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Potassium 3-formyl-[1,1′-biphenyl]-4-olate monohydrate

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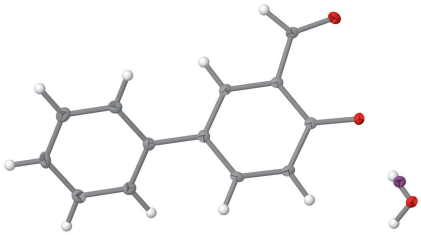
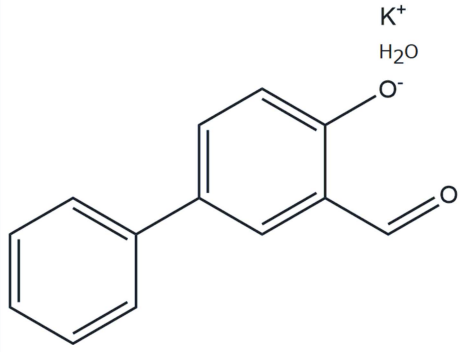
The title salt, $K^{+}\cdot C_{13}H_9O_2^{-}\cdot H_2O$, was synthesized from 5-bromosalicylaldehyde and a phenylboronic acid derivative using the Suzuki–Miyaura cross-coupling reaction (Miyaura & Suzuki, 1979). In addition to the intermolecular interactions between the charged species, two O—H···O hydrogen bonds involving the isolated water molecules further stabilize the crystal packing of the title salt leading to the formation of a three-dimensional framework structure.

3D view



Chemical scheme



Structure description

Biaryl is an important basic skeleton for various kinds of molecules: physiologically active substances (*e.g.* diflunisal, which shows analgesic and anti-inflammatory action) and liquid crystals (*e.g.* 4-alkyl 4′-cyanobiphenyl). In addition, phenylphenol comprising a biaryl skeleton, is used as reagent, reactant (Kikushima & Nishina, 2013; Hall *et al.*, 2017; Yuan *et al.*, 2017) and drug (Jiratthiya *et al.* 2015).

In the crystal structure of the title compound (Fig. 1), the O atom of the formyl group is tilted towards the phenoxide O atom: the torsion angle C10—C9—C13—O2 is 3.0 (2)° and the torsion angle O2—C13—C9—C8 is −179.71 (13)°. The K^{+} cations are surrounded by seven O atoms from three isolated water molecules and three different $[C_{13}H_9O_2]^{-}$ anions. The seven K···O distances are in the range of 2.717 (1)–2.960 (1) Å. Two O—H···O hydrogen bonds (Table 1) involving the isolated water molecules further stabilize the crystal packing of the title salt (Fig. 2) leading to the formation of a three-dimensional framework structure.

Synthesis and crystallization

Treatment of 5-bromosalicylaldehyde (0.402 g, 2.00 mmol), phenylboronic acid (0.366 g, 3.00 mmol), K_2CO_3 (0.553 g, 4.00 mmol) and $Pd(PPh_3)_4$ (0.5 mol%) in EtOH–H_2O (4:1 *v*/

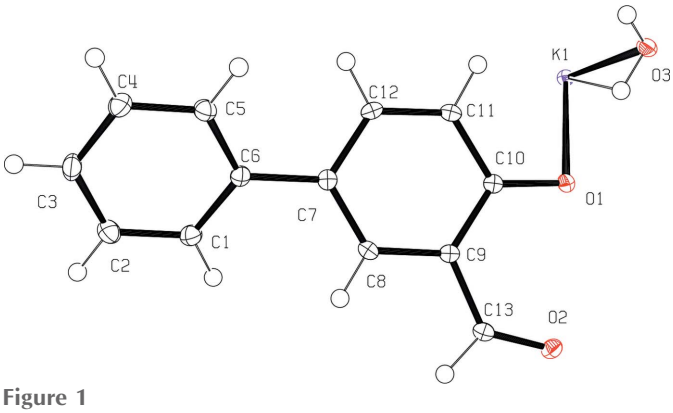


Figure 1
The structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

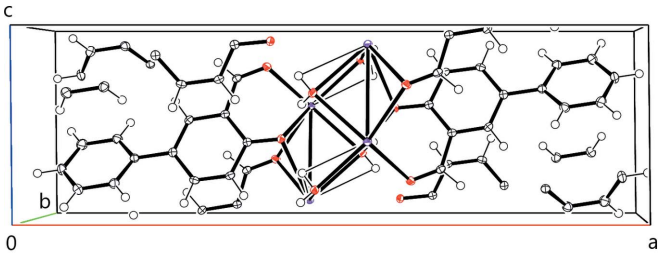


Figure 2
A packing diagram of the title compound.

