

## Poly[*bis*( $\mu_2$ -pyridine-2,6-dicarboxylato)-cobalt(II)disodium(I)]

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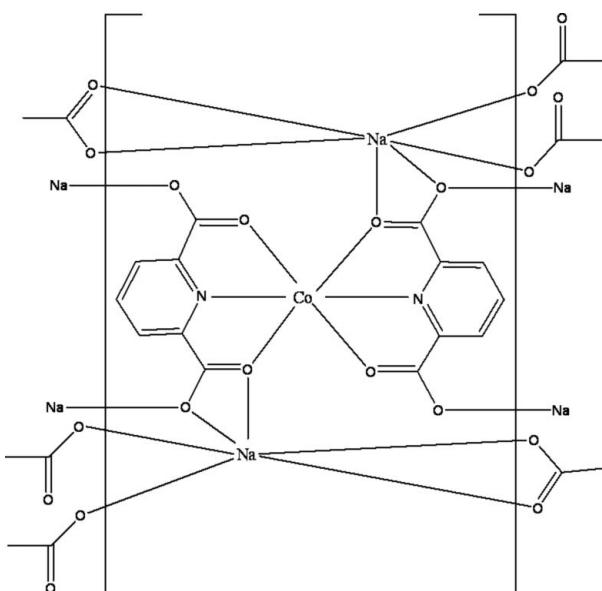
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.003$  Å;  
 $R$  factor = 0.029;  $wR$  factor = 0.069; data-to-parameter ratio = 11.3.

The title compound,  $[Na_2Co(C_7H_3NO_4)_2]_n$ , is isostructural with the nickel(II) analog. In the crystal structure, the Co cation is coordinated by two N atoms and four O atoms of two pyridine-2,6-dicarboxylate groups with a strongly distorted octahedral geometry. The Na cations are coordinated by six O atoms of pyridine-2,6-dicarboxylate anions in an irregular geometry. The bis(pyridine-2,6-dicarboxylato)cobalt complexes are connected by the sodium cations into a three-dimensional coordination network.

### Related literature

For the nickel(II) analog, see: Xiang *et al.* (2006).



### Experimental

#### Crystal data

$[Na_2Co(C_7H_3NO_4)_2]$	$V = 1504.0 (5)$ Å <sup>3</sup>
$M_r = 435.12$	$Z = 4$
Orthorhombic, $Pnna$	Mo $K\alpha$ radiation
$a = 14.476 (3)$ Å	$\mu = 1.25$ mm <sup>-1</sup>
$b = 12.643 (3)$ Å	$T = 293 (2)$ K
$c = 8.2179 (16)$ Å	$0.5 \times 0.4 \times 0.4$ mm

#### Data collection

Bruker SMART CCD area-detector diffractometer	12550 measured reflections
Absorption correction: multi-scan ( <i>SADABS</i> ; Bruker, 1998)	1401 independent reflections
$T_{\min} = 0.560$ , $T_{\max} = 0.611$	1288 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.045$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$	124 parameters
$wR(F^2) = 0.069$	H-atom parameters constrained
$S = 1.16$	$\Delta\rho_{\max} = 0.25$ e Å <sup>-3</sup>
1401 reflections	$\Delta\rho_{\min} = -0.28$ e Å <sup>-3</sup>

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT* and *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; 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: NC2057).

### References

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## **supplementary materials**

*Acta Cryst.* (2007). E63, m2557 [doi:10.1107/S1600536807044121]

## Poly[ $\mu_2$ -pyridine-2,6-dicarboxylato)cobalt(II)disodium(I)]

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### Comment

Poly[bis(pyridine-2,6-dicarboxylato) cobalt(II)disodium(I)] (I) is isostructural with the nickel(II) analogs, whose structures has been reported recently (Xiang *et al.*, 2006). In the crystal structure the Co cation is coordinated by two nitrogen atoms and four oxygen atoms of two pyridine-2,6-dicarboxylato groups within an strongly distorted octahedra (Fig. 1). The Na cations are coordinated by six oxygen atoms of the pyridine-2,6-dicarboxylato anions in irregula geometry. The bis(pyridine-2,6-dicarboxylato) cobalt complexes are connected by the sodium cations into a three-dimensional coordination network.

