

X-Ray Crystallography

In crystals of complexes **2** and **3** two kinds of compounds with a slightly different formula were observed, $[\text{Co}^{\text{II}}_7\text{L}_9(\text{OH})_2(\text{OAc})_3(\text{H}_2\text{O})]\cdot 4.6\text{MeOH}\cdot 3.6\text{H}_2\text{O}$ and $[\text{Co}^{\text{II}}_7\text{L}_9(\text{OH})_2(\text{OAc})_2(\text{MeO})(\text{H}_2\text{O})]\cdot 4.6\text{MeOH}\cdot 3.6\text{H}_2\text{O}$ for **2**; $[\text{Co}^{\text{II}}_{10}\text{L}_{14}(\text{OH})_4](\text{ClO}_4)_2\cdot 8.5\text{MeOH}\cdot 5.75\text{H}_2\text{O}$ and $[\text{Co}^{\text{II}}_{10}\text{L}_{14}(\text{OH})_3(\text{MeO})](\text{ClO}_4)_2\cdot 8.5\text{MeOH}\cdot 5.75\text{H}_2\text{O}$ for **3**. Because the metallic core remains exactly the same for both components in clusters **2** and **3**, only the major complex is described.

In a case of complex **7** two kinds of crystals with different amount of solvent molecules were obtained. For the clarity only the crystal $7\cdot 6.8\text{MeOH}\cdot 7\text{H}_2\text{O}$ is discussed in this paper.

During final cycle of refining of crystal **3** high ($1.5\text{ e}/\text{\AA}^3$) residual electron density was found around $3\text{ \AA}$ from Co1, Co3 and Co10. Therefore another model of the structure was introduced in which additional Co atom was added. In such case it was assumed that there were two complexes in crystal structure occupying same position one containing 10 Co atoms (95%) and another one with 11 Co atoms (5%). In a discussion only model with 10 cobalt atoms was used, but CIFs for the two models have been deposited at the CCDC.

Table S1. Crystallographic data for complexes **1-7**.

[illegible]

$D_c/\text{g cm}^{-3}$	1.577	1.502	1.478	1.461	1.528	1.420	1.504	1.560
$\mu(\text{Mo-K}\alpha)/\text{mm}^{-1}$	1.11	0.92	0.88	0.90	0.76	0.71	0.90	1.00
Meas./indep. (R_{int}) refl.	9952 / 4711 (0.069)	63201 / 26415 (0.230)	87729 / 41142 (0.077)	22089 / 7338 (0.331)	21768 / 6826 (0.045)	45060 / 18761 (0.058)	42673 / 21724 (0.055)	36057 / 17925 (0.066)
Obs. refl. [$I > 2\sigma(I)$]	2431	5745	19457	2145	4882	10712	9693	6864
$wR2$ (all data) ^c	0.168	0.085	0.3258	0.231	0.085	0.208	0.179	0.121
$R1$ (obs. data) ^d	0.080	0.062	0.101	0.120	0.039	0.078	0.070	0.065
Goodness of fit on F^2	1.02	0.690	1.05	1.00	1.00	1.02	1.04	1.02
$\Delta\rho_{\text{max,min}}/\text{e}\text{\AA}^{-3}$	0.60, -0.45	0.50, -0.53	1.57, -0.74	0.58, -0.61	0.51, -0.33	0.85, -0.70	0.94, -0.79	0.68, -0.46

^a Including solvate molecules. ^b Mo-K α radiation, graphite monochromator. ^c $wR2 = \{\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]\}^{1/2}$. ^d $R1 = \sum||F_o| - |F_c|| / \sum|F_o|$.

Table S2. Selected bond distances (Å) and angles (°) for **1**·0.5MeOH·0.2H₂O

Co1—O	1.8648 (14)	Co1—O1 ⁱ	1.983 (3)
Co1—O3 ⁱ	1.886 (11)	Co1—N1	1.987 (3)
Co1—O2	1.963 (8)	Co1—N2	2.106 (4)
O—Co1—O3 ⁱ	90.3 (4)	O2—Co1—O1 ⁱ	179.3 (3)
O—Co1—O2	87.5 (3)	O—Co1—N1	87.84 (14)
O3 ⁱ —Co1—O2	85.8 (6)	O3 ⁱ —Co1—N1	176.2 (5)
O—Co1—N2	169.29 (17)	O2—Co1—N1	90.9 (4)
O3 ⁱ —Co1—N2	99.7 (4)	O1 ⁱ —Co1—N1	88.84 (13)
O2—Co1—N2	97.2 (3)	O1 ⁱ —Co1—N2	83.48(12)
O—Co1—O1 ⁱ	91.83 (14)	N1—Co1—N2	82.46(14)
O3 ⁱ —Co1—O1 ⁱ	94.5 (5)		

Symmetry codes: (i) $-y+1, x-y+1, z$; (ii) $-x+y, -x+1, z$.

