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Crystal structure of *catena*-poly[[potassium-tri- μ -dimethylacetamide- κ^6 O:O] iodide]

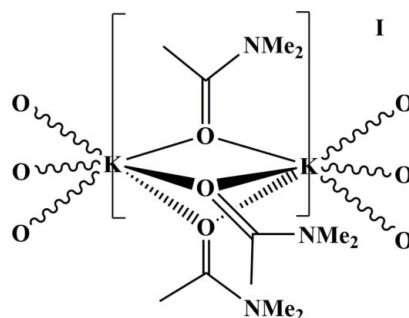
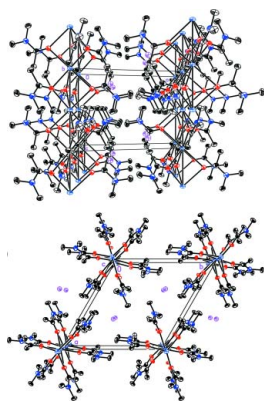
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The structure of *catena*-poly[[potassium-tri- μ -dimethylacetamide- κ^6 O:O] iodide], $[\{K(C_4H_9NO)_3\}I]_n$, at 120 K has trigonal ($P\bar{3}$) symmetry. The structure adopts a linear chain motif parallel to the crystallographic c axis. Two crystallographically independent K^+ cations are present in the asymmetric unit located on threefold rotoinversion axes at $[0, 0, 0]$ and $[0, 0, \frac{1}{2}]$ and are bridged by the O atoms of the acetamide moiety. This is an example of a rare μ_2 -bridging mode for dimethylacetamide O atoms. The iodide counter-ion resides on a threefold rotation axis in the channel formed by the $[K(C_4H_9NO)]^+$ chains.

1. Chemical context

Coordination of dimethylacetamide (DMA) to metal centers has been observed previously in a number of metal complexes, but μ_2 -coordination of the O atom has only been reported in two crystallographically confirmed structures. Tikhonova *et al.* (2001) crystallized a bis(μ_3 - N,N -dimethylacetamide)tris(μ_2 -perfluoro-*o*-phenylene)trimercury(II) complex and found Hg–O(DMA) bond lengths in the range 2.776 (2)–2.989 (2) Å. Dias *et al.* (1995) synthesized bis{(μ_2 -dimethylacetamido- O,O)}(μ_2 -hydrogen tris[3,5-bis(trifluoromethyl)pyrazoly]borate)potassium}, in which the O atom is μ_2 -bridging between two K^+ cations and the K–O bond length is 2.703 (2) Å. In the KI·3DMA structure reported here, the K–O bond lengths are in the range 2.763 (2)–2.774 (3) Å, slightly longer than in the closely related potassium complex synthesized by Dias *et al.* (1995).



2. Structural commentary

The cation of title compound consists of two crystallographically independent potassium cations. Each K^+ cation is octahedrally coordinated by six O atoms from the DMA moieties, with each oxygen adopting a μ_2 -bridging mode (Fig. 1 and Table 1). The C=O distance is comparable with that in free dimethylacetamide (see *Database survey*). The iodide