### Experimental

A mixture of  $\text{Co}(\text{NO}_3)_2 \cdot 6 \text{ H}_2\text{O}$ (0.145 g, 0.5 mmol),  $\text{NaN}_3$ (0.038 g, 0.5 mmol), pyridyl-2,6-dicarboxylic acid(0.085 g, 0.5 mmol) and  $\text{H}_2\text{O}$ (18 g, 1 mol) in a ratio of 1:1:1:2000 was sealed in a Teflon-lined autoclave and heated at 413k for 72 h. On cooling to room temperature purple coloured crystals have grown. Yield, 30%, based on cobalt.

### Refinement

The H atoms were positioned with idealized geometry and were refined isotropic with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$  using a riding model with  $\text{C}—\text{H} = 0.93 \text{ \AA}$ .

### Figures

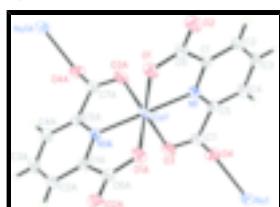


Fig. 1. Crystal structure of compound (I) with labeling and displacement ellipsoids drawn at the 50% probability level. Symmetry codes: A =  $x, -y + 3/2, -z - 3/2$ .

## Poly[ $\mu_2$ -pyridine-2,6-dicarboxylato)cobalt(II)disodium(I)]

### Crystal data

$[\text{Na}_2\text{Co}(\text{C}_7\text{H}_3\text{NO}_4)_2]$

$D_x = 1.922 \text{ Mg m}^{-3}$

$M_r = 435.12$

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{ \AA}$

Orthorhombic,  $Pnma$

Cell parameters from 12804 reflections

$a = 14.476 (3) \text{ \AA}$

$\theta = 3.2\text{--}27.6^\circ$

$b = 12.643 (3) \text{ \AA}$

$\mu = 1.25 \text{ mm}^{-1}$

$c = 8.2179 (16) \text{ \AA}$

$T = 293 (2) \text{ K}$

# supplementary materials

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$V = 1504.0 (5) \text{ \AA}^3$	Prism, purple
$Z = 4$	$0.5 \times 0.4 \times 0.4 \text{ mm}$
$F_{000} = 868$	

## Data collection

Bruker SMART CCD area-detector diffractometer	1401 independent reflections
Radiation source: fine-focus sealed tube	1288 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.045$
$T = 293(2) \text{ K}$	$\theta_{\text{max}} = 25.5^\circ$
$\varphi$ and $\omega$ scan	$\theta_{\text{min}} = 3.2^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -17 \rightarrow 17$
$T_{\text{min}} = 0.560, T_{\text{max}} = 0.611$	$k = -15 \rightarrow 15$
12550 measured reflections	$l = -9 \rightarrow 9$

## Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.029$	$w = 1/[\sigma^2(F_o^2) + (0.0255P)^2 + 1.1266P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.069$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.16$	$\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
1401 reflections	$\Delta\rho_{\text{min}} = -0.28 \text{ e \AA}^{-3}$
124 parameters	Extinction correction: SHELXL97, $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0131 (9)
Secondary atom site location: difference Fourier map	