Table S3. Selected bond distances (Å) and angles (°) for **2**·4.6MeOH·3.6 H₂O

Co1—O1	2.034 (4)	Co4—O15	2.083 (14)
Co1—O2	2.037 (5)	Co4—O1	2.101 (4)
Co1—N16	2.155 (6)	Co4—N24	2.283 (6)
Co1—N19	2.197 (7)	Co5—O18	2.004 (5)
Co1—O11	2.198 (5)	Co5—O1	2.036 (4)
Co1—O14	2.247 (5)	Co5—N1K	2.069 (8)
Co2—O2	2.039 (4)	Co5—O15	2.089 (12)
Co2—O13	2.043 (5)	Co5—O2B	2.090 (5)
Co2—O1A	2.056 (6)	Co5—N25	2.223 (6)
Co2—N11	2.107 (7)	Co5—O16	2.244 (5)
Co2—O3	2.166 (5)	Co6—O19	2.057 (5)
Co2—N21	2.198 (6)	Co6—O16	2.071 (4)
Co3—O14	2.027 (5)	Co6—N17	2.132 (7)
Co3—O11	2.113 (5)	Co6—N18	2.138 (6)
Co3—N12	2.143 (7)	Co6—N28	2.240 (6)
Co3—N13	2.153 (7)	Co6—N27	2.258 (7)
Co3—N22	2.241 (6)	Co7—O17	2.026 (6)
Co3—N23	2.255 (6)	Co7—O2	2.053 (4)
Co4—O1B	2.019 (5)	Co7—O3	2.229 (5)
Co4—O1K	2.038 (11)	Co7—O1C	2.081 (5)
Co4—O12	2.066 (5)	Co7—O2A	2.082 (7)
Co4—N14	2.083 (6)	Co7—O19	2.110 (5)
O1—Co1—O2	179.21 (18)	N14—Co4—O1	89.3 (2)
O1—Co1—N16	87.8 (2)	O15—Co4—O1	75.0 (3)
O2—Co1—N16	92.7 (2)	O1B—Co4—N24	94.1 (2)
O1—Co1—N19	92.1 (2)	O1K—Co4—N24	74.2 (3)
O2—Co1—N19	87.3 (2)	O12—Co4—N24	106.33 (18)
N16—Co1—N19	93.5 (2)	N14—Co4—N24	79.3 (3)
O1—Co1—O11	91.06 (19)	O15—Co4—N24	88.5 (4)
O2—Co1—O11	88.40 (19)	O1—Co4—N24	158.25 (18)
N16—Co1—O11	174.9 (2)	O18—Co5—O1	110.67 (19)
N19—Co1—O11	91.5 (2)	O18—Co5—N1K	145.6 (3)
O1—Co1—O14	89.83 (17)	O1—Co5—N1K	102.0 (3)
O2—Co1—O14	90.66 (19)	O18—Co5—O15	170.5 (4)

