3-hydroxy-2-(2-hydroxybenzylideneamino)propionato]potassium]

### Crystal data

[K(C <sub>10</sub> H <sub>10</sub> NO <sub>4</sub> )]	$F_{000} = 512$
$M_r = 247.29$	$D_x = 1.504 \text{ Mg m}^{-3}$
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation
Hall symbol: P 2c -2ac	$\lambda = 0.71073 \text{ \AA}$
$a = 7.9571 (6) \text{ \AA}$	Cell parameters from 1145 reflections
$b = 17.7596 (13) \text{ \AA}$	$\theta = 3.0\text{--}25.1^\circ$
$c = 7.7258 (6) \text{ \AA}$	$\mu = 0.48 \text{ mm}^{-1}$
$V = 1091.77 (14) \text{ \AA}^3$	$T = 291 (2) \text{ K}$
$Z = 4$	Block, yellow
	$0.16 \times 0.12 \times 0.10 \text{ mm}$

### Data collection

Bruker SMART CCD area-detector diffractometer	1782 independent reflections
Radiation source: fine-focus sealed tube	1689 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.027$
$T = 291(2) \text{ K}$	$\theta_{\text{max}} = 26.0^\circ$
$\varphi$ and $\omega$ scans	$\theta_{\text{min}} = 2.3^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.927$ , $T_{\text{max}} = 0.953$	$k = -20 \rightarrow 21$
5642 measured reflections	$l = -9 \rightarrow 7$

### Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.024$	$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.0126P]$
$wR(F^2) = 0.068$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{\text{max}} = 0.002$
1782 reflections	$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
153 parameters	$\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 630 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: $-0.06 (4)$

*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>	$U_{\text{iso}}^*/U_{\text{eq}}$
K1	0.91131 (5)	1.03625 (2)	1.40599 (7)	0.04057 (13)
O1	0.86842 (16)	1.08264 (8)	1.0595 (2)	0.0402 (3)
O2	1.13102 (19)	1.09544 (8)	1.1450 (2)	0.0440 (4)
O3	1.0429 (2)	1.10354 (8)	0.70054 (19)	0.0427 (4)
H3	1.141 (3)	1.1124 (14)	0.700 (4)	0.053 (8)*
O4	1.49653 (19)	1.22892 (9)	0.8458 (2)	0.0483 (4)
H4A	1.400 (4)	1.2107 (18)	0.872 (6)	0.087 (11)*
N1	1.18204 (19)	1.22190 (8)	0.9470 (2)	0.0345 (4)
C1	1.0058 (2)	1.11657 (10)	1.0608 (3)	0.0309 (4)
C2	1.0143 (2)	1.18757 (11)	0.9488 (3)	0.0339 (4)
H2	0.9347	1.2244	0.9955	0.041*
C3	0.9613 (3)	1.16839 (12)	0.7653 (3)	0.0387 (5)
H3A	0.8408	1.1603	0.7628	0.046*
H3B	0.9864	1.2108	0.6904	0.046*
C4	1.1984 (2)	1.28810 (11)	1.0049 (3)	0.0392 (5)
H4	1.1057	1.3115	1.0546	0.047*
C5	1.3570 (3)	1.32923 (11)	0.9967 (3)	0.0405 (5)
C6	1.4980 (2)	1.29850 (11)	0.9128 (3)	0.0412 (4)
C7	1.6432 (3)	1.34175 (13)	0.8968 (5)	0.0607 (6)
H7	1.7358	1.3227	0.8378	0.073*
C8	1.6498 (4)	1.41259 (15)	0.9681 (5)	0.0789 (10)
H8	1.7470	1.4411	0.9560	0.095*
C9	1.5147 (4)	1.44216 (14)	1.0573 (6)	0.0828 (10)
H9	1.5219	1.4897	1.1070	0.099*
C10	1.3691 (3)	1.40066 (12)	1.0720 (5)	0.0609 (7)
H10	1.2780	1.4203	1.1324	0.073*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
K1	0.0396 (2)	0.0493 (2)	0.0329 (2)	0.00844 (17)	0.00437 (19)	0.0037 (2)
O1	0.0326 (7)	0.0483 (8)	0.0398 (8)	-0.0112 (6)	-0.0002 (7)	0.0046 (6)

