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A mixed-valence $[Co^{II}_4Co^{III}_2]$ cluster with defect disk-shaped topology

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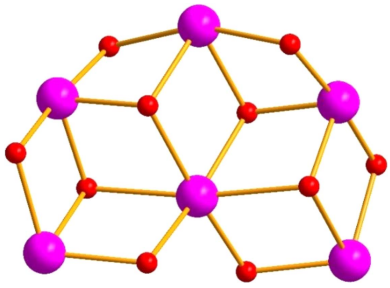
The employment of the new Schiff base ligand 2-[(4-chloro-2-hydroxybenzylideneamino)methyl]phenol (H_2L) bearing O_2N donors for the preparation of a novel Co_6 cluster is reported. The hexanuclear cobalt complex, namely, di-μ_2-acetatotetrakis{μ_2-2-[(4-chloro-2-oxidobenzylideneamino)methyl]phenolato}tetra-μ_3-methanolato-tetracobalt(II)dicobalt(III), $[Co^{II}_4Co^{III}_2(C_{14}H_{10}ClNO_2)_4(CH_3COO)_2(CH_3O)_4]$, was obtained using $Co(CH_3COO)_2{\cdot}4H_2O$ and H_2L as starting materials in MeOH under solvothermal conditions. The six metal ions are linked together by the μ_3-O atoms of four deprotonated MeOH molecules, two CH_3COO^- units and six phenolate O atoms of four L^{2-} ligands to form a defect disk-shaped topology. DC magnetic susceptibility investigations revealed the existence of antiferromagnetic interactions in the Co_6 cluster.

1. Introduction

Polynuclear coordination compounds of 3*d* transition metals have attracted continued attention for several decades due to their structural novelty, interesting catalytic (Dastidar & Chattopadhyay, 2022; Shul'pin & Shul'pina, 2021; Nesterov & Nesterova, 2018; Jing *et al.*, 2020) and biological properties (Hazari *et al.*, 2017; Amtul *et al.*, 2002; Azizian *et al.*, 2012; Tanaka *et al.*, 2003), and their potential as single-molecule magnets (SMMs) (Radu *et al.*, 2017; Pattacini *et al.*, 2011). Among numerous polynuclear 3*d* complexes, cobalt clusters have received particular interest because of their pleasing topological aesthetics (Brechin *et al.*, 1997; Cao *et al.*, 2013), their relevance to dioxygen reduction (Monte-Pérez *et al.*, 2017) and their fascinating magnetic properties (Liu *et al.*, 2020; Sarto *et al.*, 2018; Li *et al.*, 2020; Ma *et al.*, 2012).

Several synthetic methodologies towards polynuclear cobalt clusters were established and one of the most efficient approaches involves the employment of hydroxy-containing Schiff base ligands. Schiff base ligands are easy to synthesize and their steric properties can be tuned by varying the size of the amine or carbonyl substituents (Qin *et al.*, 2017, 2018; Ge *et al.*, 2018; Li *et al.*, 2021). More importantly, the hydroxy moieties of the Schiff base ligands can combine many metal ions with μ-O bridges, resulting in the formation of large polynuclear clusters.

In the present work, we utilized the hydroxy-containing Schiff base 2-[(4-chloro-2-hydroxybenzylideneamino)methyl]phenol (H_2L) (Huang *et al.*, 2019) as a ligand to assemble a polynuclear cobalt cluster. The hexanuclear cobalt compound $[Co_4^{II}Co_2^{III}(L)_4(CH_3COO)_2(MeO)_4]$ (**1**) was obtained successfully and we report its structural diversity and discuss its magnetic properties.



2. Experimental

2.1. Materials and physical measurements

All chemicals were of reagent grade, purchased from commercial suppliers and used without further purification. All manipulations were conducted under aerobic and solvothermal conditions. H_2L was synthesized following the literature procedure of Huang *et al.* (2019). Elemental analyses for C, H and N were performed with a Carlo-Erba EA1110 CHNO-S analyser. The FT–IR spectrum was determined on a Nicolet MagNa-IR 500 spectrometer using KBr pellets in the range 400–4000 cm^{-1}. DC magnetic susceptibilities were measured in the temperature range 2–300 K in a field of 1000 Oe using a Quantum Design MPMS-7 SQUID magnetometer.

2.2. Synthesis and crystallization

To a Pyrex tube (10 ml) was added a mixture of H_2L (0.0291 g, 0.1 mmol), $Co(CH_3COO)_2{\cdot}4H_2O$ (0.0249 g, 0.1 mmol), Et_3N (0.0202 g, 0.2 mmol) and MeOH (1.5 ml). The tube was sealed and heated at 80 °C for 48 h under autogenous pressure. It was then cooled to room temperature and dark-red needle-like crystals were obtained. The crystals were collected, washed with MeOH (2 ml) and dried in air (yield: 0.020 g; 48% based on cobalt). Analysis calculated (%) for $C_{64}H_{58}Cl_4Co_6N_4O_{16}$: C 47.03, H 3.58, N 3.43; found (%): C 46.18, H 4.048, N 3.280. Selected IR data for **1** (cm^{-1}): 1637 (*s*), 1590 (*s*), 1523 (*s*), 1450 (*m*), 1419 (*m*), 1286 (*w*), 1248 (*s*), 1185 (*s*), 1089 (*m*), 1021 (*m*), 933 (*s*), 874 (*m*), 852 (*w*), 755 (*s*).

2.3. Structure determination

Crystal data, data collection and structure refinement details are summarized in Table 1. The crystal structure contained disordered solvent that could not be satisfactorily refined. The SQUEEZE (Spek, 2015) routine of *PLATON* (Spek, 2020) was used in the treatment of the crystallographic data. All H atoms were placed in geometrically idealized positions, with C—H = 0.95–0.99 Å. The H atoms of the CH_2, aromatic and amide groups were constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of CH_3 groups were refined as rotating groups, with $U_{iso}(H) = 1.5U_{eq}(C)$.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Co_6(C_{14}H_{10}ClNO_2)_4(C_2H_3O_2)_2(CH_3O)_4]$
M_r	1634.52
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	120
a, *b*, *c* (Å)	15.4873 (10), 16.2116 (11), 28.1099 (19)
V (Å^3)	7057.7 (8)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	1.60
Crystal size (mm)	0.4 × 0.2 × 0.2
Data collection	
Diffractometer	Bruker SMART APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.612, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	78040, 16170, 11376
R_{int}	0.094
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.057, 0.174, 1.04
No. of reflections	16170
No. of parameters	853
No. of restraints	12
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.65, −0.78
Absolute structure	Flack *x* determined using 4303 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.011 (8)

Computer programs: *SAINT* (Bruker, 2016), *APEX2* (Bruker, 2016), *olex2.solve* (Bourhis *et al.*, 2015), *SHELXL* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *PLATON* (Spek, 2020).

3. Results and discussion

3.1. Synthesis of complex 1 and IR spectral analysis

The reaction of H_2L and $Co(CH_3COO)_2{\cdot}4H_2O$ in MeOH in the presence of NEt_3 under solvothermal conditions led to the isolation of **1** in moderate yield. $Co(CH_3COO)_2{\cdot}4H_2O$ is a good starting material because it not only serves as a convenient metal source, but also provides CH_3COO^- bridging ligands. In the solid state, complex **1** is stable in air and its elemental analysis is consistent with the given molecular formula.

The vibrational bands in the IR spectrum agree well with the formulation of complex **1** (see Fig. S1 in the supporting information). The signals of the carboxyl $\nu_{as}(CO_2)$ and $\nu_s(CO_2)$ vibrations were found in the 1637–1419 cm^{-1} range. The vibrations of the C═N bond appear at 1450 cm^{-1}. Several bands in the 1286–1185 cm^{-1} range were assigned to the vibrations of the aromatic rings. The sharp signals in the 979–766 cm^{-1} range were ascribed to the vibrations of C—H bonds.

3.2. Structure description of 1

Single crystals of **1** were obtained from MeOH under solvothermal conditions. Complex **1** crystallized in the orthorhombic space group $P2_12_12_1$. The structure is shown in Fig. 1. The structure analysis shows that complex **1** is composed of six cobalt ions, four 2-[(4-chloro-2-oxidobenzylideneamino)methyl]phenolate (L^{2-}) ligands, two acetate ligands and four methanol-solvent-derived MeO^- ligands. There exists an approximate C_2 symmetry in the molecule. The imine N atom and both phenolate O-atom donors of each L^{2-} ligand coordinate each cobalt centre. Bond valence calculations (Brese & O'Keeffe, 1991; Brown & Altermatt, 1985) gave valence parameters of 1.90, 2.32, 3.60, 2.12, 3.64 and 2.31 for the Co1–Co6 ions, respectively, indicating that the Co3 and Co5 ions are in 3+ valence states, and that the Co1, Co2, Co4