N16—Co1—O14	94.4 (2)	O1—Co5—O15	76.3 (4)
N19—Co1—O14	171.9 (2)	O18—Co5—O2B	89.7 (2)
O11—Co1—O14	80.60 (17)	O1—Co5—O2B	91.86 (18)
O2—Co2—O13	99.2 (2)	N1K—Co5—O2B	99.8 (3)
O2—Co2—O1A	101.0 (2)	O15—Co5—O2B	96.7 (3)
O13—Co2—O1A	85.2 (2)	O18—Co5—N25	94.3 (3)
O2—Co2—N11	85.1 (2)	O1—Co5—N25	155.0 (2)
O13—Co2—N11	93.6 (2)	O15—Co5—N25	78.9 (5)
O1A—Co2—N11	173.9 (3)	O2B—Co5—N25	88.5 (3)
O2—Co2—O3	81.53 (18)	O18—Co5—O16	88.59 (19)
O13—Co2—O3	173.3 (2)	O1—Co5—O16	86.18 (18)
O1A—Co2—O3	88.1 (2)	N1K—Co5—O16	83.2 (3)
N11—Co2—O3	93.0 (2)	O15—Co5—O16	85.3 (3)
O2—Co2—N21	158.5 (2)	O2B—Co5—O16	176.73 (18)
O13—Co2—N21	95.5 (2)	N25—Co5—O16	94.4 (3)
O1A—Co2—N21	95.7 (3)	O19—Co6—O16	96.11 (19)
N11—Co2—N21	78.4 (3)	O19—Co6—N17	84.9 (3)
O3—Co2—N21	85.7 (2)	O16—Co6—N17	94.7 (2)
O14—Co3—O11	87.96 (18)	O19—Co6—N18	93.9 (2)
O14—Co3—N12	100.8 (2)	O16—Co6—N18	84.2 (2)
O11—Co3—N12	86.4 (2)	N17—Co6—N18	178.3 (3)
O14—Co3—N13	87.5 (2)	O19—Co6—N28	89.6 (2)
O11—Co3—N13	102.1 (3)	O16—Co6—N28	164.1 (2)
N12—Co3—N13	168.3 (3)	N17—Co6—N28	100.6 (3)
O14—Co3—N22	176.8 (2)	N18—Co6—N28	80.7 (3)
O11—Co3—N22	90.2 (2)	O19—Co6—N27	162.3 (2)
N12—Co3—N22	81.6 (3)	O16—Co6—N27	95.5 (2)
N13—Co3—N22	90.3 (3)	N17—Co6—N27	80.9 (3)
O14—Co3—N23	89.7 (2)	N18—Co6—N27	100.5 (3)
O11—Co3—N23	176.7 (2)	N28—Co6—N27	82.8 (2)
N12—Co3—N23	91.8 (3)	O17—Co7—O2	104.2 (2)
N13—Co3—N23	80.1 (3)	O17—Co7—O1C	90.4 (2)
N22—Co3—N23	92.2 (2)	O2—Co7—O1C	165.3 (2)
O1B—Co4—O1K	97.6 (3)	O17—Co7—O2A	83.3 (3)
O1B—Co4—O12	85.4 (2)	O2—Co7—O2A	92.8 (2)
O1K—Co4—O12	176.9 (3)	O1C—Co7—O2A	89.2 (3)
O1B—Co4—N14	172.4 (2)	O17—Co7—O19	92.0 (2)

O1K—Co4—N14	84.4 (3)	O2—Co7—O19	89.76 (19)
O12—Co4—N14	92.7 (2)	O1C—Co7—O19	89.4 (2)
O1B—Co4—O15	84.2 (4)	O2A—Co7—O19	175.1 (2)
O12—Co4—O15	162.5 (4)	O17—Co7—O3	172.9 (2)
N14—Co4—O15	99.4 (4)	O2—Co7—O3	79.71 (18)
O1B—Co4—O1	98.12 (19)	O1C—Co7—O3	85.7 (2)
O1K—Co4—O1	86.4 (3)	O2A—Co7—O3	90.7 (2)
O12—Co4—O1	92.60 (17)	O19—Co7—O3	93.9 (2)

Table S4. Selected bond distances (Å) and angles (°) for **3**·8.5MeOH· 5.75H₂O

Co1—O1A	2.075 (5)	Co3—O1A	2.178 (6)
Co1—O1C	2.100 (5)	Co3—N3O	2.218 (7)
Co1—O1B	2.107 (5)	Co3—N3E	2.279 (9)
Co1—O1	2.125 (5)	Co4—O1M	1.943 (6)
Co1—O1D	2.172 (6)	Co4—N1H	2.114 (7)
Co1—O1E	2.179 (7)	Co4—N1A	2.128 (7)
Co2—O3	2.051 (5)	Co4—O1B	2.187 (5)
Co2—O1	2.057 (5)	Co4—N3H	2.301 (7)
Co2—O1G	2.103 (6)	Co4—N3A	2.377 (7)
Co2—N1C	2.118 (6)	Co5—O1M	1.942 (6)
Co2—O2	2.121 (6)	Co5—O1	2.035 (5)
Co2—O1F	2.226 (5)	Co5—O2	2.045 (5)
Co3—O1H	1.997 (6)	Co5—O1I	2.127 (7)
Co3—N1E	2.031 (9)	Co5—N1B	2.144 (6)
Co3—N1O	2.081 (8)	Co6—O2	2.021 (5)
Co6—N3I	2.424 (9)	Co6—N1I	2.041 (9)
Co7—O1K	1.925 (6)	Co6—N1J	2.119 (7)
Co7—O1J	2.008 (7)	Co6—N3J	2.188 (8)
Co7—O1F	2.024 (6)	Co6—O1F	2.252 (6)

