

Syntheses and crystal structures of three novel oxalate coordination compounds: $\text{Rb}_2\text{Co}(\text{C}_2\text{O}_4)_2 \cdot 4\text{H}_2\text{O}$, $\text{Rb}_2\text{CoCl}_2(\text{C}_2\text{O}_4)$ and $\text{K}_2\text{Li}_2\text{Cu}(\text{C}_2\text{O}_4)_3 \cdot 2\text{H}_2\text{O}$

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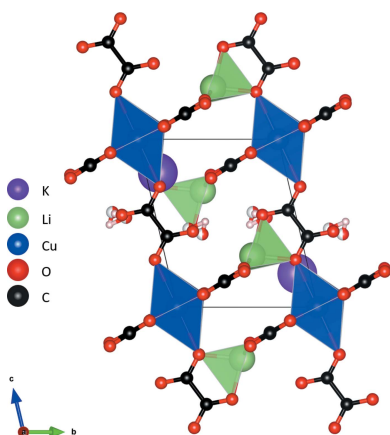
Single crystals of three novel transition-metal oxalates, dirubidium diaqua-dioxalatocobalt(II) dihydrate or dirubidium cobalt(II) bis(oxalate) tetrahydrate, $\text{Rb}_2[\text{Co}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$, (I), *catena*-poly[*dirubidium* [[dichlorido-cobalt(II)]- μ -oxalato]] or dirubidium cobalt(II) dichloride oxalate, $\{\text{Rb}_2[\text{CoCl}_2(\text{C}_2\text{O}_4)]\}_n$, (II), and poly[*dipotassium* [tri- μ -oxalato-copper(II) dilithium] dihydrate] or dipotassium dilithium copper(II) tris(oxalate) dihydrate, $\{\text{K}_2[\text{Li}_2\text{Cu}(\text{C}_2\text{O}_4)_3] \cdot 2\text{H}_2\text{O}\}_n$, (III), have been grown under hydrothermal conditions and their crystal structures determined using single-crystal X-ray diffraction. The structure of (I) exhibits isolated octahedral $[\text{Co}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$ units, whereas (II) consists of *trans* chains of Co^{2+} ions bridged by bidentate oxalato ligands and (III) displays a novel tri-periodic network of Li^+ and Cu^{2+} ions linked by oxalato bridging ligands.

1. Chemical context

Oxalate-based transition-metal complexes have long attracted interest because of their promising magnetic and electrochemical properties. Their magnetic properties are in part due to the oxalato ligand, which is known to facilitate magnetic exchange between transition-metal cations, and the compounds are known to exhibit both ferro- and anti-ferromagnetic interactions (Miller & Drillon, 2002; Baran, 2014). In addition to their magnetic properties, there have also been numerous studies concerning their electrochemical properties, which have shown promising results (Pramanik *et al.*, 2022; Cai *et al.*, 2020; Yao *et al.*, 2019). Part of the appeal of oxalate-based coordination compounds is due to their high degree of structural diversity, as a result of the oxalate ligand, which can adopt 17 different coordination modes and act as a mono-, bi-, tri- or tetradentate ligand (Rao *et al.*, 2004). This has led to a vast compositional area, which is yet to be fully explored. In this context, the crystal structures of three new oxalate-based coordination compounds are reported and discussed herein.

2. Structural commentary

$\text{Rb}_2\text{Co}(\text{C}_2\text{O}_4)_2 \cdot 4\text{H}_2\text{O}$ (I) consists of isolated $[\text{Co}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$ octahedra. The Co^{2+} cation lies on the $2c$ Wyckoff position with a site symmetry of $\bar{1}$, leading to a *trans* disposition of the bidentate oxalato and aqua ligands (Fig. 1). The



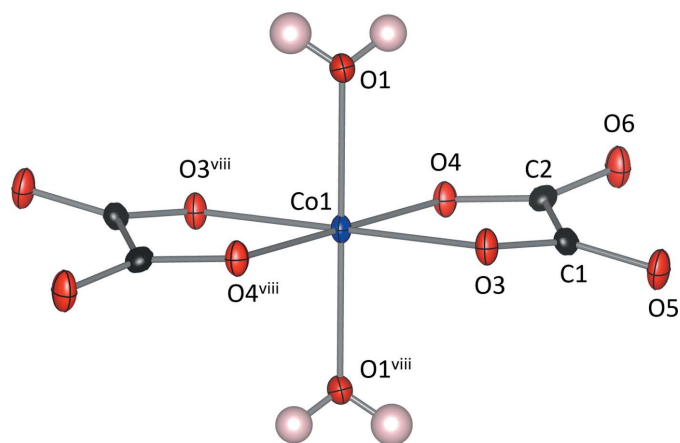


Figure 1
Coordination environment of Co^{2+} in $\text{Rb}_2\text{Co}(\text{C}_2\text{O}_4)_2 \cdot 4\text{H}_2\text{O}$ (I). Colour code: Co (blue), C (black), O (red) and H (light pink). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (viii) $-x + 1, -y, -z + 1$].

average Co—O bond length was determined as 2.080 Å, with a calculated bond-valence sum of 2.10 valence units. The Rb^+ cation has a coordination number of 11, defined by oxalate O atoms and water molecules. While the water molecule involving O1 coordinates to both Rb^+ and Co^{2+} , the second water

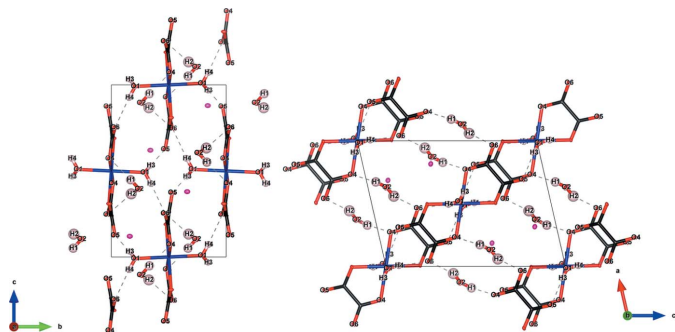


Figure 2
The hydrogen-bonding network of $\text{Rb}_2\text{Co}(\text{C}_2\text{O}_4)_2 \cdot 2\text{H}_2\text{O}$ (I) viewed along the *a* and *b* axes. Displacement ellipsoids are drawn at the 30% probability level. The hydrogen bonds are shown as dashed lines. Colour code: Rb (pink), Co (blue), C (black), O (red) and H (light pink).

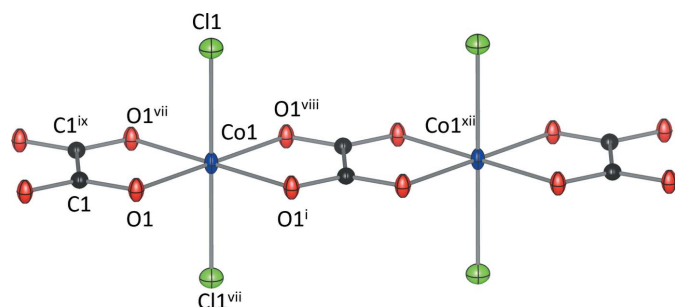


Figure 3
Coordination environment of Co^{2+} in $\text{Rb}_2\text{CoCl}_2(\text{C}_2\text{O}_4)$ (II). Colour code: Co (blue), Cl (green), C (black) and O (red). Displacement ellipsoids are drawn at 50% probability level. [Symmetry codes: (i) $-x + 1, y, -z + 1$; (vii) $x, -y + 2, z$; (viii) $-x + 1, -y + 2, -z + 1$; (ix) $-x + 2, -y + 2, -z + 1$; (xii) $x - 1, y, z$].

