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# Poly[[diaqua[$\mu_5$-(*R*,*S*)-2-({2-[(1,2-dicarboxylatoethyl)amino]ethyl}amino)butanedioato]cobaltate(III)sodium] dihydrate]

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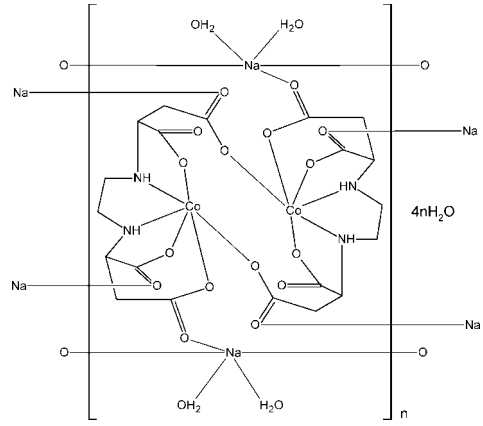
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.029; $wR$ factor = 0.065; data-to-parameter ratio = 11.9.

In the asymmetric unit of the title coordination polymer, $\{[CoNa(C_{10}H_{12}N_2O_8)(H_2O)_2]\cdot 2H_2O\}_n$, the $Co^{II}$ ion is coordinated in a distorted octahedral environment, defined by two N atoms and four carboxylate O atoms. Two $Co^{II}$ ions and two 2-({2-[(1,2-dicarboxylatoethyl)amino]ethyl}amino)butanedioate (EDDS) ligands form a dimeric complex dianion $[Co_2(EDDS)_2]$. These dimeric units are connected *via* $Na^+$ ions, forming a three-dimensional polymeric structure. In the crystal, the ligand N—H groups and the coordinated and solvent water molecules are involved in intermolecular N—H···O and O—H···O hydrogen bonding, reinforcing the three-dimensional polymeric structure.

## Related literature

For the synthesis and applications of EDDS and its complexes, see: Jones & Williams (2001); Kos & Leštan (2003); Mazurenko & Trunova (2001); Meers *et al.* (2005); Shadchina *et al.* (2008); Tandy *et al.* (2004, 2006); Vandevivere *et al.* (2001). For related structures, see: Horn *et al.* (1993); Pavelčík *et al.* (1980). For standard bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$[CoNa(C_{10}H_{12}N_2O_8)(H_2O)_2]\cdot 2H_2O$
$M_r$ = 442.20
Orthorhombic, *Pbca*
$a$ = 10.0207 (2) Å
$b$ = 15.6475 (2) Å
$c$ = 20.3837 (4) Å
$V$ = 3196.14 (10) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 1.17 mm$^{-1}$
$T$ = 100 K
0.32 × 0.28 × 0.13 mm

### Data collection

Bruker SMART APEXII diffractometer
Absorption correction: numerical (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.706, $T_{max}$ = 0.863
11219 measured reflections
3161 independent reflections
2549 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.065
$S$ = 0.97
3161 reflections
265 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.50 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*···O7$^{i}$ | 0.84 (2) | 2.21 (2) | 2.830 (2) | 130.6 (18) |
| N2—H2*N*···O6$^{ii}$ | 0.82 (2) | 2.16 (2) | 2.809 (2) | 137.0 (18) |
| O9—H91···O11 | 0.84 (2) | 1.92 (2) | 2.741 (2) | 166 (2) |
| O9—H92···O2$^{iii}$ | 0.80 (3) | 2.08 (3) | 2.853 (2) | 162 (3) |
| O10—H101···O8 | 0.83 (2) | 2.18 (3) | 2.972 (2) | 160 (2) |
| O10—H102···O2$^{iv}$ | 0.82 (3) | 2.04 (3) | 2.853 (2) | 175 (3) |
| O11—H111···O1 | 0.79 (3) | 2.26 (3) | 3.004 (2) | 158 (3) |
| O11—H112···O12$^{iii}$ | 0.96 (3) | 1.77 (3) | 2.706 (3) | 164 (2) |
| O12—H121···O1 | 0.77 (3) | 2.05 (3) | 2.793 (2) | 161 (3) |
| O12—H122···O4$^{v}$ | 0.76 (3) | 2.04 (3) | 2.788 (2) | 167 (3) |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2010); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5329).

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# supporting information

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## Poly[[diaqua[$\mu_5$-(*R*,*S*)-2-({2-[(1,2-dicarboxylatoethyl)amino]ethyl}amino)butanedioato]cobaltate(III)sodium] dihydrate]

**Olena K. Trunova, Anatolij V. Dudko, Tamara O. Makotryk, Olena V. Osadcha, Vasily I. Pekhnyo and Ganna V. Shovkova**

### S1. Comment

Ethylenediamine-N,*N*′-disuccinic acid and its coordination compounds with different 3 d-metals have attracted much interest due to their potential and practical applications in biochemistry. EDDS can be applied for some technical purposes: for the extraction of heavy metals from soils as an efficient biodegradable chelating agents (Tandy *et al.*, 2004; Tandy *et al.*, 2006), in replacement of edta in soil washing and phytoextraction (Vandevivere *et al.*, 2001; Kos & Leštan, 2003; Meers *et al.* 2005) or for radionuclide decontamination in the pulp and paper-making industry (Jones & Williams, 2001). Biologically active complexes are widely used in plant growing and animal industries (Mazurenko & Trunova 2001; Shadchina *et al.* 2008). The biodegradable strong transition metal chelant [S,*S*] stereoisomer of ethylenediamine disuccinate was investigated for its applicability for the washing extraction of heavy metals from soil, sewage sludge, and harbor sediment (Vandevivere *et al.*, 2001).