## 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 ( $\text{\AA}^2$ )

$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
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Co1	0.48472 (3)	0.7500	-0.7500	0.02158 (17)
Na1	0.26971 (6)	0.64416 (7)	-0.10636 (11)	0.0271 (2)
N1	0.46109 (12)	0.59694 (13)	-0.6959 (2)	0.0184 (4)
O3	0.38369 (11)	0.75524 (11)	-0.5514 (2)	0.0323 (4)
C5	0.39461 (13)	0.57119 (16)	-0.5917 (2)	0.0187 (4)
C2	0.48779 (15)	0.41704 (17)	-0.7593 (3)	0.0229 (5)
H2A	0.5199	0.3657	-0.8174	0.027*
C1	0.50857 (14)	0.52354 (17)	-0.7765 (2)	0.0186 (5)
C4	0.37083 (15)	0.46689 (17)	-0.5658 (3)	0.0242 (5)
H4A	0.3247	0.4489	-0.4920	0.029*
C3	0.41763 (16)	0.38953 (17)	-0.6527 (3)	0.0271 (5)
H3A	0.4018	0.3188	-0.6394	0.033*
O4	0.29805 (11)	0.65269 (13)	-0.39208 (19)	0.0290 (4)
C7	0.35443 (14)	0.66626 (16)	-0.5038 (3)	0.0219 (5)
O1	0.59125 (11)	0.66942 (12)	-0.87976 (19)	0.0272 (4)
C6	0.58828 (14)	0.56926 (16)	-0.8724 (3)	0.0204 (5)
O2	0.64704 (10)	0.50923 (12)	-0.9290 (2)	0.0307 (4)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.0246 (3)	0.0128 (2)	0.0274 (3)	0.000	0.000	-0.00046 (17)
Na1	0.0257 (5)	0.0220 (4)	0.0336 (5)	-0.0015 (4)	0.0005 (4)	-0.0036 (4)
N1	0.0182 (9)	0.0156 (9)	0.0215 (9)	0.0007 (7)	-0.0011 (7)	-0.0013 (7)
O3	0.0372 (9)	0.0189 (8)	0.0408 (10)	-0.0002 (7)	0.0139 (8)	-0.0046 (7)
C5	0.0165 (10)	0.0207 (11)	0.0190 (10)	-0.0004 (8)	-0.0016 (8)	-0.0009 (9)
C2	0.0242 (11)	0.0176 (11)	0.0269 (12)	0.0026 (9)	-0.0038 (9)	-0.0047 (9)
C1	0.0186 (10)	0.0172 (11)	0.0200 (11)	0.0021 (8)	-0.0041 (8)	-0.0013 (8)
C4	0.0225 (11)	0.0221 (11)	0.0280 (12)	-0.0035 (9)	0.0009 (9)	0.0028 (9)
C3	0.0306 (12)	0.0150 (10)	0.0357 (13)	-0.0049 (9)	-0.0031 (10)	0.0010 (9)
O4	0.0253 (8)	0.0332 (9)	0.0284 (9)	-0.0032 (7)	0.0080 (7)	-0.0075 (7)
C7	0.0172 (10)	0.0234 (11)	0.0250 (11)	0.0003 (9)	-0.0015 (9)	-0.0046 (10)
O1	0.0262 (8)	0.0189 (8)	0.0365 (9)	-0.0022 (6)	0.0074 (7)	-0.0010 (7)
C6	0.0194 (10)	0.0218 (11)	0.0201 (11)	0.0018 (9)	-0.0031 (9)	-0.0012 (9)
O2	0.0245 (8)	0.0277 (8)	0.0398 (10)	0.0075 (7)	0.0074 (7)	-0.0022 (7)

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

Co1—N1 <sup>i</sup>	2.0149 (17)	O3—Na1 <sup>iii</sup>	2.4538 (17)
Co1—N1	2.0149 (17)	C5—C4	1.379 (3)
Co1—O1 <sup>i</sup>	2.1338 (16)	C5—C7	1.518 (3)
Co1—O1	2.1338 (16)	C2—C3	1.386 (3)
Co1—O3 <sup>i</sup>	2.1923 (16)	C2—C1	1.387 (3)
Co1—O3	2.1923 (16)	C2—H2A	0.9300
Na1—O2 <sup>ii</sup>	2.3017 (18)	C1—C6	1.512 (3)
Na1—O4	2.3860 (19)	C4—C3	1.388 (3)
Na1—O3 <sup>iii</sup>	2.4538 (17)	C4—H4A	0.9300