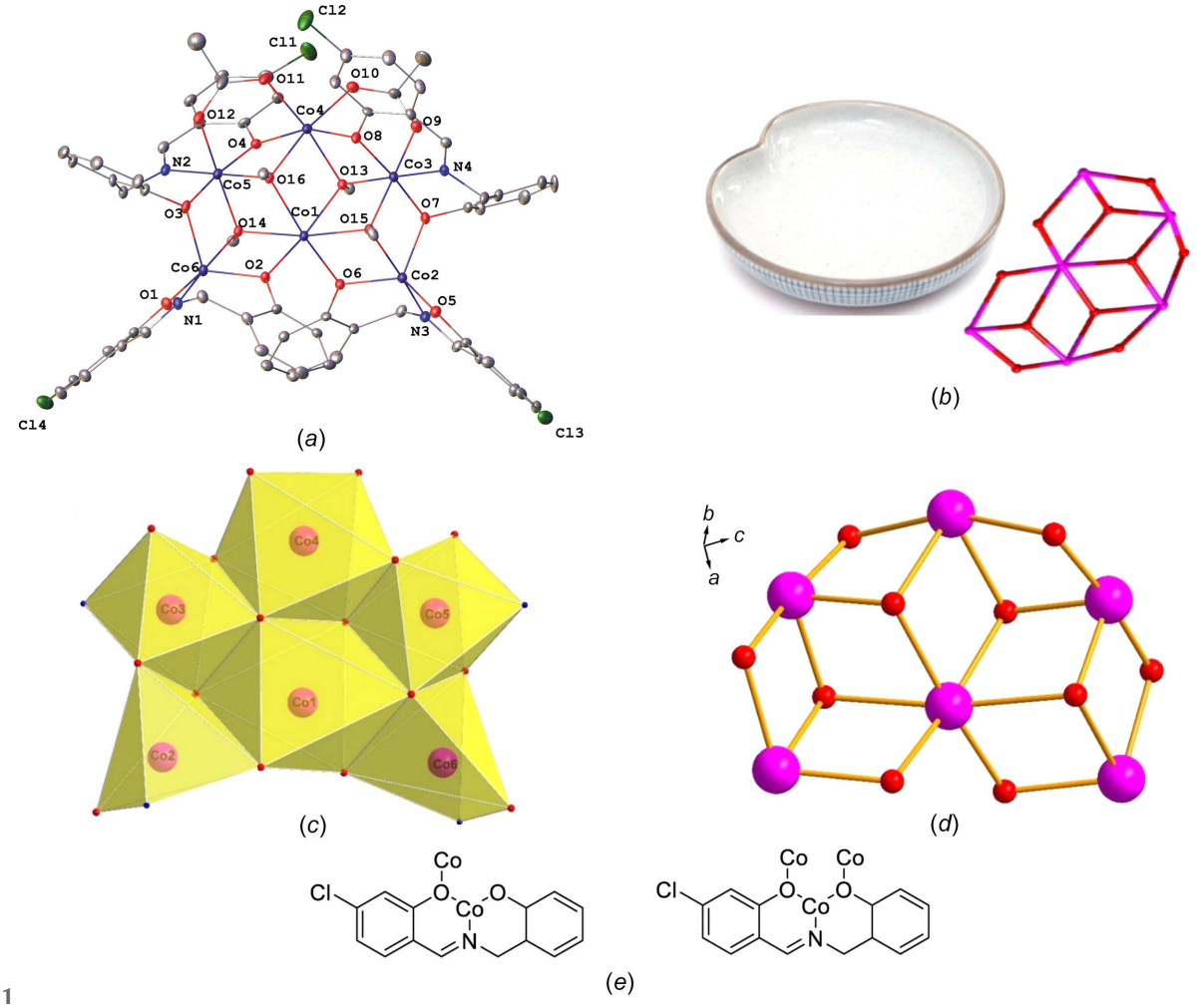


Figure 1
(*a*) The molecular structure of **1**, (*b*) the defect disk-shaped topology, (*c*) the coordination polyhedra of the Co atoms, (*d*) the metal framework, with the H atoms omitted for clarity, and (*e*) the coordination modes of the H_2L ligand.

and Co6 ions are in 2+ oxidation states. The formation of four fused defect cubes confirms the involvement of four methanol-solvent-derived μ_3-O^- groups, giving the Co_6O_{10} structure. Thus, the molecular structure of **1** displays a defect disk-shaped topology [Fig. 1(*b*)]. Of the six cobalt centres, the Co1, Co3, Co4 and Co5 ions are six-coordinated, and the Co2 and Co6 ions are five-coordinated. The coordination environments of the Co2 and Co6 ions, and the Co3 and Co5 ions are individually identical. The Co1 centre is present in a distorted octahedral O_6 coordination environment, among which two O atoms are from two μ_2-κ^4O:O,O',N L^{2-} ligands and four O atoms are from four μ_3-O^- MeO^- ligands. The Co2 centre is enclosed by the N and O atoms of one μ_2-κ^4O:O,O',N L^{2-} ligand, one O atom of a μ_3-κ^5O:O,N,O':O' L^{2-} ligand and one O atom of one μ_3-O^- MeO^- ligand. The six-coordinate NO_5 environment around the Co3 ion is accomplished by two μ_3-O^- MeO^- groups, one O atom from one acetate bridge and the N and O atoms of one μ_3-κ^5O:O,N,O':O' L^{2-} ligand. The six O-donor atoms around the Co6 centre originate from bridging acetate ligands, two μ_3-O^- MeO^- groups and two μ_3-κ^5O:O,N,O':O' L^{2-} ligands. The H_2L ligand exhibits two types of coordination mode.

The geometries of the five-coordinated Co2 and Co6 atoms were analyzed with the program *SHAPE* (Version 2.0; Pinsky & Avnir, 1998). The calculated values revealed trigonal bipyramid (D_{3h}) geometry for both atoms, with a minimum CShM (contunuous shape measure) value of 1.065 for Co2 and 1.172 for Co6.

Complex **1** joins a small family of Co_6 clusters. Hexanuclear cobalt complexes mainly exhibit wheel, cage and ring topologies (Shi *et al.*, 2021; Zou *et al.*, 2014; Wang *et al.*, 2013; Guo *et al.*, 2013; Lazzarini *et al.*, 2012; Chen *et al.*, 2010; Malassa *et al.*, 2010; Tudor *et al.*, 2010; Colacio *et al.*, 2009; Jones *et al.*, 2009; Shiga & Oshio, 2007; Alley *et al.*, 2006; Murrie *et al.*, 2003; Kumagai *et al.*, 2003; Gutschke *et al.*, 1999). Complex **1** is a rare example that displays a defect disk-shaped structure.

3.3. Magnetic properties of 1

Magnetic susceptibility data as a function of temperature for complex **1** are shown in Fig. 2. The room temperature $\chi_M T$ value is 10.96 cm^3 mol^{-1} K, which is greater than the value of 7.50 cm^3 mol^{-1} K for four uncoupled S = 3/2 Co^{II} centres, possibly owing to the orbital contributions of the metal ions

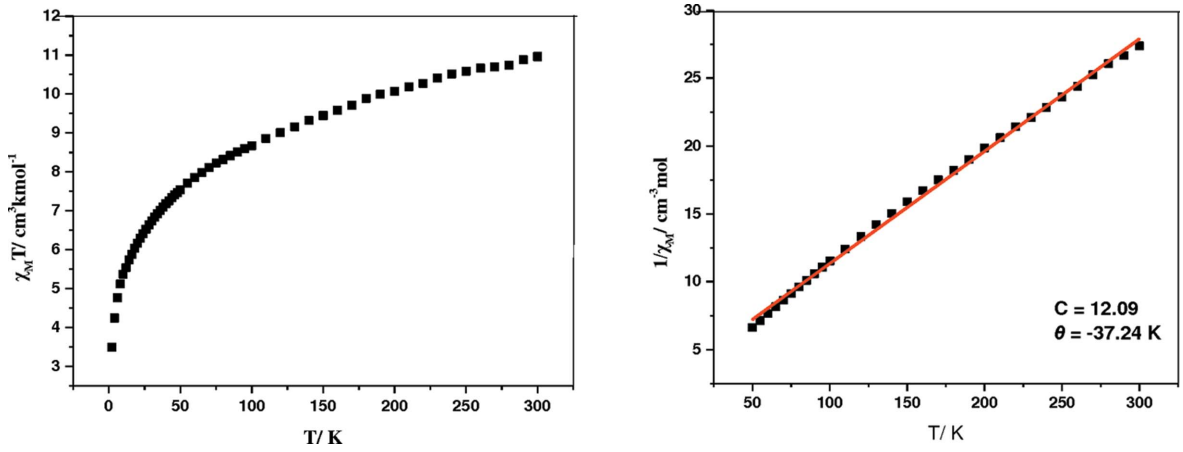


Figure 2
Temperature dependence of magnetic susceptibilities in the forms of (*a*) $\chi_M T$ *versus* T and (*b*) $1/\chi_M$ *versus* T for **1** at 1 kOe. The red solid line corresponds to the best fit of the magnetic data.

(Cao *et al.*, 2013). Upon lowering the temperature, the $\chi_M T$ value drops slightly to a minimum value of 3.49 cm^3 mol^{-1} K at 2 K, which suggests possible antiferromagnetic couplings between the unpaired spins. The data of $1/\chi_M$ in the temperature range 2–300 K were fitted by the Curie–Weiss Law of $1/\chi_M = (T - \theta)/C$. The Curie constant C = 12.09 cm^3 mol^{-1} K and the Weiss constant $\theta = -37.24$ K were obtained. The negative θ value proves the antiferromagnetic interactions.

The magnetic dynamic behaviour of **1** was also explored. The ac magnetic susceptibilities for **1** at 1000 Hz under a zero-dc field in the temperature range 2–25 K were shown in Fig. S2 (see supporting information). The χ'' susceptibilities at 1000 Hz did not increase upon lowering the temperature and no peaks were determined. These phenomena revealed that complex **1** is not a single-molecule magnet.

4. Conclusion

A hexanuclear cobalt complex of composition $[Co_2^{III}Co_4^{II}(L)_4(CH_3COO)_2(MeO)_4]$ (**1**), based on the hydroxy-containing Schiff base ligand 2-[(4-chloro-2-hydroxybenzylideneamino)methyl]phenol (H_2L) was prepared and characterized. Complex **1** exhibits a defect disk-shaped topology. Four cobalt ions are six-coordinated and two cobalt ions are five-coordinated. An investigation of the magnetic properties revealed that there exist antiferromagnetic interactions between the Co^{II} ions.

Funding information

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References

Alley, K. G., Bircher, R., Waldmann, O., Ochsenbein, S. T., Güdel, H. U., Moubaraki, B., Murray, K. S., Fernandez-Alonso, F., Abrahams, B. F. & Boskovic, C. (2006). *Inorg. Chem.* **45**, 8950–8957.
Amtul, Z., Atta-ur-Rahman, B. S. P., Siddiqui, R. A. & Choudhary, M. I. (2002). *Curr. Med. Chem.* **9**, 1323–1348.
Azizian, H., Nabati, F., Sharifi, A., Siavoshi, F., Mahdavi, M. & Amanlou, M. (2012). *J. Mol. Model.* **18**, 2917–2927.
Bourhis, L. J., Dolomanov, O. V., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2015). *Acta Cryst.* A**71**, 59–75.
Brechin, E. K., Harris, S. G., Harrison, A., Parsons, S., Gavin Whittaker, A. & Winpenny, R. E. P. (1997). *Chem. Commun.* pp. 653–654.
Brese, N. E. & O'Keeffe, M. (1991). *Acta Cryst.* B**47**, 192–197.
Brown, I. D. & Altermatt, D. (1985). *Acta Cryst.* B**41**, 244–247.
Bruker (2016). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cao, Y. Y., Chen, Y. M., Li, L., Gao, D. D., Liu, W., Hu, H. L., Li, W. & Li, Y. H. (2013). *Dalton Trans.* **42**, 10912–10918.
Chen, Q., Zeng, M. H., Wei, L. Q. & Kurmoo, M. (2010). *Chem. Mater.* **22**, 4328–4334.
Colacio, E., Aouryaghal, H., Mota, A. J., Cano, J., Sillanpää, R. & Rodríguez-Diéguez, A. (2009). *CrystEngComm*, **11**, 2054–2064.
Dastidar, T. G. & Chattopadhyay, S. (2022). *Polyhedron*, **211**, 115511–115536.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Ge, Y., Qin, Y. R., Cui, Y. F., Pan, Y. D., Huang, Y., Li, Y. H., Liu, W. & Zhang, Y. Q. (2018). *Chem. Asian J.* **13**, 3753–3761.
Guo, J. Y., Zhang, D., Chen, L., Song, Y., Zhu, D. R. & Xu, Y. (2013). *Dalton Trans.* **42**, 8454–8459.
Gutschke, S. O. H., Price, D. I., Powell, A. K. & Wood, P. T. (1999). *Angew. Chem. Int. Ed.* **38**, 1088–1090.
Hazari, A., Das, A., Mahapatra, P. & Ghosh, A. (2017). *Polyhedron*, **134**, 99–106.
Huang, Y., Qin, Y. R., Ge, Y., Cui, Y. F., Zhang, X. M., Li, Y. H. & Yao, J. L. (2019). *New J. Chem.* **43**, 19344–19354.
Jing, Y., Zhang, X. M., Cui, Y. F., Li, D. W., Sun, H., Ge, Y. & Li, Y. H. (2020). *Chin. J. Struct. Chem.* **39**, 1057–1062.
Jones, L. F., Kilner, C. A. & Halcrow, M. A. (2009). *Chem. Eur. J.* **15**, 4667–4675.
Kumagai, H., Oka, Y., Kawata, S., Ohba, M., Inoue, K., Kurmoo, M. & Ōkawa, H. (2003). *Polyhedron*, **22**, 1917–1920.
Lazzarini, I. C., Carrella, L., Rentschler, E. & Alborés, P. (2012). *Polyhedron*, **31**, 779–788.