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O2}-\text{H1} \cdots \text{O4}$	0.89 (4)	2.00 (4)	2.880 (2)	171 (4)
$\text{O2}-\text{H2} \cdots \text{O4}^{\text{i}}$	0.85 (5)	2.47 (5)	3.187 (2)	143 (4)
$\text{O2}-\text{H2} \cdots \text{O6}^{\text{i}}$	0.85 (5)	2.20 (5)	3.008 (2)	159 (4)
$\text{O1}-\text{H3} \cdots \text{O5}^{\text{ii}}$	0.76 (3)	1.98 (3)	2.736 (2)	174 (3)
$\text{O1}-\text{H4} \cdots \text{O6}^{\text{iii}}$	0.78 (3)	2.05 (3)	2.825 (2)	172 (3)

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

molecule involving O2 solely bonds to the alkali metal cation. The $[\text{Co}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$ octahedra are interlinked by hydrogen bonding of both types of water molecules, as shown in Fig. 2. The mutually *trans* coordinating water molecules (H3, O1, H4) form hydrogen bonds with the oxalate ligands of the neighbouring $[\text{Co}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$ octahedra, whilst the second type of water molecule (H1, O2, H2) forms hydrogen bonds (in part bifurcated) with the oxalate ligands of two separate $[\text{Co}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$ octahedra. Numerical data for the hydrogen-bonding interactions are given in Table 1.

$\text{Rb}_2\text{CoCl}_2(\text{C}_2\text{O}_4)$ (II) consists of octahedrally coordinated Co^{2+} cations. They are linked by bis-bidentate oxalate ligands to form chains extending parallel to the *a* axis, as shown in Fig. 3. The oxalate ligands are mutually *trans* to one another whilst the Cl^- anions cap each side of the octahedron. Co—O bond lengths are 2.0616 (17) Å and longer for the Co—Cl bond at 2.4863 (9) Å, with a calculated bond-valence sum of 2.03 valence units for Co. The Rb^+ cation has a coordination number of eight and lies between the layers formed by the Co^{2+} chains (Fig. 4), with no direct connectivity between the chains. Each of the atoms lies on a special position within the unit cell with Wyckoff positions/site symmetries: Rb^+

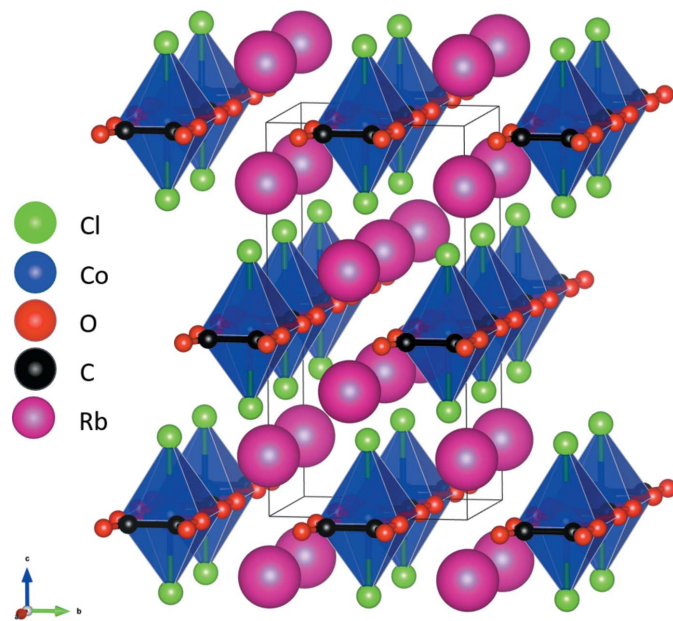
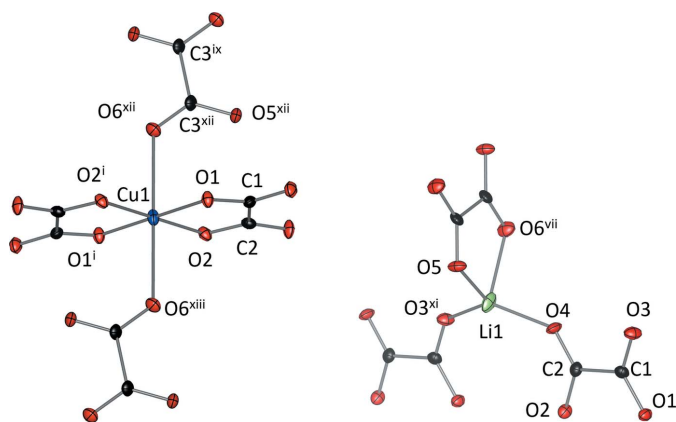


Figure 4
The crystal structure of $\text{Rb}_2\text{CoCl}_2(\text{C}_2\text{O}_4)$ (II) in a view approximately along the *a* axis.


Figure 5

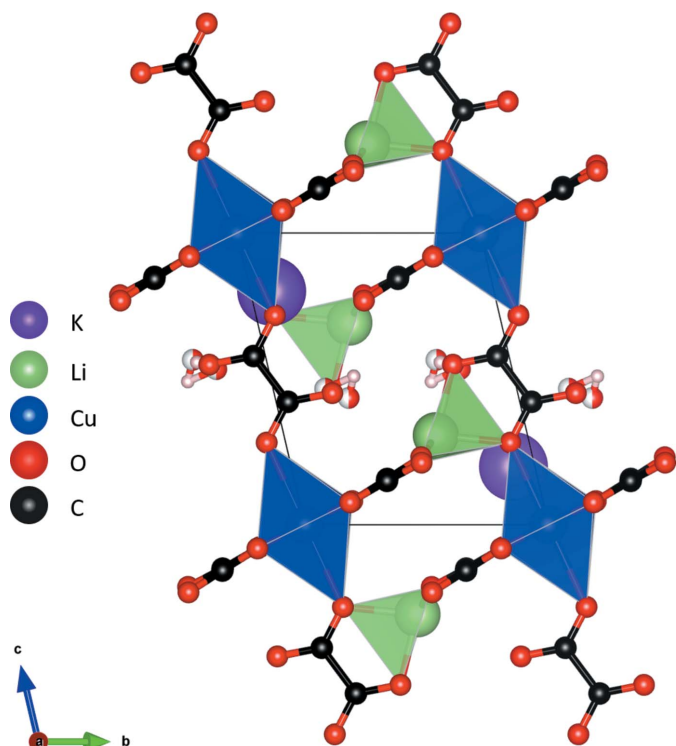
Coordination environments of Cu^{2+} and of Li^{+} in the crystal structure of $\text{K}_2\text{Li}_2\text{Cu}(\text{C}_2\text{O}_4)_3 \cdot 2\text{H}_2\text{O}$ (III). Colour code: Li (green), Cu (Blue), C (black) and O (red). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $-x + 2, -y + 2, -z + 2$; (vii) $-x, -y, -z + 1$; (ix) $x + 1, y + 1, z$; (xi) $x - 1, y, z$; (xii) $-x + 1, -y + 1, -z + 1$; (xiii) $x + 1, y + 1, z + 1$].