v) for 5 h at 353 K in degassed N_2 (Morris & Nguyen, 2001) gave rise to a yellow precursor after evaporation and was dried in a desiccator for several days (68% yield). This crude yellow compound was filtered off and recrystallized by slow evaporation from a methanol solution to give yellow prismatic single crystals.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The formyl H atom and the water H atoms were located and freely refined, while the other aromatic H atoms were placed in calculated positions.

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Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H14···O1^{i}	0.82 (3)	1.96 (3)	2.7751 (15)	168 (2)
O3—H15···O1	0.86 (2)	1.87 (2)	2.7136 (15)	168 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$K^+\cdot C_{13}H_9O_2^-\cdot HO$
M_r	254.32
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	103
a, b, c (Å)	23.213 (5), 6.7398 (15), 7.2711 (16)
β (°)	90.593 (3)
V (Å^3)	1137.5 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.46
Crystal size (mm)	0.27 × 0.18 × 0.10
Data collection	
Diffractometer	Bruker APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.886, 0.957
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5890, 2532, 2402
R_{int}	0.024
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.073, 1.12
No. of reflections	2532
No. of parameters	170
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.25

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *SHELXTL* (Sheldrick, 2008).

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full crystallographic data

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Potassium 3-formyl-[1,1′-biphenyl]-4-olate monohydrate

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Potassium 3-formyl-[1,1′-biphenyl]-4-olate monohydrate