## supplementary materials

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Na1—O2 <sup>iv</sup>	2.4795 (18)	C3—H3A	0.9300
Na1—O4 <sup>iii</sup>	2.6009 (19)	O4—C7	1.240 (3)
Na1—O1 <sup>iv</sup>	2.6056 (18)	O4—Na1 <sup>iii</sup>	2.6009 (19)
Na1—C6 <sup>iv</sup>	2.797 (2)	C7—Na1 <sup>iii</sup>	2.840 (2)
Na1—C7 <sup>iii</sup>	2.840 (2)	O1—C6	1.268 (3)
Na1—Na1 <sup>iii</sup>	3.5686 (18)	O1—Na1 <sup>vi</sup>	2.6056 (18)
Na1—Na1 <sup>v</sup>	3.6896 (18)	C6—O2	1.231 (3)
N1—C5	1.329 (3)	C6—Na1 <sup>vi</sup>	2.797 (2)
N1—C1	1.331 (3)	O2—Na1 <sup>ii</sup>	2.3017 (18)
O3—C7	1.264 (3)	O2—Na1 <sup>vi</sup>	2.4795 (18)
N1 <sup>i</sup> —Co1—N1	160.46 (10)	O2 <sup>ii</sup> —Na1—Na1 <sup>v</sup>	41.28 (4)
N1 <sup>i</sup> —Co1—O1 <sup>i</sup>	76.97 (6)	O4—Na1—Na1 <sup>v</sup>	94.08 (4)
N1—Co1—O1 <sup>i</sup>	118.09 (6)	O3 <sup>iii</sup> —Na1—Na1 <sup>v</sup>	128.03 (5)
N1 <sup>i</sup> —Co1—O1	118.09 (6)	O2 <sup>iv</sup> —Na1—Na1 <sup>v</sup>	37.77 (4)
N1—Co1—O1	76.97 (6)	O4 <sup>iii</sup> —Na1—Na1 <sup>v</sup>	179.67 (5)
O1 <sup>i</sup> —Co1—O1	87.44 (9)	O1 <sup>iv</sup> —Na1—Na1 <sup>v</sup>	88.15 (5)
N1 <sup>i</sup> —Co1—O3 <sup>i</sup>	75.60 (6)	C6 <sup>iv</sup> —Na1—Na1 <sup>v</sup>	61.34 (5)
N1—Co1—O3 <sup>i</sup>	91.27 (6)	C7 <sup>iii</sup> —Na1—Na1 <sup>v</sup>	154.22 (5)
O1 <sup>i</sup> —Co1—O3 <sup>i</sup>	150.29 (6)	Na1 <sup>iii</sup> —Na1—Na1 <sup>v</sup>	137.81 (3)
O1—Co1—O3 <sup>i</sup>	95.49 (6)	C5—N1—C1	121.60 (18)
N1 <sup>i</sup> —Co1—O3	91.27 (6)	C5—N1—Co1	120.04 (14)
N1—Co1—O3	75.60 (6)	C1—N1—Co1	118.15 (14)
O1 <sup>i</sup> —Co1—O3	95.49 (6)	C7—O3—Co1	115.29 (13)
O1—Co1—O3	150.29 (6)	C7—O3—Na1 <sup>iii</sup>	94.14 (13)
O3 <sup>i</sup> —Co1—O3	96.31 (10)	Co1—O3—Na1 <sup>iii</sup>	149.04 (8)
O2 <sup>ii</sup> —Na1—O4	94.15 (6)	N1—C5—C4	120.97 (19)
O2 <sup>ii</sup> —Na1—O3 <sup>iii</sup>	91.02 (6)	N1—C5—C7	112.96 (18)
O4—Na1—O3 <sup>iii</sup>	112.39 (7)	C4—C5—C7	126.00 (19)
O2 <sup>ii</sup> —Na1—O2 <sup>iv</sup>	77.32 (6)	C3—C2—C1	117.9 (2)
O4—Na1—O2 <sup>iv</sup>	105.64 (6)	C3—C2—H2A	121.1
O3 <sup>iii</sup> —Na1—O2 <sup>iv</sup>	140.91 (7)	C1—C2—H2A	121.1
O2 <sup>ii</sup> —Na1—O4 <sup>iii</sup>	138.59 (6)	N1—C1—C2	120.92 (19)
O4—Na1—O4 <sup>iii</sup>	85.61 (6)	N1—C1—C6	112.77 (18)
O3 <sup>iii</sup> —Na1—O4 <sup>iii</sup>	52.03 (5)	C2—C1—C6	126.14 (19)
O2 <sup>iv</sup> —Na1—O4 <sup>iii</sup>	142.46 (6)	C5—C4—C3	118.2 (2)
O2 <sup>ii</sup> —Na1—O1 <sup>iv</sup>	128.90 (6)	C5—C4—H4A	120.9
O4—Na1—O1 <sup>iv</sup>	97.00 (6)	C3—C4—H4A	120.9
O3 <sup>iii</sup> —Na1—O1 <sup>iv</sup>	128.78 (6)	C2—C3—C4	120.4 (2)
O2 <sup>iv</sup> —Na1—O1 <sup>iv</sup>	51.64 (5)	C2—C3—H3A	119.8
O4 <sup>iii</sup> —Na1—O1 <sup>iv</sup>	92.02 (5)	C4—C3—H3A	119.8
O2 <sup>ii</sup> —Na1—C6 <sup>iv</sup>	102.37 (7)	C7—O4—Na1	147.97 (14)