(4i, $mm2$), Co^{2+} (2d, mmm), Cl^- (4j, $mm2$), O ($8n, .m$) and C (4h, $m2m$). The presence of the oxalate-bridged Co^{2+} chain could allow for magnetic exchange (García-Couceiro *et al.*, 2004), hence the magnetic properties of the compound should also be investigated in the future.

The Cu^{2+} and Li^{+} binding environments of $\text{K}_2\text{Li}_2\text{Cu}(\text{C}_2\text{O}_4)_3 \cdot 2\text{H}_2\text{O}$ (III) are shown in Fig. 5. The d^9 Cu^{2+} cations display classic Jahn–Teller distortion with elongation of the axial Cu–O bonds. The equatorial Cu–O bond lengths are 1.938 (3) (O2) and 1.942 (3) (O1) Å whilst the axial bonds are significantly longer at 2.473 (4) Å (O6). The Cu^{2+} ion lies on a special position with Wyckoff position and site symmetry of $6b$ and $\bar{3}$, respectively. The Cu^{2+} coordination environment consists of four oxalate ligands, two of which act as bidentate bridging ligands and two of which are axially oriented and bind to four metal cations with a tricoordinate oxygen atom. The Li^{+} cation is tetrahedrally coordinated by three oxalate molecules, one of which is bidentate whilst the other two are monodentate. The Cu^{2+} and Li^{+} -centred polyhedra are interconnected into a tri-periodic network, as shown in Fig. 6. The coordination environment of the K^{+} cation lies within this network and consists of eight oxygen atoms from the oxalate ligands and two water molecules. These water molecules exhibit disorder of the O7 atom, which is split into two positions. The interatomic distances between the water molecules is ~ 3.7 Å, which is too far apart to facilitate hydrogen bonding.

3. Database survey

Database surveys were carried out using the Cambridge Structural Database (CSD, last update November 2022; Groom *et al.*, 2016) for compounds with structural similarities to the three new oxalate coordination compounds reported here. For (I), a search for first-row transition metals with the


Figure 6

The crystal structure of $\text{K}_2\text{Li}_2\text{Cu}(\text{C}_2\text{O}_4)_3 \cdot 2\text{H}_2\text{O}$ (III) viewed along the a axis.

same coordination environment produced numerous results for a range of transition metals. The most similar is DIHXID [dipotassium bis(oxalato)diaquacobalt(II) tetrahydrate; Chylewska *et al.*, 2013], which has the same formula type and coordination environment as (I) although with K^{+} rather Rb^{+} cations, but is not isostructural. For (II), there are several compounds containing transition-metal oxalate chains with the same binding environment, although with quite different cations involved. For example BEJHOQ {catena-[bis(2-(5,6-dihydro-2H-[1,3]dithiolo[4,5-b][1,4]dithiin-2-ylidene)-5,6-dihydro-2H-[1,3]dithiolo[4,5-b][1,4]dithiin-1-ium) bis(μ -oxalato)tetrachlorodiiron(III) dichloromethane solvate]} and EYALIB {catena-[bis(2-(5,6-dihydro-2H-[1,3]diselenolo[4,5-b][1,4]dithiin-2-ylidene)-5,6-dihydro-2H-[1,3]diselenolo[4,5-b][1,4]dithiin-1-ium) bis(μ -oxalato)tetrachlorodiiron(III)]}; Zhang, 2016, 2017). The database survey of compounds with similar binding environments to (III) focused on first-row transition metals with two bidentate and two mutually *trans* monodentate oxalate ligands, containing a tricoordinating oxygen atom. The search revealed evidence of only two similar compounds, *viz.* ADAJUL [octaammonium hexakis(μ_2 -oxalato- O, O, O')bis(oxalato- O, O')diaquatetrapropylcopper(II) tetrahydrate] and ASOXOV {bis[1,4-diazoniabicyclo(2.2.2)octane]bis(μ_2 -oxalato)diaquabis(oxalato)dipropylcopper(II) tetrahydrate; Kadir *et al.*, 2006; Keene *et al.*, 2004}. These contain similar types of linkages, although with only one type of cation and only as discrete molecules rather than coordination polymers. Hence, (III) represents the first example of this type of binding environment.

Table 2
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	Rb ₂ [Co(C ₂ O ₄) ₂ (H ₂ O) ₂]-2H ₂ O	Rb ₂ [CoCl ₂ (C ₂ O ₄)]	K ₂ [Li ₂ Cu(C ₂ O ₄) ₃]-2H ₂ O
<i>M_r</i>	477.97	388.79	455.71
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>	Orthorhombic, <i>Immm</i>	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	173	173	173
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.8434 (5), 7.0795 (4), 10.9133 (7)	5.3445 (3), 6.4380 (4), 12.5866 (8)	6.1847 (4), 7.2575 (5), 8.1795 (5)
α , β , γ (°)	90, 102.836 (8), 90	90, 90, 90	101.327 (11), 91.723 (11), 113.563 (11)
<i>V</i> (Å ³)	590.84 (7)	433.08 (5)	327.56 (5)
<i>Z</i>	2	2	1
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	9.70	13.73	2.39
Crystal size (mm)	0.21 × 0.16 × 0.08	0.20 × 0.15 × 0.07	0.14 × 0.14 × 0.07
Data collection			
Diffractometer	Rigaku Mercury2 (2x2 bin mode)	Rigaku Mercury2 (2x2 bin mode)	Rigaku Mercury2 (2x2 bin mode)
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} – <i>T</i> _{max}	0.681, 1.00	0.671, 1.00	0.610, 1.00
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	5799, 1343, 1169	2218, 310, 296	3403, 1500, 1077
<i>R</i> _{int}	0.039	0.034	0.095
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.650	0.649	0.651
Refinement			
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> [<i>F</i> ²], <i>S</i>	0.021, 0.050, 0.97	0.018, 0.043, 1.11	0.045, 0.114, 0.94
No. of reflections	1343	310	1500
No. of parameters	104	22	132
H-atom treatment	All H-atom parameters refined	–	All H-atom parameters refined
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.65, –0.64	0.63, –0.53	1.03, –1.01

Computer programs: *CrystalClear* (Rigaku, 2015), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *ORTEP* for Windows and *WinGX* (Farrugia, 2012).

