Synthesis and structure of hexaaquacobalt bis(2-methyl-1H-imidazol-3-ium) tetraaquabis(benzene-1,3,5-tricarboxylato-κO)cobalt

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The title compound, \((\text{C}_4\text{H}_7\text{N}_2)_2[\text{Co(H}_2\text{O})_6][\text{Co(C}_9\text{H}_3\text{O}_6)_2(\text{H}_2\text{O})_4]\) (1), was synthesized from cobalt(II) chloride, 1,3,5-benzene tricarboxylic acid (Hbtc) and 2-methyl-imidazole (H-2mIm) under ambient conditions. The structure of 1 is here reported and compared with the parent complex hexaaquacobalt bis(1H-imidazol-3-iun) tetraaquabis(benzene-1,3,5-tricarboxylato)cobalt (2).

1. Chemical context

Effective bifunctional electrocatalysts for oxygen reduction/evolution reactions (ORR/OER) are indispensable for the development of energy storage and conversion systems, such as fuel cells and rechargeable metal-air batteries (Cai et al., 2017; Wang et al., 2014). Currently, platinum-based materials are considered the most effective due to their superior catalytic activity and stability. However, their high cost, caused by the scarcity of the metal, rules them out for scale-up development. Therefore, a great deal of effort has been devoted to the development of cost-effective and earth-abundant replacements for platinum-based catalysts. Among the different substitute materials, a hexaaquacobalt bis(1H-imidazol-3-iun) tetraaquabis(benzene-1,3,5-tricarboxylato)cobalt complex, 2, has shown excellent bifunctional catalytic activity and durability for both the oxygen-reduction reaction and oxygen-evolution reaction in alkaline media (Wang et al., 2020). Unfortunately, the solvothermal synthesis required to produce the material hinders its implementation on a large scale.

Herein, we present the synthesis and structure of a hexaaquacobalt bis(1H-2-methyl-imidazol-3-iun) tetraaquabis(-
2. Structural commentary

The complete molecule of 1 (Fig. 1) is generated by a crystallographic centre of symmetry. Both Co-containing ions lie about an inversion centre, and therefore only half of the coordinating ions and molecules are crystallographically independent. One of the two metal centres (Co1) is coordinated by six water molecules to constitute a hexaquo-cobalt cation, while the second (Co2) binds with four water molecules and two carboxylate oxygen atoms from two btc^2− ligands to form a [Co(H2O)4(btc)]^{2−} anion. Charge neutrality of the molecule is provided by the presence of two 1-H-2-methyl-imidazol-3-ium cations. The observed Co−O(carboxylate) bond length is 2.0835 (9) Å and the C−Owater bond lengths are in the range 2.0576 (9)−2.1196 (9) Å. To estimate the distortion from the ideal octahedral geometry, the parameters Σ (Halcrow, 2011) and Θ (Marchivie et al., 2005) were calculated using the OctaDist program (Ketkaew et al., 2021). While Σ summarizes the deviation of the cis O−Cu−O angles from 90°, Θ indicates the degree of twist from a perfect octahedron towards a trigonal prism. Both parameters are equal to zero for an ideal octahedron. The calculated values of the distortion parameters Σ/Θ for Co1 and Co2 are equal to 19°/62° and 11°/31°, respectively. Both parameters indicate a slight distortion of the coordination environment of both metal centres.

3. Supramolecular features

A packing diagram of the compound as viewed down [010] is shown in Fig. 2. The figure shows layers parallel to the (111)
plane formed by all ions. Each ion interacts with others via hydrogen bonds of the O–H⋯O or N–H⋯O type. A summary of the hydrogen-bonding interactions is given in Table 1. The table demonstrates that all possible donor and acceptor groups are involved in moderate hydrogen bonds. The presence of various hydrogen bonds in 1 results in characteristic arrays that may be described by graph-set analysis (Etter et al., 1990; Bernstein et al., 1995). In the structure of 1, there are 27 possible motifs involved in discrete D (types a–f and k–l) and intermolecular S (type h) motifs, as well as rings R (types g, i and j) and chains C (types k–f). It is worth noting that while hydrogen bonds b, c and i hold the aforementioned layers together through $C_2^g(20)$ and D arrays, other hydrogen bonds, such as type a and e, form $C_2^e(20)$ arrays, which generates a three-dimensional network with channels along the a and c axes in which the imidazolium ions are located (Fig. 3).