O4—Na1—C6 <sup>iv</sup>	96.62 (6)	C7—O4—Na1 <sup>iii</sup>	87.91 (13)
O3 <sup>iii</sup> —Na1—C6 <sup>iv</sup>	147.12 (7)	Na1—O4—Na1 <sup>iii</sup>	91.28 (6)
O2 <sup>iv</sup> —Na1—C6 <sup>iv</sup>	26.11 (6)	O4—C7—O3	125.0 (2)
O4 <sup>iii</sup> —Na1—C6 <sup>iv</sup>	118.82 (6)	O4—C7—C5	119.65 (19)
O1 <sup>iv</sup> —Na1—C6 <sup>iv</sup>	26.86 (5)	O3—C7—C5	115.38 (18)
O2 <sup>ii</sup> —Na1—C7 <sup>iii</sup>	116.40 (7)	O4—C7—Na1 <sup>iii</sup>	66.22 (12)
O4—Na1—C7 <sup>iii</sup>	101.61 (7)	O3—C7—Na1 <sup>iii</sup>	59.51 (11)
O3 <sup>iii</sup> —Na1—C7 <sup>iii</sup>	26.35 (6)	C5—C7—Na1 <sup>iii</sup>	170.10 (15)
O2 <sup>iv</sup> —Na1—C7 <sup>iii</sup>	148.47 (7)	C6—O1—Co1	115.36 (14)
O4 <sup>iii</sup> —Na1—C7 <sup>iii</sup>	25.87 (5)	C6—O1—Na1 <sup>vi</sup>	85.03 (12)
O1 <sup>iv</sup> —Na1—C7 <sup>iii</sup>	109.79 (6)	Co1—O1—Na1 <sup>vi</sup>	142.84 (8)
C6 <sup>iv</sup> —Na1—C7 <sup>iii</sup>	135.31 (7)	O2—C6—O1	125.0 (2)
O2 <sup>ii</sup> —Na1—Na1 <sup>iii</sup>	135.68 (5)	O2—C6—C1	119.25 (19)
O4—Na1—Na1 <sup>iii</sup>	46.77 (4)	O1—C6—C1	115.61 (18)
O3 <sup>iii</sup> —Na1—Na1 <sup>iii</sup>	87.76 (5)	O2—C6—Na1 <sup>vi</sup>	62.38 (12)
O2 <sup>iv</sup> —Na1—Na1 <sup>iii</sup>	126.41 (5)	O1—C6—Na1 <sup>vi</sup>	68.12 (12)
O4 <sup>iii</sup> —Na1—Na1 <sup>iii</sup>	41.95 (4)	C1—C6—Na1 <sup>vi</sup>	151.45 (14)
O1 <sup>iv</sup> —Na1—Na1 <sup>iii</sup>	83.06 (4)	C6—O2—Na1 <sup>ii</sup>	146.43 (15)
C6 <sup>iv</sup> —Na1—Na1 <sup>iii</sup>	102.27 (5)	C6—O2—Na1 <sup>vi</sup>	91.51 (13)
C7 <sup>iii</sup> —Na1—Na1 <sup>iii</sup>	65.04 (5)	Na1 <sup>ii</sup> —O2—Na1 <sup>vi</sup>	100.95 (6)