4. Synthesis and crystallization

The samples were synthesized *via* hydrothermal syntheses in the temperature range 433–463 K over four days, from commercially available starting reagents. Compounds (I) and (II) were synthesized as by-products from the reaction of rubidium carbonate, sodium carbonate, cobalt chloride hexahydrate and oxalic acid dihydrate in molar ratios of 2:2:1:1.5 and 1:1.5:1:1.5 at 433 and 463 K, respectively. Compound (III) was synthesized by the reaction of potassium carbonate, lithium carbonate, copper chloride dihydrate and oxalic acid dihydrate (1:3:1:3) at 463 K. Single crystals were isolated from a mixture of products for further analysis. The resulting crystals were filtered and dried overnight at 323 K prior to analysis by X-ray diffraction.

5. Refinement

Crystal data and refinement details of the three compounds are summarized in Table 2. The H atoms in (I) and (III) were allowed to refine freely. The disordered oxygen atom in compound III (O7) was split over two positions with their occupancies fixed at 0.5 while their atomic coordinates and *U*^{ij}s were refined independently.

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Syntheses and crystal structures of three novel oxalate coordination compounds: $\text{Rb}_2\text{Co}(\text{C}_2\text{O}_4)_2 \cdot 4\text{H}_2\text{O}$, $\text{Rb}_2\text{CoCl}_2(\text{C}_2\text{O}_4)$ and $\text{K}_2\text{Li}_2\text{Cu}(\text{C}_2\text{O}_4)_3 \cdot 2\text{H}_2\text{O}$

Rebecca Clulow and Philip Lightfoot

Computing details

For all structures, data collection: *CrystalClear* (Rigaku, 2015); cell refinement: *CrystalClear* (Rigaku, 2015); data reduction: *CrystalClear* (Rigaku, 2015); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *ORTEP* for Windows (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Dirubidium diaquadioxalatocobalt(II) dihydrate (I)

Crystal data

$\text{Rb}_2[\text{Co}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$

$M_r = 477.97$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 7.8434$ (5) Å

$b = 7.0795$ (4) Å

$c = 10.9133$ (7) Å

$\beta = 102.836$ (8)°

$V = 590.84$ (7) Å³

$Z = 2$

$F(000) = 458$

$D_x = 2.687$ Mg m⁻³

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

Cell parameters from 935 reflections

$\theta = 1.9$ – 27.5 °

$\mu = 9.70$ mm⁻¹

$T = 173$ K

Prism, orange

$0.21 \times 0.16 \times 0.08$ mm

Data collection

Rigaku Mercury2 (2x2 bin mode)
diffractometer

Radiation source: Sealed Tube

Detector resolution: 13.6612 pixels mm⁻¹
profile data from ω -scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.681$, $T_{\max} = 1.00$

5799 measured reflections

1343 independent reflections

1169 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 2.9$ °

$h = -10 \rightarrow 10$

$k = -9 \rightarrow 9$

$l = -14 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.021$

$wR(F^2) = 0.050$

$S = 0.97$

1343 reflections

104 parameters

0 restraints

Hydrogen site location: difference Fourier map

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2]$

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

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

$\Delta\rho_{\max} = 0.65$ e Å⁻³

$\Delta\rho_{\min} = -0.64$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Rb1	0.81534 (3)	0.66030 (3)	0.37962 (2)	0.01935 (9)
Co1	0.500000	0.000000	0.500000	0.01014 (11)
O1	0.5165 (2)	0.2912 (2)	0.49112 (17)	0.0160 (3)
O2	0.8705 (2)	0.2408 (3)	0.39553 (17)	0.0236 (4)
O3	0.50631 (18)	0.0198 (2)	0.69060 (13)	0.0143 (3)
O4	0.77067 (18)	−0.0152 (2)	0.57235 (13)	0.0139 (3)
O5	0.6916 (2)	−0.0314 (2)	0.87422 (14)	0.0186 (3)
O6	0.96271 (19)	0.0330 (2)	0.75326 (14)	0.0191 (3)
C1	0.6578 (3)	−0.0014 (3)	0.75938 (19)	0.0118 (4)
C2	0.8121 (3)	0.0076 (3)	0.69128 (19)	0.0122 (4)
H1	0.828 (5)	0.168 (5)	0.449 (4)	0.056 (11)*
H2	0.942 (6)	0.173 (6)	0.367 (4)	0.079 (15)*
H3	0.594 (4)	0.342 (4)	0.532 (3)	0.023 (8)*
H4	0.494 (4)	0.345 (4)	0.427 (3)	0.029 (9)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb1	0.01880 (14)	0.02412 (14)	0.01580 (13)	0.00190 (8)	0.00529 (9)	0.00010 (8)
Co1	0.0105 (2)	0.01303 (19)	0.00658 (19)	0.00024 (14)	0.00112 (15)	−0.00043 (14)
O1	0.0195 (9)	0.0142 (7)	0.0118 (8)	−0.0033 (6)	−0.0020 (7)	0.0004 (6)
O2	0.0248 (10)	0.0268 (9)	0.0231 (9)	−0.0002 (8)	0.0138 (8)	0.0007 (7)
O3	0.0123 (7)	0.0216 (7)	0.0083 (7)	0.0009 (6)	0.0011 (6)	−0.0011 (6)
O4	0.0121 (7)	0.0202 (7)	0.0093 (7)	0.0010 (6)	0.0024 (6)	−0.0012 (6)
O5	0.0180 (8)	0.0291 (8)	0.0081 (7)	0.0000 (6)	0.0016 (6)	0.0021 (6)
O6	0.0126 (8)	0.0305 (9)	0.0126 (7)	−0.0007 (7)	−0.0009 (6)	0.0005 (7)
C1	0.0138 (10)	0.0119 (9)	0.0099 (9)	−0.0008 (7)	0.0031 (8)	−0.0019 (8)
C2	0.0134 (10)	0.0103 (9)	0.0130 (10)	0.0020 (8)	0.0032 (8)	0.0014 (8)

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

Rb1—O2	3.0003 (18)	Co1—O1 ^{viii}	2.0690 (16)
Rb1—O5 ⁱ	3.0209 (16)	Co1—O1	2.0690 (16)
Rb1—O3 ⁱⁱ	3.0819 (15)	Co1—O3 ^{viii}	2.0744 (14)
Rb1—O2 ⁱⁱⁱ	3.0856 (19)	Co1—O3	2.0744 (14)
Rb1—O5 ⁱⁱ	3.1023 (16)	Co1—O4	2.0969 (14)
Rb1—O6 ^{iv}	3.1190 (15)	Co1—O4 ^{viii}	2.0969 (14)
Rb1—O2 ^v	3.1461 (19)	O3—C1	1.265 (2)
Rb1—O4 ^{vi}	3.1862 (15)	O4—C2	1.276 (3)