Co7—N3F	2.084 (7)	Co10—O1O	1.983 (7)
Co7—O3	2.095 (5)	Co10—N1N	2.067 (8)
Co8—O1L	1.963 (7)	Co10—O1D	2.071 (5)
Co8—O3	1.980 (5)	Co10—N3D	2.192 (7)
Co8—N1K	2.056 (8)	Co10—N3N	2.294 (7)
Co8—N3L	2.078 (8)	Co10—O1E	2.324 (8)
Co9—O1N	1.997 (7)		

O1A—Co1—O1C	171.6 (2)	O1M—Co5—N1B	82.1 (2)
O1A—Co1—O1B	90.0 (2)	O1—Co5—N1B	88.0 (2)
O1C—Co1—O1B	97.9 (2)	O2—Co5—N1B	100.9 (2)
O1A—Co1—O1	92.2 (2)	O1I—Co5—N1B	163.2 (3)
O1C—Co1—O1	85.3 (2)	O2—Co6—N1I	93.9 (3)
O1B—Co1—O1	87.83 (19)	O2—Co6—N1J	102.9 (2)
O1A—Co1—O1D	92.7 (2)	N1I—Co6—N1J	162.7 (3)
O1C—Co1—O1D	79.9 (2)	O2—Co6—N3J	96.4 (2)
O1B—Co1—O1D	171.26 (19)	N1I—Co6—N3J	102.4 (3)
O1—Co1—O1D	100.36 (19)	N1J—Co6—N3	80.3 (3)
O1A—Co1—O1E	88.5 (3)	O2—Co6—O1F	79.9 (2)
O1C—Co1—O1E	93.9 (3)	N1I—Co6—O1F	87.5 (3)
O1B—Co1—O1E	93.3 (2)	N1J—Co6—O1F	91.1 (3)
O1—Co1—O1E	178.6 (3)	N3J—Co6—O1F	169.7 (2)
O1D—Co1—O1E	78.5 (2)	O2—Co6—N3I	167.0 (3)
O3—Co2—O1	172.4 (2)	N1I—Co6—N3I	76.8 (4)
O3—Co2—O1G	79.9 (2)	N1J—Co6—N3I	85.9 (3)
O1—Co2—O1G	96.5 (2)	N3J—Co6—N3I	94.5 (3)
O3—Co2—N1C	96.8 (2)	O1F—Co6—N3I	90.5 (2)
O1—Co2—N1C	89.5 (2)	O1K—Co7—O1J	119.5 (3)
O1G—Co2—N1C	85.7 (2)	O1K—Co7—O1F	133.8 (3)
O3—Co2—O2	98.6 (2)	O1J—Co7—O1F	106.4 (3)
O1—Co2—O2	84.6 (2)	O1K—Co7—N3F	86.8 (3)
O1G—Co2—O2	176.4 (2)	O1J—Co7—N3F	98.9 (3)
N1C—Co2—O2	97.7 (2)	O1F—Co7—N3F	91.1 (3)
O3—Co2—O1F	78.4 (2)	O1K—Co7—O3	93.9 (2)
O1—Co2—O1F	95.6 (2)	O1J—Co7—O3	88.4 (2)
O1G—Co2—O1F	98.1 (2)	O1F—Co7—O3	82.1 (2)
N1C—Co2—O1F	173.2 (2)	N3F—Co7—O3	171.3 (3)
O2—Co2—O1F	78.5 (2)	O1L—Co8—O3	117.8 (2)