In the course of our investigations the title compound was prepared and structurally characterized. The asymmetric unit of the title compound is shown in Fig. 1. The $Co^{II}$ ion forms a distorted octahedral [$CoN_2O_4$] environment defined by sets of three five-membered (Co1/O1/C1/C2/N1;/Co1/N1/C3/C4/N2; Co1/N2/C5/C6/O3) and a six-membered (Co1/N2/C5/C7/C8/O5) metallocycle. The sixth O donor from a centrosymmetrically related $[Co(edds)]^-$ complex ion forms a 12-membered macrocycle, as a result a dimeric unit is produced (Fig. 2). The Co-O, Co-N, Na-O bond lengths are in normal ranges and have a good correlation with literature data (Allen *et al.*, 1987; Pavelčík *et al.*, 1980; Horn *et al.*, 1993). The Co1···Co1(-x, -y+1, -z) distance is 5.265 Å, which excludes the possibility of any interaction between the ions. In the crystal the compound exists as a polymeric structure, in which the monomers are interconnected by $Na^+$ ions (Fig. 2). The $Na^+$ ions are five-coordinate, with a distorted trigonal-bipyramidal coordination geometry formed by oxygen atoms, two of which belong to water molecules and the other three to oxygen atoms of the ligand which do not take part in the coordination of the $Co^{ii}$ ion. Intermolecular N—H···O and O—H···O hydrogen bonds in the crystal structure form a three-dimensional supramolecular network which stabilizes the structure (Fig.3, Table 1).

### S2. Experimental

A mixture of $CoCl_2.6H_2O$ (2.38 g, 10 mmol) and EDDS (2.92 g, 10 mmol) were dissolved in distilled water (10 ml). The pH was then adjusted to 4.5 by concentrated NaOH solution. Reaction mixture was refluxed with stirring for 24 h. After cooling to room temperature diethyl ether was added into the solution giving a powder crude product. Precipitate was filtered of and washed with methanol for several times (yield 86%). The resulting residue was dissolved in water and was stored in a dark place for slow evaporation. After 4 days suitable crystals for X-ray data collection were obtained.

### S3. Refinement

H atoms bonded to O and N atoms were located in a difference Fourier map. Their positions were refined freely whereas thermal parameters were fixed to $U_{iso}$(H) = 1.5$U_{eq}$(N,*O*). To avoid short contacts between H91 and H112 they were refined with distance restraint (H···H= 2.3 ±0.02 Å). H atoms bonded to C were positioned geometrically and refined using a riding model with C—H = 0.99 Å for $CH_2$ and C—H = 1.00 Å for CH with $U_{iso}$(H) = 1.2$U_{eq}$(C).

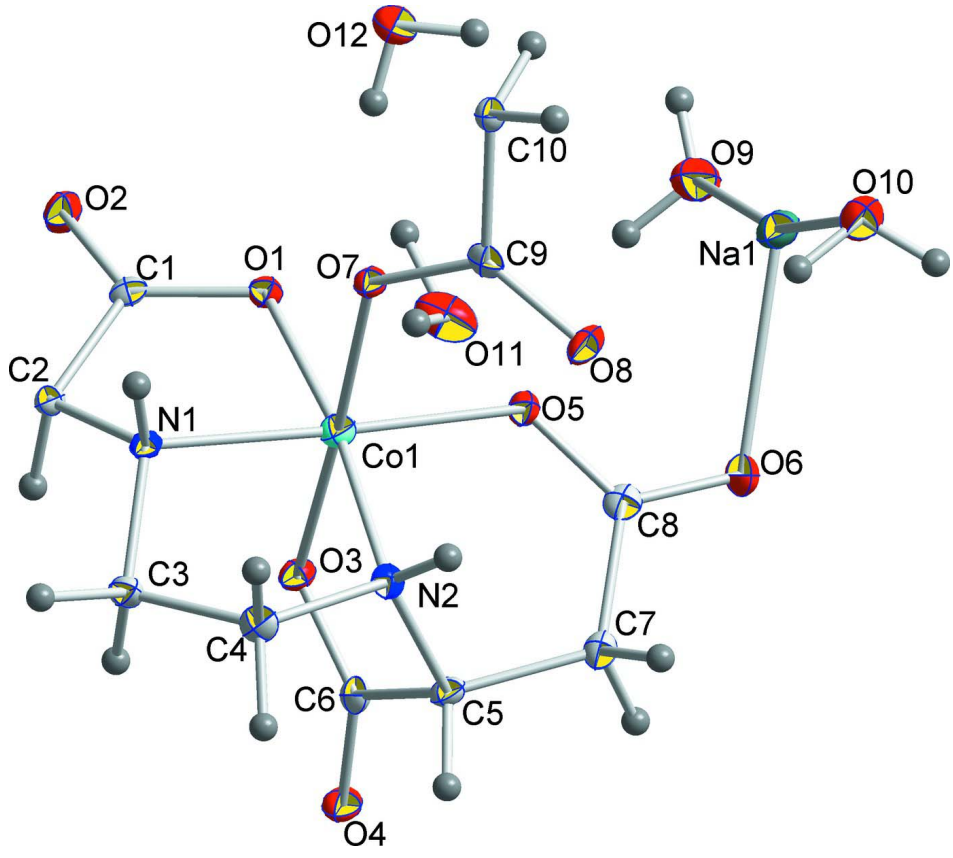


**Figure 1**

The asymmetric unit of the title compound with ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