4. Database survey

A search of the Cambridge Structural Database (CSD version 5.41, update of August 2020; Groom et al., 2016) for hexaquacobalt and the ditrimesate tetraaquacobalt moiety revealed only one hit, namely refcode: VUHQIA (imidazolium)$_2$[Co(H$_2$O)$_6$][Co(H$_2$O)$_4$(btc)$_2$], 2, (Wang et al., 2020). Compounds 1 and 2 crystallize in the triclinic system, space group P$ar{T}$. The Co⋯O$_\text{carboxylate}$ and C⋯O$_\text{water}$ bond lengths are similar in both complexes. The coordination polyhedra of compound 2 are slightly more distorted. The calculated values of $\Sigma/\Theta$ for compound 2 are equal to 21°/63° for Co1 and 10°/39° for Co2 – that is, the trigonal distortion ($\Theta$) in 2 is higher by 1° and 8° for Co1 and Co2, respectively. The slightly different distortion of the metal centres in 2 and the introduction of the imidazolium allow for shorter hydrogen bonds with distances between 1.73 and 2.00 Å. Other complexes with a low degree of similarity to the title compound were also found, for example refcodes DOWFUS (Clegg & Holcroft, 2014), IQOZUK (Li et al., 2011) and SETQOX (Wolodkiewicz et al., 1996). However, these compounds are polymeric and/or incorporate a different organic ligand than btc. Additionally, none of them contain the imidazolium anion. These changes in chemical composition may provide them with totally different properties that those desired for ORR and OER, and therefore, they will not be discussed further.

![Figure 3](https://example.com/figure3.png)

**Figure 3**
The three-dimensional supramolecular network with one-dimensional channels along the (a) a and (b) c axes showing O–H⋯O hydrogen bonds of type a and e in the magnified area. Imidazolium ions are drawn in green for clarity.
5. Synthesis and crystallization
In a typical synthesis, H-2mIm (160 mg, 1.96 mmol), Hbtc (412, 1.96 mmol) and cobalt chloride (127 mg, 0.95mmol) were dissolved in 160 ml of a 1:1:1 mixture of deionized water, ethanol and dimethylformamide by stirring for 10 min at room temperature. After 5 minutes, light-pink crystals of 1 were obtained. The product was collected by filtration and washed three times with ethanol.

6. Refinement
Crystal data, data collection and structure refinement details are summarized in Table 2. Positions of remaining non-H atoms were found from the electron density difference maps. The positions of hydrogen atoms were refined with $U_{iso}(H) = 1.5U_{eq}(C$ or $N)$ for CH and NH groups and $U_{iso}(H) = 1.5U_{eq}(C$ or $O)$ for others. The O—H and H···H distances in the water molecules as well as the N—H distances were restrained to be approximately equal within each type (SHELXL instruction SADI). The protons of the methyl group were refined as disordered over two geometrically idealized positions.

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Synthesis and structure of hexaaquacobalt bis(2-methyl-1H-imidazol-3-ium) tetraaquabis(benzene-1,3,5-tricarboxylato-κO)cobalt

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Computing details
Data collection: APEX2 (Bruker, 2016); cell refinement: SAINT (Bruker, 2016); data reduction: SAINT (Bruker, 2016); program(s) used to solve structure: SHELXT2018/2 (Sheldrick, 2018); program(s) used to refine structure: SHELXL2019/2 (Sheldrick, 2015); molecular graphics: OLEX2 (Dolomanov et al., 2009); software used to prepare material for publication: OLEX2 (Dolomanov et al., 2009).

Hexaaquacobalt bis(2-methyl-1H-imidazol-3-ium) tetraaquabis(benzene-1,3,5-tricarboxylato-κO)cobalt

Crystal data
(C4H7N2)2[Co(H2O)6][Co(C9H3O6)2(H2O)4] Z = 1
Mr = 878.48
Triclinic, P̅1
a = 9.2008 (4) Å
b = 9.3137 (4) Å
c = 10.6470 (4) Å
α = 86.551 (2)°
β = 79.378 (2)°
γ = 72.369 (2)°
V = 854.61 (6) Å³

Data collection
Bruker CCD area detector
diffraction; phi and ω scans
Absorption correction: multi-scan
(SADABS; Krause et al., 2015)
Tmin = 0.699, Tmax = 0.746
26203 measured reflections
5250 independent reflections
4605 reflections with I > 2σ(I)
Rint = 0.026
θmax = 30.7°, θmin = 2.0°
h = −13→13
k = −13→12
l = −15→14

