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A two-dimensional Co^{II} coordination polymer with the ligand 1,1′-bis[(1*H*-1,2,4-triazol-1-yl)methyl]ferrocene

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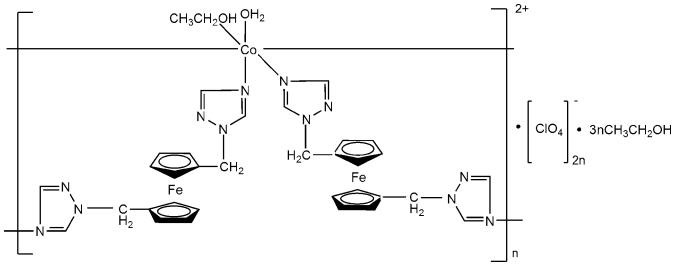
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.009 Å; R factor = 0.057; wR factor = 0.190; data-to-parameter ratio = 15.3.

In the title polymer, poly[[aquabis{μ_2-1,1′-bis[(1*H*-1,2,4-triazol-1-yl)methyl]ferrocene-κ^2N^4:$N^{4'}$}ethanolcobalt(II)] bis(perchlorate) ethanol trisolvate], $\{[CoFe_2(C_8H_8N_3)_4(C_2H_6O)(H_2O)](ClO_4)_2\cdot 3C_6H_6O\}_n$ or $\{[Co(btmf)_2(EtOH)(H_2O)](ClO_4)_2\cdot 3EtOH\}_n$, where btmf is the ferrocene-containing ligand, the Co^{II} ion is six-coordinated by four N atoms from btmf ligands, one O atom from a water molecule and one O atom from an ethanol molecule. The btmf ligands connect the Co^{II} ions to form layers and these layers are organized by hydrogen bonds, expanding the crystal structure to a three-dimensional supramolecular network.

Related literature

For related literature, see: Chen *et al.* (2005); Gao *et al.* (2004, 2006); Dong *et al.* (2003); Han *et al.* (2005); Jia *et al.* (2007); Li *et al.* (2003); Wilkes *et al.* (1995).



Experimental

Crystal data

$[CoFe_2(C_8H_8N_3)_4(C_2H_6O)(H_2O)](ClO_4)_2\cdot 3C_6H_6O[$
M_r = 1156.51
Monoclinic, $P2_1/n$
a = 17.3708 (11) Å
b = 14.2250 (9) Å
c = 21.2747 (14) Å
β = 94.224 (1)°
V = 5242.7 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.03 mm^{-1}
T = 291 (2) K
0.20 × 0.15 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.817, T_{max} = 0.919
27120 measured reflections
9696 independent reflections
6313 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.190
S = 1.02
9696 reflections
635 parameters
720 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1D···O2	0.93	1.74	2.665 (6)	174
O2—H2D···Cl2^{i}	0.82	2.87	3.620 (6)	153
O3—H3D···O8	0.85	2.08	2.906 (12)	162
O3—H3D···Cl1	0.85	2.90	3.687 (8)	153
O4—H4D···N5^{ii}	0.84	2.05	2.871 (8)	164
O13—H1W···O3	0.85	1.92	2.677 (7)	148
O13—H2W···O4	0.90	2.06	2.622 (7)	119

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2097).

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supplementary materials

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A two-dimensional Co^{II} coordination polymer with the ligand 1,1'-bis[(1*H*-1,2,4-triazol-1-yl)methyl]ferrocene