Li, D. W., Ding, M. M., Huang, Y., Tello Yepes, D. F., Li, H. Y., Li, Y. H., Zhang, Y. Q. & Yao, J. L. (2021). *Dalton Trans.* **50**, 217–228.
Li, X., Guo, Y., Xu, T., Fang, M., Xu, Q., Zhang, F., Wu, Z., Li, C. & Zhu, W. (2020). *J. Chin. Chem. Soc.* **67**, 1070–1077.
Liu, Y. N., Hou, J. L., Wang, Z., Gupta, R. K., Jagličić, Z., Jagodič, M., Wang, W. G., Tung, C. H. & Sun, D. (2020). *Inorg. Chem.* **59**, 5683–5693.
Ma, Y. S., Xue, F. F., Tang, X. Y., Chen, B. & Yuan, R. X. (2012). *Inorg. Chem. Commun.* **15**, 285–287.
Malassa, A., Agthe, C., Görls, H., Podewitz, M., Yu, L., Herrmann, C., Reiher, M. & Westerhausen, M. (2010). *Eur. J. Inorg. Chem.* **2010**, 1777–1790.
Monte-Pérez, I., Kundu, S., Chandra, A., Craigo, K. E., Chernev, P., Kuhlmann, U., Dau, H., Hildebrandt, P., Greco, C., Van Stappen, C., Lehnert, N. & Ray, K. (2017). *J. Am. Chem. Soc.* **139**, 15033–15042.
Murrie, M., Teat, S. J., Stoeckli-Evans, H. & Güdel, H. U. (2003). *Angew. Chem. Int. Ed.* **42**, 4653–4656.
Nesterov, D. S. & Nesterova, O. V. (2018). *Catalysts*, **8**, 602–623.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Pattacini, R., Teo, P., Zhang, J., Lan, Y. H., Powell, A. K., Nehrkorn, J., Waldmann, O., Hor, T. S. A. & Braunstein, P. (2011). *Dalton Trans.* **40**, 10526–10534.
Pinsky, M. & Avnir, D. (1998). *Inorg. Chem.* **37**, 5575–5582.
Qin, Y., Zhang, H. F., Sun, H., Pan, Y. D., Ge, Y., Li, Y. H. & Zhang, Y. Q. (2017). *Chem. Asian J.* **12**, 2834–2844.
Qin, Y. R., Jing, Y., Ge, Y., Liu, W., Li, Y. H. & Zhang, Y. Q. (2018). *Dalton Trans.* **47**, 15197–15205.
Radu, I., Kravtsov, V. Ch., Ostrovsky, S. M., Reu, O. S., Krämer, K., Decurtins, S., Liu, S. X., Klokishner, S. I. & Baca, S. G. (2017). *Inorg. Chem.* **56**, 2662–2676.
Sarto, C., Rouzières, M., Liu, J. L., Bamberger, H., van Slageren, J., Clérac, R. & Alborés, P. (2018). *Dalton Trans.* **47**, 17055–17066.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Shi, Z. H., Huang, Y., Wu, Y. Z., Chen, X. L. & Yang, H. (2021). *Chin. J. Struct. Chem.* **40**, 495–500.
Shiga, T. & Oshio, H. (2007). *Polyhedron*, **26**, 1881–1884.
Shul'pin, G. B. & Shul'pina, L. S. (2021). *Catalysts*, **11**, 186–223.
Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.
Spek, A. L. (2015). *Acta Cryst.* C**71**, 9–18.
Tanaka, T., Kawase, M. & Tani, S. (2003). *Life Sci.* **73**, 2985–2990.
Tudor, V., Madalan, A., Lupu, V., Lloret, F., Julve, M. & Andruh, M. (2010). *Inorg. Chim. Acta*, **363**, 823–826.
Wang, J., Jian, F. F., Huang, B. X. & Bai, Z. S. (2013). *J. Solid State Chem.* **204**, 272–277.
Zou, J. Y., Shi, W., Gao, H. L., Cui, J. Z. & Cheng, P. (2014). *Wuji Huaxue Xuebao*, **30**, 149–154.

supporting information

Acta Cryst. (2022). C**78**, 488-492 [https://doi.org/10.1107/S2053229622005885]

A mixed-valence [$Co^{II}_4Co^{III}_2$] cluster with defect disk-shaped topology

Hua Yang, Yu-Pei Fu, Yuan Huang, Xiao-Li Chen, Dan Qiao and Hua-Li Cui

Computing details

Data collection: *SAINT* (Bruker, 2016); cell refinement: *APEX2* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: olex2.solve (Bourhis *et al.*, 2015); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009) and *PLATON* (Spek, 2020).

Di-μ_2-acetato-tetrakis{μ_2-2-[(4-chloro-2-oxidobenzylideneamino)methyl]phenolato}tetra-μ_3-methanolato-tetracobalt(II)dicobalt(III)

Crystal data

$[Co_6(C_{14}H_{10}ClNO_2)_4(C_2H_3O_2)_2(CH_3O)_4]$
M_r = 1634.52
Orthorhombic, $P2_12_12_1$
a = 15.4873 (10) Å
b = 16.2116 (11) Å
c = 28.1099 (19) Å
V = 7057.7 (8) Å^3
Z = 4
$F(000)$ = 3312
D_x = 1.538 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9807 reflections
θ = 2.3–25.0°
μ = 1.60 mm^{-1}
T = 120 K
Block, red
0.4 × 0.2 × 0.2 mm

Data collection

Bruker SMART APEXII diffractometer
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.612, T_{max} = 0.746
78040 measured reflections
16170 independent reflections
11376 reflections with $I > 2\sigma(I)$
R_{int} = 0.094
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −16→20
k = −21→20
l = −36→36

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.174
S = 1.04
16170 reflections
853 parameters
12 restraints
Primary atom site location: iterative
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0906P)^2 + 7.497P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}
Absolute structure: Flack x determined using 4303 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.011 (8)

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. SQUEEZE, constraints & restraints, applied to the data, 17 reflections OMITted
Data for **1** was collected on a Bruker *SMART* APEXII diffractometer equipped with a graphite monochromator utilizing Mo *Kα* radiation (λ = 0.71073). The crystal structure of **1** was solved with the *OLEX2* program (Dolomanov *et al.*, 2009) and refined by *SHELXL* package (Sheldrick, 2015). The crystal structure of **1** contained disordered solvent that could not be satisfactorily refined. The SQUEEZE routine of *PLATON* was used in the treatment of the crystallographic data. CCDC-1991979 (**1**) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge *via* www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Centre, 12 Union Road, Cambridge CB21EZ, UK; Fax: (+44) 1223–336-033; or deposit@ccdc.cam.ac.uk). The crystallographic data was shown in Table 1. Selected bond lengths and bond angles of **1** are listed in Table 2.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.76532 (7)	0.48030 (7)	0.63042 (4)	0.0272 (3)
Co2	0.75457 (8)	0.37642 (7)	0.53446 (4)	0.0310 (3)
Co3	0.64711 (8)	0.53340 (8)	0.54249 (4)	0.0308 (3)
Co4	0.60975 (9)	0.60947 (8)	0.63671 (4)	0.0339 (3)
Co5	0.71075 (8)	0.57569 (8)	0.72480 (4)	0.0309 (3)
Co6	0.88399 (8)	0.48935 (8)	0.72294 (4)	0.0311 (3)
Cl1	0.27968 (19)	0.4953 (3)	0.70412 (13)	0.0880 (13)
Cl2	0.6728 (4)	0.94857 (19)	0.58576 (13)	0.0949 (15)
Cl3	1.0115 (2)	0.2814 (2)	0.34231 (10)	0.0618 (8)
Cl4	1.0081 (2)	0.2435 (2)	0.91102 (11)	0.0657 (9)
O1	0.8938 (4)	0.4073 (4)	0.7727 (2)	0.0380 (15)
O2	0.8905 (4)	0.4868 (4)	0.6523 (2)	0.0312 (13)
O3	0.8270 (4)	0.5965 (4)	0.7389 (2)	0.0360 (15)
O4	0.5975 (4)	0.5510 (4)	0.7035 (2)	0.0328 (14)
O5	0.8388 (5)	0.3739 (4)	0.4831 (2)	0.0409 (16)
O6	0.7686 (4)	0.3639 (4)	0.6037 (2)	0.0326 (14)
O7	0.6375 (4)	0.4225 (4)	0.5223 (2)	0.0352 (15)
O8	0.6589 (4)	0.6401 (4)	0.5695 (2)	0.0344 (14)
O9	0.5259 (4)	0.5511 (4)	0.5349 (2)	0.0422 (16)
O10	0.4897 (5)	0.6094 (5)	0.6053 (2)	0.0453 (17)
O11	0.5940 (6)	0.7169 (4)	0.6734 (2)	0.052 (2)
O12	0.6775 (5)	0.6864 (4)	0.7377 (2)	0.0432 (17)
O13	0.6353 (4)	0.4952 (4)	0.6070 (2)	0.0298 (13)
O14	0.7492 (4)	0.4674 (4)	0.70863 (19)	0.0289 (13)
O15	0.7654 (4)	0.5070 (4)	0.5537 (2)	0.0288 (13)
O16	0.7373 (4)	0.5983 (4)	0.6593 (2)	0.0301 (13)
N1	1.0097 (5)	0.5200 (5)	0.7269 (3)	0.0342 (17)
N2	0.6850 (5)	0.5540 (5)	0.7906 (3)	0.0364 (19)
N3	0.7286 (5)	0.2548 (5)	0.5280 (3)	0.0352 (18)
N4	0.6619 (5)	0.5716 (5)	0.4782 (3)	0.0364 (18)
C1	0.4468 (6)	0.5296 (7)	0.7069 (4)	0.045 (3)