Refinement
Refinement on F²
Least-squares matrix: full
R(F² > 2σ(F²)) = 0.026
wR(F²) = 0.069
S = 1.04
5250 reflections
285 parameters
47 restraints
Primary atom site location: difference Fourier map
Secondary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
w = 1/[σ²(Fo²) + (0.0331P)² + 0.4935P]
where P = (Fo² + 2Fe²)/3
(Δ/σ)max < 0.001
Δρmax = 0.60 e Å⁻³
Δρmin = −0.42 e Å⁻³

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Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

| Atom | x       | y       | z       | Uiso (Å²) | Occ. (<1) |
|------|---------|---------|---------|-----------|-----------|
| Co1  | 1.000000| 0.500000| 0.500000| 0.00661 (6)|           |
| Co2  | 1.000000| 0.000000| 1.000000| 0.00734 (6)|           |
| O1   | 1.09226 (11)| -0.04186 (11)| 0.80639 (9)| 0.01446 (19)|       |
| H1A  | 1.128 (2) | -0.1158 (16) | 0.7654 (16) | 0.022*    |           |
| H1B  | 1.0319 (19)| 0.0150 (17) | 0.7699 (17) | 0.022*    |           |
| O2   | 1.06874 (11)| 0.19677 (11)| 0.98183 (10)| 0.01395 (18)|       |
| H2A  | 1.107 (2)  | 0.215 (2)  | 1.0361 (15) | 0.021*    |           |
| H2B  | 1.0153 (19)| 0.2726 (17)| 0.9590 (17) | 0.021*    |           |
| O3   | 0.78549 (10)| 0.12296 (10)| 0.95554 (8) | 0.01077 (17)|       |
| O4   | 0.85774 (10)| 0.18407 (10)| 0.75266 (8) | 0.01246 (18)|       |
| O5   | 0.23219 (10)| 0.29950 (10)| 1.15378 (8) | 0.01007 (16)|       |
| O6   | 0.10354 (10)| 0.53500 (10)| 1.10793 (8) | 0.01151 (17)|       |
| O7   | 0.24698 (10)| 0.69230 (10)| 0.65394 (8) | 0.00982 (16)|       |
| O8   | 0.49974 (10)| 0.65513 (10)| 0.58167 (8) | 0.01243 (18)|       |
| O9   | 0.91967 (10)| 0.31282 (10)| 0.53041 (9) | 0.01031 (17)|       |
| H9A  | 0.898 (2)  | 0.278 (2)  | 0.5975 (12) | 0.015*    |           |
| H9B  | 0.8655 (19)| 0.302 (2)  | 0.4862 (14) | 0.015*    |           |
| O10  | 1.09204 (10)| 0.46619 (10)| 0.67157 (8) | 0.00996 (16)|       |
| H10A | 1.1344 (18)| 0.5265 (17) | 0.6797 (16) | 0.015*    |           |
| H10B | 1.0313 (17)| 0.4689 (19) | 0.7355 (13) | 0.015*    |           |
| O11  | 1.20606 (10)| 0.36656 (11)| 0.40161 (9) | 0.01061 (17)|       |
| H11A | 1.2898 (16)| 0.368 (2)  | 0.4028 (16) | 0.016*    |           |
| H11B | 1.2048 (19)| 0.350 (2)  | 0.3281 (17) | 0.016*    |           |
| N1   | 0.50458 (13)| 0.14060 (12)| 0.61249 (10)| 0.0119 (2) |           |
| H1   | 0.510 (2)  | 0.2077 (18)| 0.5469 (15) | 0.014*    |           |
| N2   | 0.57535 (12)| -0.03974 (12)| 0.74458 (10)| 0.0119 (2) |           |
| H2   | 0.6351 (19)| -0.1208 (18)| 0.7785 (16) | 0.014*    |           |
| C1   | 0.76058 (13)| 0.19797 (13)| 0.85484 (11)| 0.0081 (2) |           |
| C2   | 0.60272 (13)| 0.31087 (13)| 0.85916 (11)| 0.0074 (2) |           |
| C3   | 0.57120 (13)| 0.41453 (13)| 0.76032 (11)| 0.0082 (2) |           |
| H3   | 0.647875  | 0.413232   | 0.689599   | 0.010*    |           |
| C4   | 0.42546 (13)| 0.52015 (13)| 0.76680 (11)| 0.0079 (2) |           |
| C5   | 0.31078 (13)| 0.52211 (13)| 0.87313 (11)| 0.0082 (2) |           |
| H5   | 0.213899  | 0.593210   | 0.878284   | 0.010*    |           |
| C6   | 0.34094 (13)| 0.41785 (13)| 0.97165 (11)| 0.0076 (2) |           |
| C7   | 0.48664 (13)| 0.31248 (13)| 0.96411 (11)| 0.0081 (2) |           |
| H7   | 0.506641  | 0.242605   | 1.029673   | 0.010*    |           |
| C8   | 0.21698 (13)| 0.41903 (13)| 1.08554 (11)| 0.0078 (2) |           |
| C9   | 0.38899 (13)| 0.63054 (13)| 0.65934 (11)| 0.0081 (2) |           |
### Atomic displacement parameters (Å²)