Crystal data

$K^+ \cdot C_{13}H_9O_2^- \cdot HO$
$M_r = 254.32$
Monoclinic, $P2_1/c$
$a = 23.213$ (5) Å
$b = 6.7398$ (15) Å
$c = 7.2711$ (16) Å
$\beta = 90.593$ (3)°
$V = 1137.5$ (4) Å^3
$Z = 4$
$F(000) = 528$
$D_x = 1.485$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4464 reflections
$\theta = 1.8$–27.5°
$\mu = 0.46$ mm^{-1}
$T = 103$ K
Prism, orange
0.27 × 0.18 × 0.10 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
$T_{min} = 0.886$, $T_{max} = 0.957$
5890 measured reflections
2532 independent reflections
2402 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
$h = -18 \rightarrow 29$
$k = -7 \rightarrow 8$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.073$
$S = 1.12$
2532 reflections
170 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0255P)^2 + 0.8435P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.59348 (4)	0.52653 (14)	0.58043 (13)	0.0108 (2)
O3	0.53358 (4)	0.72835 (16)	0.83869 (14)	0.0128 (2)
O2	0.61886 (4)	0.43723 (15)	0.20229 (13)	0.0127 (2)
C10	0.64935 (6)	0.52030 (19)	0.59788 (18)	0.0095 (3)
C12	0.73524 (6)	0.5543 (2)	0.79525 (18)	0.0115 (3)
H12	0.7511	0.5843	0.913	0.014*
C11	0.67639 (6)	0.5623 (2)	0.77061 (19)	0.0115 (3)
C9	0.68751 (6)	0.4706 (2)	0.45135 (18)	0.0099 (3)
C8	0.74752 (6)	0.4621 (2)	0.48228 (19)	0.0111 (3)
H8	0.7717	0.4267	0.3828	0.013*
C7	0.77284 (6)	0.5032 (2)	0.65162 (19)	0.0108 (3)
C13	0.66859 (6)	0.4365 (2)	0.26244 (19)	0.0112 (3)
C6	0.83627 (6)	0.4996 (2)	0.68178 (19)	0.0118 (3)
C5	0.86217 (6)	0.6294 (2)	0.8087 (2)	0.0150 (3)
H5	0.8389	0.7199	0.875	0.018*
C1	0.87173 (6)	0.3692 (2)	0.5851 (2)	0.0151 (3)
H1	0.8551	0.2796	0.4987	0.018*
C4	0.92142 (6)	0.6274 (2)	0.8388 (2)	0.0174 (3)
H4	0.9382	0.7151	0.9265	0.021*
C3	0.95605 (6)	0.4978 (2)	0.7413 (2)	0.0178 (3)
H3	0.9966	0.4968	0.7613	0.021*
C2	0.93100 (7)	0.3692 (2)	0.6139 (2)	0.0182 (3)
H2	0.9546	0.2809	0.5461	0.022*
H11	0.6529 (7)	0.601 (3)	0.873 (2)	0.015 (4)*
H13	0.7009 (7)	0.408 (3)	0.178 (2)	0.012 (4)*
H14	0.5538 (10)	0.807 (4)	0.897 (3)	0.040 (7)*
H15	0.5545 (9)	0.680 (3)	0.753 (3)	0.027 (5)*
K1	0.55412 (2)	0.31194 (4)	0.91130 (4)	0.01045 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0090 (5)	0.0120 (5)	0.0113 (4)	0.0002 (4)	0.0007 (3)	−0.0005 (4)
O3	0.0108 (5)	0.0155 (5)	0.0122 (5)	−0.0005 (4)	0.0019 (4)	−0.0030 (4)
O2	0.0127 (5)	0.0142 (5)	0.0111 (5)	−0.0022 (4)	−0.0012 (4)	0.0005 (4)
C10	0.0120 (6)	0.0056 (6)	0.0109 (6)	−0.0008 (5)	0.0005 (5)	0.0011 (5)
C12	0.0152 (7)	0.0104 (6)	0.0088 (6)	−0.0013 (5)	−0.0015 (5)	−0.0003 (5)
C11	0.0137 (7)	0.0112 (6)	0.0097 (6)	−0.0005 (5)	0.0022 (5)	−0.0008 (5)
C9	0.0125 (6)	0.0075 (6)	0.0097 (6)	−0.0008 (5)	0.0008 (5)	0.0005 (5)
C8	0.0118 (6)	0.0102 (6)	0.0115 (6)	−0.0001 (5)	0.0028 (5)	−0.0006 (5)
C7	0.0113 (6)	0.0085 (6)	0.0126 (6)	−0.0007 (5)	0.0001 (5)	0.0007 (5)
C13	0.0133 (7)	0.0094 (6)	0.0109 (6)	−0.0012 (5)	0.0023 (5)	0.0002 (5)
C6	0.0120 (7)	0.0124 (6)	0.0110 (6)	−0.0003 (5)	0.0000 (5)	0.0025 (5)
C5	0.0146 (7)	0.0152 (7)	0.0153 (7)	−0.0002 (6)	0.0012 (5)	−0.0025 (6)
C1	0.0156 (7)	0.0158 (7)	0.0140 (7)	0.0013 (6)	−0.0013 (5)	−0.0022 (6)

C4	0.0154 (7)	0.0201 (7)	0.0166 (7)	−0.0032 (6)	−0.0015 (6)	−0.0021 (6)
C3	0.0105 (7)	0.0239 (8)	0.0192 (7)	0.0007 (6)	−0.0019 (5)	0.0026 (6)
C2	0.0166 (7)	0.0202 (7)	0.0178 (7)	0.0046 (6)	0.0017 (6)	−0.0013 (6)
K1	0.01107 (15)	0.01123 (15)	0.00905 (15)	0.00107 (11)	0.00014 (10)	−0.00008 (11)

Geometric parameters (Å, º)