H1	0.4423	0.5343	0.6733	0.054*
C2	0.3754 (7)	0.5145 (9)	0.7339 (4)	0.060 (3)
C3	0.3781 (7)	0.5108 (8)	0.7839 (4)	0.053 (3)
H3	0.3270	0.5027	0.8020	0.064*
C4	0.4559 (7)	0.5190 (7)	0.8052 (4)	0.049 (3)
H4	0.4588	0.5150	0.8389	0.058*
C5	0.5320 (6)	0.5333 (6)	0.7801 (4)	0.039 (2)
C6	0.5283 (6)	0.5380 (6)	0.7300 (4)	0.037 (2)
C7	0.6097 (7)	0.5405 (6)	0.8072 (3)	0.038 (2)
H7	0.6048	0.5348	0.8408	0.045*
C8	0.7583 (7)	0.5597 (6)	0.8253 (3)	0.036 (2)
H8A	0.7351	0.5577	0.8581	0.043*
H8B	0.7970	0.5117	0.8209	0.043*
C9	0.8089 (7)	0.6371 (6)	0.8189 (3)	0.038 (2)
C10	0.8217 (8)	0.6933 (7)	0.8549 (4)	0.048 (3)
H10	0.7953	0.6842	0.8850	0.058*
C11	0.8722 (8)	0.7628 (7)	0.8482 (4)	0.052 (3)
H11	0.8810	0.8008	0.8734	0.062*
C12	0.9110 (8)	0.7766 (7)	0.8028 (4)	0.052 (3)
H12	0.9468	0.8234	0.7980	0.062*
C13	0.8968 (8)	0.7219 (6)	0.7656 (4)	0.045 (2)
H13	0.9209	0.7312	0.7350	0.054*
C14	0.8449 (7)	0.6517 (6)	0.7750 (3)	0.039 (2)
C15	0.9556 (7)	0.3343 (7)	0.8366 (4)	0.044 (2)
H15	0.9028	0.3052	0.8403	0.052*
C16	0.9615 (6)	0.3927 (6)	0.8002 (3)	0.035 (2)
C17	1.0425 (6)	0.4339 (6)	0.7952 (3)	0.035 (2)
C18	1.0999 (7)	0.3583 (8)	0.8636 (4)	0.051 (3)
H18	1.1452	0.3475	0.8855	0.062*
C19	1.1099 (7)	0.4154 (7)	0.8276 (4)	0.047 (3)
H19	1.1636	0.4432	0.8244	0.057*
C20	1.0212 (7)	0.3171 (7)	0.8668 (4)	0.044 (2)
C21	1.0635 (6)	0.4918 (6)	0.7579 (3)	0.035 (2)
H21	1.1215	0.5106	0.7561	0.043*
C22	1.0409 (7)	0.5708 (7)	0.6875 (3)	0.040 (2)
H22A	1.1000	0.5907	0.6944	0.048*
H22B	1.0029	0.6194	0.6834	0.048*
C23	1.0413 (6)	0.5210 (7)	0.6432 (3)	0.039 (2)
C24	1.1158 (7)	0.5121 (6)	0.6156 (4)	0.042 (2)
H24	1.1665	0.5412	0.6248	0.050*
C25	1.1186 (7)	0.4631 (7)	0.5759 (3)	0.044 (2)
H25	1.1704	0.4593	0.5579	0.052*
C26	1.0474 (7)	0.4197 (7)	0.5621 (4)	0.043 (2)
H26	1.0499	0.3850	0.5349	0.051*
C27	0.9702 (6)	0.4266 (6)	0.5882 (3)	0.036 (2)
H27	0.9207	0.3960	0.5788	0.043*
C28	0.9662 (6)	0.4782 (6)	0.6278 (3)	0.034 (2)
C29	0.8365 (6)	0.2853 (6)	0.6654 (3)	0.037 (2)

H29	0.8709	0.3318	0.6734	0.044*
C30	0.8427 (7)	0.2144 (6)	0.6922 (4)	0.043 (2)
H30	0.8797	0.2121	0.7192	0.052*
C31	0.7947 (7)	0.1476 (7)	0.6794 (4)	0.048 (3)
H31	0.7971	0.0989	0.6981	0.057*
C32	0.7422 (7)	0.1498 (6)	0.6391 (4)	0.045 (2)
H32	0.7105	0.1019	0.6304	0.054*
C33	0.7353 (6)	0.2198 (6)	0.6117 (3)	0.033 (2)
C34	0.7802 (6)	0.2900 (5)	0.6267 (3)	0.032 (2)
C35	0.6792 (6)	0.2187 (6)	0.5677 (3)	0.037 (2)
H35A	0.6624	0.1614	0.5599	0.044*
H35B	0.6260	0.2512	0.5733	0.044*
C36	0.7550 (6)	0.2086 (6)	0.4935 (3)	0.036 (2)
H36	0.7351	0.1532	0.4929	0.044*
C37	0.8119 (6)	0.2338 (6)	0.4560 (3)	0.036 (2)
C38	0.8302 (7)	0.1754 (7)	0.4205 (3)	0.043 (2)
H38	0.8014	0.1236	0.4217	0.052*
C39	0.8873 (7)	0.1895 (7)	0.3846 (3)	0.047 (3)
H39	0.8966	0.1497	0.3603	0.056*
C40	0.9318 (7)	0.2643 (8)	0.3847 (3)	0.047 (3)
C41	0.9149 (7)	0.3239 (7)	0.4177 (4)	0.042 (2)
H41	0.9455	0.3745	0.4162	0.050*
C42	0.8532 (6)	0.3123 (6)	0.4540 (3)	0.035 (2)
C43	0.5196 (6)	0.3442 (7)	0.4902 (4)	0.042 (2)
H43	0.5135	0.3150	0.5194	0.051*
C44	0.5833 (6)	0.4050 (6)	0.4854 (3)	0.035 (2)
C45	0.4645 (7)	0.3265 (8)	0.4515 (4)	0.055 (3)
H45	0.4230	0.2835	0.4535	0.066*
C46	0.4723 (7)	0.3731 (9)	0.4106 (4)	0.056 (3)
H46	0.4342	0.3632	0.3847	0.068*
C47	0.5346 (8)	0.4342 (8)	0.4064 (4)	0.053 (3)
H47	0.5384	0.4660	0.3781	0.064*
C48	0.5921 (7)	0.4488 (6)	0.4441 (3)	0.040 (2)
C49	0.6648 (7)	0.5090 (6)	0.4405 (3)	0.041 (2)
H49A	0.7203	0.4788	0.4425	0.049*
H49B	0.6624	0.5367	0.4092	0.049*
C50	0.6674 (6)	0.6489 (6)	0.4657 (3)	0.036 (2)
H50	0.6716	0.6603	0.4327	0.043*
C51	0.6675 (6)	0.7168 (6)	0.4969 (3)	0.036 (2)
C52	0.6742 (7)	0.7961 (6)	0.4756 (4)	0.045 (3)
H52	0.6781	0.7998	0.4420	0.054*
C53	0.6754 (8)	0.8669 (7)	0.5016 (4)	0.054 (3)
H53	0.6802	0.9192	0.4866	0.064*
C54	0.6692 (8)	0.8603 (7)	0.5515 (4)	0.051 (3)
C55	0.6638 (8)	0.7861 (6)	0.5741 (4)	0.045 (3)
H55	0.6612	0.7836	0.6078	0.055*
C56	0.6622 (6)	0.7123 (6)	0.5466 (3)	0.036 (2)
C57	0.4733 (7)	0.5833 (8)	0.5639 (4)	0.053 (3)

C58	0.3814 (8)	0.5903 (13)	0.5464 (6)	0.096 (5)
H58A	0.3655	0.6487	0.5440	0.144*
H58B	0.3427	0.5626	0.5689	0.144*
H58C	0.3765	0.5643	0.5151	0.144*
C59	0.6256 (11)	0.7309 (7)	0.7142 (4)	0.062 (4)
C60	0.6036 (12)	0.8124 (10)	0.7369 (6)	0.094 (5)
H60A	0.6531	0.8497	0.7344	0.140*
H60B	0.5893	0.8038	0.7705	0.140*
H60C	0.5538	0.8368	0.7206	0.140*
C61	0.5769 (6)	0.4302 (6)	0.6171 (3)	0.036 (2)
H61A	0.6032	0.3774	0.6082	0.055*
H61B	0.5236	0.4382	0.5989	0.055*
H61C	0.5636	0.4299	0.6512	0.055*
C62	0.7050 (6)	0.3996 (6)	0.7304 (3)	0.036 (2)
H62A	0.6429	0.4043	0.7242	0.054*
H62B	0.7153	0.4003	0.7648	0.054*
H62C	0.7265	0.3476	0.7170	0.054*
C63	0.7956 (7)	0.6638 (6)	0.6484 (3)	0.037 (2)
H63A	0.8550	0.6457	0.6543	0.055*
H63B	0.7825	0.7116	0.6684	0.055*
H63C	0.7894	0.6791	0.6148	0.055*
C64	0.8312 (6)	0.5582 (6)	0.5321 (4)	0.040 (2)
H64A	0.8213	0.6159	0.5408	0.060*
H64B	0.8288	0.5524	0.4975	0.060*
H64C	0.8882	0.5409	0.5436	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0306 (6)	0.0269 (6)	0.0242 (6)	0.0002 (5)	−0.0015 (5)	−0.0026 (5)
Co2	0.0346 (6)	0.0300 (6)	0.0283 (6)	0.0024 (5)	−0.0027 (5)	−0.0032 (5)
Co3	0.0349 (6)	0.0329 (7)	0.0247 (6)	0.0038 (5)	−0.0031 (5)	−0.0006 (5)
Co4	0.0406 (7)	0.0336 (6)	0.0275 (6)	0.0086 (6)	0.0001 (5)	−0.0009 (5)
Co5	0.0384 (7)	0.0304 (6)	0.0240 (6)	0.0010 (5)	0.0017 (5)	−0.0028 (5)
Co6	0.0315 (6)	0.0358 (6)	0.0261 (6)	−0.0023 (5)	−0.0015 (5)	−0.0027 (5)
Cl1	0.0342 (14)	0.163 (4)	0.067 (2)	0.013 (2)	0.0036 (13)	0.009 (2)
Cl2	0.189 (5)	0.0361 (16)	0.060 (2)	−0.007 (2)	0.005 (2)	−0.0041 (14)
Cl3	0.0632 (18)	0.078 (2)	0.0436 (15)	0.0168 (16)	0.0178 (14)	0.0156 (15)
Cl4	0.0634 (19)	0.077 (2)	0.0562 (18)	0.0193 (16)	0.0140 (15)	0.0292 (16)
O1	0.032 (3)	0.045 (4)	0.038 (4)	−0.004 (3)	−0.005 (3)	0.001 (3)
O2	0.029 (3)	0.041 (3)	0.024 (3)	−0.001 (3)	0.000 (2)	−0.001 (3)
O3	0.048 (4)	0.037 (4)	0.023 (3)	−0.008 (3)	0.004 (3)	−0.007 (3)
O4	0.033 (3)	0.036 (3)	0.029 (3)	0.006 (3)	0.004 (3)	0.002 (3)
O5	0.050 (4)	0.037 (4)	0.036 (3)	0.003 (3)	−0.001 (3)	−0.004 (3)
O6	0.040 (4)	0.029 (3)	0.028 (3)	0.002 (3)	−0.004 (3)	−0.001 (3)
O7	0.037 (3)	0.042 (4)	0.028 (3)	−0.001 (3)	−0.008 (3)	−0.003 (3)
O8	0.052 (4)	0.028 (3)	0.024 (3)	0.003 (3)	−0.001 (3)	0.003 (3)
O9	0.040 (4)	0.052 (4)	0.034 (4)	0.005 (3)	−0.002 (3)	0.003 (3)