Rb1—O1 ^{vii}	3.2421 (17)	O5—C1	1.240 (3)
Rb1—O6 ^v	3.3122 (16)	O6—C2	1.237 (3)
Rb1—O3 ^{vii}	3.3497 (15)	C1—C2	1.556 (3)
O2—Rb1—O5 ⁱ	62.28 (5)	O2 ⁱⁱⁱ —Rb1—O3 ^{vii}	58.91 (4)
O2—Rb1—O3 ⁱⁱ	62.87 (4)	O5 ⁱⁱ —Rb1—O3 ^{vii}	149.98 (4)
O5 ⁱ —Rb1—O3 ⁱⁱ	121.12 (4)	O6 ^{iv} —Rb1—O3 ^{vii}	69.30 (4)
O2—Rb1—O2 ⁱⁱⁱ	105.67 (5)	O2 ^v —Rb1—O3 ^{vii}	116.60 (4)
O5 ⁱ —Rb1—O2 ⁱⁱⁱ	148.26 (5)	O4 ^{vi} —Rb1—O3 ^{vii}	58.39 (4)
O3 ⁱⁱ —Rb1—O2 ⁱⁱⁱ	67.65 (4)	O1 ^{vii} —Rb1—O3 ^{vii}	52.51 (4)
O2—Rb1—O5 ⁱⁱ	65.45 (5)	O6 ^v —Rb1—O3 ^{vii}	84.20 (4)
O5 ⁱ —Rb1—O5 ⁱⁱ	95.16 (4)	O1 ^{viii} —Co1—O1	180.0
O3 ⁱⁱ —Rb1—O5 ⁱⁱ	42.24 (4)	O1 ^{viii} —Co1—O3 ^{viii}	89.52 (6)
O2 ⁱⁱⁱ —Rb1—O5 ⁱⁱ	106.35 (5)	O1—Co1—O3 ^{viii}	90.48 (6)
O2—Rb1—O6 ^{iv}	72.16 (5)	O1 ^{viii} —Co1—O3	90.48 (6)
O5 ⁱ —Rb1—O6 ^{iv}	90.38 (4)	O1—Co1—O3	89.52 (6)
O3 ⁱⁱ —Rb1—O6 ^{iv}	92.16 (4)	O3 ^{viii} —Co1—O3	180.0
O2 ⁱⁱⁱ —Rb1—O6 ^{iv}	58.00 (5)	O1 ^{viii} —Co1—O4	89.98 (6)
O5 ⁱⁱ —Rb1—O6 ^{iv}	128.06 (4)	O1—Co1—O4	90.02 (6)
O2—Rb1—O2 ^v	95.58 (5)	O3 ^{viii} —Co1—O4	99.83 (6)
O5 ⁱ —Rb1—O2 ^v	64.67 (5)	O3—Co1—O4	80.17 (6)
O3 ⁱⁱ —Rb1—O2 ^v	101.60 (4)	O1 ^{viii} —Co1—O4 ^{viii}	90.02 (6)
O2 ⁱⁱⁱ —Rb1—O2 ^v	146.79 (5)	O1—Co1—O4 ^{viii}	89.98 (6)
O5 ⁱⁱ —Rb1—O2 ^v	59.77 (4)	O3 ^{viii} —Co1—O4 ^{viii}	80.17 (6)
O6 ^{iv} —Rb1—O2 ^v	155.02 (4)	O3—Co1—O4 ^{viii}	99.83 (6)
O2—Rb1—O4 ^{vi}	135.32 (4)	O4—Co1—O4 ^{viii}	180.0
O5 ⁱ —Rb1—O4 ^{vi}	73.17 (4)	Co1—O1—Rb1 ^{vii}	91.19 (6)
O3 ⁱⁱ —Rb1—O4 ^{vi}	151.80 (4)	Rb1—O2—Rb1 ^{ix}	95.49 (5)
O2 ⁱⁱⁱ —Rb1—O4 ^{vi}	114.32 (4)	Rb1—O2—Rb1 ^v	84.42 (4)
O5 ⁱⁱ —Rb1—O4 ^{vi}	117.99 (4)	Rb1 ^{ix} —O2—Rb1 ^v	156.77 (7)
O6 ^{iv} —Rb1—O4 ^{vi}	113.04 (4)	C1—O3—Co1	113.38 (13)
O2 ^v —Rb1—O4 ^{vi}	60.44 (4)	C1—O3—Rb1 ^x	94.92 (12)
O2—Rb1—O1 ^{vii}	101.48 (5)	Co1—O3—Rb1 ^x	137.42 (6)
O5 ⁱ —Rb1—O1 ^{vii}	59.06 (4)	C1—O3—Rb1 ^{vii}	140.90 (12)
O3 ⁱⁱ —Rb1—O1 ^{vii}	153.07 (4)	Co1—O3—Rb1 ^{vii}	88.13 (5)
O2 ⁱⁱⁱ —Rb1—O1 ^{vii}	98.78 (5)	Rb1 ^x —O3—Rb1 ^{vii}	88.83 (4)
O5 ⁱⁱ —Rb1—O1 ^{vii}	153.95 (4)	C2—O4—Co1	112.61 (13)
O6 ^{iv} —Rb1—O1 ^{vii}	61.33 (4)	C2—O4—Rb1 ^{xi}	136.21 (12)
O2 ^v —Rb1—O1 ^{vii}	101.68 (5)	Co1—O4—Rb1 ^{xi}	92.24 (5)
O4 ^{vi} —Rb1—O1 ^{vii}	54.53 (4)	C1—O5—Rb1 ^{xii}	141.22 (13)
O2—Rb1—O6 ^v	126.25 (5)	C1—O5—Rb1 ^x	94.51 (12)
O5 ⁱ —Rb1—O6 ^v	143.03 (4)	Rb1 ^{xii} —O5—Rb1 ^x	84.84 (4)
O3 ⁱⁱ —Rb1—O6 ^v	66.26 (4)	C2—O6—Rb1 ^{xiii}	145.41 (13)
O2 ⁱⁱⁱ —Rb1—O6 ^v	68.49 (4)	C2—O6—Rb1 ^v	112.75 (13)
O5 ⁱⁱ —Rb1—O6 ^v	65.79 (4)	Rb1 ^{xiii} —O6—Rb1 ^v	88.88 (4)
O6 ^{iv} —Rb1—O6 ^v	126.49 (2)	O5—C1—O3	125.57 (19)
O2 ^v —Rb1—O6 ^v	78.39 (4)	O5—C1—C2	118.35 (18)
O4 ^{vi} —Rb1—O6 ^v	87.81 (4)	O3—C1—C2	116.07 (17)

O1 ^{vii} —Rb1—O6 ^v	132.20 (4)	O6—C2—O4	124.8 (2)
O2—Rb1—O3 ^{vii}	140.70 (5)	O6—C2—C1	119.63 (18)
O5 ⁱ —Rb1—O3 ^{vii}	110.22 (4)	O4—C2—C1	115.52 (18)
O3 ⁱⁱ —Rb1—O3 ^{vii}	125.45 (2)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H1 \cdots O4	0.89 (4)	2.00 (4)	2.880 (2)	171 (4)
O2—H2 \cdots O4 ^{xiv}	0.85 (5)	2.47 (5)	3.187 (2)	143 (4)
O2—H2 \cdots O6 ^{xiv}	0.85 (5)	2.20 (5)	3.008 (2)	159 (4)
O1—H3 \cdots O5 ⁱ	0.76 (3)	1.98 (3)	2.736 (2)	174 (3)
O1—H4 \cdots O6 ^{iv}	0.78 (3)	2.05 (3)	2.825 (2)	172 (3)

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

catena-Poly[dirubidium [[dichloridocobalt(II)]- μ -oxalato]] (II)