|      | $U^{11}$  | $U^{22}$  | $U^{33}$  | $U^{12}$  | $U^{13}$  | $U^{23}$  |
|------|-----------|-----------|-----------|-----------|-----------|-----------|
| Co1  | 0.00602 (10) | 0.00746 (11) | 0.00589 (10) | −0.00185 (8) | −0.00054 (7) | 0.00102 (7) |
| Co2  | 0.00718 (10) | 0.00685 (11) | 0.00737 (10) | −0.00111 (8) | −0.00184 (7) | 0.00140 (8) |
| O1   | 0.0144 (4)  | 0.0133 (5)  | 0.0109 (4)  | 0.0036 (4)   | −0.0031 (3)  | −0.0002 (3)  |
| O2   | 0.0155 (4)  | 0.0092 (4)  | 0.0193 (5)  | −0.0037 (3)  | −0.0097 (4)  | 0.0036 (3)   |
| O3   | 0.0100 (4)  | 0.0115 (4)  | 0.0088 (4)  | −0.0005 (3)  | −0.0021 (3)  | 0.0035 (3)   |
| O4   | 0.0111 (4)  | 0.0131 (4)  | 0.0089 (4)  | 0.0006 (3)   | 0.0006 (3)   | 0.0002 (3)   |
| O5   | 0.0123 (4)  | 0.0081 (4)  | 0.0085 (4)  | −0.0021 (3)  | −0.0008 (3)  | 0.0027 (3)   |
| O6   | 0.0101 (4)  | 0.0103 (4)  | 0.0105 (4)  | 0.0001 (3)   | 0.0013 (3)   | 0.0021 (3)   |
| O7   | 0.0078 (4)  | 0.0110 (4)  | 0.0099 (4)  | −0.0013 (3)  | −0.0029 (3)  | 0.0019 (3)   |
| O8   | 0.0091 (4)  | 0.0151 (4)  | 0.0116 (4)  | −0.0030 (3)  | −0.0012 (3)  | 0.0066 (3)   |
| O9   | 0.0123 (4)  | 0.0129 (4)  | 0.0077 (4)  | −0.0067 (3)  | −0.0029 (3)  | 0.0038 (3)   |
| O10  | 0.0089 (4)  | 0.0138 (4)  | 0.0077 (4)  | −0.0047 (3)  | −0.0011 (3)  | 0.0016 (3)   |
| O11  | 0.0077 (4)  | 0.0144 (4)  | 0.0092 (4)  | −0.0028 (3)  | −0.0006 (3)  | −0.0009 (3)  |
| N1   | 0.0147 (5)  | 0.0096 (5)  | 0.0111 (5)  | −0.0029 (4)  | −0.0036 (4)  | 0.0030 (4)   |
| N2   | 0.0116 (5)  | 0.0096 (5)  | 0.0127 (5)  | −0.0012 (4)  | −0.0017 (4)  | 0.0031 (4)   |
| C1   | 0.0081 (5)  | 0.0075 (5)  | 0.0086 (5)  | −0.0020 (4)  | −0.0021 (4)  | 0.0009 (4)   |
| C2   | 0.0073 (5)  | 0.0067 (5)  | 0.0080 (5)  | −0.0016 (4)  | −0.0021 (4)  | 0.0004 (4)   |
| C3   | 0.0082 (5)  | 0.0083 (5)  | 0.0079 (5)  | −0.0026 (4)  | −0.0014 (4)  | 0.0011 (4)   |
| C4   | 0.0089 (5)  | 0.0084 (5)  | 0.0068 (5)  | −0.0033 (4)  | −0.0020 (4)  | 0.0018 (4)   |
| C5   | 0.0081 (5)  | 0.0082 (5)  | 0.0082 (5)  | −0.0022 (4)  | −0.0018 (4)  | 0.0005 (4)   |
| C6   | 0.0084 (5)  | 0.0079 (5)  | 0.0066 (5)  | −0.0028 (4)  | −0.0010 (4)  | 0.0007 (4)   |
| C7   | 0.0095 (5)  | 0.0073 (5)  | 0.0074 (5)  | −0.0022 (4)  | −0.0024 (4)  | 0.0014 (4)   |
| C8   | 0.0086 (5)  | 0.0094 (5)  | 0.0067 (5)  | −0.0039 (4)  | −0.0027 (4)  | 0.0005 (4)   |
| C9   | 0.0099 (5)  | 0.0072 (5)  | 0.0077 (5)  | −0.0025 (4)  | −0.0026 (4)  | 0.0003 (4)   |
| C10  | 0.0121 (5)  | 0.0126 (6)  | 0.0171 (6)  | −0.0020 (4)  | −0.0028 (4)  | 0.0015 (5)   |
| C11  | 0.0123 (5)  | 0.0136 (6)  | 0.0134 (6)  | −0.0030 (5)  | 0.0000 (4)   | 0.0017 (4)   |
| C12  | 0.0140 (5)  | 0.0082 (5)  | 0.0113 (5)  | −0.0042 (4)  | −0.0022 (4)  | 0.0005 (4)   |
| C13  | 0.0148 (6)  | 0.0137 (6)  | 0.0168 (6)  | −0.0046 (5)  | 0.0023 (5)   | −0.0015 (5)  |
Geometric parameters (Å, °)

| Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|-----------------------|--------------|-----------------------|--------------|
| Co1—O11               | 2.0576 (9)   | N1—C12                | 1.3289 (16)  |
| Co1—O11^i             | 2.0576 (9)   | N1—C10                | 1.3854 (16)  |
| Co1—O9^i              | 2.0772 (9)   | N1—H1                 | 0.913 (15)   |
| Co1—O9                | 2.0772 (9)   | N2—C12                | 1.3375 (15)  |
| Co1—O10               | 2.1196 (9)   | N2—C11                | 1.3832 (16)  |
| Co1—O10^i             | 2.1196 (9)   | N2—H2                 | 0.890 (15)   |
| Co2—O3^ii             | 2.0835 (9)   | C1—C2                 | 1.5078 (16)  |
| Co2—O3                | 2.0835 (9)   | C2—C7                 | 1.3934 (15)  |
| Co2—O1^ii             | 2.0912 (9)   | C2—C3                 | 1.3944 (16)  |
| Co2—O1                | 2.0912 (9)   | C3—C4                 | 1.3948 (16)  |
| Co2—O2^ii             | 2.1000 (9)   | C3—H3                 | 0.9300       |
| Co2—O2                | 2.1000 (9)   | C4—C5                 | 1.3949 (15)  |
| O1—H1A                | 0.787 (12)   | C4—C9                 | 1.5066 (16)  |
| O1—H1B                | 0.785 (12)   | C5—C6                 | 1.3934 (15)  |
| O2—H2A                | 0.778 (12)   | C5—H5                 | 0.9300       |
| O2—H2B                | 0.783 (12)   | C6—C7                 | 1.3926 (16)  |
| O3—C1                 | 1.2624 (14)  | C6—C8                 | 1.5019 (15)  |
| O4—C1                 | 1.2601 (14)  | C7—H7                 | 0.9300       |
| O5—C8                 | 1.2777 (14)  | C10—C11               | 1.3537 (17)  |
| O6—C8                 | 1.2526 (15)  | C10—H10               | 0.9300       |
| O7—C9                 | 1.2687 (14)  | C11—H11               | 0.9300       |
| O8—C9                 | 1.2580 (14)  | C12—C13               | 1.4818 (17)  |
| O9—H9A                | 0.785 (12)   | C13—H13A              | 0.9600       |
| O9—H9B                | 0.775 (12)   | C13—H13B              | 0.9600       |
| O10—H10A              | 0.791 (12)   | C13—H13C              | 0.9600       |
| O10—H10B              | 0.793 (12)   | C13—H13D              | 0.9600       |
| O11—H11A              | 0.778 (12)   | C13—H13E              | 0.9600       |
| O11—H11B              | 0.809 (17)   | C13—H13F              | 0.9600       |
| O11—Co1—O11^i         | 180.0        | C7—C2—C3              | 119.40 (10)  |
| O11—Co1—O9^i          | 90.60 (4)    | C7—C2—C1              | 119.49 (10)  |
| O11^i—Co1—O9^i        | 89.40 (4)    | C3—C2—C1              | 121.11 (10)  |
| O11—Co1—O9            | 89.40 (4)    | C2—C3—C4              | 120.45 (10)  |
| O11^i—Co1—O9          | 90.60 (4)    | C2—C3—H3              | 119.8        |
| O9^i—Co1—O9           | 180.0        | C4—C3—H3              | 119.8        |
| O11—Co1—O10           | 90.76 (4)    | C3—C4—C5              | 119.66 (10)  |
| O11^i—Co1—O10         | 89.24 (4)    | C3—C4—C9              | 120.93 (10)  |
| O9^i—Co1—O10          | 86.64 (3)    | C5—C4—C9              | 119.40 (10)  |