O10	0.045 (4)	0.052 (4)	0.040 (4)	0.012 (3)	0.001 (3)	0.004 (3)
O11	0.085 (6)	0.037 (4)	0.034 (4)	0.021 (4)	0.003 (4)	−0.001 (3)
O12	0.067 (5)	0.033 (4)	0.029 (3)	0.001 (3)	0.005 (3)	−0.001 (3)
O13	0.035 (3)	0.028 (3)	0.026 (3)	0.000 (3)	−0.001 (2)	0.001 (2)
O14	0.034 (3)	0.031 (3)	0.022 (3)	−0.003 (3)	0.002 (2)	−0.001 (2)
O15	0.032 (3)	0.029 (3)	0.026 (3)	−0.001 (3)	−0.002 (2)	−0.004 (2)
O16	0.036 (3)	0.029 (3)	0.026 (3)	−0.003 (3)	−0.001 (3)	−0.003 (2)
N1	0.039 (4)	0.034 (4)	0.030 (4)	−0.007 (4)	−0.006 (3)	0.000 (3)
N2	0.051 (5)	0.032 (4)	0.026 (4)	0.002 (4)	0.000 (3)	−0.004 (3)
N3	0.044 (4)	0.031 (4)	0.031 (4)	0.002 (3)	−0.002 (3)	−0.003 (3)
N4	0.034 (4)	0.046 (5)	0.029 (4)	0.004 (4)	−0.005 (3)	−0.005 (4)
C1	0.037 (5)	0.066 (7)	0.032 (5)	0.014 (5)	0.007 (4)	−0.002 (5)
C2	0.035 (6)	0.083 (9)	0.061 (7)	0.009 (6)	0.010 (5)	−0.004 (7)
C3	0.038 (6)	0.070 (8)	0.051 (6)	0.001 (5)	0.016 (5)	−0.012 (6)
C4	0.052 (6)	0.053 (7)	0.040 (6)	0.008 (6)	0.014 (5)	−0.009 (5)
C5	0.040 (5)	0.039 (5)	0.039 (5)	0.005 (4)	0.007 (4)	−0.002 (5)
C6	0.031 (5)	0.040 (5)	0.040 (5)	0.003 (4)	0.015 (4)	−0.006 (4)
C7	0.046 (6)	0.037 (5)	0.031 (5)	−0.002 (5)	0.009 (4)	0.000 (4)
C8	0.043 (5)	0.041 (5)	0.024 (4)	−0.004 (4)	0.000 (4)	−0.002 (4)
C9	0.052 (6)	0.044 (6)	0.018 (4)	0.001 (5)	−0.005 (4)	−0.002 (4)
C10	0.062 (7)	0.053 (6)	0.030 (5)	0.006 (6)	−0.006 (5)	−0.014 (5)
C11	0.058 (7)	0.046 (6)	0.051 (6)	0.004 (5)	−0.011 (6)	−0.021 (5)
C12	0.063 (7)	0.038 (6)	0.055 (7)	−0.006 (5)	−0.009 (6)	−0.008 (5)
C13	0.060 (7)	0.035 (5)	0.040 (6)	−0.011 (5)	0.000 (5)	−0.007 (4)
C14	0.051 (6)	0.035 (5)	0.031 (5)	−0.001 (4)	−0.004 (5)	−0.010 (4)
C15	0.043 (6)	0.049 (6)	0.039 (6)	0.007 (5)	0.008 (5)	0.007 (5)
C16	0.036 (5)	0.042 (5)	0.027 (4)	0.007 (4)	0.003 (4)	−0.005 (4)
C17	0.039 (5)	0.037 (5)	0.028 (4)	−0.002 (4)	−0.001 (4)	−0.001 (4)
C18	0.045 (6)	0.071 (8)	0.038 (6)	0.012 (6)	−0.005 (5)	0.007 (6)
C19	0.040 (6)	0.055 (7)	0.047 (6)	0.004 (5)	−0.010 (5)	−0.001 (5)
C20	0.047 (6)	0.056 (6)	0.029 (5)	0.018 (5)	0.001 (4)	0.005 (5)
C21	0.030 (5)	0.039 (5)	0.038 (5)	−0.003 (4)	0.000 (4)	0.001 (4)
C22	0.044 (6)	0.042 (6)	0.034 (5)	−0.005 (5)	−0.003 (4)	0.007 (4)
C23	0.034 (5)	0.045 (6)	0.038 (5)	−0.007 (4)	−0.004 (4)	0.010 (5)
C24	0.041 (5)	0.039 (5)	0.046 (6)	0.000 (5)	0.008 (4)	0.014 (5)
C25	0.038 (5)	0.058 (7)	0.035 (5)	0.003 (5)	0.012 (4)	0.015 (5)
C26	0.044 (6)	0.047 (6)	0.037 (5)	0.019 (5)	0.010 (4)	0.007 (5)
C27	0.037 (5)	0.039 (5)	0.032 (5)	0.011 (4)	−0.004 (4)	0.002 (4)
C28	0.037 (5)	0.037 (5)	0.026 (4)	0.008 (4)	0.005 (4)	0.001 (4)
C29	0.041 (5)	0.036 (5)	0.033 (5)	0.002 (4)	0.001 (4)	−0.002 (4)
C30	0.050 (6)	0.042 (6)	0.037 (5)	0.010 (5)	0.001 (5)	0.009 (5)
C31	0.055 (7)	0.038 (6)	0.050 (6)	−0.001 (5)	−0.006 (5)	0.003 (5)
C32	0.061 (7)	0.026 (4)	0.048 (6)	−0.007 (5)	0.000 (5)	0.003 (4)
C33	0.044 (5)	0.029 (4)	0.027 (4)	0.005 (4)	−0.001 (4)	0.004 (4)
C34	0.037 (5)	0.023 (4)	0.035 (5)	0.006 (4)	−0.003 (4)	−0.004 (4)
C35	0.042 (5)	0.035 (5)	0.034 (5)	−0.007 (4)	0.005 (4)	−0.006 (4)
C36	0.040 (5)	0.032 (5)	0.038 (5)	−0.004 (4)	0.001 (4)	−0.011 (4)
C37	0.040 (5)	0.042 (5)	0.024 (4)	0.009 (4)	−0.007 (4)	−0.003 (4)

C38	0.045 (6)	0.051 (6)	0.033 (5)	−0.001 (5)	0.004 (4)	−0.006 (5)
C39	0.055 (7)	0.056 (7)	0.029 (5)	0.013 (6)	−0.004 (5)	−0.006 (5)
C40	0.049 (6)	0.067 (8)	0.024 (5)	0.019 (6)	0.002 (4)	0.011 (5)
C41	0.044 (6)	0.040 (6)	0.041 (6)	0.002 (5)	0.007 (5)	0.009 (5)
C42	0.036 (5)	0.040 (5)	0.031 (5)	0.011 (4)	0.002 (4)	0.000 (4)
C43	0.037 (5)	0.049 (6)	0.041 (6)	−0.009 (5)	−0.010 (4)	−0.004 (5)
C44	0.031 (5)	0.041 (5)	0.031 (5)	0.003 (4)	−0.005 (4)	−0.010 (4)
C45	0.038 (6)	0.074 (8)	0.055 (7)	−0.007 (6)	−0.007 (5)	−0.021 (6)
C46	0.046 (6)	0.094 (10)	0.029 (5)	−0.016 (7)	−0.014 (5)	−0.016 (6)
C47	0.059 (7)	0.072 (8)	0.028 (5)	0.015 (6)	−0.010 (5)	−0.010 (5)
C48	0.048 (6)	0.047 (6)	0.024 (4)	0.004 (5)	−0.001 (4)	−0.007 (4)
C49	0.063 (6)	0.038 (5)	0.021 (4)	0.006 (5)	−0.002 (4)	0.000 (4)
C50	0.033 (5)	0.041 (5)	0.034 (5)	0.003 (4)	0.001 (4)	0.004 (4)
C51	0.037 (5)	0.044 (6)	0.027 (5)	0.004 (4)	−0.002 (4)	0.006 (4)
C52	0.056 (6)	0.042 (6)	0.037 (5)	−0.010 (5)	−0.011 (5)	0.012 (5)
C53	0.075 (8)	0.036 (6)	0.049 (7)	−0.010 (6)	−0.003 (6)	0.011 (5)
C54	0.072 (8)	0.041 (6)	0.041 (6)	−0.003 (6)	−0.005 (5)	0.004 (5)
C55	0.071 (7)	0.030 (5)	0.035 (5)	0.000 (5)	−0.009 (5)	0.004 (4)
C56	0.040 (5)	0.033 (5)	0.034 (5)	0.013 (4)	−0.002 (4)	0.010 (4)
C57	0.047 (6)	0.071 (8)	0.040 (6)	0.028 (6)	0.000 (5)	0.003 (6)
C58	0.039 (7)	0.162 (15)	0.087 (10)	0.037 (9)	−0.015 (7)	−0.024 (11)
C59	0.121 (12)	0.038 (6)	0.027 (5)	0.021 (7)	0.005 (6)	−0.002 (4)
C60	0.098 (5)	0.091 (5)	0.092 (5)	0.004 (3)	−0.001 (3)	−0.001 (3)
C61	0.032 (5)	0.040 (5)	0.038 (5)	−0.007 (4)	−0.002 (4)	0.001 (4)
C62	0.033 (5)	0.034 (5)	0.041 (5)	−0.004 (4)	0.005 (4)	0.003 (4)
C63	0.050 (6)	0.026 (5)	0.035 (5)	−0.005 (4)	−0.003 (4)	0.001 (4)
C64	0.043 (5)	0.040 (5)	0.038 (5)	−0.011 (4)	−0.010 (4)	0.011 (4)