O1H—Co3—N1E	93.1 (4)	O1L—Co8—N1K	138.5 (3)
O1H—Co3—N1O	170.2 (3)	O3—Co8—N1K	96.3 (3)
N1E—Co3—N1O	93.9 (4)	O1L—Co8—N3L	95.4 (3)
O1H—Co3—O1A	102.5 (2)	O3—Co8—N3L	94.6 (3)
N1E—Co3—O1A	86.7 (4)	N1K—Co8—N3L	105.4 (3)
N1O—Co3—O1A	84.7 (3)	O1N—Co9—O1G	170.0 (3)
O1H—Co3—N3O	92.2 (3)	O1N—Co9—O1C	85.2 (3)
N1E—Co3—N3O	174.1 (4)	O1G—Co9—O1C	86.9 (2)
N1O—Co3—N3O	80.5 (3)	O1N—Co9—O1L	97.1 (3)
O1A—Co3—N3O	94.6 (2)	O1G—Co9—O1L	77.3 (2)
O1H—Co3—N3E	79.2 (3)	O1C—Co9—O1L	93.1 (2)
N1E—Co3—N3E	80.0 (4)	O1N—Co9—N3G	101.8 (3)
N1O—Co3—N3E	95.3 (3)	O1G—Co9—N3G	86.6 (2)
O1A—Co3—N3E	166.7 (3)	O1C—Co9—N3G	171.8 (2)
N3O—Co3—N3E	98.5 (3)	O1L—Co9—N3G	90.3 (3)
O1M—Co4—N1H	169.6 (3)	O1N—Co9—O1D	91.7 (3)
O1M—Co4—N1A	100.8 (2)	O1G—Co9—O1D	92.6 (2)
N1H—Co4—N1A	89.5 (3)	O1C—Co9—O1D	77.9 (2)
O1M—Co4—O1B	88.8 (2)	O1L—Co9—O1D	166.9 (2)
N1H—Co4—O1B	93.0 (2)	N3G—Co9—O1D	97.4 (2)
N1A—Co4—O1B	83.8 (2)	O1O—Co10—N1N	172.0 (3)
O1M—Co4—N3H	90.9 (3)	O1O—Co10—O1D	98.1 (3)
N1H—Co4—N3H	78.8 (3)	N1N—Co10—O1D	89.2 (3)
N1A—Co4—N3H	167.7 (3)	O1O—Co10—N3D	78.2 (3)
O1B—Co4—N3H	93.0 (2)	N1N—Co10—N3D	99.1 (3)
O1M—Co4—N3A	84.4 (2)	O1D—Co10—N3D	87.0 (2)
N1H—Co4—N3A	97.7 (3)	O1O—Co10—N3N	94.6 (3)
N1A—Co4—N3A	75.9 (3)	N1N—Co10—N3N	78.8 (3)
O1B—Co4—N3A	156.9 (2)	O1D—Co10—N3N	163.7 (3)
N3H—Co4—N3A	109.1 (3)	N3D—Co10—N3N	105.6 (3)
O1M—Co5—O1	125.1 (2)	O1O—Co10—O1E	104.9 (3)
O1M—Co5—O2	147.8 (2)	N1N—Co10—O1E	79.8 (3)
O1—Co5—O2	87.2 (2)	O1D—Co10—O1E	77.3 (2)
O1M—Co5—O1I	81.3 (3)	N3D—Co10—O1E	164.3 (3)
O1—Co5—O1I	99.3 (2)	N3N—Co10—O1E	89.6 (3)
O2—Co5—O1I	94.6 (3)		