N1 <sup>i</sup> —Co1—N1—C5	−41.45 (15)	O1 <sup>iv</sup> —Na1—O4—Na1 <sup>iii</sup>	73.59 (6)
O1 <sup>i</sup> —Co1—N1—C5	96.22 (16)	C6 <sup>iv</sup> —Na1—O4—Na1 <sup>iii</sup>	100.64 (6)
O1—Co1—N1—C5	176.12 (16)	C7 <sup>iii</sup> —Na1—O4—Na1 <sup>iii</sup>	−38.34 (7)
O3 <sup>i</sup> —Co1—N1—C5	−88.54 (16)	Na1 <sup>v</sup> —Na1—O4—Na1 <sup>iii</sup>	162.22 (3)
O3—Co1—N1—C5	7.66 (15)	Na1—O4—C7—O3	−79.0 (4)
N1 <sup>i</sup> —Co1—N1—C1	133.33 (15)	Na1 <sup>iii</sup> —O4—C7—O3	10.1 (2)
O1 <sup>i</sup> —Co1—N1—C1	−88.99 (16)	Na1—O4—C7—C5	99.9 (3)
O1—Co1—N1—C1	−9.10 (15)	Na1 <sup>iii</sup> —O4—C7—C5	−171.07 (17)
O3 <sup>i</sup> —Co1—N1—C1	86.25 (16)	Na1—O4—C7—Na1 <sup>iii</sup>	−89.1 (2)
O3—Co1—N1—C1	−177.56 (16)	Co1—O3—C7—O4	179.17 (17)
N1 <sup>i</sup> —Co1—O3—C7	161.39 (16)	Na1 <sup>iii</sup> —O3—C7—O4	−10.7 (2)
N1—Co1—O3—C7	−3.95 (16)	Co1—O3—C7—C5	0.3 (2)
O1 <sup>i</sup> —Co1—O3—C7	−121.58 (16)	Na1 <sup>iii</sup> —O3—C7—C5	170.39 (15)
O1—Co1—O3—C7	−27.1 (2)	Co1—O3—C7—Na1 <sup>iii</sup>	−170.12 (15)
O3 <sup>i</sup> —Co1—O3—C7	85.74 (16)	N1—C5—C7—O4	−173.18 (18)
N1 <sup>i</sup> —Co1—O3—Na1 <sup>iii</sup>	0.83 (17)	C4—C5—C7—O4	3.7 (3)
N1—Co1—O3—Na1 <sup>iii</sup>	−164.51 (18)	N1—C5—C7—O3	5.8 (3)
O1 <sup>i</sup> —Co1—O3—Na1 <sup>iii</sup>	77.86 (17)	C4—C5—C7—O3	−177.3 (2)
O1—Co1—O3—Na1 <sup>iii</sup>	172.34 (12)	N1—C5—C7—Na1 <sup>iii</sup>	62.5 (9)
O3 <sup>i</sup> —Co1—O3—Na1 <sup>iii</sup>	−74.82 (16)	C4—C5—C7—Na1 <sup>iii</sup>	−120.5 (8)
C1—N1—C5—C4	−1.4 (3)	N1 <sup>i</sup> —Co1—O1—C6	−162.89 (14)