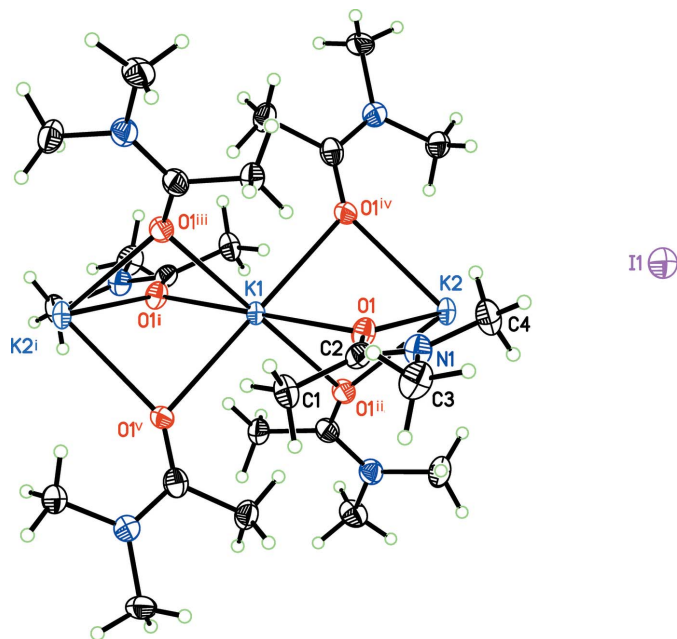


Figure 1
The atom-labeling scheme for KI·3DMA, with displacement ellipsoids depicted at the 50% probability level. [Symmetry codes: (i) $-x, -y, -z$; (ii) $y, -x + y, -z$; (iii) $-y, x - y, z$; (iv) $x - y, x, -z$; (v) $-x + y, -x, z$; (vi) $x, y, z - 1$.]

anion is independent of the one-dimensional chain and does not form any covalent contacts to the cation.

The extended structure forms a chain of K^+ cations, bridged by μ_2 -*O*-dimethylacetamide moieties. The two independent K^+ cations are located at $[0, 0, 0]$ and $[0, 0, \frac{1}{2}]$ (Wyckoff positions *a* and *b*, respectively) and the iodine is located at $[\frac{2}{3}, \frac{1}{3}, z]$ (Wyckoff position *d*). In the primary structure, each K^+ cation adopts a slightly distorted octahedral coordination sphere (key bond lengths and angles are given in Table 1).

3. Supramolecular features

The μ_2 -*O*-dimethylacetamide bridging the two K^+ cations forms a linear $[K(DMA)_3]^+$ chain parallel to the *c* axis. The application of the $\bar{3}$ symmetry results in an aesthetically pleasing ‘snowflake’ configuration when viewed along the *c* axis (Fig. 2). The iodide counter-ion resides in the channels formed by the $[K(DMA)_3]^+$ chains. With regards to the extended structure, there are very weak $C-H \cdots I$ interactions within the lattice (Table 2). These serve to locate the iodine in a pocket within the structure.

Table 1
Selected geometric parameters (Å, °).

K1—O1	2.7438 (16)	O1—C2	1.254 (3)
K1—K2	3.6728 (4)	O1—K2	2.7627 (16)
O1 ⁱ —K1—O1	180.0	O1 ⁱⁱⁱ —K1—O1	80.70 (5)
O1 ⁱⁱ —K1—O1	99.30 (5)		