Geometric parameters (Å, º)

Co1—O2	2.036 (6)	C16—C17	1.428 (14)
Co1—O6	2.031 (6)	C17—C19	1.416 (14)
Co1—O13	2.132 (6)	C17—C21	1.444 (13)
Co1—O14	2.222 (5)	C18—H18	0.9500
Co1—O15	2.201 (6)	C18—C19	1.381 (15)
Co1—O16	2.123 (6)	C18—C20	1.393 (16)
Co2—O5	1.945 (7)	C19—H19	0.9500
Co2—O6	1.969 (6)	C21—H21	0.9500
Co2—O7	1.991 (6)	C22—H22A	0.9900
Co2—O15	2.191 (6)	C22—H22B	0.9900
Co2—N3	2.021 (8)	C22—C23	1.482 (14)
Co3—O7	1.890 (7)	C23—C24	1.399 (14)
Co3—O8	1.898 (6)	C23—C28	1.422 (13)
Co3—O9	1.910 (7)	C24—H24	0.9500
Co3—O13	1.925 (6)	C24—C25	1.372 (14)
Co3—O15	1.907 (6)	C25—H25	0.9500
Co3—N4	1.923 (8)	C25—C26	1.365 (15)
Co4—O4	2.111 (6)	C26—H26	0.9500

Co4—O8	2.097 (6)	C26—C27	1.408 (13)
Co4—O10	2.057 (7)	C27—H27	0.9500
Co4—O11	2.039 (7)	C27—C28	1.396 (13)
Co4—O13	2.070 (6)	C29—H29	0.9500
Co4—O16	2.083 (6)	C29—C30	1.378 (14)
Co5—O3	1.874 (7)	C29—C34	1.397 (13)
Co5—O4	1.897 (6)	C30—H30	0.9500
Co5—O12	1.902 (7)	C30—C31	1.362 (15)
Co5—O14	1.909 (6)	C31—H31	0.9500
Co5—O16	1.921 (6)	C31—C32	1.394 (15)
Co5—N2	1.924 (8)	C32—H32	0.9500
Co6—O1	1.937 (6)	C32—C33	1.376 (13)
Co6—O2	1.989 (6)	C33—C34	1.399 (13)
Co6—O3	2.000 (7)	C33—C35	1.511 (13)
Co6—O14	2.156 (6)	C35—H35A	0.9900
Co6—N1	2.012 (8)	C35—H35B	0.9900
Cl1—C2	1.731 (12)	C36—H36	0.9500
Cl2—C54	1.727 (11)	C36—C37	1.433 (14)
Cl3—C40	1.738 (11)	C37—C38	1.404 (13)
Cl4—C20	1.734 (11)	C37—C42	1.425 (14)
O1—C16	1.324 (11)	C38—H38	0.9500
O2—C28	1.367 (10)	C38—C39	1.362 (15)
O3—C14	1.380 (11)	C39—H39	0.9500
O4—C6	1.322 (11)	C39—C40	1.394 (16)
O5—C42	1.311 (11)	C40—C41	1.366 (15)
O6—C34	1.373 (10)	C41—H41	0.9500
O7—C44	1.364 (10)	C41—C42	1.410 (13)
O8—C56	1.336 (11)	C43—H43	0.9500
O9—C57	1.265 (12)	C43—C44	1.400 (14)
O10—C57	1.264 (13)	C43—C45	1.414 (14)
O11—C59	1.268 (13)	C44—C48	1.369 (13)
O12—C59	1.265 (14)	C45—H45	0.9500
O13—C61	1.417 (11)	C45—C46	1.381 (17)
O14—C62	1.432 (10)	C46—H46	0.9500
O15—C64	1.447 (11)	C46—C47	1.387 (17)
O16—C63	1.428 (11)	C47—H47	0.9500
N1—C21	1.290 (12)	C47—C48	1.405 (14)
N1—C22	1.462 (12)	C48—C49	1.493 (15)
N2—C7	1.274 (12)	C49—H49A	0.9900
N2—C8	1.500 (12)	C49—H49B	0.9900
N3—C35	1.473 (12)	C50—H50	0.9500
N3—C36	1.294 (11)	C50—C51	1.407 (14)
N4—C49	1.469 (12)	C51—C52	1.420 (14)
N4—C50	1.304 (13)	C51—C56	1.403 (13)
C1—H1	0.9500	C52—H52	0.9500
C1—C2	1.363 (15)	C52—C53	1.361 (15)
C1—C6	1.426 (14)	C53—H53	0.9500
C2—C3	1.407 (16)	C53—C54	1.408 (15)

C3—H3	0.9500	C54—C55	1.364 (14)
C3—C4	1.352 (16)	C55—H55	0.9500
C4—H4	0.9500	C55—C56	1.424 (14)
C4—C5	1.393 (14)	C57—C58	1.509 (16)
C5—C6	1.411 (14)	C58—H58A	0.9800
C5—C7	1.431 (14)	C58—H58B	0.9800
C7—H7	0.9500	C58—H58C	0.9800
C8—H8A	0.9900	C59—C60	1.507 (19)
C8—H8B	0.9900	C60—H60A	0.9800
C8—C9	1.490 (14)	C60—H60B	0.9800
C9—C10	1.375 (14)	C60—H60C	0.9800
C9—C14	1.377 (13)	C61—H61A	0.9800
C10—H10	0.9500	C61—H61B	0.9800
C10—C11	1.385 (16)	C61—H61C	0.9800
C11—H11	0.9500	C62—H62A	0.9800
C11—C12	1.428 (16)	C62—H62B	0.9800
C12—H12	0.9500	C62—H62C	0.9800
C12—C13	1.388 (14)	C63—H63A	0.9800
C13—H13	0.9500	C63—H63B	0.9800
C13—C14	1.417 (14)	C63—H63C	0.9800
C15—H15	0.9500	C64—H64A	0.9800
C15—C16	1.396 (14)	C64—H64B	0.9800
C15—C20	1.354 (14)	C64—H64C	0.9800

O2—Co1—O13	170.5 (2)	C14—C13—H13	121.2
O2—Co1—O14	79.2 (2)	O3—C14—C13	119.9 (9)
O2—Co1—O15	106.6 (2)	C9—C14—O3	117.8 (9)
O2—Co1—O16	91.9 (2)	C9—C14—C13	122.3 (9)
O6—Co1—O2	97.8 (3)	C16—C15—H15	118.3
O6—Co1—O13	90.8 (2)	C20—C15—H15	118.3
O6—Co1—O14	106.3 (2)	C20—C15—C16	123.4 (10)
O6—Co1—O15	79.6 (2)	O1—C16—C15	119.8 (9)
O6—Co1—O16	169.5 (3)	O1—C16—C17	123.6 (8)
O13—Co1—O14	102.1 (2)	C15—C16—C17	116.6 (9)
O13—Co1—O15	71.1 (2)	C16—C17—C21	125.0 (8)
O15—Co1—O14	171.3 (2)	C19—C17—C16	119.0 (9)
O16—Co1—O13	79.8 (2)	C19—C17—C21	116.0 (9)
O16—Co1—O14	71.5 (2)	C19—C18—H18	121.1
O16—Co1—O15	101.4 (2)	C19—C18—C20	117.8 (10)
O5—Co2—O6	131.1 (3)	C20—C18—H18	121.1
O5—Co2—O7	119.4 (3)	C17—C19—H19	119.0
O5—Co2—O15	98.7 (3)	C18—C19—C17	122.1 (11)
O5—Co2—N3	92.7 (3)	C18—C19—H19	119.0
O6—Co2—O7	108.0 (3)	C15—C20—Cl4	120.3 (9)
O6—Co2—O15	81.2 (2)	C15—C20—C18	121.1 (10)
O6—Co2—N3	90.6 (3)	C18—C20—Cl4	118.6 (8)
O7—Co2—O15	75.5 (2)	N1—C21—C17	125.1 (9)
O7—Co2—N3	99.8 (3)	N1—C21—H21	117.4