Table S5. Selected bond distances (Å) and angles (°) for **4**·MeOH·H₂O

Co1—O23	2.053 (8)	Co2—O14	1.983 (8)
Co1—O1M	2.055 (8)	Co2—O13	2.065 (8)
Co1—O12	2.058 (7)	Co2—O11	2.064 (7)
Co1—O11	2.133 (8)	Co2—N12 ⁱ	2.153 (10)
Co1—N11	2.185 (10)	Co2—N32 ⁱ	2.240 (10)
Co1—N31	2.246 (9)	Co2—O12	2.244 (8)
O23—Co1—O1M	93.5 (3)	O14—Co2—O13	97.7 (4)
O23—Co1—O12	85.4 (3)	O14—Co2—O11	92.7 (3)
O1M—Co1—O12	88.8 (3)	O13—Co2—O11	87.7 (3)
O23—Co1—O11	88.8 (3)	O14—Co2—N12 ⁱ	100.5 (4)
O1M—Co1—O11	171.8 (3)	O13—Co2—N12 ⁱ	158.5 (4)
O23—Co1—N31	95.1 (3)	O11—Co2—N12 ⁱ	102.5 (4)
O1M—Co1—N31	91.3 (3)	O14—Co2—N32 ⁱ	85.6 (4)
O12—Co1—N31	179.4 (4)	O13—Co2—N32 ⁱ	91.1 (3)
O11—Co1—N31	96.4 (3)	O11—Co2—N32 ⁱ	177.8 (4)
N11—Co1—N31	77.9 (4)	N12 ⁱ —Co2—N32 ⁱ	79.3 (4)
O12—Co1—O11	83.5 (3)	O14—Co2—O12	173.2 (3)
O23—Co1—N11	172.5 (4)	O13—Co2—O12	83.4 (3)
O1M—Co1—N11	89.3 (4)	O11—Co2—O12	80.7 (3)
O12—Co1—N11	101.6 (4)	N12—Co2—O12	79.8 (3)
O11—Co1—N11	89.3 (3)	N32—Co2—O12	101.1 (3)

Symmetry code: (i) -x+1, y, -z+1/2.

Table S6. Selected bond distances (Å) and angles (°) for **5**·3H₂O

Co—O13	1.8774 (13)	Co—N11	1.9591 (17)
Co—O12	1.9093 (12)	Co—N21	1.9998 (16)
Co—N13	1.9308 (15)	Co—O14	1.86 (2)
Co—N12	1.9429 (15)		
O13—Co—O12	89.33 (6)	O13—Co—N21	175.15 (6)
O13—Co—N13	86.07 (6)	O12—Co—N21	94.85 (6)
O12—Co—N13	89.52 (6)	N13—Co—N21	91.52 (6)
O13—Co—N12	90.24 (6)	N11—Co—N21	84.79 (8)
O12—Co—N12	85.08 (6)	O14—Co—N21	107.1 (8)
N13—Co—N12	173.50 (6)	O14—Co—N12	94.7 (7)
N12—Co—N21	92.54 (6)	O14—Co—O12	158.0 (8)
O13—Co—N11	91.28 (7)	O14—Co—N13	89.0 (7)
O12—Co—N11	174.46 (6)	O14—Co—O13	68.7 (8)
N13—Co—N11	96.01 (7)		
N12—Co—N11	89.41 (6)		

Table S7. Selected bond distances (Å) and angles (°) for **6**·7.9MeOH

Co1—O1A	1.894 (3)	Co2—N12	2.074 (5)
Co1—O12	1.910 (5)	Co2—N23	2.184 (11)
Co1—N1A	1.913 (4)	Co2—N22	2.299 (4)
Co1—O1	1.920 (3)	Co3—O13	1.830 (8)
Co1—N11	1.944 (4)	Co3—O1B	1.883(3)
Co1—N21	2.006 (4)	Co3—O2	1.909 (3)
Co2—O2	2.023 (3)	Co3—N1B	1.928 (4)
Co2—O1	2.025 (3)	Co3—N14	1.955 (4)
Co2—N13	2.047 (9)	Co3—N24	1.996 (4)
O1A—Co1—O12	84.93 (17)	N13—Co2—N22	102.4 (4)
O1A—Co1—N1A	84.66 (15)	N12—Co2—N22	78.82 (18)
O12—Co1—N1A	87.7 (3)	N23—Co2—N22	84.5 (4)
O1A—Co1—O1	176.43 (15)	O2—Co2—N23	160.3 (3)
O12—Co1—O1	93.76 (17)	O1—Co2—N23	92.6 (3)
N1A—Co1—O1	91.98 (15)	N13—Co2—N23	81.4 (4)
N11—Co1—N21	85.61 (16)	N12—Co2—N23	101.7(3)
O1A—Co1—N21	89.99 (15)	O13—Co3—O2	91.5 (2)
O12—Co1—N21	97.8 (3)	O13—Co3—N1B	92.5 (3)
N1A—Co1—N21	171.96 (16)	O2—Co3—N1B	92.10 (15)
O1—Co1—N21	93.48 (15)	O13—Co3—N14	178.9 (2)
O1A—Co1—N11	92.64 (14)	O2—Co3—N14	89.58 (15)
O12—Co1—N11	175.8 (2)	N1B—Co3—N14	87.85 (18)
N1A—Co1—N11	88.64 (16)	O13—Co3—N24	94.3 (3)
O1—Co1—N11	88.46 (14)	O2—Co3—N24	93.57 (14)
O2—Co2—O1	94.79 (13)	N1B—Co3—N24	170.99 (17)
O2—Co2—N13	79.5 (3)	N14—Co3—N24	85.20 (17)
O1—Co2—N13	97.7 (3)	O13—Co3—O1B	87.1(2)
O1—Co2—N12	81.51 (16)	O1B—Co3—O2	176.70(16)
N13—Co2—N12	176.8 (4)	O1B—Co3—N1B	84.99(16)
O2—Co2—N12	97.5 (3)	O1B—Co3—N14	91.86(15)
O2—Co2—N22	94.8 (3)	O1B—Co3—N24	89.51(16)
O1—Co2—N22	159.1 (2)		