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

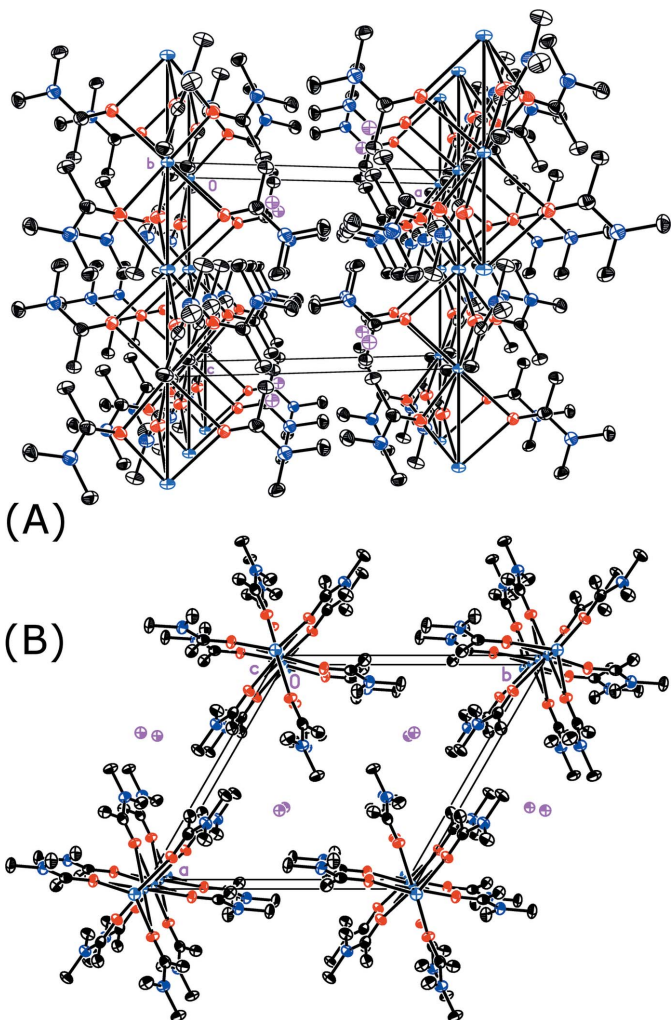


Figure 2
(A) Packing diagram viewed along the *b* axis. (B) View along the *c* axis. Legend: black = carbon, dark blue = nitrogen, light blue = potassium, magenta = iodine, and red = oxygen. H atoms have been omitted for clarity.

4. Database survey

A search in the Cambridge Structure Database (CSD, Version 5.35, November 2013 plus three updates; Allen, 2002) for structures in which K^+ is triple bridged in a μ_2 -fashion by three O atoms returns 17 results, but only 3 of them are relevant to the structure reported herein. Gonzalez-Rodriguez *et al.* (2009) have shown a complex guanosine-derived nucleoside to crystallize as an acetone solvate monohydrate in which the six bridging K^+ cations are each coordinated to eight O atoms from eight guanosine ligands, and the two terminal K^+ cations

Table 2
Hydrogen-bond geometry (Å, °).

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C1—H1A \cdots I1 ^{iv}	0.98	3.20	4.178 (3)	177
C3—H3A \cdots I1 ^{iv}	0.98	3.20	4.178 (3)	174
C4—H4C \cdots I1	0.98	3.00	3.967 (3)	170

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

Table 3
Experimental details.

Crystal data	
Chemical formula	[K(C ₄ H ₉ NO) ₃]I
<i>M_r</i>	427.37
Crystal system, space group	Trigonal, <i>P</i> $\bar{3}$
Temperature (K)	120
<i>a</i> , <i>c</i> (Å)	11.9776 (8), 7.3455 (7)
<i>V</i> (Å ³)	912.62 (15)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	1.99
Crystal size (mm)	0.20 × 0.09 × 0.06
Data collection	
Diffractionmeter	Bruker APEX
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2012)
<i>T_{min}</i> , <i>T_{max}</i>	0.615, 0.745
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	11940, 1248, 1194
<i>R_{int}</i>	0.026
(sin θ/λ) _{max} (Å ⁻¹)	0.623
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.024, 0.059, 1.07
No. of reflections	1248
No. of parameters	65
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	1.14, -0.43

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS97*, *SHELXL2013* and *XP* in *SHELXTL* (Sheldrick, 2013) and *pubCIF* (Westrip, 2010).

are coordinated to eight O atoms from four guanosine ligands and either four acetone molecules or four water molecules. Cunningham *et al.* (2000) crystallized *catena*-[tetrakis[*N,N'*-bis(3-methoxysalicylidene)propane-1,3-diaminoato]iodido-nickel(II)potassium], where K⁺ is bridged by four μ₂-*O*, one μ₂-*N*, and one μ₂-*I*. In fact, both of these structures contain four μ₂-*O* atoms bridging K⁺ cations. No close K⋯K contacts were observed: the K⋯K distances are in the range 3.451 (2)–3.567 (2) Å. Most closely related is the structure of *catena*-[tris(μ₂-dimethylformamide-*O,O*)potassium iodide], reported by Batsanov & Struchkov (1994), with a K⋯K distance of 3.4170 (10) Å and a K–O distance of 2.6570 (13) Å. In the KI·3DMA structure reported herein, the K1⋯K2 distance is 3.6728 (4) Å, which is longer by approximately 0.106 Å. In the Gonzalez-Rodriguez and Cunningham structures, iodine is found to form bonds to the K⁺ cations, while it is located in a channel within the Batsanov structure and not covalently bound. In the title compound, the iodine is not covalently bonded to the cation chain.