X.-L. Zhou, X.-R. Meng and H.-W. Hou

Comment

Within the research field of metal-organic compounds, ferrocene derivatives have attracted much attention in the construction of metal-organic polymers and supramolecular architectures, due to their potential applications: electrochemical sensors, potential antitumor agents, monomers for extended stacked complexes, and even units for self-assembly (Li *et al.*, 2003). We use ferrocene-containing ligand 1,1'-bis[(1*H*-1,2,4-triazol-1-yl)methyl]ferrocene, btmf, to construct ferrocene-containing metal-organic polymers (Gao *et al.*, 2004, 2006). It is suggested that introducing ferrocene groups into coordination polymers can lead to interesting assembled structures, because of their conformational flexibility. The ferrocene groups usually behave as the ball-joints, and so the bidentate representatives can adapt as chelating or bridging groups to different geometric requirements of the metal centers (Dong *et al.*, 2003). Herein, we describe a metal-organic polymer of Co^{II} with btmf, in which ferrocene-based ligands behave as bridges connecting the adjacent Co^{II} ions to form a two dimensional network. Fig. 1 depicts the coordination geometry of the Co^{II} center. Each Co^{II} ion is coordinated by four N atoms from btmf ligands [N1, N7, N6^{i} and N12^{ii}; symmetry codes: (i) 3/2 − *x*, 1/2 + *y*, 1/2 - *z;* (ii) 3/2 − *x*, 1/2 + *y*, 3/2 − *z*], one O atom (O13) from water molecule and one O atom (O1) from an ethanol molecule, leading to an slightly distorted octahedral geometry. The Co1—N bond lengths range from 2.149 (4) to 2.157 (4) Å (see deposited Table), and they are all within the range of those reported for related complexes (Han *et al.* 2005, Chen *et al.*, 2005). The Co1—O1 bond length of 2.118 (3) Å and Co1—O13 = 2.093 (4) Å are also close to those reported in analogous compounds (*e.g.* Jia *et al.*, 2007). *Cis* and *trans* angles around Co^{II} ion range from 88.06 (15)° to 93.51 (15) and 177.00 (16) to 178.09 (16)°. Fig. 2 displays the packing arrangement of the title compound, in which the btmf bridging ligands connect the Co^{II} ions to form layers parallel to the *bc* plane. The repeating unit of the two dimensional network possesses a 8-membered grid (size *ca*. 12.701×12.922 Å^2) which is composed of four btmf groups acting as four edges and four Co^{II} ions representing the four vertexes. These two dimensional layers are interconnected by extensive hydrogen bonds, leading to a three dimensional supramolecular framework (Fig. 3).

Experimental

Dichloromethane was distilled from P_2O_5. Other chemicals (A·*R*. Grade) were obtained commercially without further purification. The preparation of btmf followed a published method (Wilkes *et al.*, 1995) and was modified by us. The title polymer was synthesized as follows: A solution of btmf (3.5 mg, 0.01 mmol) in ethanol (5 cm^3) was slowly added to a solution of $Co(ClO_4)_2$ (2.6 mg, 0.01 mmol) in ethanol (3 cm^3) and water. The mixture was sealed in a small glass vial and allowed to stand over 36 h. Orange single crystals appeared after this time. Yield: 49%. Anal. Calcd for $C_{40}H_{58}Cl_2CoFe_2N_{12}O_{13}$: C 41.54, H 5.05, N 14.53%. Found: C 41.50, H 4.96, N 14.52%.

Refinement

Hydroxy H atoms of the water and ethanol molecules were located in a difference map and refined with isotropic displacement parameters fixed to U_{iso}(H) = 1.5U_{eq}(carrier O). Other H atoms were included in calculated positions and refined using a riding model, with C—H = 0.93–0.98 Å, and U_{iso}(H) = 1.5U_{eq}(carrier C) for methyl groups and U_{iso}(H) = 1.2U_{eq}(carrier C) otherwise.

Figures

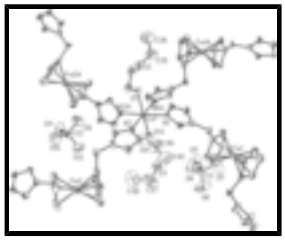


Fig. 1. Coordination geometry of the Co^{II} center in the title polymer with atom numbering, showing 30% displacement ellipsoids. H atoms have been omitted for clarity.

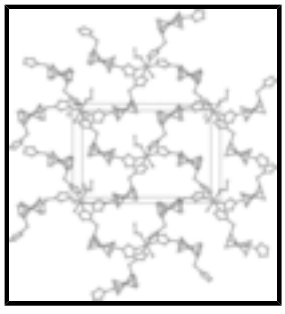


Fig. 2. Two dimensional layered structure of the title polymer, in which all H atoms, lattice solvents and counterions are omitted for clarity.