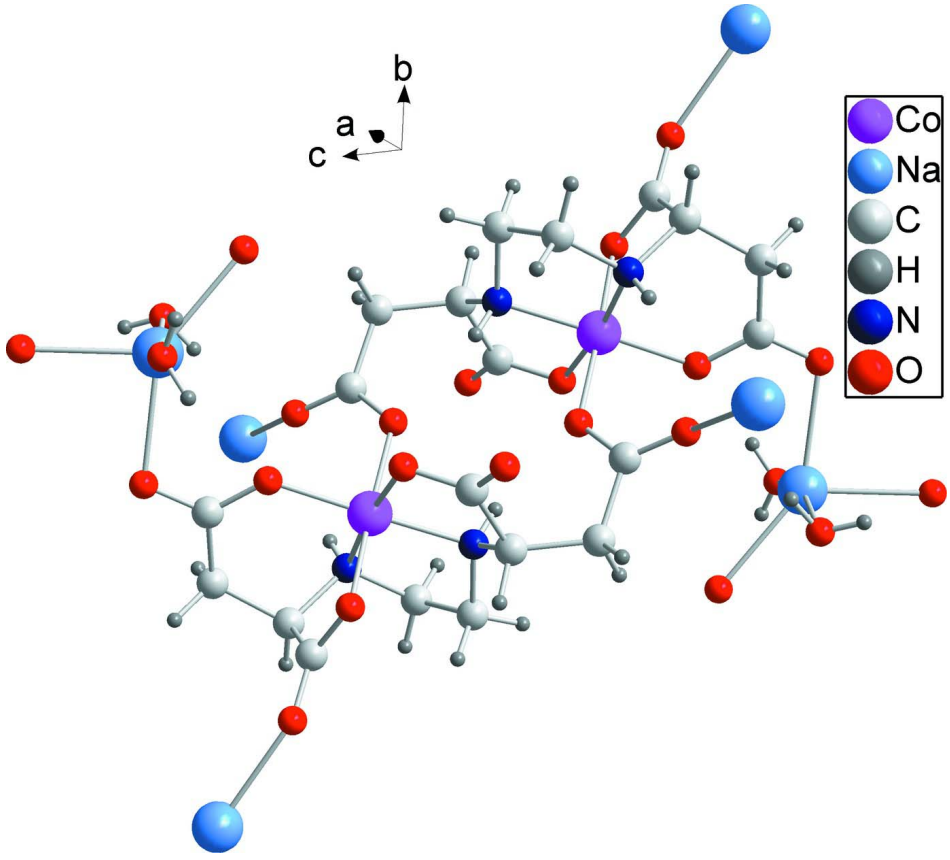


**Figure 2**

Part of the polymeric structure of the title compound formed by sodium ions.

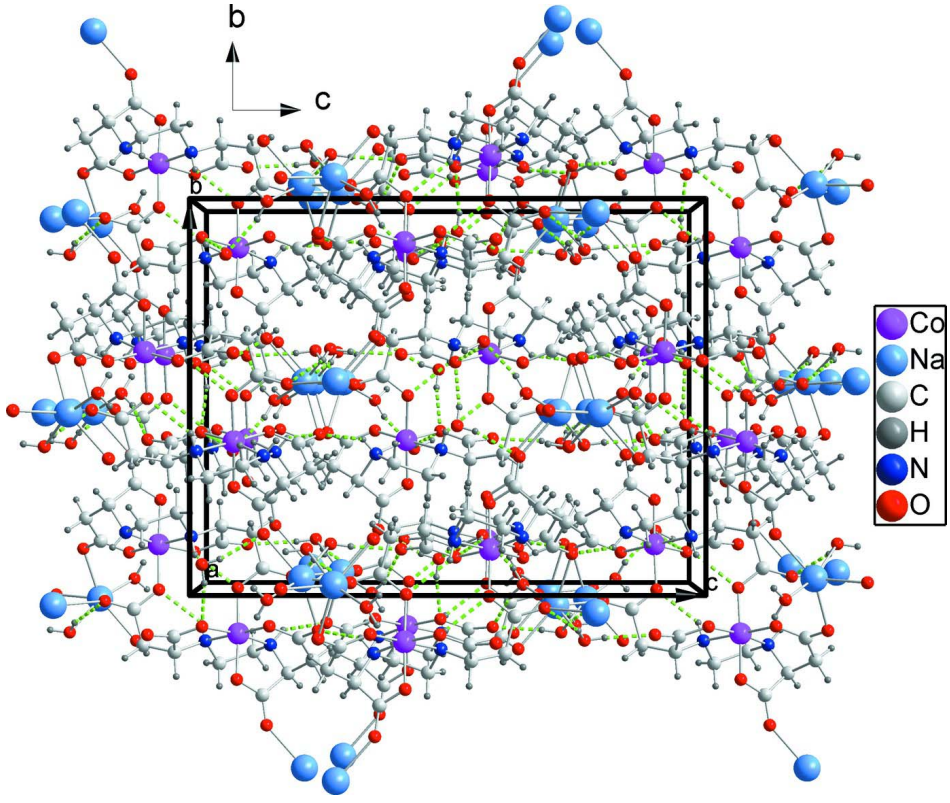


**Figure 3**

Crystal packing of title compound, projected along the *a* axis. Dashed lines indicate hydrogen bonds.