## supplementary materials

O2	0.0336 (7)	0.0456 (8)	0.0527 (10)	-0.0037 (6)	-0.0075 (7)	0.0111 (7)
O3	0.0347 (7)	0.0539 (9)	0.0396 (9)	-0.0066 (7)	0.0036 (7)	-0.0091 (7)
O4	0.0450 (9)	0.0563 (10)	0.0435 (9)	-0.0054 (7)	0.0029 (7)	-0.0065 (7)
N1	0.0340 (8)	0.0359 (8)	0.0335 (10)	-0.0056 (6)	0.0020 (6)	0.0014 (6)
C1	0.0285 (9)	0.0362 (9)	0.0279 (10)	-0.0004 (7)	0.0023 (8)	-0.0031 (8)
C2	0.0297 (9)	0.0363 (9)	0.0356 (11)	-0.0003 (7)	0.0040 (7)	0.0007 (8)
C3	0.0352 (10)	0.0464 (11)	0.0346 (11)	-0.0021 (8)	-0.0007 (8)	0.0062 (9)
C4	0.0395 (11)	0.0370 (11)	0.0411 (12)	-0.0005 (8)	0.0036 (9)	0.0045 (8)
C5	0.0464 (11)	0.0328 (10)	0.0424 (12)	-0.0067 (8)	-0.0073 (9)	0.0062 (8)
C6	0.0413 (11)	0.0452 (10)	0.0371 (11)	-0.0061 (7)	-0.0066 (10)	0.0115 (10)
C7	0.0429 (11)	0.0652 (14)	0.0741 (17)	-0.0118 (10)	-0.0057 (15)	0.0092 (16)
C8	0.0565 (15)	0.0589 (16)	0.121 (3)	-0.0256 (12)	-0.0184 (18)	0.0143 (15)
C9	0.0706 (19)	0.0418 (14)	0.136 (3)	-0.0157 (12)	-0.021 (2)	-0.0080 (18)
C10	0.0587 (14)	0.0380 (12)	0.086 (2)	-0.0021 (10)	-0.0047 (15)	-0.0068 (12)

### Geometric parameters (Å, °)

K1—O1 <sup>i</sup>	2.6533 (14)	C4—N1	1.265 (2)
K1—O3 <sup>ii</sup>	2.7755 (16)	C4—C5	1.460 (3)
K1—O1	2.8215 (16)	C4—H4	0.9300
K1—O2	2.8685 (17)	C5—C10	1.399 (3)
K1—O3 <sup>iii</sup>	2.9691 (16)	C5—C6	1.406 (3)
K1—O1 <sup>iii</sup>	2.9896 (15)	C6—O4	1.340 (3)
K1—O2 <sup>iii</sup>	2.9986 (17)	C6—C7	1.393 (3)
K1—C1 <sup>iii</sup>	3.0384 (19)	C7—C8	1.374 (4)
K1—K1 <sup>iv</sup>	4.1817 (4)	C7—H7	0.9300
K1—K1 <sup>v</sup>	4.1817 (4)	C8—C9	1.380 (5)
K1—K1 <sup>vi</sup>	4.3095 (4)	C8—H8	0.9300
K1—K1 <sup>iii</sup>	4.3095 (4)	C9—C10	1.378 (4)
C1—O2	1.248 (2)	C9—H9	0.9300
C1—O1	1.248 (2)	C10—H10	0.9300
C1—C2	1.531 (3)	O1—K1 <sup>vii</sup>	2.6533 (14)
C1—K1 <sup>vi</sup>	3.0384 (19)	O1—K1 <sup>vi</sup>	2.9896 (15)
C2—N1	1.468 (2)	O2—K1 <sup>vi</sup>	2.9986 (17)
C2—C3	1.517 (3)	O3—K1 <sup>viii</sup>	2.7755 (16)
C2—H2	0.9800	O3—K1 <sup>vi</sup>	2.9691 (16)
C3—O3	1.414 (3)	O3—H3	0.79 (3)
C3—H3A	0.9700	O4—H4A	0.85 (3)
C3—H3B	0.9700		
O1 <sup>i</sup> —K1—O3 <sup>ii</sup>	79.42 (5)	O2 <sup>iii</sup> —K1—K1 <sup>iii</sup>	41.57 (3)
O1 <sup>i</sup> —K1—O1	103.41 (4)	C1 <sup>iii</sup> —K1—K1 <sup>iii</sup>	46.30 (4)
O3 <sup>ii</sup> —K1—O1	134.25 (4)	K1 <sup>iv</sup> —K1—K1 <sup>iii</sup>	102.687 (14)
O1 <sup>i</sup> —K1—O2	135.38 (4)	K1 <sup>v</sup> —K1—K1 <sup>iii</sup>	66.196 (10)
O3 <sup>ii</sup> —K1—O2	100.87 (5)	K1 <sup>vi</sup> —K1—K1 <sup>iii</sup>	127.367 (19)
O1—K1—O2	45.55 (4)	O2—C1—O1	123.94 (19)