Table S8. Selected bond distances (Å) and angles (°) for 7·6.8MeOH·7H₂O

Co1—O1M	2.078 (3)	Co3—O15	1.988 (3)
Co1—O11	2.086 (3)	Co3—O26	2.081 (3)
Co1—O14 ⁱ	2.094 (3)	Co3—N22	2.102 (4)
Co1—O1M ⁱ	2.098 (3)	Co3—N16	2.107 (4)
Co1—O26	2.115 (3)	Co3—O12	2.158 (3)
Co1—O12	2.160 (3)	Co4—O12	2.101 (3)
Co2—O13 ⁱ	1.990 (3)	Co4—N15	2.125 (4)
Co2—N14	2.056 (4)	Co4—O14 ⁱ	2.134 (3)
Co2—O1M	2.087 (3)	Co4—N13	2.174 (4)
Co2—O16	2.094 (3)	Co4—N25	2.197 (4)
Co2—O11	2.185 (3)	Co4—N23	2.223 (4)
Co2—N24	2.306 (4)		
O1M—Co1—O11	90.20 (12)	N14—Co2—O16	174.16 (16)
O1M—Co1—O14 ⁱ	103.25 (12)	O1M—Co2—O16	93.86 (12)
O11—Co1—O14 ⁱ	163.90 (12)	O26—Co3—N16	80.52 (13)
O1M—Co1—O1M ⁱ	80.44 (12)	N22—Co3—N16	106.66 (16)
O11—Co1—O1M ⁱ	98.18 (12)	O15—Co3—O12	94.43 (12)
O14 ⁱ —Co1—O1M ⁱ	92.83 (13)	O26—Co3—O12	83.45 (12)
O1M—Co1—O26	91.57 (12)	N22—Co3—O12	87.36 (14)
O11—Co1—O26	83.94 (12)	N16—Co3—O12	163.18 (14)
O14 ⁱ —Co1—O26	86.83 (13)	O15—Co3—O26	95.03 (13)
O1M ⁱ —Co1—O26	171.71 (12)	O15—Co3—N22	100.87 (15)
O1M—Co1—O12	173.10 (12)	O26—Co3—N22	162.20 (14)
O11—Co1—O12	85.54 (12)	O15—Co3—N16	92.03 (14)
O14 ⁱ —Co1—O12	80.20 (12)	O12—Co4—N15	86.20 (14)
O1M ⁱ —Co1—O12	105.51 (12)	O12—Co4—O14 ⁱ	80.66 (12)
O26—Co1—O12	82.60 (12)	N15—Co4—O14 ⁱ	85.15 (14)
O13 ⁱ —Co2—O11	178.64 (12)	O12—Co4—N13	96.43 (13)
N14—Co2—O11	86.36 (14)	O12—Co4—N25	165.44 (13)
O1M—Co2—O11	87.29 (12)	N15—Co4—N25	80.59 (14)
O16—Co2—O11	90.05 (12)	O14 ⁱ —Co4—N25	92.07 (14)
O13 ⁱ —Co2—N24	96.43 (14)	N13—Co4—N25	97.01 (14)
N14—Co2—N24	78.11 (17)	O12—Co4—N23	86.32 (13)
O1M—Co2—N24	165.60 (13)	N15—Co4—N23	98.06 (14)
O16—Co2—N24	96.90 (14)	O14 ⁱ —Co4—N23	166.37 (13)