Crystal data

Rb₂[CoCl₂(C₂O₄)]

$M_r = 388.79$

Orthorhombic, *Immm*

Hall symbol: $-I\ 2\ 2$

$a = 5.3445$ (3) \AA

$b = 6.4380$ (4) \AA

$c = 12.5866$ (8) \AA

$V = 433.08$ (5) \AA^3

$Z = 2$

$F(000) = 358$

$D_x = 2.981$ Mg m⁻³

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

Cell parameters from 800 reflections

$\theta = 3.2\text{--}27.5^\circ$

$\mu = 13.73$ mm⁻¹

$T = 173$ K

Prism, purple

$0.20 \times 0.15 \times 0.07$ mm

Data collection

Rigaku Mercury2 (2x2 bin mode)
diffractometer

Radiation source: Sealed Tube

Detector resolution: 13.6612 pixels mm⁻¹

profile data from ω -scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.671, T_{\max} = 1.00$

2218 measured reflections

310 independent reflections

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

$R_{\text{int}} = 0.034$

$\theta_{\max} = 27.5^\circ, \theta_{\min} = 3.2^\circ$

$h = -6 \rightarrow 6$

$k = -8 \rightarrow 8$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.018$

$wR(F^2) = 0.043$

$S = 1.11$

310 reflections

22 parameters

0 restraints

$w = 1/[\sigma^2(F_o^2) + (0.0276P)^2]$

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

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

$\Delta\rho_{\max} = 0.63$ e \AA^{-3}

$\Delta\rho_{\min} = -0.53$ e \AA^{-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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Rb1	0.500000	0.500000	0.34642 (3)	0.01924 (15)
Co1	0.500000	1.000000	0.500000	0.01332 (18)
Cl1	0.500000	1.000000	0.30247 (7)	0.0198 (2)
O1	0.7911 (3)	0.7898 (2)	0.500000	0.0154 (4)
C1	1.000000	0.8775 (5)	0.500000	0.0123 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb1	0.0230 (2)	0.0136 (2)	0.0211 (2)	0.000	0.000	0.000
Co1	0.0072 (3)	0.0105 (3)	0.0222 (3)	0.000	0.000	0.000
Cl1	0.0233 (4)	0.0172 (4)	0.0190 (4)	0.000	0.000	0.000
O1	0.0106 (9)	0.0106 (7)	0.0251 (8)	−0.0006 (6)	0.000	0.000
C1	0.0119 (16)	0.0125 (16)	0.0125 (14)	0.000	0.000	0.000

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

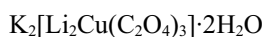
Rb1—O1	3.1045 (13)	Co1—O1 ^{vii}	2.0616 (17)
Rb1—O1 ⁱ	3.1045 (13)	Co1—O1 ⁱ	2.0616 (17)
Rb1—O1 ⁱⁱ	3.1045 (13)	Co1—O1 ^{viii}	2.0616 (17)
Rb1—O1 ⁱⁱⁱ	3.1045 (13)	Co1—O1	2.0616 (17)
Rb1—Cl1 ^{iv}	3.2639 (6)	Co1—Cl1 ^{viii}	2.4863 (9)
Rb1—Cl1 ^v	3.2639 (6)	Co1—Cl1	2.4863 (9)
Rb1—Cl1 ^{vi}	3.2662 (3)	O1—C1	1.251 (2)
Rb1—Cl1	3.2662 (3)	C1—C1 ^{ix}	1.577 (6)
O1—Rb1—O1 ⁱ	60.14 (6)	O1 ^{vii} —Co1—O1	82.03 (9)
O1—Rb1—O1 ⁱⁱ	73.89 (5)	O1 ⁱ —Co1—O1	97.97 (9)
O1 ⁱ —Rb1—O1 ⁱⁱ	102.98 (4)	O1 ^{viii} —Co1—O1	180.0
O1—Rb1—O1 ⁱⁱⁱ	102.98 (4)	O1 ^{vii} —Co1—Cl1 ^{viii}	90.0
O1 ⁱ —Rb1—O1 ⁱⁱⁱ	73.89 (5)	O1 ⁱ —Co1—Cl1 ^{viii}	90.0
O1 ⁱⁱ —Rb1—O1 ⁱⁱⁱ	60.14 (6)	O1 ^{viii} —Co1—Cl1 ^{viii}	90.0
O1—Rb1—Cl1 ^{iv}	140.15 (3)	O1—Co1—Cl1 ^{viii}	90.0
O1 ⁱ —Rb1—Cl1 ^{iv}	86.98 (3)	O1 ^{vii} —Co1—Cl1	90.0
O1 ⁱⁱ —Rb1—Cl1 ^{iv}	140.15 (3)	O1 ⁱ —Co1—Cl1	90.0
O1 ⁱⁱⁱ —Rb1—Cl1 ^{iv}	86.98 (3)	O1 ^{viii} —Co1—Cl1	90.0
O1—Rb1—Cl1 ^v	86.98 (3)	O1—Co1—Cl1	90.0
O1 ⁱ —Rb1—Cl1 ^v	140.15 (3)	Cl1 ^{viii} —Co1—Cl1	180.0
O1 ⁱⁱ —Rb1—Cl1 ^v	86.98 (3)	Co1—Cl1—Rb1 ^{iv}	125.042 (14)

O1 ⁱⁱⁱ —Rb1—Cl1 ^v	140.15 (3)	Co1—Cl1—Rb1 ^v	125.042 (14)
Cl1 ^{iv} —Rb1—Cl1 ^v	109.92 (3)	Rb1 ^{iv} —Cl1—Rb1 ^v	109.92 (3)
O1—Rb1—Cl1 ^{vi}	134.25 (3)	Co1—Cl1—Rb1	80.247 (16)
O1 ⁱ —Rb1—Cl1 ^{vi}	134.25 (3)	Rb1 ^{iv} —Cl1—Rb1	95.582 (8)
O1 ⁱⁱ —Rb1—Cl1 ^{vi}	60.86 (3)	Rb1 ^v —Cl1—Rb1	95.582 (8)
O1 ⁱⁱⁱ —Rb1—Cl1 ^{vi}	60.86 (3)	Co1—Cl1—Rb1 ^x	80.246 (16)
Cl1 ^{iv} —Rb1—Cl1 ^{vi}	84.419 (8)	Rb1 ^{iv} —Cl1—Rb1 ^x	95.582 (8)
Cl1 ^v —Rb1—Cl1 ^{vi}	84.419 (8)	Rb1 ^v —Cl1—Rb1 ^x	95.582 (8)
O1—Rb1—Cl1	60.86 (3)	Rb1—Cl1—Rb1 ^x	160.49 (3)
O1 ⁱ —Rb1—Cl1	60.86 (3)	C1—O1—Co1	112.18 (16)
O1 ⁱⁱ —Rb1—Cl1	134.25 (3)	C1—O1—Rb1 ⁱⁱⁱ	135.91 (8)
O1 ⁱⁱⁱ —Rb1—Cl1	134.25 (3)	Co1—O1—Rb1 ⁱⁱⁱ	90.94 (5)
Cl1 ^{iv} —Rb1—Cl1	84.418 (8)	C1—O1—Rb1	135.91 (8)
Cl1 ^v —Rb1—Cl1	84.418 (8)	Co1—O1—Rb1	90.94 (5)
Cl1 ^{vi} —Rb1—Cl1	160.49 (3)	Rb1 ⁱⁱⁱ —O1—Rb1	77.02 (4)
O1 ^{vii} —Co1—O1 ⁱ	180.0	O1 ^{xi} —C1—O1	126.4 (3)
O1 ^{vii} —Co1—O1 ^{viii}	97.97 (9)	O1 ^{xi} —C1—C1 ^{ix}	116.81 (15)
O1 ⁱ —Co1—O1 ^{viii}	82.03 (9)	O1—C1—C1 ^{ix}	116.81 (15)