O1 <sup>i</sup> —K1—O3 <sup>iii</sup>	126.98 (5)	O2—C1—C2	120.46 (16)
O3 <sup>ii</sup> —K1—O3 <sup>iii</sup>	138.77 (3)	O1—C1—C2	115.60 (16)
O1—K1—O3 <sup>iii</sup>	75.63 (4)	O2—C1—K1 <sup>vi</sup>	76.29 (11)
O2—K1—O3 <sup>iii</sup>	81.71 (4)	O1—C1—K1 <sup>vi</sup>	75.87 (11)
O1 <sup>i</sup> —K1—O1 <sup>iii</sup>	122.26 (6)	C2—C1—K1 <sup>vi</sup>	120.25 (12)
O3 <sup>ii</sup> —K1—O1 <sup>iii</sup>	75.97 (4)	N1—C2—C3	109.69 (15)
O1—K1—O1 <sup>iii</sup>	130.81 (4)	N1—C2—C1	112.83 (15)
O2—K1—O1 <sup>iii</sup>	100.39 (4)	C3—C2—C1	109.32 (16)
O3 <sup>iii</sup> —K1—O1 <sup>iii</sup>	63.23 (4)	N1—C2—H2	108.3
O1 <sup>i</sup> —K1—O2 <sup>iii</sup>	82.69 (4)	C3—C2—H2	108.3
O3 <sup>ii</sup> —K1—O2 <sup>iii</sup>	82.73 (5)	C1—C2—H2	108.3
O1—K1—O2 <sup>iii</sup>	142.97 (4)	O3—C3—C2	112.71 (17)
O2—K1—O2 <sup>iii</sup>	141.92 (2)	O3—C3—H3A	109.0
O3 <sup>iii</sup> —K1—O2 <sup>iii</sup>	71.99 (4)	C2—C3—H3A	109.0
O1 <sup>iii</sup> —K1—O2 <sup>iii</sup>	43.17 (4)	O3—C3—H3B	109.0
O1 <sup>i</sup> —K1—C1 <sup>iii</sup>	106.48 (5)	C2—C3—H3B	109.0
O3 <sup>ii</sup> —K1—C1 <sup>iii</sup>	88.85 (5)	H3A—C3—H3B	107.8
O1—K1—C1 <sup>iii</sup>	131.34 (5)	N1—C4—C5	122.61 (18)
O2—K1—C1 <sup>iii</sup>	118.14 (5)	N1—C4—H4	118.7
O3 <sup>iii</sup> —K1—C1 <sup>iii</sup>	55.73 (5)	C5—C4—H4	118.7
O1 <sup>iii</sup> —K1—C1 <sup>iii</sup>	23.88 (4)	C10—C5—C6	119.3 (2)
O2 <sup>iii</sup> —K1—C1 <sup>iii</sup>	23.85 (4)	C10—C5—C4	119.7 (2)
O1 <sup>i</sup> —K1—K1 <sup>iv</sup>	45.37 (3)	C6—C5—C4	121.05 (18)
O3 <sup>ii</sup> —K1—K1 <sup>iv</sup>	119.44 (3)	O4—C6—C7	118.8 (2)
O1—K1—K1 <sup>iv</sup>	88.56 (3)	O4—C6—C5	121.93 (17)
O2—K1—K1 <sup>iv</sup>	133.84 (3)	C7—C6—C5	119.3 (2)
O3 <sup>iii</sup> —K1—K1 <sup>iv</sup>	81.91 (3)	C8—C7—C6	120.0 (3)
O1 <sup>iii</sup> —K1—K1 <sup>iv</sup>	109.90 (3)	C8—C7—H7	120.0
O2 <sup>iii</sup> —K1—K1 <sup>iv</sup>	69.70 (3)	C6—C7—H7	120.0
C1 <sup>iii</sup> —K1—K1 <sup>iv</sup>	86.08 (4)	C7—C8—C9	121.2 (2)
O1 <sup>i</sup> —K1—K1 <sup>v</sup>	153.35 (3)	C7—C8—H8	119.4
O3 <sup>ii</sup> —K1—K1 <sup>v</sup>	76.91 (3)	C9—C8—H8	119.4
O1—K1—K1 <sup>v</sup>	101.83 (3)	C10—C9—C8	119.5 (3)
O2—K1—K1 <sup>v</sup>	62.16 (3)	C10—C9—H9	120.2
O3 <sup>iii</sup> —K1—K1 <sup>v</sup>	68.03 (3)	C8—C9—H9	120.2
O1 <sup>iii</sup> —K1—K1 <sup>v</sup>	39.17 (3)	C9—C10—C5	120.6 (3)
O2 <sup>iii</sup> —K1—K1 <sup>v</sup>	82.34 (3)	C9—C10—H10	119.7
C1 <sup>iii</sup> —K1—K1 <sup>v</sup>	61.21 (3)	C5—C10—H10	119.7
K1 <sup>iv</sup> —K1—K1 <sup>v</sup>	144.13 (2)	C4—N1—C2	118.45 (16)
O1 <sup>i</sup> —K1—K1 <sup>vi</sup>	140.20 (4)	C1—O1—K1 <sup>vii</sup>	152.63 (14)
O3 <sup>ii</sup> —K1—K1 <sup>vi</sup>	137.73 (4)	C1—O1—K1	91.58 (12)