O1—C10	1.3026 (17)	C7—C6	1.4864 (19)
O1—K1^{i}	2.7437 (11)	C13—K1^{i}	3.3310 (15)
O1—K1	2.9597 (11)	C13—H13	0.992 (17)
O3—K1^{ii}	2.7567 (11)	C6—C1	1.399 (2)
O3—K1^{iii}	2.7730 (12)	C6—C5	1.402 (2)
O3—K1	2.8943 (13)	C5—C4	1.391 (2)
O3—H14	0.82 (3)	C5—H5	0.95
O3—H15	0.86 (2)	C1—C2	1.390 (2)
O2—C13	1.2302 (17)	C1—H1	0.95
O2—K1^{iv}	2.7170 (11)	C4—C3	1.387 (2)
O2—K1^{i}	2.7268 (11)	C4—H4	0.95
C10—C11	1.4266 (19)	C3—C2	1.391 (2)
C10—C9	1.4324 (19)	C3—H3	0.95
C10—K1^{i}	3.4175 (14)	C2—H2	0.95
C10—K1	3.4866 (14)	K1—O2^{v}	2.7171 (11)
C12—C11	1.377 (2)	K1—O2^{vi}	2.7269 (11)
C12—C7	1.4107 (19)	K1—O1^{vi}	2.7437 (11)
C12—H12	0.95	K1—O3^{ii}	2.7566 (11)
C11—K1	3.4656 (15)	K1—O3^{vii}	2.7730 (12)
C11—H11	0.962 (18)	K1—C13^{vi}	3.3311 (15)
C9—C8	1.4098 (19)	K1—C10^{vi}	3.4175 (14)
C9—C13	1.4561 (19)	K1—K1^{vi}	3.7302 (8)
C8—C7	1.3869 (19)	K1—H11	3.022 (18)
C8—H8	0.95	K1—H15	2.74 (2)
C10—O1—K1^{i}	110.09 (8)	O1^{vi}—K1—O3	160.29 (3)
C10—O1—K1	102.74 (8)	O3^{ii}—K1—O3	95.42 (3)
K1^{i}—O1—K1	81.60 (3)	O3^{vii}—K1—O3	87.65 (2)
K1^{ii}—O3—K1^{iii}	84.84 (3)	O2^{v}—K1—O1	107.95 (3)
K1^{ii}—O3—K1	84.58 (3)	O2^{vi}—K1—O1	70.82 (3)
K1^{iii}—O3—K1	115.79 (4)	O1^{vi}—K1—O1	131.80 (4)
K1^{ii}—O3—H14	98.1 (16)	O3^{ii}—K1—O1	145.13 (3)
K1^{iii}—O3—H14	128.3 (16)	O3^{vii}—K1—O1	78.29 (3)
K1—O3—H14	115.9 (16)	O3—K1—O1	55.22 (3)
K1^{ii}—O3—H15	150.4 (14)	O2^{v}—K1—C13^{vi}	88.43 (4)
K1^{iii}—O3—H15	90.9 (14)	O2^{vi}—K1—C13^{vi}	20.48 (3)
K1—O3—H15	71.0 (14)	O1^{vi}—K1—C13^{vi}	57.63 (3)
H14—O3—H15	107 (2)	O3^{ii}—K1—C13^{vi}	139.62 (4)
C13—O2—K1^{iv}	141.72 (9)	O3^{vii}—K1—C13^{vi}	105.52 (4)
C13—O2—K1^{i}	108.66 (8)	O3—K1—C13^{vi}	123.96 (3)
K1^{iv}—O2—K1^{i}	86.51 (3)	O1—K1—C13^{vi}	74.19 (3)