**Poly[[diaqua[$\mu_5$-(*R*,*S*)-2-({2-[(1,2- dicarboxylatoethyl)amino]ethyl}amino)butanedioate]cobaltate(III)sodium] dihydrate]**

*Crystal data*

$[CoNa(C_{10}H_{12}N_2O_8)(H_2O)_2]\cdot 2H_2O$
$M_r = 442.20$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 10.0207\ (2)$ Å
$b = 15.6475\ (2)$ Å
$c = 20.3837\ (4)$ Å
$V = 3196.14\ (10)$ Å$^3$
$Z = 8$
$F(000) = 1824$
$D_x = 1.838$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4049 reflections
$\theta = 2.6$–$26.1°$
$\mu = 1.17$ mm$^{-1}$
$T = 100$ K
Diamond, violet
0.32 × 0.28 × 0.13 mm

*Data collection*

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: numerical (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.706$, $T_{max} = 0.863$
11219 measured reflections
3161 independent reflections
2549 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 26.1°$, $\theta_{min} = 2.0°$
$h = -7 \rightarrow 12$
$k = -19 \rightarrow 19$
$l = -25 \rightarrow 21$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.065$
$S = 0.97$
3161 reflections
265 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0324P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å$^{-3}$
$\Delta\rho_{min} = -0.50$ 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.
**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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co1 | 0.09689 (3) | 0.387117 (14) | 0.083088 (13) | 0.00826 (9) |
| Na1 | 0.39217 (9) | 0.53940 (5) | 0.21505 (4) | 0.0178 (2) |
| C1 | 0.1871 (2) | 0.38312 (11) | −0.04223 (10) | 0.0104 (4) |
| C2 | 0.0531 (2) | 0.33752 (11) | −0.04526 (9) | 0.0100 (4) |
| H2 | 0.0712 | 0.2749 | −0.0414 | 0.012* |
| C3 | −0.1234 (2) | 0.29948 (11) | 0.03843 (10) | 0.0120 (5) |
| H3A | −0.0830 | 0.2418 | 0.0400 | 0.014* |
| H3B | −0.2034 | 0.2975 | 0.0099 | 0.014* |
| C4 | −0.1601 (2) | 0.32957 (12) | 0.10675 (10) | 0.0130 (5) |
| H4A | −0.2192 | 0.3801 | 0.1038 | 0.016* |
| H4B | −0.2088 | 0.2838 | 0.1302 | 0.016* |
| C5 | 0.0280 (2) | 0.28136 (11) | 0.18052 (10) | 0.0111 (4) |
| H5 | −0.0412 | 0.2455 | 0.2027 | 0.013* |
| C6 | 0.1054 (2) | 0.22824 (12) | 0.13122 (10) | 0.0118 (4) |
| C7 | 0.1248 (2) | 0.31881 (11) | 0.23126 (10) | 0.0123 (5) |
| H7A | 0.0714 | 0.3483 | 0.2653 | 0.015* |
| H7B | 0.1714 | 0.2707 | 0.2529 | 0.015* |
| C8 | 0.2302 (2) | 0.38128 (11) | 0.20641 (10) | 0.0124 (5) |
| C9 | 0.0287 (2) | 0.55445 (11) | 0.13005 (10) | 0.0106 (4) |
| C10 | 0.0175 (2) | 0.64820 (11) | 0.11074 (10) | 0.0111 (4) |
| H10A | 0.1083 | 0.6729 | 0.1082 | 0.013* |
| H10B | −0.0317 | 0.6792 | 0.1455 | 0.013* |
| N1 | −0.02558 (17) | 0.36314 (9) | 0.01328 (8) | 0.0087 (4) |
| H1N | −0.065 (2) | 0.4093 (12) | 0.0043 (10) | 0.010* |