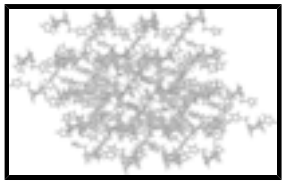


Fig. 3. Packing diagram of the title compound, showing the three-dimensional supramolecular network.

poly[[aquabis{μ$_2$-1,1'-bis[(1*H*-1,2,4-triazol-1-yl)methyl]\ ferrocene-κ$^2N^4$:$N^{4'}$}ethanolcobalt(II)] bis(perchlorate) ethanol trisolvate]

Crystal data

$[CoFe_2(C_8H_8N_3)_4(C_2H_6O)(H_2O)](ClO_4)_2·C_6H_6O$	F_{000} = 2396
M_r = 1156.51	D_x = 1.465 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 4968 reflections
a = 17.3708 (11) Å	θ = 2.4–23.7º
b = 14.2250 (9) Å	μ = 1.03 mm^{-1}
c = 21.2747 (14) Å	T = 291 (2) K
β = 94.224 (1)º	Block, orange

V = 5242.7 (6) Å^3
Z = 4

0.20 × 0.15 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
T = 291(2) K
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.817, T_{max} = 0.919
27120 measured reflections

9696 independent reflections
6313 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.5º
θ_{min} = 2.4º
h = −21→20
k = −17→17
l = −16→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.190
S = 1.02
9696 reflections
635 parameters
720 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0987P)^2 + 5.0582P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}
Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.76780 (4)	0.47416 (4)	0.50420 (3)	0.04369 (19)
Fe1	0.99384 (4)	0.41748 (5)	0.16723 (3)	0.0454 (2)
Fe2	0.98856 (4)	0.00490 (5)	0.66848 (3)	0.0572 (2)
Cl1	0.73105 (11)	0.25768 (14)	0.22650 (10)	0.0969 (6)
Cl2	0.79526 (10)	0.25124 (11)	0.75988 (8)	0.0780 (4)
O1	0.8175 (2)	0.5938 (2)	0.55053 (15)	0.0562 (8)
H1D	0.7822	0.6420	0.5547	0.084*
O2	0.7185 (4)	0.7314 (4)	0.5717 (3)	0.136 (2)
H2D	0.6989	0.7381	0.6053	0.204*
O3	0.7871 (4)	0.2248 (5)	0.3956 (3)	0.157 (3)
H3D	0.7918	0.2335	0.3563	0.236*
O4	0.5688 (3)	0.3181 (6)	0.4625 (3)	0.176 (3)
H4D	0.5396	0.3464	0.4862	0.265*
O5	0.6616 (5)	0.2462 (6)	0.2507 (5)	0.204 (4)

O6	0.7527 (4)	0.1720 (6)	0.2071 (5)	0.204 (4)
O7	0.7274 (6)	0.3137 (11)	0.1764 (6)	0.324 (7)
O8	0.7851 (7)	0.2927 (8)	0.2667 (4)	0.257 (5)
O9	0.8093 (3)	0.3400 (4)	0.7360 (3)	0.130 (2)
O10	0.8577 (4)	0.2163 (5)	0.7989 (3)	0.159 (3)
O11	0.7290 (3)	0.2535 (5)	0.7933 (3)	0.143 (2)
O12	0.7806 (5)	0.1913 (5)	0.7054 (3)	0.162 (3)
O13	0.7150 (2)	0.3602 (3)	0.45607 (17)	0.0675 (10)
H1W	0.7436	0.3120	0.4518	0.101*
H2W	0.6720	0.3603	0.4295	0.101*
N1	0.8276 (2)	0.5102 (3)	0.42227 (17)	0.0453 (9)
N2	0.9179 (3)	0.5739 (3)	0.36527 (18)	0.0625 (12)
N3	0.8726 (2)	0.5145 (3)	0.32994 (17)	0.0485 (9)
N4	0.9068 (2)	0.1511 (3)	0.08487 (18)	0.0511 (9)
N5	0.9494 (3)	0.1182 (4)	0.0387 (2)	0.0713 (13)
N6	0.8300 (2)	0.0581 (3)	0.02814 (18)	0.0487 (9)
N7	0.8620 (2)	0.3837 (3)	0.53572 (18)	0.0544 (10)
N8	0.9633 (3)	0.2874 (3)	0.5306 (2)	0.0655 (12)
N9	0.9364 (2)	0.2847 (3)	0.58887 (19)	0.0540 (10)
N10	0.8390 (2)	−0.0544 (3)	0.82146 (18)	0.0545 (10)
N11	0.8619 (3)	−0.1382 (3)	0.8469 (2)	0.0640 (12)
N12	0.7895 (2)	−0.0588 (3)	0.91196 (18)	0.0516 (10)
C1	0.8884 (3)	0.5698 (4)	0.4198 (2)	0.0561 (12)
H1	0.9075	0.6049	0.4544	0.067*
C2	0.8196 (3)	0.4775 (3)	0.3636 (2)	0.0482 (11)
H2A	0.7821	0.4348	0.3486	0.058*
C3	0.8832 (3)	0.5020 (4)	0.2620 (2)	0.0562 (12)
H3A	0.8753	0.5618	0.2406	0.067*
H3B	0.8447	0.4583	0.2441	0.067*
C4	0.9617 (3)	0.4658 (3)	0.2511 (2)	0.0461 (10)
C5	0.9874 (3)	0.3713 (3)	0.2567 (2)	0.0502 (11)
H5	0.9569	0.3177	0.2697	0.060*
C6	1.0645 (3)	0.3680 (4)	0.2406 (2)	0.0623 (12)
H6	1.0967	0.3115	0.2399	0.075*
C7	1.0873 (3)	0.4598 (4)	0.2249 (2)	0.0657 (13)
H7	1.1379	0.4779	0.2112	0.079*
C8	1.0251 (3)	0.5204 (4)	0.2321 (2)	0.0580 (12)
H8	1.0246	0.5882	0.2241	0.070*
C9	0.9514 (3)	0.3123 (3)	0.1103 (2)	0.0492 (10)
C10	1.0205 (3)	0.3492 (4)	0.0875 (2)	0.0648 (13)
H10	1.0679	0.3138	0.0821	0.078*
C11	1.0089 (4)	0.4445 (5)	0.0746 (2)	0.0776 (16)
H11	1.0471	0.4876	0.0590	0.093*
C12	0.9338 (4)	0.4684 (4)	0.0882 (3)	0.0806 (16)
H12	0.9105	0.5311	0.0837	0.097*
C13	0.8974 (3)	0.3874 (4)	0.1104 (2)	0.0617 (12)
H13	0.8446	0.3836	0.1234	0.074*
C14	0.9399 (3)	0.2152 (4)	0.1339 (2)	0.0551 (12)
H14A	0.9892	0.1905	0.1507	0.066*