A search in the Cambridge Structure Database for free acetamide returned 180 results, featuring C=O bond lengths between 1.123 Å (Patra & Goldberg, 2013) and 1.67 Å (Gole *et al.*, 2011), with a mean of 1.259 Å (std. dev. 0.059), which is

very close to the C=O bond length reported herein [1.254 (3) Å]

5. Synthesis and crystallization

A carbon–carbon Heck coupling reaction catalyzed by a Pd^{II} diphosphane precatalyst was performed using conditions established previously by Brase & de Meijere (1998). In a typical synthesis, 1-iodo-4-nitrobenzene (IC₆H₄NO₂; 102.1 mg, 0.41 mmol) was mixed with 2 equivalents of *n*-butyl acrylate [CH₂=CHCOO(CH₂)₃CH₃; 105.6 mg, 0.82 mmol] in the presence of K₂CO₃ (63.6 mg, 0.46 mmol) and *n*-Bu₄NBr (13 mg, 0.041 mmol) in dimethylacetamide (DMA) over a period of 4 h at 413 K. The title compound formed and was recrystallized from the filtered reaction mixture at room temperature. The target Pd^{II} complex of the reaction has been reported (Comanescu & Iluc, 2014).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were included in a riding model and allowed to rotate to minimize electron-density contribution. C–H distances were set at 0.98 Å, with *U*_{iso}(H) = 1.5*U*_{eq}(C).

Acknowledgements

CCC thanks Professor Vlad Iluc for insightful discussions.

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Crystal structure of *catena*-poly[[potassium-tri- μ -dimethylacetamide- κ^6 O:O] iodide]

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Computing details

Data collection: APEXII (Bruker, 2012); cell refinement: *SAINTE* (Bruker, 2012); data reduction: *SAINTE* (Bruker, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

catena-Poly[[potassium-tri- μ -dimethylacetamide- κ^6 O:O] iodide]

Crystal data

[K(C₄H₉NO)₃]I
 $M_r = 427.37$
 Trigonal, $P\bar{3}$
 $a = 11.9776$ (8) Å
 $c = 7.3455$ (7) Å
 $V = 912.62$ (15) Å³
 $Z = 2$
 $F(000) = 432$

$D_x = 1.555$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 7529 reflections
 $\theta = 2.7$ – 26.3°
 $\mu = 1.99$ mm⁻¹
 $T = 120$ K
 Block, colorless
 0.20 × 0.09 × 0.06 mm

Data collection

Bruker APEX
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 8.33 pixels mm⁻¹
 combination of ω and ϕ -scans
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2012)
 $T_{\min} = 0.615$, $T_{\max} = 0.745$

11940 measured reflections
 1248 independent reflections
 1194 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$
 $\theta_{\max} = 26.3^\circ$, $\theta_{\min} = 2.0^\circ$
 $h = -14 \rightarrow 14$
 $k = -14 \rightarrow 14$
 $l = -9 \rightarrow 9$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.059$
 $S = 1.07$
 1248 reflections
 65 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
 $w = 1/[\sigma^2(F_o^2) + (0.0227P)^2 + 1.7319P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.14$ e Å⁻³
 $\Delta\rho_{\min} = -0.43$ e Å⁻³