O1—C10—C11	120.53 (12)	O2^{v}—K1—C10^{vi}	62.89 (3)
O1—C10—C9	123.92 (12)	O2^{vi}—K1—C10^{vi}	57.30 (3)
C11—C10—C9	115.55 (12)	O1^{vi}—K1—C10^{vi}	20.97 (3)
O1—C10—K1^{i}	48.94 (6)	O3^{ii}—K1—C10^{vi}	98.79 (4)
C11—C10—K1^{i}	139.15 (9)	O3^{vii}—K1—C10^{vi}	126.48 (3)
C9—C10—K1^{i}	87.36 (8)	O3—K1—C10^{vi}	144.33 (3)
O1—C10—K1	55.89 (6)	O1—K1—C10^{vi}	116.04 (3)
C11—C10—K1	77.33 (8)	C13^{vi}—K1—C10^{vi}	44.33 (3)
C9—C10—K1	142.48 (9)	O2^{v}—K1—C11	68.31 (3)
K1^{i}—C10—K1	65.40 (3)	O2^{vi}—K1—C11	71.19 (3)
C11—C12—C7	122.26 (12)	O1^{vi}—K1—C11	105.50 (3)
C11—C12—H12	118.9	O3^{ii}—K1—C11	148.79 (3)
C7—C12—H12	118.9	O3^{vii}—K1—C11	120.22 (4)
C12—C11—C10	122.25 (13)	O3—K1—C11	66.92 (3)
C12—C11—K1	139.20 (9)	O1—K1—C11	42.39 (3)
C10—C11—K1	78.99 (8)	C13^{vi}—K1—C11	59.36 (4)
C12—C11—H11	118.6 (10)	C10^{vi}—K1—C11	84.71 (4)
C10—C11—H11	119.1 (10)	O2^{v}—K1—C10	91.98 (3)
K1—C11—H11	55.2 (11)	O2^{vi}—K1—C10	61.77 (3)
C8—C9—C10	120.56 (12)	O1^{vi}—K1—C10	114.67 (3)
C8—C9—C13	115.60 (12)	O3^{ii}—K1—C10	161.48 (3)
C10—C9—C13	123.75 (12)	O3^{vii}—K1—C10	96.86 (4)
C7—C8—C9	122.86 (13)	O3—K1—C10	66.08 (3)
C7—C8—H8	118.6	O1—K1—C10	21.37 (3)
C9—C8—H8	118.6	C13^{vi}—K1—C10	58.45 (3)
C8—C7—C12	116.50 (12)	C10^{vi}—K1—C10	96.40 (4)
C8—C7—C6	122.53 (12)	C11—K1—C10	23.68 (3)
C12—C7—C6	120.95 (12)	O2^{v}—K1—K1^{vi}	46.86 (2)
O2—C13—C9	127.42 (13)	O2^{vi}—K1—K1^{vi}	114.26 (3)
O2—C13—K1^{i}	50.86 (7)	O1^{vi}—K1—K1^{vi}	51.71 (2)
C9—C13—K1^{i}	90.38 (8)	O3^{ii}—K1—K1^{vi}	47.76 (2)
O2—C13—H13	119.7 (10)	O3^{vii}—K1—K1^{vi}	125.88 (3)
C9—C13—H13	112.9 (10)	O3—K1—K1^{vi}	113.15 (2)
K1^{i}—C13—H13	135.7 (10)	O1—K1—K1^{vi}	154.79 (2)
C1—C6—C5	118.17 (13)	C13^{vi}—K1—K1^{vi}	102.25 (3)
C1—C6—C7	121.55 (13)	C10^{vi}—K1—K1^{vi}	58.19 (2)
C5—C6—C7	120.28 (13)	C11—K1—K1^{vi}	113.89 (2)
C4—C5—C6	120.96 (14)	C10—K1—K1^{vi}	137.19 (2)
C4—C5—H5	119.5	O2^{v}—K1—H11	57.2 (3)
C6—C5—H5	119.5	O2^{vi}—K1—H11	85.5 (4)
C2—C1—C6	120.73 (14)	O1^{vi}—K1—H11	109.1 (3)
C2—C1—H1	119.6	O3^{ii}—K1—H11	133.7 (4)
C6—C1—H1	119.6	O3^{vii}—K1—H11	128.5 (3)
C3—C4—C5	120.20 (14)	O3—K1—H11	58.8 (3)
C3—C4—H4	119.9	O1—K1—H11	50.9 (3)
C5—C4—H4	119.9	C13^{vi}—K1—H11	71.6 (3)
C4—C3—C2	119.47 (14)	C10^{vi}—K1—H11	88.3 (3)
C4—C3—H3	120.3	C11—K1—H11	15.2 (3)