| | | | | |
|---|---|---|---|---|
| N2 | −0.03629 (17) | 0.35219 (10) | 0.14370 (8) | 0.0102 (4) |
| H2N | −0.057 (2) | 0.3904 (12) | 0.1691 (11) | 0.012* |
| O1 | 0.22354 (14) | 0.41008 (8) | 0.01494 (6) | 0.0105 (3) |
| O2 | 0.25654 (16) | 0.39053 (8) | −0.09163 (7) | 0.0163 (3) |
| O3 | 0.15026 (14) | 0.27071 (7) | 0.08149 (6) | 0.0113 (3) |
| O4 | 0.12621 (15) | 0.15144 (8) | 0.14003 (7) | 0.0158 (3) |
| O5 | 0.22710 (14) | 0.41130 (8) | 0.14795 (7) | 0.0119 (3) |
| O6 | 0.31703 (15) | 0.40383 (8) | 0.24573 (7) | 0.0184 (4) |
| O7 | 0.04285 (14) | 0.50388 (7) | 0.08043 (6) | 0.0107 (3) |
| O8 | 0.02390 (15) | 0.53288 (8) | 0.18835 (7) | 0.0156 (3) |
| O9 | 0.56412 (18) | 0.49111 (10) | 0.15130 (8) | 0.0245 (4) |
| H91 | 0.537 (3) | 0.4471 (15) | 0.1319 (11) | 0.037* |
| H92 | 0.605 (3) | 0.5215 (16) | 0.1272 (14) | 0.037* |
| O10 | 0.22692 (18) | 0.62299 (10) | 0.26905 (8) | 0.0214 (4) |
| H101 | 0.162 (3) | 0.5949 (15) | 0.2558 (12) | 0.032* |
| H102 | 0.229 (3) | 0.6165 (15) | 0.3088 (13) | 0.032* |
| O11 | 0.49078 (18) | 0.36011 (9) | 0.06961 (9) | 0.0253 (4) |
| H111 | 0.415 (3) | 0.3726 (17) | 0.0657 (14) | 0.038* |
| H112 | 0.539 (3) | 0.3836 (15) | 0.0329 (11) | 0.038* |
| O12 | 0.33610 (19) | 0.57331 (10) | 0.01853 (8) | 0.0241 (4) |
| H121 | 0.320 (3) | 0.5253 (16) | 0.0228 (13) | 0.036* |
| H122 | 0.348 (3) | 0.5872 (17) | 0.0539 (14) | 0.036* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 0.00957 (17) | 0.00764 (12) | 0.00757 (14) | 0.00002 (11) | −0.00016 (12) | 0.00084 (11) |
| Na1 | 0.0234 (5) | 0.0147 (4) | 0.0153 (4) | 0.0012 (4) | 0.0001 (4) | 0.0032 (3) |
| C1 | 0.0113 (12) | 0.0080 (8) | 0.0119 (10) | 0.0028 (8) | −0.0009 (9) | 0.0029 (8) |
| C2 | 0.0141 (12) | 0.0078 (8) | 0.0082 (10) | 0.0000 (8) | 0.0013 (9) | −0.0007 (8) |
| C3 | 0.0110 (12) | 0.0123 (8) | 0.0126 (11) | −0.0031 (8) | −0.0009 (9) | 0.0017 (8) |
| C4 | 0.0081 (12) | 0.0163 (9) | 0.0145 (11) | −0.0004 (9) | −0.0002 (9) | 0.0017 (8) |
| C5 | 0.0118 (12) | 0.0109 (8) | 0.0105 (10) | 0.0002 (8) | −0.0009 (9) | 0.0036 (8) |
| C6 | 0.0103 (12) | 0.0137 (9) | 0.0114 (10) | −0.0008 (9) | −0.0040 (9) | 0.0008 (8) |
| C7 | 0.0142 (13) | 0.0125 (9) | 0.0103 (10) | 0.0026 (9) | −0.0011 (9) | −0.0008 (8) |
| C8 | 0.0142 (13) | 0.0097 (8) | 0.0134 (11) | 0.0043 (8) | −0.0005 (10) | 0.0002 (8) |
| C9 | 0.0048 (12) | 0.0128 (9) | 0.0143 (11) | −0.0016 (8) | −0.0008 (9) | 0.0000 (8) |
| C10 | 0.0135 (13) | 0.0106 (9) | 0.0092 (10) | −0.0004 (8) | 0.0006 (9) | −0.0007 (8) |