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

Poly[dipotassium [tri- μ -oxalatocopper(II)dilithium] dihydrate] (III)

Crystal data



$M_r = 455.71$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 6.1847$ (4) Å

$b = 7.2575$ (5) Å

$c = 8.1795$ (5) Å

$\alpha = 101.327$ (11)°

$\beta = 91.723$ (11)°

$\gamma = 113.563$ (11)°

$V = 327.56$ (5) Å³

$Z = 1$

$F(000) = 225$

$D_x = 2.310$ Mg m⁻³

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

Cell parameters from 888 reflections

$\theta = 2.5\text{--}27.5^\circ$

$\mu = 2.38$ mm⁻¹

$T = 173$ K

Prism, blue

$0.14 \times 0.14 \times 0.07$ mm

Data collection

Rigaku Mercury2 (2x2 bin mode)
diffractometer

Radiation source: Sealed Tube

Detector resolution: 13.6612 pixels mm⁻¹

profile data from ω -scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.610$, $T_{\max} = 1.00$

3403 measured reflections

1500 independent reflections

1077 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.095$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.6^\circ$

$h = -8 \rightarrow 8$

$k = -9 \rightarrow 9$

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.114$

$S = 0.94$

1500 reflections

132 parameters

0 restraints

Hydrogen site location: difference Fourier map

All H-atom parameters refined

$$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 1.03 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.01 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cu1	1.000000	1.000000	1.000000	0.0141 (2)	
K1	0.53561 (17)	0.08774 (15)	0.80051 (12)	0.0182 (2)	
O1	1.1046 (5)	0.7828 (4)	0.9188 (4)	0.0139 (6)	
O2	0.6795 (5)	0.7931 (5)	0.9232 (4)	0.0139 (6)	
O3	0.9423 (5)	0.4577 (5)	0.7685 (4)	0.0166 (7)	
O4	0.5056 (5)	0.4613 (4)	0.7870 (4)	0.0168 (7)	
O5	0.1518 (5)	0.2387 (4)	0.4512 (4)	0.0174 (7)	
O6	-0.0303 (6)	-0.0777 (5)	0.2817 (4)	0.0194 (7)	
O7A	0.3910 (18)	-0.2142 (15)	0.5335 (14)	0.028 (2)	0.5
O7B	0.3555 (18)	-0.3016 (16)	0.5653 (14)	0.027 (2)	0.5
C1	0.9305 (7)	0.6178 (6)	0.8431 (5)	0.0125 (8)	
C2	0.6818 (7)	0.6206 (6)	0.8495 (5)	0.0129 (8)	
C3	0.0359 (7)	0.0482 (6)	0.4216 (6)	0.0138 (8)	
Li1	0.1867 (13)	0.3767 (13)	0.6931 (10)	0.0205 (17)	
H1	0.481 (15)	-0.288 (12)	0.557 (10)	0.06 (3)*	
H2	0.283 (15)	-0.343 (13)	0.491 (11)	0.07 (3)*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0105 (4)	0.0100 (4)	0.0191 (4)	0.0037 (3)	0.0009 (3)	-0.0015 (3)
K1	0.0195 (5)	0.0173 (5)	0.0177 (5)	0.0079 (4)	0.0026 (4)	0.0031 (4)
O1	0.0106 (14)	0.0118 (14)	0.0176 (16)	0.0044 (11)	0.0000 (11)	0.0000 (12)
O2	0.0119 (14)	0.0156 (15)	0.0133 (15)	0.0064 (12)	0.0018 (11)	-0.0001 (12)
O3	0.0171 (15)	0.0116 (14)	0.0204 (17)	0.0064 (12)	0.0047 (13)	0.0005 (12)
O4	0.0108 (14)	0.0102 (14)	0.0229 (17)	0.0003 (12)	-0.0022 (12)	-0.0014 (12)
O5	0.0223 (16)	0.0086 (14)	0.0159 (16)	0.0012 (12)	0.0031 (13)	0.0018 (12)
O6	0.0236 (17)	0.0182 (16)	0.0121 (16)	0.0051 (13)	0.0001 (13)	0.0014 (13)
O7A	0.026 (5)	0.012 (4)	0.043 (6)	0.012 (4)	-0.003 (4)	-0.011 (4)
O7B	0.019 (5)	0.014 (5)	0.036 (6)	0.007 (4)	-0.009 (4)	-0.017 (4)
C1	0.014 (2)	0.0117 (19)	0.013 (2)	0.0048 (16)	0.0038 (16)	0.0050 (16)
C2	0.013 (2)	0.016 (2)	0.0092 (19)	0.0061 (17)	0.0011 (15)	0.0027 (16)
C3	0.016 (2)	0.011 (2)	0.017 (2)	0.0089 (17)	0.0019 (17)	0.0034 (17)
Li1	0.010 (3)	0.029 (4)	0.021 (4)	0.010 (3)	0.000 (3)	-0.002 (3)

Geometric parameters (Å, °)