H14B	0.9059	0.2176	0.1680	0.066*
C15	0.8369 (3)	0.1150 (3)	0.0778 (2)	0.0495 (11)
H15	0.7976	0.1276	0.1040	0.059*
C16	0.9004 (3)	0.0642 (4)	0.0058 (3)	0.0668 (15)
H16	0.9132	0.0324	−0.0302	0.080*
C17	0.9174 (3)	0.3469 (4)	0.5008 (2)	0.0608 (14)
H17	0.9219	0.3632	0.4588	0.073*
C18	0.8777 (3)	0.3420 (4)	0.5913 (2)	0.0584 (13)
H18	0.8508	0.3521	0.6268	0.070*
C19	0.9713 (3)	0.2233 (4)	0.6387 (3)	0.0625 (13)
H19A	0.9432	0.2291	0.6762	0.075*
H19B	1.0243	0.2422	0.6493	0.075*
C20	0.9691 (3)	0.1234 (4)	0.6165 (2)	0.0581 (12)
C21	0.9044 (4)	0.0643 (4)	0.6106 (2)	0.0677 (13)
H21	0.8525	0.0805	0.6222	0.081*
C22	0.9267 (5)	−0.0235 (5)	0.5860 (3)	0.0943 (19)
H22	0.8930	−0.0779	0.5775	0.113*
C23	1.0045 (6)	−0.0184 (5)	0.5759 (3)	0.102 (2)
H23	1.0352	−0.0694	0.5596	0.123*
C24	1.0319 (4)	0.0703 (5)	0.5934 (3)	0.0826 (17)
H24	1.0851	0.0924	0.5913	0.099*
C25	0.9410 (3)	−0.0312 (3)	0.7488 (2)	0.0508 (11)
C26	0.9810 (4)	−0.1091 (4)	0.7249 (3)	0.0728 (15)
H26	0.9581	−0.1698	0.7123	0.087*
C27	1.0590 (4)	−0.0837 (6)	0.7222 (3)	0.101 (2)
H27	1.0998	−0.1234	0.7070	0.122*
C28	1.0678 (4)	0.0085 (7)	0.7445 (3)	0.101 (2)
H28	1.1160	0.0446	0.7474	0.122*
C29	0.9945 (4)	0.0420 (5)	0.7609 (2)	0.0704 (14)
H29	0.9836	0.1043	0.7778	0.084*
C30	0.8570 (3)	−0.0280 (4)	0.7572 (2)	0.0609 (13)
H30A	0.8381	0.0351	0.7482	0.073*
H30B	0.8304	−0.0704	0.7273	0.073*
C31	0.7960 (3)	−0.0093 (4)	0.8605 (2)	0.0545 (12)
H31	0.7734	0.0492	0.8525	0.065*
C32	0.8304 (3)	−0.1372 (4)	0.9008 (2)	0.0580 (13)
H32	0.8358	−0.1866	0.9294	0.070*
C33	0.8870 (4)	0.6021 (4)	0.5903 (3)	0.0772 (17)
H33A	0.9258	0.5611	0.5745	0.093*
H33B	0.8773	0.5808	0.6323	0.093*
C34	0.9180 (4)	0.7002 (5)	0.5943 (3)	0.089 (2)
H34A	0.9209	0.7250	0.5526	0.134*
H34B	0.9686	0.6997	0.6158	0.134*
H34C	0.8844	0.7389	0.6172	0.134*
C35	0.7069 (9)	0.8145 (6)	0.5347 (5)	0.191 (6)
H35A	0.6646	0.8028	0.5033	0.229*
H35B	0.7528	0.8246	0.5122	0.229*
C36	0.6903 (9)	0.9023 (6)	0.5674 (6)	0.214 (5)
H36A	0.6492	0.8919	0.5943	0.320*