| O9—Co1—O10            | 93.36 (4)    | C6—C5—C4              | 120.20 (11)  |
| O11—Co1—O10^i         | 89.24 (4)    | C6—C5—H5              | 119.9        |
| O11^i—Co1—O10^i       | 90.76 (4)    | C4—C5—H5              | 119.9        |
| O9^i—Co1—O10^i        | 93.36 (3)    | C7—C6—C5              | 119.71 (10)  |
| O9—Co1—O10^i          | 86.64 (4)    | C7—C6—C8              | 120.09 (10)  |
| O10—Co1—O10^i         | 180.0        | C5—C6—C8              | 120.19 (10)  |
| O3^ii—Co2—O3          | 180.00 (5)   | C6—C7—C2              | 120.56 (10)  |
| O3^ii—Co2—O1^ii       | 90.97 (4)    | C6—C7—H7              | 119.7        |
O3—Co2—O1 89.03 (4)  C2—C7—H7 119.7
O3—Co2—O1 89.03 (4)  O6—C8—O5 123.36 (11)
O3—Co2—O1 90.97 (4)  O6—C8—C6 118.94 (10)
O1—Co2—O1 180.0  O5—C8—C6 117.70 (10)
O3—Co2—O2 89.79 (4)  O8—C9—O7 124.60 (11)
O3—Co2—O2 90.21 (4)  O8—C9—C4 118.45 (10)
O1—Co2—O2 89.38 (4)  O7—C9—C4 116.95 (10)
O1—Co2—O2 91.62 (4)  C11—C10—N1 106.62 (11)
O3—Co2—O2 90.21 (4)  C11—C10—H10 126.7
O3—Co2—O2 89.79 (4)  N1—C10—H10 126.7
O1—Co2—O2 91.62 (4)  C10—C11—N2 106.72 (11)
O1—Co2—O2 88.38 (4)  C10—C11—H11 126.6
O2—Co2—O2 180.0  N2—C11—H11 126.6
Co2—O1—H1A 133.6 (14)  N1—C12—N2 107.33 (11)
Co2—O1—H1B 104.8 (13)  N1—C12—C13 125.58 (11)
H1A—O1—H1B 107.5 (16)  N2—C12—C13 127.07 (11)
Co2—O2—H2A 117.6 (14)  C12—C13—H13A 109.5
Co2—O2—H2B 121.0 (13)  C12—C13—H13B 109.5
H2A—O2—H2B 108.3 (16)  H13A—C13—H13B 109.5
C1—O3—Co2 126.90 (8)  C12—C13—H13C 109.5
Co1—O9—H9A 125.1 (13)  H13A—C13—H13D 109.5
Co1—O9—H9B 117.8 (13)  H13C—C13—H13E 35.5
H9A—O9—H9B 108.5 (16)  H13D—C13—H13E 135.3
Co1—O10—H10A 111.8 (12)  H13A—C13—H13D 135.3
Co1—O10—H10B 115.7 (13)  H13B—C13—H13E 76.7
H10A—O10—H10B 106.0 (15)  H13C—C13—H13D 35.5
Co1—O11—H11A 128.6 (13)  C12—C13—H13E 109.5
Co1—O11—H11B 114.9 (12)  H13A—C13—H13E 35.5
H11A—O11—H11B 105.6 (16)  H13B—C13—H13E 135.3
C12—N1—C10 109.77 (10)  H13C—C13—H13E 76.7
C12—N1—H1 124.4 (11)  H13D—C13—H13E 109.5
C10—N1—H1 125.7 (11)  C12—C13—H13F 109.5
C12—N2—C11 109.55 (11)  H13A—C13—H13F 76.7
C12—N2—H2 123.4 (11)  H13B—C13—H13F 35.5
C11—N2—H2 127.0 (11)  H13C—C13—H13F 135.3
O4—C1—O3 124.51 (11)  H13D—C13—H13F 109.5
O4—C1—C2 118.73 (10)  H13E—C13—H13F 109.5
O3—C1—C2 116.76 (10)  H13F—C13—H13E 109.5
Co2—O3—C1—O4 16.76 (18)  C1—C2—C7—C6 178.56 (11)
Co2—O3—C1—C2 −163.49 (8)  C7—C6—C8—O6 161.30 (11)
O4—C1—C2—C7 170.61 (11)  C5—C6—C8—O6 −18.68 (17)
O3—C1—C2—C7 −9.15 (17)  C7—C6—C8—O5 −19.76 (17)
O4—C1—C2—C3 −9.89 (17)  C5—C6—C8—O5 160.27 (11)
O3—C1—C2—C3 170.35 (11)  C3—C4—C9—O8 −19.45 (17)
C7—C2—C3—C4 0.72 (18)  C5—C4—C9—O8 161.70 (11)
C1—C2—C3—C4 −178.78 (11)  C3—C4—C9—O7 160.47 (11)
C2—C3—C4—C5 0.16 (18)  C5—C4—C9—O7 −18.38 (17)
C2—C3—C4—C9  -178.68 (11)  C12—N1—C10—C11  -0.03 (15)
C3—C4—C5—C6  -0.83 (18)  N1—C10—C11—C12  0.19 (15)
C9—C4—C5—C6  178.03 (11)  C12—N2—C11—C10  -0.29 (15)
C4—C5—C6—C7  0.61 (18)  C10—N1—C12—N2  -0.15 (15)
C4—C5—C6—C8  -179.42 (11)  C10—N1—C12—C13  178.19 (12)
C5—C6—C7—C2  0.29 (18)  C11—N2—C12—C13  0.27 (15)
C8—C6—C7—C2  -179.69 (11)  C11—N2—C12—N1  -0.27 (15)
C3—C2—C7—C6  -0.95 (18)