| N1 | 0.0099 (10) | 0.0072 (7) | 0.0089 (9) | 0.0014 (7) | −0.0001 (7) | 0.0011 (7) |
| N2 | 0.0103 (10) | 0.0099 (7) | 0.0104 (9) | 0.0017 (7) | −0.0001 (8) | −0.0010 (7) |
| O1 | 0.0091 (8) | 0.0117 (6) | 0.0107 (7) | −0.0014 (6) | 0.0005 (6) | 0.0008 (6) |
| O2 | 0.0159 (9) | 0.0223 (7) | 0.0107 (8) | −0.0029 (6) | 0.0031 (7) | −0.0004 (6) |
| O3 | 0.0126 (8) | 0.0099 (6) | 0.0114 (7) | 0.0018 (6) | 0.0007 (6) | 0.0014 (6) |
| O4 | 0.0241 (10) | 0.0095 (6) | 0.0138 (8) | 0.0018 (6) | −0.0011 (7) | 0.0015 (6) |
| O5 | 0.0116 (9) | 0.0137 (6) | 0.0103 (7) | −0.0014 (6) | −0.0021 (6) | 0.0013 (6) |
| O6 | 0.0203 (9) | 0.0198 (7) | 0.0153 (8) | −0.0051 (6) | −0.0078 (7) | 0.0024 (6) |
| O7 | 0.0138 (8) | 0.0086 (6) | 0.0097 (7) | 0.0011 (6) | −0.0005 (6) | 0.0008 (6) |
| O8 | 0.0229 (10) | 0.0156 (6) | 0.0083 (7) | 0.0033 (6) | 0.0017 (7) | 0.0016 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O9 | 0.0310 (12) | 0.0211 (8) | 0.0214 (9) | −0.0064 (7) | 0.0051 (8) | −0.0005 (7) |
| O10 | 0.0232 (10) | 0.0246 (8) | 0.0163 (8) | −0.0030 (7) | −0.0002 (8) | 0.0023 (7) |
| O11 | 0.0174 (10) | 0.0180 (7) | 0.0405 (11) | 0.0026 (7) | 0.0020 (9) | −0.0021 (7) |
| O12 | 0.0380 (12) | 0.0140 (7) | 0.0202 (9) | −0.0057 (7) | −0.0033 (9) | 0.0003 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Co1—O5 | 1.8957 (14) | C5—C7 | 1.534 (3) |
| Co1—O3 | 1.8987 (12) | C5—H5 | 1.0000 |
| Co1—N2 | 1.8990 (17) | C6—O4 | 1.233 (2) |
| Co1—O7 | 1.9064 (12) | C6—O3 | 1.293 (2) |
| Co1—O1 | 1.9155 (13) | C7—C8 | 1.526 (3) |
| Co1—N1 | 1.9161 (17) | C7—H7A | 0.9900 |
| Na1—O9 | 2.2866 (19) | C7—H7B | 0.9900 |
| Na1—O4$^{i}$ | 2.3336 (15) | C8—O6 | 1.234 (2) |
| Na1—O6 | 2.3363 (15) | C8—O5 | 1.281 (2) |
| Na1—O8$^{ii}$ | 2.3728 (16) | C9—O8 | 1.236 (2) |
| Na1—O10 | 2.3800 (19) | C9—O7 | 1.292 (2) |
| Na1—O5 | 2.9368 (15) | C9—C10 | 1.523 (2) |
| Na1—H101 | 2.60 (3) | C10—C2$^{iii}$ | 1.527 (3) |
| C1—O2 | 1.229 (2) | C10—H10A | 0.9900 |
| C1—O1 | 1.292 (2) | C10—H10B | 0.9900 |
| C1—C2 | 1.522 (3) | N1—H1N | 0.84 (2) |
| C2—N1 | 1.485 (2) | N2—H2N | 0.82 (2) |
| C2—C10$^{iii}$ | 1.527 (3) | O4—Na1$^{iv}$ | 2.3336 (15) |
| C2—H2 | 1.0000 | O8—Na1$^{v}$ | 2.3728 (16) |
| C3—N1 | 1.489 (2) | O9—H91 | 0.84 (2) |
| C3—C4 | 1.515 (3) | O9—H92 | 0.80 (3) |
| C3—H3A | 0.9900 | O10—H101 | 0.83 (2) |
| C3—H3B | 0.9900 | O10—H102 | 0.82 (3) |
| C4—N2 | 1.494 (3) | O11—H111 | 0.79 (3) |
| C4—H4A | 0.9900 | O11—H112 | 0.96 (3) |
| C4—H4B | 0.9900 | O12—H121 | 0.77 (3) |
| C5—N2 | 1.486 (2) | O12—H122 | 0.76 (3) |
| C5—C6 | 1.517 (3) | | |