C2—C3—H3	120.3	C10—K1—H11	36.3 (3)
C1—C2—C3	120.46 (14)	K1^{vi}—K1—H11	104.0 (3)
C1—C2—H2	119.8	O2^{v}—K1—H15	92.4 (4)
C3—C2—H2	119.8	O2^{vi}—K1—H15	108.6 (5)
O2^{v}—K1—O2^{vi}	108.77 (4)	O1^{vi}—K1—H15	160.1 (4)
O2^{v}—K1—O1^{vi}	74.36 (3)	O3^{ii}—K1—H15	111.9 (5)
O2^{vi}—K1—O1^{vi}	63.57 (3)	O3^{vii}—K1—H15	85.0 (4)
O2^{v}—K1—O3^{ii}	85.61 (4)	O3—K1—H15	17.2 (5)
O2^{vi}—K1—O3^{ii}	136.21 (3)	O1—K1—H15	38.0 (5)
O1^{vi}—K1—O3^{ii}	82.37 (3)	C13^{vi}—K1—H15	108.3 (5)
O2^{v}—K1—O3^{vii}	165.93 (3)	C10^{vi}—K1—H15	139.2 (4)
O2^{vi}—K1—O3^{vii}	85.10 (3)	C11—K1—H15	55.1 (4)
O1^{vi}—K1—O3^{vii}	111.33 (3)	C10—K1—H15	49.8 (5)
O3^{ii}—K1—O3^{vii}	82.54 (3)	K1^{vi}—K1—H15	127.9 (5)
O2^{v}—K1—O3	85.95 (3)	H11—K1—H15	51.1 (5)
O2^{vi}—K1—O3	125.89 (3)		

K1^{i}—O1—C10—C11	−130.61 (11)	C13—C9—C8—C7	175.89 (13)
K1—O1—C10—C11	−45.02 (13)	C9—C8—C7—C12	0.2 (2)
K1^{i}—O1—C10—C9	48.75 (14)	C9—C8—C7—C6	−178.19 (13)
K1—O1—C10—C9	134.34 (11)	C11—C12—C7—C8	0.4 (2)
K1—O1—C10—K1^{i}	85.59 (5)	C11—C12—C7—C6	178.84 (13)
K1^{i}—O1—C10—K1	−85.59 (5)	K1^{iv}—O2—C13—C9	−161.18 (10)
C7—C12—C11—C10	−0.3 (2)	K1^{i}—O2—C13—C9	−52.27 (16)
C7—C12—C11—K1	112.39 (15)	K1^{iv}—O2—C13—K1^{i}	−108.92 (14)
O1—C10—C11—C12	178.99 (12)	C8—C9—C13—O2	−179.71 (13)
C9—C10—C11—C12	−0.42 (19)	C10—C9—C13—O2	−3.0 (2)
K1^{i}—C10—C11—C12	117.93 (14)	C8—C9—C13—K1^{i}	142.45 (11)
K1—C10—C11—C12	142.10 (13)	C10—C9—C13—K1^{i}	−40.80 (13)
O1—C10—C11—K1	36.89 (11)	C8—C7—C6—C1	−32.3 (2)
C9—C10—C11—K1	−142.53 (11)	C12—C7—C6—C1	149.29 (14)
K1^{i}—C10—C11—K1	−24.17 (12)	C8—C7—C6—C5	147.29 (14)
O1—C10—C9—C8	−178.37 (12)	C12—C7—C6—C5	−31.1 (2)
C11—C10—C9—C8	1.02 (19)	C1—C6—C5—C4	−0.5 (2)
K1^{i}—C10—C9—C8	−143.79 (12)	C7—C6—C5—C4	179.81 (13)
K1—C10—C9—C8	−101.90 (16)	C5—C6—C1—C2	−0.2 (2)
O1—C10—C9—C13	5.0 (2)	C7—C6—C1—C2	179.40 (13)
C11—C10—C9—C13	−175.58 (13)	C6—C5—C4—C3	0.8 (2)
K1^{i}—C10—C9—C13	39.61 (13)	C5—C4—C3—C2	−0.3 (2)
K1—C10—C9—C13	81.51 (19)	C6—C1—C2—C3	0.7 (2)
C10—C9—C8—C7	−1.0 (2)	C4—C3—C2—C1	−0.4 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H14···O1^{viii}	0.82 (3)	1.96 (3)	2.7751 (15)	168 (2)

O3—H15···O1	0.86 (2)	1.87 (2)	2.7136 (15)	168 (2)

Symmetry code: (viii) x, $-y+3/2$, $z+1/2$.