Symmetry codes: (i) −x+2, −y+1, −z+1; (ii) −x+2, −y, −z+2.

Hydrogen-bond geometry (Å, °)

| D—H···A     | D—H   | H···A   | D···A     | D—H···A |
|------------|-------|--------|-----------|--------|
| O1—H1A···O7^iii | 0.79 (1) | 2.10 (1) | 2.8789 (13) | 174 (2) |
| O1—H1B···O4   | 0.79 (1) | 1.90 (1) | 2.6401 (13) | 156 (2) |
| O2—H2A···O5^iv | 0.78 (1) | 2.17 (1) | 2.9371 (13) | 167 (2) |
| O2—H2B···O6^v | 0.78 (1) | 1.97 (1) | 2.7458 (13) | 175 (2) |
| O9—H9A···O4   | 0.79 (1) | 1.85 (1) | 2.6339 (12) | 176 (2) |
| O9—H9B···O7^vi | 0.78 (1) | 1.96 (1) | 2.7150 (13) | 166 (2) |
| O10—H10A···O7^iv | 0.79 (1) | 2.09 (1) | 2.8592 (13) | 166 (2) |
| O10—H10B···O6^v | 0.79 (1) | 1.89 (1) | 2.6835 (12) | 176 (2) |
| O11—H11A···O8^i | 0.78 (1) | 1.92 (1) | 2.6911 (13) | 172 (2) |
| O11—H11B···O5^vii | 0.81 (2) | 1.90 (2) | 2.6989 (13) | 172 (2) |
| N1—H1···O8^vii | 0.91 (2) | 1.81 (2) | 2.7214 (13) | 175 (2) |
| N2—H2···O5^viii | 0.89 (2) | 1.93 (2) | 2.8206 (14) | 178 (2) |

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