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
II	0.6667	0.3333	0.83886 (4)	0.02490 (11)
K1	0.0000	0.0000	0.0000	0.0172 (2)
O1	0.18933 (16)	0.14411 (16)	0.2481 (2)	0.0229 (4)
N1	0.3896 (2)	0.2882 (2)	0.3421 (3)	0.0262 (5)
C1	0.3288 (3)	0.3114 (3)	0.0349 (3)	0.0281 (5)
H1A	0.4093	0.3202	−0.0125	0.042*
H1B	0.3388	0.3971	0.0517	0.042*
H1C	0.2588	0.2620	−0.0516	0.042*
K2	0.0000	0.0000	0.5000	0.0227 (3)
C2	0.2970 (2)	0.2414 (2)	0.2163 (3)	0.0249 (5)
C3	0.5155 (3)	0.4036 (3)	0.3094 (4)	0.0320 (6)
H3A	0.5574	0.3884	0.2054	0.048*
H3B	0.5697	0.4223	0.4178	0.048*
H3C	0.5033	0.4770	0.2830	0.048*
C4	0.3621 (3)	0.2247 (3)	0.5200 (4)	0.0315 (6)
H4A	0.3164	0.1310	0.5031	0.047*
H4B	0.3083	0.2488	0.5913	0.047*
H4C	0.4432	0.2516	0.5848	0.047*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
II	0.02578 (13)	0.02578 (13)	0.02315 (16)	0.01289 (6)	0.000	0.000
K1	0.0195 (4)	0.0195 (4)	0.0126 (5)	0.00975 (18)	0.000	0.000
O1	0.0183 (8)	0.0237 (9)	0.0202 (8)	0.0057 (7)	−0.0003 (6)	−0.0034 (7)
N1	0.0242 (11)	0.0271 (11)	0.0237 (10)	0.0100 (9)	0.0003 (8)	−0.0003 (8)
C1	0.0284 (13)	0.0352 (14)	0.0196 (12)	0.0152 (11)	0.0012 (10)	0.0047 (10)
K2	0.0278 (4)	0.0278 (4)	0.0123 (5)	0.0139 (2)	0.000	0.000
C2	0.0291 (13)	0.0286 (13)	0.0223 (12)	0.0185 (11)	0.0013 (10)	−0.0037 (10)
C3	0.0212 (12)	0.0280 (13)	0.0336 (14)	0.0025 (11)	0.0023 (10)	−0.0045 (11)
C4	0.0325 (14)	0.0321 (14)	0.0218 (12)	0.0100 (12)	−0.0043 (11)	0.0038 (10)

Geometric parameters (\AA , $^\circ$)

K1—O1 ⁱ	2.7437 (16)	C1—H1B	0.9800
K1—O1 ⁱⁱ	2.7437 (16)	C1—H1C	0.9800
K1—O1 ⁱⁱⁱ	2.7437 (16)	K2—O1 ^{vii}	2.7627 (16)
K1—O1 ^{iv}	2.7437 (16)	K2—O1 ^v	2.7627 (16)
K1—O1 ^v	2.7437 (16)	K2—O1 ^{viii}	2.7627 (16)