N3—Co2—O15	168.6 (3)	C17—C21—H21	117.4
O7—Co3—O8	173.8 (3)	N1—C22—H22A	109.8
O7—Co3—O9	91.8 (3)	N1—C22—H22B	109.8
O7—Co3—O13	88.2 (3)	N1—C22—C23	109.3 (8)
O7—Co3—O15	84.9 (3)	H22A—C22—H22B	108.3
O7—Co3—N4	91.9 (3)	C23—C22—H22A	109.8
O8—Co3—O9	90.1 (3)	C23—C22—H22B	109.8
O8—Co3—O13	85.7 (3)	C24—C23—C22	121.7 (9)
O8—Co3—O15	92.7 (3)	C24—C23—C28	117.1 (9)
O8—Co3—N4	94.0 (3)	C28—C23—C22	121.2 (9)
O9—Co3—O13	93.4 (3)	C23—C24—H24	118.7
O9—Co3—N4	88.0 (3)	C25—C24—C23	122.5 (10)
O15—Co3—O9	174.6 (3)	C25—C24—H24	118.7
O15—Co3—O13	82.2 (2)	C24—C25—H25	119.8
O15—Co3—N4	96.4 (3)	C26—C25—C24	120.3 (9)
N4—Co3—O13	178.6 (3)	C26—C25—H25	119.8
O8—Co4—O4	160.1 (2)	C25—C26—H26	120.1
O10—Co4—O4	107.4 (3)	C25—C26—C27	119.8 (10)
O10—Co4—O8	86.6 (3)	C27—C26—H26	120.1
O10—Co4—O13	89.9 (3)	C26—C27—H27	120.0
O10—Co4—O16	170.9 (3)	C28—C27—C26	120.1 (10)
O11—Co4—O4	85.6 (3)	C28—C27—H27	120.0
O11—Co4—O8	107.3 (3)	O2—C28—C23	119.9 (8)
O11—Co4—O10	96.3 (3)	O2—C28—C27	120.1 (8)
O11—Co4—O13	172.5 (3)	C27—C28—C23	120.0 (9)
O11—Co4—O16	91.9 (3)	C30—C29—H29	119.5
O13—Co4—O4	88.5 (2)	C30—C29—C34	121.0 (10)
O13—Co4—O8	77.2 (2)	C34—C29—H29	119.5
O13—Co4—O16	82.2 (2)	C29—C30—H30	120.7
O16—Co4—O4	77.0 (2)	C31—C30—C29	118.7 (10)
O16—Co4—O8	87.2 (3)	C31—C30—H30	120.7
O3—Co5—O4	173.4 (3)	C30—C31—H31	119.5
O3—Co5—O12	92.8 (3)	C30—C31—C32	120.9 (10)
O3—Co5—O14	85.2 (3)	C32—C31—H31	119.5
O3—Co5—O16	87.9 (3)	C31—C32—H32	119.3
O3—Co5—N2	91.6 (3)	C33—C32—C31	121.4 (9)
O4—Co5—O12	90.5 (3)	C33—C32—H32	119.3
O4—Co5—O14	91.1 (3)	C32—C33—C34	117.6 (8)
O4—Co5—O16	86.3 (3)	C32—C33—C35	119.6 (9)
O4—Co5—N2	94.2 (3)	C34—C33—C35	122.8 (8)
O12—Co5—O14	176.1 (3)	O6—C34—C29	119.7 (8)
O12—Co5—O16	93.4 (3)	O6—C34—C33	120.2 (8)
O12—Co5—N2	86.2 (3)	C29—C34—C33	120.1 (8)
O14—Co5—O16	83.1 (2)	N3—C35—C33	108.4 (8)
O14—Co5—N2	97.2 (3)	N3—C35—H35A	110.0
O16—Co5—N2	179.4 (3)	N3—C35—H35B	110.0
O1—Co6—O2	134.7 (3)	C33—C35—H35A	110.0
O1—Co6—O3	118.0 (3)	C33—C35—H35B	110.0

O1—Co6—O14	95.6 (2)	H35A—C35—H35B	108.4
O1—Co6—N1	93.1 (3)	N3—C36—H36	117.2
O2—Co6—O3	105.3 (3)	N3—C36—C37	125.5 (9)
O2—Co6—O14	81.9 (2)	C37—C36—H36	117.2
O2—Co6—N1	90.6 (3)	C38—C37—C36	116.9 (9)
O3—Co6—O14	76.0 (2)	C38—C37—C42	119.0 (9)
O3—Co6—N1	101.5 (3)	C42—C37—C36	124.0 (8)
N1—Co6—O14	171.1 (3)	C37—C38—H38	118.5
C16—O1—Co6	127.4 (6)	C39—C38—C37	122.9 (11)
Co6—O2—Co1	104.8 (3)	C39—C38—H38	118.5
C28—O2—Co1	131.3 (5)	C38—C39—H39	121.1
C28—O2—Co6	123.2 (5)	C38—C39—C40	117.8 (10)
Co5—O3—Co6	102.7 (3)	C40—C39—H39	121.1
C14—O3—Co5	117.8 (6)	C39—C40—Cl3	119.3 (9)
C14—O3—Co6	129.8 (6)	C41—C40—Cl3	119.3 (10)
Co5—O4—Co4	95.9 (3)	C41—C40—C39	121.4 (10)
C6—O4—Co4	130.2 (6)	C40—C41—H41	119.1
C6—O4—Co5	127.2 (6)	C40—C41—C42	121.9 (10)
C42—O5—Co2	126.4 (6)	C42—C41—H41	119.1
Co2—O6—Co1	105.5 (3)	O5—C42—C37	125.5 (9)
C34—O6—Co1	129.8 (5)	O5—C42—C41	117.8 (9)
C34—O6—Co2	124.7 (5)	C41—C42—C37	116.8 (9)
Co3—O7—Co2	103.5 (3)	C44—C43—H43	120.2
C44—O7—Co2	127.8 (6)	C44—C43—C45	119.5 (10)
C44—O7—Co3	118.3 (6)	C45—C43—H43	120.2
Co3—O8—Co4	96.3 (3)	O7—C44—C43	120.5 (9)
C56—O8—Co3	127.6 (6)	O7—C44—C48	118.4 (9)
C56—O8—Co4	130.9 (6)	C48—C44—C43	121.2 (9)
C57—O9—Co3	128.6 (7)	C43—C45—H45	120.7
C57—O10—Co4	125.2 (7)	C46—C45—C43	118.6 (11)
C59—O11—Co4	124.4 (7)	C46—C45—H45	120.7
C59—O12—Co5	127.7 (7)	C45—C46—H46	119.3
Co3—O13—Co1	103.7 (3)	C45—C46—C47	121.5 (10)
Co3—O13—Co4	96.3 (3)	C47—C46—H46	119.3
Co4—O13—Co1	99.1 (2)	C46—C47—H47	120.1
C61—O13—Co1	117.1 (5)	C46—C47—C48	119.8 (11)
C61—O13—Co3	119.2 (5)	C48—C47—H47	120.1
C61—O13—Co4	117.6 (5)	C44—C48—C47	119.3 (10)
Co5—O14—Co1	100.6 (2)	C44—C48—C49	118.1 (8)
Co5—O14—Co6	96.1 (2)	C47—C48—C49	122.5 (10)
Co6—O14—Co1	93.5 (2)	N4—C49—C48	112.3 (8)
C62—O14—Co1	123.3 (5)	N4—C49—H49A	109.1
C62—O14—Co5	117.1 (5)	N4—C49—H49B	109.1
C62—O14—Co6	120.7 (5)	C48—C49—H49A	109.1
Co2—O15—Co1	93.0 (2)	C48—C49—H49B	109.1
Co3—O15—Co1	101.8 (3)	H49A—C49—H49B	107.9
Co3—O15—Co2	95.9 (2)	N4—C50—H50	117.1
C64—O15—Co1	121.5 (5)	N4—C50—C51	125.8 (9)

C64—O15—Co2	120.3 (6)	C51—C50—H50	117.1
C64—O15—Co3	118.6 (5)	C50—C51—C52	116.6 (8)
Co4—O16—Co1	99.0 (2)	C56—C51—C50	125.4 (9)
Co5—O16—Co1	103.8 (3)	C56—C51—C52	118.1 (9)
Co5—O16—Co4	96.1 (3)	C51—C52—H52	118.7
C63—O16—Co1	117.3 (5)	C53—C52—C51	122.6 (10)
C63—O16—Co4	118.0 (5)	C53—C52—H52	118.7
C63—O16—Co5	118.9 (5)	C52—C53—H53	121.0
C21—N1—Co6	125.1 (7)	C52—C53—C54	117.9 (10)
C21—N1—C22	119.9 (8)	C54—C53—H53	121.0
C22—N1—Co6	114.6 (6)	C53—C54—Cl2	119.3 (9)
C7—N2—Co5	125.1 (7)	C55—C54—Cl2	118.2 (8)
C7—N2—C8	117.6 (8)	C55—C54—C53	122.4 (10)
C8—N2—Co5	117.1 (6)	C54—C55—H55	120.3
C35—N3—Co2	115.0 (6)	C54—C55—C56	119.3 (9)
C36—N3—Co2	124.7 (7)	C56—C55—H55	120.3
C36—N3—C35	120.2 (8)	O8—C56—C51	121.9 (9)
C49—N4—Co3	117.3 (6)	O8—C56—C55	118.4 (8)
C50—N4—Co3	124.8 (7)	C51—C56—C55	119.7 (9)
C50—N4—C49	117.9 (8)	O9—C57—C58	115.4 (11)
C2—C1—H1	120.6	O10—C57—O9	126.9 (10)
C2—C1—C6	118.7 (9)	O10—C57—C58	117.7 (10)
C6—C1—H1	120.6	C57—C58—H58A	109.5
C1—C2—Cl1	117.2 (9)	C57—C58—H58B	109.5
C1—C2—C3	122.8 (11)	C57—C58—H58C	109.5
C3—C2—Cl1	120.0 (8)	H58A—C58—H58B	109.5
C2—C3—H3	121.2	H58A—C58—H58C	109.5
C4—C3—C2	117.6 (10)	H58B—C58—H58C	109.5
C4—C3—H3	121.2	O11—C59—C60	116.9 (12)
C3—C4—H4	118.5	O12—C59—O11	127.9 (10)
C3—C4—C5	123.0 (10)	O12—C59—C60	115.1 (11)
C5—C4—H4	118.5	C59—C60—H60A	109.5
C4—C5—C6	118.7 (9)	C59—C60—H60B	109.5
C4—C5—C7	117.1 (9)	C59—C60—H60C	109.5
C6—C5—C7	124.2 (9)	H60A—C60—H60B	109.5
O4—C6—C1	118.4 (9)	H60A—C60—H60C	109.5
O4—C6—C5	122.6 (9)	H60B—C60—H60C	109.5
C5—C6—C1	119.0 (8)	O13—C61—H61A	109.5
N2—C7—C5	126.0 (9)	O13—C61—H61B	109.5
N2—C7—H7	117.0	O13—C61—H61C	109.5
C5—C7—H7	117.0	H61A—C61—H61B	109.5
N2—C8—H8A	109.2	H61A—C61—H61C	109.5
N2—C8—H8B	109.2	H61B—C61—H61C	109.5
H8A—C8—H8B	107.9	O14—C62—H62A	109.5
C9—C8—N2	111.9 (8)	O14—C62—H62B	109.5
C9—C8—H8A	109.2	O14—C62—H62C	109.5
C9—C8—H8B	109.2	H62A—C62—H62B	109.5
C10—C9—C8	123.0 (9)	H62A—C62—H62C	109.5

C10—C9—C14	119.2 (10)	H62B—C62—H62C	109.5
C14—C9—C8	117.7 (8)	O16—C63—H63A	109.5
C9—C10—H10	119.4	O16—C63—H63B	109.5
C9—C10—C11	121.3 (10)	O16—C63—H63C	109.5
C11—C10—H10	119.4	H63A—C63—H63B	109.5
C10—C11—H11	120.4	H63A—C63—H63C	109.5
C10—C11—C12	119.2 (10)	H63B—C63—H63C	109.5
C12—C11—H11	120.4	O15—C64—H64A	109.5
C11—C12—H12	119.8	O15—C64—H64B	109.5
C13—C12—C11	120.4 (11)	O15—C64—H64C	109.5
C13—C12—H12	119.8	H64A—C64—H64B	109.5
C12—C13—H13	121.2	H64A—C64—H64C	109.5
C12—C13—C14	117.6 (10)	H64B—C64—H64C	109.5