O11—Co2—N24	83.17 (13)	N13—Co4—N23	80.05 (14)
O13 ⁱ —Co2—N14	94.83 (15)	N25—Co4—N23	101.51 (14)
O13 ⁱ —Co2—O1M	93.35 (12)	N15—Co4—N13	176.63 (15)
N14—Co2—O1M	90.58 (16)	O14 ⁱ —Co4—N13	97.33 (14)
O13 ⁱ —Co2—O16	88.71 (12)		

Symmetry code: (i) -x+1, -y+1, -z+1

Table S9. Selected bond distances (Å) and angles (°) for **7**·MeOH·3H₂O

Co1—O11	2.059 (3)	Co3—O15	1.996 (3)
Co1—O1M ⁱ	2.066 (3)	Co3—O26	2.084 (3)
Co1—O14 ⁱ	2.075 (3)	Co3—N16	2.104 (4)
Co1—O1M	2.096 (3)	Co3—N22	2.115 (5)
Co1—O26	2.116 (3)	Co3—O12	2.159 (3)
Co1—O12	2.158 (3)	Co4—O12	2.087 (3)
Co2—O13 ⁱ	1.991 (3)	Co4—N15	2.117 (4)
Co2—N14	2.054 (4)	Co4—O14 ⁱ	2.117 (3)
Co2—O16	2.080 (3)	Co4—N23	2.173 (4)
Co2—O1M ⁱ	2.082 (3)	Co4—N13	2.180 (4)
Co2—O11	2.197 (3)	Co4—N25	2.204 (4)
Co2—N24	2.330 (4)		
O11—Co1—O1M ⁱ	90.68 (12)	O1M ⁱ —Co2—N24	165.27 (13)
O11—Co1—O14 ⁱ	163.82 (12)	O11—Co2—N24	83.74 (13)
O1M ⁱ —Co1—O14 ⁱ	102.86 (12)	O15—Co3—O26	92.51 (13)
O11—Co1—O1M	97.76 (12)	O15—Co3—N16	90.90 (14)
O1M ⁱ —Co1—O1M	80.62 (12)	O26—Co3—N16	80.55 (14)
O14 ⁱ —Co1—O1M	93.20 (12)	O15—Co3—N22	98.66 (16)
O11—Co1—O26	84.44 (12)	O26—Co3—N22	165.30 (17)
O1M ⁱ —Co1—O26	91.13 (12)	N16—Co3—N22	108.65 (19)
O14 ⁱ —Co1—O26	86.46 (12)	O15—Co3—O12	93.39 (13)
O1M—Co1—O26	171.47 (12)	O26—Co3—O12	83.42 (12)
O11—Co1—O12	85.67 (12)	N16—Co3—O12	163.56 (13)
O1M ⁱ —Co1—O12	173.08 (11)	N22—Co3—O12	86.39 (18)
O14 ⁱ —Co1—O12	79.92 (12)	O12—Co4—N15	86.28 (14)
O1M—Co1—O12	105.67 (12)	O12—Co4—O14 ⁱ	80.61 (13)
O26—Co1—O12	82.68 (13)	N15—Co4—O14 ⁱ	84.47 (14)
O13 ⁱ —Co2—N14	95.18 (14)	O12—Co4—N23	88.19 (13)
O13 ⁱ —Co2—O16	88.80 (12)	N15—Co4—N23	97.21 (15)
N14—Co2—O16	174.26 (16)	O14 ⁱ —Co4—N23	168.56 (12)

O13 ⁱ —Co2—O1M ⁱ	92.61 (12)	O12—Co4—N13	96.04 (13)
N14—Co2—O1M ⁱ	89.40 (16)	N15—Co4—N13	176.90 (14)
O16—Co2—O1M ⁱ	94.56 (11)	O14 ⁱ —Co4—N13	97.92 (15)
O13 ⁱ —Co2—O11	178.80 (12)	N23—Co4—N13	80.84 (16)
N14—Co2—O11	85.63 (14)	O12—Co4—N25	166.30 (13)
O16—Co2—O11	90.46 (12)	N15—Co4—N25	80.77 (15)
O1M ⁱ —Co2—O11	86.51 (11)	O14 ⁱ —Co4—N25	93.60 (13)
O13 ⁱ —Co2—N24	97.28 (13)	N23—Co4—N25	97.83 (14)
N14—Co2—N24	78.89 (18)	N13—Co4—N25	97.06 (14)
O16—Co2—N24	96.53 (14)		

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