| | | | |
|---|---|---|---|
| O5—Co1—O3 | 90.55 (6) | N2—C5—C6 | 107.20 (16) |
| O5—Co1—N2 | 95.02 (7) | N2—C5—C7 | 109.25 (15) |
| O3—Co1—N2 | 86.16 (6) | C6—C5—C7 | 109.43 (17) |
| O5—Co1—O7 | 91.37 (6) | N2—C5—H5 | 110.3 |
| O3—Co1—O7 | 177.39 (6) | C6—C5—H5 | 110.3 |
| N2—Co1—O7 | 95.43 (6) | C7—C5—H5 | 110.3 |
| O5—Co1—O1 | 90.70 (6) | O4—C6—O3 | 123.80 (19) |
| O3—Co1—O1 | 88.91 (6) | O4—C6—C5 | 121.60 (18) |
| N2—Co1—O1 | 172.47 (6) | O3—C6—C5 | 114.56 (15) |
| O7—Co1—O1 | 89.30 (5) | C8—C7—C5 | 117.30 (17) |
| O5—Co1—N1 | 176.22 (7) | C8—C7—H7A | 108.0 |
| O3—Co1—N1 | 88.84 (6) | C5—C7—H7A | 108.0 |

| | | | |
|---|---|---|---|
| N2—Co1—N1 | 88.66 (7) | C8—C7—H7B | 108.0 |
| O7—Co1—N1 | 89.12 (6) | C5—C7—H7B | 108.0 |
| O1—Co1—N1 | 85.56 (7) | H7A—C7—H7B | 107.2 |
| O9—Na1—O4$^{i}$ | 86.29 (6) | O6—C8—O5 | 121.08 (19) |
| O9—Na1—O6 | 95.44 (6) | O6—C8—C7 | 117.10 (18) |
| O4$^{i}$—Na1—O6 | 146.32 (6) | O5—C8—C7 | 121.79 (18) |
| O9—Na1—O8$^{ii}$ | 92.19 (6) | O8—C9—O7 | 126.13 (17) |
| O4$^{i}$—Na1—O8$^{ii}$ | 128.32 (6) | O8—C9—C10 | 120.57 (17) |
| O6—Na1—O8$^{ii}$ | 85.30 (5) | O7—C9—C10 | 113.31 (16) |
| O9—Na1—O10 | 165.64 (6) | C9—C10—C2$^{iii}$ | 113.63 (15) |
| O4$^{i}$—Na1—O10 | 80.52 (6) | C9—C10—H10A | 108.8 |
| O6—Na1—O10 | 98.69 (6) | C2$^{iii}$—C10—H10A | 108.8 |
| O8$^{ii}$—Na1—O10 | 91.54 (6) | C9—C10—H10B | 108.8 |
| O9—Na1—O5 | 86.23 (5) | C2$^{iii}$—C10—H10B | 108.8 |
| O4$^{i}$—Na1—O5 | 99.39 (5) | H10A—C10—H10B | 107.7 |
| O6—Na1—O5 | 47.42 (5) | C2—N1—C3 | 116.47 (14) |
| O8$^{ii}$—Na1—O5 | 132.10 (5) | C2—N1—Co1 | 108.02 (12) |
| O10—Na1—O5 | 101.46 (6) | C3—N1—Co1 | 107.29 (12) |
| O9—Na1—H101 | 163.8 (6) | C2—N1—H1N | 107.7 (15) |
| O4$^{i}$—Na1—H101 | 83.6 (5) | C3—N1—H1N | 109.9 (14) |
| O6—Na1—H101 | 86.1 (5) | Co1—N1—H1N | 107.0 (14) |
| O8$^{ii}$—Na1—H101 | 104.0 (6) | C5—N2—C4 | 115.98 (15) |
| O10—Na1—H101 | 18.5 (5) | C5—N2—Co1 | 103.81 (12) |
| O5—Na1—H101 | 83.0 (6) | C4—N2—Co1 | 108.90 (13) |
| O2—C1—O1 | 123.23 (19) | C5—N2—H2N | 109.7 (15) |
| O2—C1—C2 | 120.69 (18) | C4—N2—H2N | 106.2 (16) |
| O1—C1—C2 | 116.04 (17) | Co1—N2—H2N | 112.4 (15) |
| N1—C2—C1 | 108.02 (15) | C1—O1—Co1 | 113.93 (13) |
| N1—C2—C10$^{iii}$ | 114.61 (16) | C6—O3—Co1 | 112.44 (12) |
| C1—C2—C10$^{iii}$ | 112.07 (16) | C6—O4—Na1$^{iv}$ | 144.52 (14) |
| N1—C2—H2 | 107.3 | C8—O5—Co1 | 126.31 (13) |
| C1—C2—H2 | 107.3 | C8—O5—Na1 | 78.66 (11) |
| C10$^{iii}$—C2—H2 | 107.3 | Co1—O5—Na1 | 148.08 (6) |
| N1—C3—C4 | 105.57 (15) | C8—O6—Na1 | 108.23 (12) |
| N1—C3—H3A | 110.6 | C9—O7—Co1 | 126.58 (12) |
| C4—C3—H3A | 110.6 | C9—O8—Na1$^{v}$ | 143.85 (14) |
| N1—C3—H3B | 110.6 | Na1—O9—H91 | 107.0 (17) |
| C4—C3—H3B | 110.6 | Na1—O9—H92 | 122.9 (19) |
| H3A—C3—H3B | 108.8 | H91—O9—H92 | 111 (2) |
| N2—C4—C3 | 109.59 (17) | Na1—O10—H101 | 95.7 (18) |
| N2—C4—H4A | 109.8 | Na1—O10—H102 | 112.1 (18) |
| C3—C4—H4A | 109.8 | H101—O10—H102 | 106 (3) |
| N2—C4—H4B | 109.8 | H111—O11—H112 | 108 (3) |
| C3—C4—H4B | 109.8 | H121—O12—H122 | 102 (3) |
| H4A—C4—H4B | 108.2 | | |

| | | | |
|---|---|---|---|
| O2—C1—C2—N1 | −161.41 (17) | N1—Co1—O1—C1 | −14.24 (13) |
| O1—C1—C2—N1 | 20.9 (2) | O4—C6—O3—Co1 | 179.19 (16) |