K1—O1	2.7438 (16)	K2—O1 ⁱⁱⁱ	2.7627 (16)
K1—K2 ^{vi}	3.6728 (4)	K2—O1 ^{ix}	2.7627 (17)
K1—K2	3.6728 (4)	K2—K1 ^x	3.6728 (4)
O1—C2	1.254 (3)	C3—H3A	0.9800
O1—K2	2.7627 (16)	C3—H3B	0.9800
N1—C2	1.333 (3)	C3—H3C	0.9800
N1—C4	1.465 (3)	C4—H4A	0.9800
N1—C3	1.468 (3)	C4—H4B	0.9800
C1—C2	1.517 (3)	C4—H4C	0.9800
C1—H1A	0.9800		
O1 ⁱ —K1—O1 ⁱⁱ	80.70 (5)	O1 ^v —K2—O1 ^{viii}	99.97 (5)
O1 ⁱ —K1—O1 ⁱⁱⁱ	99.30 (5)	O1 ^{vii} —K2—O1 ⁱⁱⁱ	99.97 (5)
O1 ⁱⁱ —K1—O1 ⁱⁱⁱ	180.00 (7)	O1 ^v —K2—O1 ⁱⁱⁱ	80.03 (5)
O1 ⁱ —K1—O1 ^{iv}	80.70 (5)	O1 ^{viii} —K2—O1 ⁱⁱⁱ	180.0
O1 ⁱⁱ —K1—O1 ^{iv}	80.70 (5)	O1 ^{vii} —K2—O1 ^{ix}	80.03 (5)
O1 ⁱⁱⁱ —K1—O1 ^{iv}	99.30 (5)	O1 ^v —K2—O1 ^{ix}	99.97 (5)
O1 ⁱ —K1—O1 ^v	99.30 (5)	O1 ^{viii} —K2—O1 ^{ix}	80.03 (5)
O1 ⁱⁱ —K1—O1 ^v	99.30 (5)	O1 ⁱⁱⁱ —K2—O1 ^{ix}	99.97 (5)
O1 ⁱⁱⁱ —K1—O1 ^v	80.70 (5)	O1 ^{vii} —K2—O1	99.97 (5)
O1 ^{iv} —K1—O1 ^v	180.00 (7)	O1 ^v —K2—O1	80.03 (5)
O1 ⁱ —K1—O1	180.0	O1 ^{viii} —K2—O1	99.96 (5)
O1 ⁱⁱ —K1—O1	99.30 (5)	O1 ⁱⁱⁱ —K2—O1	80.04 (5)
O1 ⁱⁱⁱ —K1—O1	80.70 (5)	O1 ^{ix} —K2—O1	180.0
O1 ^{iv} —K1—O1	99.30 (5)	O1 ^{vii} —K2—K1	132.06 (3)
O1 ^v —K1—O1	80.70 (5)	O1 ^v —K2—K1	47.94 (3)
O1 ⁱ —K1—K2 ^{vi}	48.39 (3)	O1 ^{viii} —K2—K1	132.06 (3)
O1 ⁱⁱ —K1—K2 ^{vi}	48.39 (3)	O1 ⁱⁱⁱ —K2—K1	47.94 (3)
O1 ⁱⁱⁱ —K1—K2 ^{vi}	131.61 (3)	O1 ^{ix} —K2—K1	132.06 (3)
O1 ^{iv} —K1—K2 ^{vi}	48.39 (3)	O1—K2—K1	47.94 (3)
O1 ^v —K1—K2 ^{vi}	131.61 (3)	O1 ^{vii} —K2—K1 ^x	47.94 (3)
O1—K1—K2 ^{vi}	131.61 (3)	O1 ^v —K2—K1 ^x	132.06 (3)
O1 ⁱ —K1—K2	131.61 (3)	O1 ^{viii} —K2—K1 ^x	47.94 (3)
O1 ⁱⁱ —K1—K2	131.61 (3)	O1 ⁱⁱⁱ —K2—K1 ^x	132.06 (3)
O1 ⁱⁱⁱ —K1—K2	48.39 (3)	O1 ^{ix} —K2—K1 ^x	47.94 (3)
O1 ^{iv} —K1—K2	131.61 (3)	O1—K2—K1 ^x	132.06 (3)
O1 ^v —K1—K2	48.39 (3)	K1—K2—K1 ^x	180.0
O1—K1—K2	48.39 (3)	O1—C2—N1	121.0 (2)
K2 ^{vi} —K1—K2	180.0	O1—C2—C1	122.3 (2)
C2—O1—K1	127.11 (15)	N1—C2—C1	116.8 (2)
C2—O1—K2	147.87 (15)	N1—C3—H3A	109.5
K1—O1—K2	83.67 (5)	N1—C3—H3B	109.5
C2—N1—C4	118.5 (2)	H3A—C3—H3B	109.5
C2—N1—C3	121.9 (2)	N1—C3—H3C	109.5
C4—N1—C3	119.6 (2)	H3A—C3—H3C	109.5
C2—C1—H1A	109.5	H3B—C3—H3C	109.5
C2—C1—H1B	109.5	N1—C4—H4A	109.5
H1A—C1—H1B	109.5	N1—C4—H4B	109.5

C2—C1—H1C	109.5	H4A—C4—H4B	109.5
H1A—C1—H1C	109.5	N1—C4—H4C	109.5
H1B—C1—H1C	109.5	H4A—C4—H4C	109.5
O1 ^{vii} —K2—O1 ^v	180.0	H4B—C4—H4C	109.5
O1 ^{vii} —K2—O1 ^{viii}	80.03 (5)		
K1—O1—C2—N1	-167.19 (17)	C4—N1—C2—O1	-1.0 (4)
K2—O1—C2—N1	32.0 (4)	C3—N1—C2—O1	-178.7 (2)
K1—O1—C2—C1	12.8 (3)	C4—N1—C2—C1	179.0 (2)
K2—O1—C2—C1	-148.1 (2)	C3—N1—C2—C1	1.4 (4)

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

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C1—H1A...I1 ^{vi}	0.98	3.20	4.178 (3)	177
C3—H3A...I1 ^{vi}	0.98	3.20	4.178 (3)	174
C4—H4C...I1	0.98	3.00	3.967 (3)	170

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