Co1—O2—C28—C23	150.5 (7)	C4—C5—C6—C1	1.2 (15)
Co1—O2—C28—C27	−30.5 (12)	C4—C5—C7—N2	−179.6 (10)
Co1—O6—C34—C29	−36.0 (12)	C6—C1—C2—Cl1	−174.2 (9)
Co1—O6—C34—C33	143.4 (7)	C6—C1—C2—C3	3.1 (19)
Co2—O5—C42—C37	−2.7 (13)	C6—C5—C7—N2	1.8 (17)
Co2—O5—C42—C41	177.4 (7)	C7—N2—C8—C9	−127.1 (9)
Co2—O6—C34—C29	142.0 (7)	C7—C5—C6—O4	−1.1 (16)
Co2—O6—C34—C33	−38.6 (11)	C7—C5—C6—C1	179.8 (10)
Co2—O7—C44—C43	94.2 (10)	C8—N2—C7—C5	179.8 (9)
Co2—O7—C44—C48	−86.5 (10)	C8—C9—C10—C11	177.2 (10)
Co2—N3—C35—C33	−67.2 (9)	C8—C9—C14—O3	4.3 (14)
Co2—N3—C36—C37	4.8 (14)	C8—C9—C14—C13	−177.7 (10)
Co3—O7—C44—C43	−126.8 (8)	C9—C10—C11—C12	0.6 (17)
Co3—O7—C44—C48	52.4 (10)	C10—C9—C14—O3	−176.6 (9)
Co3—O8—C56—C51	−7.8 (13)	C10—C9—C14—C13	1.5 (16)
Co3—O8—C56—C55	174.7 (7)	C10—C11—C12—C13	1.3 (17)
Co3—O9—C57—O10	−1.9 (19)	C11—C12—C13—C14	−1.8 (17)
Co3—O9—C57—C58	178.5 (11)	C12—C13—C14—O3	178.4 (10)
Co3—N4—C49—C48	49.1 (10)	C12—C13—C14—C9	0.4 (16)
Co3—N4—C50—C51	3.2 (14)	C14—C9—C10—C11	−2.0 (16)
Co4—O4—C6—C1	28.7 (13)	C15—C16—C17—C19	−1.9 (14)
Co4—O4—C6—C5	−150.4 (8)	C15—C16—C17—C21	175.5 (9)
Co4—O8—C56—C51	−156.0 (7)	C16—C15—C20—Cl4	180.0 (8)
Co4—O8—C56—C55	26.5 (13)	C16—C15—C20—C18	0.8 (17)
Co4—O10—C57—O9	2.0 (19)	C16—C17—C19—C18	0.6 (16)
Co4—O10—C57—C58	−178.4 (11)	C16—C17—C21—N1	6.9 (16)
Co4—O11—C59—O12	7 (2)	C19—C17—C21—N1	−175.6 (10)
Co4—O11—C59—C60	−177.1 (10)	C19—C18—C20—Cl4	178.7 (9)
Co5—O3—C14—C9	55.1 (11)	C19—C18—C20—C15	−2.1 (17)
Co5—O3—C14—C13	−123.0 (9)	C20—C15—C16—O1	−178.6 (9)
Co5—O4—C6—C1	172.9 (7)	C20—C15—C16—C17	1.3 (15)
Co5—O4—C6—C5	−6.2 (13)	C20—C18—C19—C17	1.4 (17)
Co5—O12—C59—O11	−12 (2)	C21—N1—C22—C23	104.6 (10)
Co5—O12—C59—C60	172.4 (10)	C21—C17—C19—C18	−177.0 (10)

Co5—N2—C7—C5	4.8 (15)	C22—N1—C21—C17	−172.7 (9)
Co5—N2—C8—C9	48.4 (10)	C22—C23—C24—C25	176.7 (9)
Co6—O1—C16—C15	175.9 (7)	C22—C23—C28—O2	4.2 (14)
Co6—O1—C16—C17	−4.0 (13)	C22—C23—C28—C27	−174.8 (9)
Co6—O2—C28—C23	−41.1 (11)	C23—C24—C25—C26	−0.8 (15)
Co6—O2—C28—C27	137.9 (7)	C24—C23—C28—O2	−177.7 (8)
Co6—O3—C14—C9	−84.4 (11)	C24—C23—C28—C27	3.3 (14)
Co6—O3—C14—C13	97.5 (10)	C24—C25—C26—C27	1.2 (15)
Co6—N1—C21—C17	−0.4 (14)	C25—C26—C27—C28	0.7 (15)
Co6—N1—C22—C23	−68.5 (9)	C26—C27—C28—O2	178.0 (8)
Cl1—C2—C3—C4	174.3 (10)	C26—C27—C28—C23	−3.0 (14)
Cl2—C54—C55—C56	−179.0 (9)	C28—C23—C24—C25	−1.5 (15)
Cl3—C40—C41—C42	−177.6 (8)	C29—C30—C31—C32	1.9 (17)
O1—C16—C17—C19	178.0 (9)	C30—C29—C34—O6	173.2 (9)
O1—C16—C17—C21	−4.6 (15)	C30—C29—C34—C33	−6.2 (14)
O7—C44—C48—C47	−177.3 (9)	C30—C31—C32—C33	−1.6 (17)
O7—C44—C48—C49	4.4 (13)	C31—C32—C33—C34	−2.6 (15)
O9—Co3—O7—Co2	−172.2 (3)	C31—C32—C33—C35	178.6 (10)
O9—Co3—O7—C44	40.1 (7)	C32—C33—C34—O6	−173.0 (9)
O9—Co3—O8—Co4	77.2 (3)	C32—C33—C34—C29	6.4 (14)
O9—Co3—O8—C56	−79.2 (8)	C32—C33—C35—N3	−132.3 (9)
O12—Co5—O3—Co6	−175.3 (3)	C34—C29—C30—C31	2.0 (15)
O12—Co5—O3—C14	35.4 (7)	C34—C33—C35—N3	49.0 (12)
O12—Co5—O4—Co4	76.5 (3)	C35—N3—C36—C37	−172.1 (9)
O12—Co5—O4—C6	−76.8 (7)	C35—C33—C34—O6	5.7 (14)
O13—Co3—O7—Co2	−78.8 (3)	C35—C33—C34—C29	−174.9 (9)
O13—Co3—O7—C44	133.4 (6)	C36—N3—C35—C33	109.9 (10)
O13—Co3—O8—Co4	−16.3 (3)	C36—C37—C38—C39	−175.8 (10)
O13—Co3—O8—C56	−172.6 (8)	C36—C37—C42—O5	−7.0 (15)
O14—Co5—O3—Co6	1.3 (3)	C36—C37—C42—C41	172.9 (9)
O14—Co5—O3—C14	−148.0 (7)	C37—C38—C39—C40	2.8 (16)
O14—Co5—O4—Co4	−99.9 (2)	C38—C37—C42—O5	176.1 (9)
O14—Co5—O4—C6	106.8 (7)	C38—C37—C42—C41	−4.0 (13)
O15—Co3—O7—Co2	3.5 (3)	C38—C39—C40—Cl3	174.8 (8)
O15—Co3—O7—C44	−144.3 (7)	C38—C39—C40—C41	−4.2 (15)
O15—Co3—O8—Co4	−98.2 (3)	C39—C40—C41—C42	1.4 (16)
O15—Co3—O8—C56	105.4 (8)	C40—C41—C42—O5	−177.4 (9)
O16—Co5—O3—Co6	−82.0 (3)	C40—C41—C42—C37	2.7 (14)
O16—Co5—O3—C14	128.8 (6)	C42—C37—C38—C39	1.4 (15)
O16—Co5—O4—Co4	−16.9 (2)	C43—C44—C48—C47	1.9 (15)
O16—Co5—O4—C6	−170.2 (7)	C43—C44—C48—C49	−176.3 (9)
N1—C22—C23—C24	−125.0 (10)	C43—C45—C46—C47	2.4 (18)
N1—C22—C23—C28	53.1 (12)	C44—C43—C45—C46	−3.4 (17)
N2—Co5—O3—Co6	98.4 (3)	C44—C48—C49—N4	−57.7 (12)
N2—Co5—O3—C14	−50.9 (7)	C45—C43—C44—O7	−179.5 (10)
N2—Co5—O4—Co4	162.8 (3)	C45—C43—C44—C48	1.2 (15)
N2—Co5—O4—C6	9.5 (8)	C45—C46—C47—C48	0.8 (18)
N2—C8—C9—C10	123.2 (10)	C46—C47—C48—C44	−3.0 (16)

N2—C8—C9—C14	−57.7 (12)	C46—C47—C48—C49	175.2 (10)
N3—C36—C37—C38	−177.4 (10)	C47—C48—C49—N4	124.2 (10)
N3—C36—C37—C42	5.6 (16)	C49—N4—C50—C51	−178.7 (9)
N4—Co3—O7—Co2	99.8 (3)	C50—N4—C49—C48	−129.2 (9)
N4—Co3—O7—C44	−48.0 (7)	C50—C51—C52—C53	−179.8 (11)
N4—Co3—O8—Co4	165.1 (3)	C50—C51—C56—O8	1.9 (15)
N4—Co3—O8—C56	8.8 (8)	C50—C51—C56—C55	179.4 (10)
N4—C50—C51—C52	179.8 (10)	C51—C52—C53—C54	−0.3 (18)
N4—C50—C51—C56	0.4 (16)	C52—C51—C56—O8	−177.5 (9)
C1—C2—C3—C4	−3 (2)	C52—C51—C56—C55	−0.1 (15)
C2—C1—C6—O4	178.7 (11)	C52—C53—C54—Cl2	178.6 (10)
C2—C1—C6—C5	−2.1 (16)	C52—C53—C54—C55	1.2 (19)
C2—C3—C4—C5	1.9 (19)	C53—C54—C55—C56	−1.6 (19)
C3—C4—C5—C6	−1.1 (17)	C54—C55—C56—O8	178.5 (10)
C3—C4—C5—C7	−179.8 (11)	C54—C55—C56—C51	1.0 (16)
C4—C5—C6—O4	−179.7 (9)	C56—C51—C52—C53	−0.3 (16)