## supplementary materials

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O1—K1—K1 <sup>vi</sup>	43.65 (3)	K1 <sup>vii</sup> —O1—K1	115.78 (5)
O2—K1—K1 <sup>vi</sup>	43.92 (3)	C1—O1—K1 <sup>vi</sup>	80.25 (10)
O3 <sup>iii</sup> —K1—K1 <sup>vi</sup>	39.72 (3)	K1 <sup>vii</sup> —O1—K1 <sup>vi</sup>	95.46 (4)
O1 <sup>iii</sup> —K1—K1 <sup>vi</sup>	87.28 (3)	K1—O1—K1 <sup>vi</sup>	95.69 (4)
O2 <sup>iii</sup> —K1—K1 <sup>vi</sup>	110.83 (3)	C1—O2—K1	89.42 (12)
C1 <sup>iii</sup> —K1—K1 <sup>vi</sup>	90.85 (4)	C1—O2—K1 <sup>vi</sup>	79.86 (11)
K1 <sup>iv</sup> —K1—K1 <sup>vi</sup>	102.687 (14)	K1—O2—K1 <sup>vi</sup>	94.51 (4)
K1 <sup>v</sup> —K1—K1 <sup>vi</sup>	66.196 (10)	C3—O3—K1 <sup>viii</sup>	117.90 (12)
O1 <sup>i</sup> —K1—K1 <sup>iii</sup>	88.10 (3)	C3—O3—K1 <sup>vi</sup>	123.25 (12)
O3 <sup>ii</sup> —K1—K1 <sup>iii</sup>	43.13 (3)	K1 <sup>viii</sup> —O3—K1 <sup>vi</sup>	97.15 (4)
O1—K1—K1 <sup>iii</sup>	167.76 (3)	C3—O3—H3	106.8 (18)
O2—K1—K1 <sup>iii</sup>	122.68 (4)	K1 <sup>viii</sup> —O3—H3	117 (2)
O3 <sup>iii</sup> —K1—K1 <sup>iii</sup>	100.91 (3)	K1 <sup>vi</sup> —O3—H3	92.8 (18)
O1 <sup>iii</sup> —K1—K1 <sup>iii</sup>	40.65 (3)	C6—O4—H4A	106 (2)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 $\cdots$ O2 <sup>ix</sup>	0.80 (2)	1.89 (2)	2.634 (2)	156 (3)
O4—H4A $\cdots$ N1	0.86 (3)	1.84 (3)	2.625 (2)	151 (3)

Symmetry codes: (ix)  $-x+5/2, y, z-1/2$ .



Fig. 1

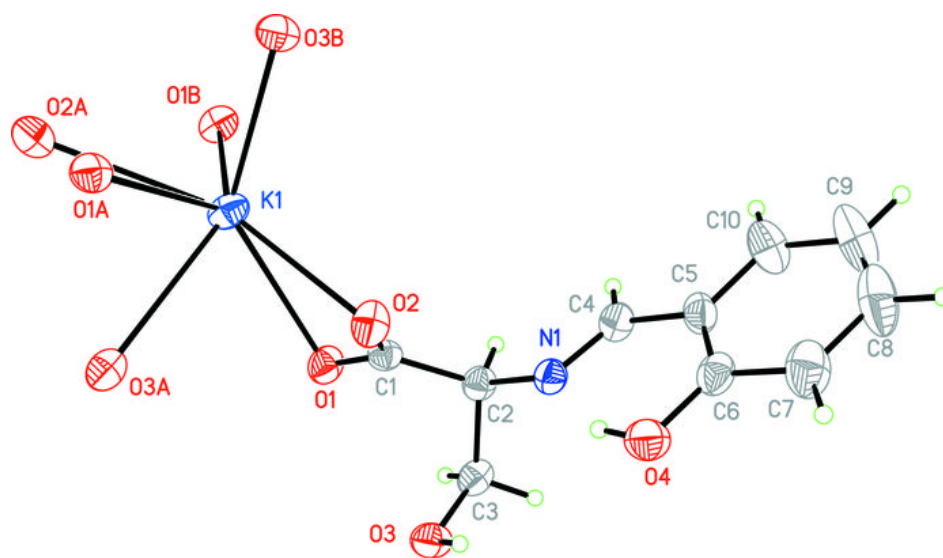


Fig. 2