Cu1—O2	1.938 (3)	O2—C2	1.284 (5)
Cu1—O2 ⁱ	1.938 (3)	O3—C1	1.233 (5)
Cu1—O1 ⁱ	1.942 (3)	O3—Li1 ^{viii}	1.907 (8)
Cu1—O1	1.942 (3)	O4—C2	1.230 (5)
K1—O7A	2.609 (10)	O4—Li1	1.901 (8)
K1—O4	2.814 (3)	O5—C3	1.245 (5)
K1—O2 ⁱⁱ	2.821 (3)	O5—Li1	1.997 (9)
K1—O7B	2.854 (10)	O6—C3	1.255 (5)
K1—O1 ⁱⁱⁱ	2.878 (3)	O6—Li1 ^{vii}	2.049 (9)
K1—O3	2.919 (3)	O7A—H1	0.95 (8)
K1—O2 ^{iv}	2.946 (3)	O7A—H2	0.89 (9)
K1—O1 ^v	3.036 (3)	O7B—H1	0.75 (8)
K1—O7A ^{vi}	3.039 (12)	O7B—H2	0.68 (9)
K1—O6 ^{vii}	3.146 (3)	C1—C2	1.549 (6)
K1—O6 ^{vi}	3.178 (3)	C3—C3 ^{vii}	1.571 (9)
O1—C1	1.271 (5)		
O2—Cu1—O2 ⁱ	180.0	O1 ⁱⁱⁱ —K1—O6 ^{vi}	63.34 (8)
O2—Cu1—O1 ⁱ	93.40 (12)	O3—K1—O6 ^{vi}	58.18 (8)
O2 ⁱ —Cu1—O1 ⁱ	86.60 (12)	O2 ^{iv} —K1—O6 ^{vi}	61.26 (8)
O2—Cu1—O1	86.60 (12)	O1 ^v —K1—O6 ^{vi}	131.85 (9)
O2 ⁱ —Cu1—O1	93.40 (12)	O7A ^{vi} —K1—O6 ^{vi}	75.66 (19)
O1 ⁱ —Cu1—O1	180.00 (9)	O6 ^{vii} —K1—O6 ^{vi}	155.90 (12)
O7A—K1—O4	119.6 (2)	C1—O1—Cu1	110.8 (3)
O7A—K1—O2 ⁱⁱ	134.7 (2)	C1—O1—K1 ⁱⁱⁱ	137.7 (3)
O4—K1—O2 ⁱⁱ	70.35 (9)	Cu1—O1—K1 ⁱⁱⁱ	94.37 (11)
O7A—K1—O7B	13.6 (3)	C1—O1—K1 ^{ix}	133.0 (3)
O4—K1—O7B	131.3 (3)	Cu1—O1—K1 ^{ix}	90.46 (11)
O2 ⁱⁱ —K1—O7B	127.0 (2)	K1 ⁱⁱⁱ —O1—K1 ^{ix}	77.56 (8)
O7A—K1—O1 ⁱⁱⁱ	133.6 (2)	C2—O2—Cu1	110.7 (3)
O4—K1—O1 ⁱⁱⁱ	101.72 (9)	C2—O2—K1 ⁱⁱ	133.6 (3)
O2 ⁱⁱ —K1—O1 ⁱⁱⁱ	76.43 (9)	Cu1—O2—K1 ⁱⁱ	97.23 (11)
O7B—K1—O1 ⁱⁱⁱ	125.6 (2)	C2—O2—K1 ^x	132.4 (3)
O7A—K1—O3	114.9 (3)	Cu1—O2—K1 ^x	92.37 (11)
O4—K1—O3	56.61 (8)	K1 ⁱⁱ —O2—K1 ^x	79.95 (8)
O2 ⁱⁱ —K1—O3	106.84 (9)	C1—O3—Li1 ^{viii}	136.6 (4)
O7B—K1—O3	125.5 (2)	C1—O3—K1	112.5 (3)
O1 ⁱⁱⁱ —K1—O3	70.04 (9)	Li1 ^{viii} —O3—K1	107.9 (3)
O7A—K1—O2 ^{iv}	80.2 (2)	C2—O4—Li1	139.7 (4)
O4—K1—O2 ^{iv}	159.58 (9)	C2—O4—K1	116.4 (3)
O2 ⁱⁱ —K1—O2 ^{iv}	100.05 (8)	Li1—O4—K1	103.7 (3)
O7B—K1—O2 ^{iv}	69.0 (2)	C3—O5—Li1	113.3 (4)
O1 ⁱⁱⁱ —K1—O2 ^{iv}	57.99 (8)	C3—O6—Li1 ^{vii}	111.7 (4)
O3—K1—O2 ^{iv}	112.41 (9)	C3—O6—K1 ^{vii}	100.4 (3)
O7A—K1—O1 ^v	80.5 (3)	Li1 ^{vii} —O6—K1 ^{vii}	89.8 (2)
O4—K1—O1 ^v	113.85 (9)	C3—O6—K1 ^{vi}	99.4 (3)

O2 ⁱⁱ —K1—O1 ^v	57.50 (8)	Li1 ^{vii} —O6—K1 ^{vi}	95.6 (2)
O7B—K1—O1 ^v	70.1 (2)	K1 ^{vii} —O6—K1 ^{vi}	155.90 (12)
O1 ⁱⁱⁱ —K1—O1 ^v	102.44 (8)	K1—O7A—K1 ^{vi}	115.8 (4)
O3—K1—O1 ^v	164.28 (9)	K1—O7A—H1	100 (5)
O2 ^{iv} —K1—O1 ^v	72.19 (8)	K1 ^{vi} —O7A—H1	113 (5)
O7A—K1—O7A ^{vi}	64.2 (4)	K1—O7A—H2	144 (6)
O4—K1—O7A ^{vi}	64.04 (18)	K1 ^{vi} —O7A—H2	96 (6)
O2 ⁱⁱ —K1—O7A ^{vi}	132.00 (18)	H1—O7A—H2	81 (7)
O7B—K1—O7A ^{vi}	77.7 (4)	K1—O7B—H1	89 (6)
O1 ⁱⁱⁱ —K1—O7A ^{vi}	126.0 (2)	K1—O7B—H2	135 (8)
O3—K1—O7A ^{vi}	58.7 (2)	H1—O7B—H2	113 (9)
O2 ^{iv} —K1—O7A ^{vi}	127.94 (18)	O3—C1—O1	126.1 (4)
O1 ^v —K1—O7A ^{vi}	131.4 (2)	O3—C1—C2	118.0 (4)
O7A—K1—O6 ^{vii}	82.2 (2)	O1—C1—C2	115.9 (4)
O4—K1—O6 ^{vii}	61.81 (9)	O4—C2—O2	125.6 (4)
O2 ⁱⁱ —K1—O6 ^{vii}	63.59 (8)	O4—C2—C1	118.7 (4)
O7B—K1—O6 ^{vii}	84.8 (2)	O2—C2—C1	115.7 (3)
O1 ⁱⁱⁱ —K1—O6 ^{vii}	139.77 (9)	O5—C3—O6	128.1 (4)
O3—K1—O6 ^{vii}	116.35 (9)	O5—C3—C3 ^{vii}	116.4 (5)
O2 ^{iv} —K1—O6 ^{vii}	131.16 (9)	O6—C3—C3 ^{vii}	115.6 (5)
O1 ^v —K1—O6 ^{vii}	60.12 (8)	O4—Li1—O3 ^{xi}	131.6 (5)
O7A ^{vi} —K1—O6 ^{vii}	81.9 (2)	O4—Li1—O5	108.5 (4)
O7A—K1—O6 ^{vi}	80.2 (2)	O3 ^{xi} —Li1—O5	117.8 (4)
O4—K1—O6 ^{vi}	114.08 (9)	O4—Li1—O6 ^{vii}	102.2 (4)
O2 ⁱⁱ —K1—O6 ^{vi}	139.69 (9)	O3 ^{xi} —Li1—O6 ^{vii}	97.4 (4)
O7B—K1—O6 ^{vi}	82.0 (2)	O5—Li1—O6 ^{vii}	82.4 (3)

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

Cu—O bond Lengths of Compound III

Bond	Bond distance (Å)
Cu—O1	1.942 (3)
Cu—O1 ⁱ	1.942 (3)
Cu—O2	1.938 (3)
Cu—O2 ⁱ	1.938 (3)
Cu—O6	2.473 (4)
Cu—O6 ⁱ	2.473 (4)

Symmetry codes: (i) $-x + 2, -y + 2, -z + 2$.