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|---|---|---|---|
| O2—C1—C2—C10$^{iii}$ | −34.2 (2) | C5—C6—O3—Co1 | −3.1 (2) |
| O1—C1—C2—C10$^{iii}$ | 148.05 (16) | O5—Co1—O3—C6 | 76.97 (13) |
| N1—C3—C4—N2 | −46.74 (19) | N2—Co1—O3—C6 | −18.03 (14) |
| N2—C5—C6—O4 | −152.14 (19) | O1—Co1—O3—C6 | 167.66 (13) |
| C7—C5—C6—O4 | 89.5 (2) | N1—Co1—O3—C6 | −106.76 (14) |
| N2—C5—C6—O3 | 30.1 (2) | O3—C6—O4—Na1$^{iv}$ | 169.60 (14) |
| C7—C5—C6—O3 | −88.3 (2) | C5—C6—O4—Na1$^{iv}$ | −7.9 (4) |
| N2—C5—C7—C8 | −53.7 (2) | O6—C8—O5—Co1 | −177.17 (13) |
| C6—C5—C7—C8 | 63.4 (2) | C7—C8—O5—Co1 | 0.7 (3) |
| C5—C7—C8—O6 | −172.07 (17) | O6—C8—O5—Na1 | −19.22 (17) |
| C5—C7—C8—O5 | 10.0 (3) | C7—C8—O5—Na1 | 158.64 (18) |
| O8—C9—C10—C2$^{iii}$ | −146.6 (2) | O3—Co1—O5—C8 | −64.38 (16) |
| O7—C9—C10—C2$^{iii}$ | 33.4 (2) | N2—Co1—O5—C8 | 21.81 (16) |
| C1—C2—N1—C3 | −150.78 (16) | O7—Co1—O5—C8 | 117.39 (15) |
| C10$^{iii}$—C2—N1—C3 | 83.5 (2) | O1—Co1—O5—C8 | −153.29 (15) |
| C1—C2—N1—Co1 | −30.05 (16) | O3—Co1—O5—Na1 | 159.72 (13) |
| C10$^{iii}$—C2—N1—Co1 | −155.76 (12) | N2—Co1—O5—Na1 | −114.09 (13) |
| C4—C3—N1—C2 | 164.59 (16) | O7—Co1—O5—Na1 | −18.51 (13) |
| C4—C3—N1—Co1 | 43.47 (17) | O1—Co1—O5—Na1 | 70.80 (13) |
| O3—Co1—N1—C2 | −64.06 (11) | O9—Na1—O5—C8 | 112.60 (12) |
| N2—Co1—N1—C2 | −150.24 (12) | O4$^{i}$—Na1—O5—C8 | −161.79 (12) |
| O7—Co1—N1—C2 | 114.30 (11) | O6—Na1—O5—C8 | 11.67 (11) |
| O1—Co1—N1—C2 | 24.94 (11) | O8$^{ii}$—Na1—O5—C8 | 23.07 (14) |
| O3—Co1—N1—C3 | 62.25 (12) | O10—Na1—O5—C8 | −79.65 (12) |
| N2—Co1—N1—C3 | −23.93 (12) | O9—Na1—O5—Co1 | −102.28 (13) |
| O7—Co1—N1—C3 | −119.39 (12) | O4$^{i}$—Na1—O5—Co1 | −16.67 (14) |
| O1—Co1—N1—C3 | 151.24 (12) | O6—Na1—O5—Co1 | 156.79 (15) |
| C6—C5—N2—C4 | 78.7 (2) | O8$^{ii}$—Na1—O5—Co1 | 168.18 (11) |
| C7—C5—N2—C4 | −162.84 (17) | O10—Na1—O5—Co1 | 65.47 (14) |
| C6—C5—N2—Co1 | −40.72 (17) | O5—C8—O6—Na1 | 25.3 (2) |
| C7—C5—N2—Co1 | 77.76 (16) | C7—C8—O6—Na1 | −152.67 (13) |
| C3—C4—N2—C5 | −88.7 (2) | O9—Na1—O6—C8 | −92.30 (14) |
| C3—C4—N2—Co1 | 27.91 (17) | O4$^{i}$—Na1—O6—C8 | −0.8 (2) |
| O5—Co1—N2—C5 | −57.29 (12) | O8$^{ii}$—Na1—O6—C8 | 175.94 (14) |
| O3—Co1—N2—C5 | 32.93 (12) | O10—Na1—O6—C8 | 85.10 (14) |
| O7—Co1—N2—C5 | −149.15 (12) | O5—Na1—O6—C8 | −12.52 (12) |
| N1—Co1—N2—C5 | 121.86 (12) | O8—C9—O7—Co1 | −14.0 (3) |
| O5—Co1—N2—C4 | 178.59 (11) | C10—C9—O7—Co1 | 165.99 (13) |
| O3—Co1—N2—C4 | −91.20 (12) | O5—Co1—O7—C9 | −40.90 (16) |
| O7—Co1—N2—C4 | 86.72 (12) | N2—Co1—O7—C9 | 54.28 (17) |
| O2—C1—O1—Co1 | −178.47 (14) | O1—Co1—O7—C9 | −131.58 (16) |
| C2—C1—O1—Co1 | −0.80 (19) | N1—Co1—O7—C9 | 142.85 (17) |
| O5—Co1—O1—C1 | 165.23 (12) | O7—C9—O8—Na1$^{v}$ | −123.2 (2) |
| O3—Co1—O1—C1 | 74.69 (13) | C10—C9—O8—Na1$^{v}$ | 56.8 (3) |
| O7—Co1—O1—C1 | −103.41 (13) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*···O7$^{iii}$ | 0.84 (2) | 2.21 (2) | 2.830 (2) | 130.6 (18) |
| N2—H2*N*···O6$^{v}$ | 0.82 (2) | 2.16 (2) | 2.809 (2) | 137.0 (18) |
| O9—H91···O11 | 0.84 (2) | 1.92 (2) | 2.741 (2) | 166 (2) |
| O9—H92···O2$^{vi}$ | 0.80 (3) | 2.08 (3) | 2.853 (2) | 162 (3) |
| O10—H101···O8 | 0.83 (2) | 2.18 (3) | 2.972 (2) | 160 (2) |
| O10—H102···O2$^{vii}$ | 0.82 (3) | 2.04 (3) | 2.853 (2) | 175 (3) |
| O11—H111···O1 | 0.79 (3) | 2.26 (3) | 3.004 (2) | 158 (3) |
| O11—H112···O12$^{vi}$ | 0.96 (3) | 1.77 (3) | 2.706 (3) | 164 (2) |
| O12—H121···O1 | 0.77 (3) | 2.05 (3) | 2.793 (2) | 161 (3) |
| O12—H122···O4$^{i}$ | 0.76 (3) | 2.04 (3) | 2.788 (2) | 167 (3) |

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