## supplementary materials

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Co1—N1—C5—C4	173.17 (16)	N1—Co1—O1—C6	3.74 (15)
C1—N1—C5—C7	175.65 (18)	O1 <sup>i</sup> —Co1—O1—C6	123.35 (17)
Co1—N1—C5—C7	−9.7 (2)	O3 <sup>i</sup> —Co1—O1—C6	−86.29 (15)
C5—N1—C1—C2	2.5 (3)	O3—Co1—O1—C6	26.7 (2)
Co1—N1—C1—C2	−172.17 (16)	N1 <sup>i</sup> —Co1—O1—Na1 <sup>vi</sup>	79.30 (13)
C5—N1—C1—C6	−172.97 (17)	N1—Co1—O1—Na1 <sup>vi</sup>	−114.07 (13)
Co1—N1—C1—C6	12.3 (2)	O1 <sup>i</sup> —Co1—O1—Na1 <sup>vi</sup>	5.54 (7)
C3—C2—C1—N1	−1.5 (3)	O3 <sup>i</sup> —Co1—O1—Na1 <sup>vi</sup>	155.90 (12)
C3—C2—C1—C6	173.37 (19)	O3—Co1—O1—Na1 <sup>vi</sup>	−91.06 (16)
N1—C5—C4—C3	−0.6 (3)	Co1—O1—C6—O2	−174.52 (17)
C7—C5—C4—C3	−177.3 (2)	Na1 <sup>vi</sup> —O1—C6—O2	−27.0 (2)
C1—C2—C3—C4	−0.6 (3)	Co1—O1—C6—C1	1.4 (2)
C5—C4—C3—C2	1.6 (3)	Na1 <sup>vi</sup> —O1—C6—C1	149.01 (16)
O2 <sup>ii</sup> —Na1—O4—C7	−68.3 (3)	Co1—O1—C6—Na1 <sup>vi</sup>	−147.57 (12)
O3 <sup>iii</sup> —Na1—O4—C7	24.6 (3)	N1—C1—C6—O2	167.43 (19)
O2 <sup>iv</sup> —Na1—O4—C7	−146.3 (3)	C2—C1—C6—O2	−7.8 (3)
O4 <sup>iii</sup> —Na1—O4—C7	70.2 (3)	N1—C1—C6—O1	−8.8 (3)
O1 <sup>iv</sup> —Na1—O4—C7	161.7 (3)	C2—C1—C6—O1	176.0 (2)
C6 <sup>iv</sup> —Na1—O4—C7	−171.3 (3)	N1—C1—C6—Na1 <sup>vi</sup>	82.2 (3)
C7 <sup>iii</sup> —Na1—O4—C7	49.8 (3)	C2—C1—C6—Na1 <sup>vi</sup>	−93.1 (3)
Na1 <sup>iii</sup> —Na1—O4—C7	88.1 (3)	O1—C6—O2—Na1 <sup>ii</sup>	140.9 (2)
Na1 <sup>v</sup> —Na1—O4—C7	−109.7 (3)	C1—C6—O2—Na1 <sup>ii</sup>	−35.0 (4)
O2 <sup>ii</sup> —Na1—O4—Na1 <sup>iii</sup>	−156.38 (5)	Na1 <sup>vi</sup> —C6—O2—Na1 <sup>ii</sup>	112.5 (3)
O3 <sup>iii</sup> —Na1—O4—Na1 <sup>iii</sup>	−63.55 (7)	O1—C6—O2—Na1 <sup>vi</sup>	28.3 (2)
O2 <sup>iv</sup> —Na1—O4—Na1 <sup>iii</sup>	125.64 (5)	C1—C6—O2—Na1 <sup>vi</sup>	−147.49 (16)
O4 <sup>iii</sup> —Na1—O4—Na1 <sup>iii</sup>	−17.91 (7)		

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

Fig. 1