H36B	0.6752	0.9498	0.5369	0.320*
H36C	0.7356	0.9225	0.5922	0.320*
C37	0.7846 (8)	0.1253 (7)	0.4087 (7)	0.228 (7)
H37A	0.8335	0.0972	0.3997	0.274*
H37B	0.7445	0.0965	0.3809	0.274*
C38	0.7694 (10)	0.1044 (11)	0.4748 (6)	0.262 (7)
H38A	0.8096	0.1313	0.5026	0.393*
H38B	0.7683	0.0376	0.4809	0.393*
H38C	0.7206	0.1308	0.4838	0.393*
C39	0.5220 (7)	0.2888 (11)	0.4075 (5)	0.208 (5)
H39A	0.4998	0.3446	0.3872	0.250*
H39B	0.4797	0.2515	0.4213	0.250*
C40	0.5592 (12)	0.2351 (14)	0.3605 (6)	0.311 (11)
H40A	0.6037	0.2686	0.3484	0.467*
H40B	0.5237	0.2261	0.3243	0.467*
H40C	0.5747	0.1751	0.3777	0.467*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0492 (4)	0.0446 (4)	0.0386 (3)	0.0021 (3)	0.0122 (3)	0.0050 (3)
Fe1	0.0553 (4)	0.0462 (4)	0.0354 (3)	−0.0015 (3)	0.0081 (3)	−0.0022 (3)
Fe2	0.0660 (5)	0.0577 (5)	0.0497 (4)	0.0107 (4)	0.0176 (4)	0.0195 (3)
Cl1	0.0853 (12)	0.0957 (13)	0.1141 (15)	−0.0164 (10)	0.0376 (11)	−0.0268 (11)
Cl2	0.0777 (10)	0.0695 (9)	0.0881 (11)	0.0086 (8)	0.0156 (8)	0.0049 (8)
O1	0.061 (2)	0.058 (2)	0.0497 (19)	0.0000 (16)	0.0043 (16)	−0.0076 (16)
O2	0.187 (6)	0.125 (4)	0.095 (4)	0.063 (4)	0.010 (4)	−0.025 (3)
O3	0.183 (7)	0.130 (5)	0.160 (6)	0.035 (5)	0.024 (5)	−0.029 (4)
O4	0.084 (4)	0.269 (9)	0.176 (6)	−0.020 (5)	0.006 (4)	−0.042 (6)
O5	0.163 (6)	0.190 (7)	0.278 (10)	−0.035 (6)	0.136 (7)	−0.055 (7)
O6	0.147 (6)	0.183 (6)	0.288 (10)	−0.009 (5)	0.058 (7)	−0.119 (6)
O7	0.208 (10)	0.428 (14)	0.338 (12)	0.004 (10)	0.029 (8)	0.257 (13)
O8	0.312 (10)	0.295 (11)	0.165 (7)	−0.214 (10)	0.026 (6)	−0.073 (6)
O9	0.125 (5)	0.101 (4)	0.167 (6)	−0.016 (3)	0.032 (4)	0.032 (4)
O10	0.145 (5)	0.164 (6)	0.160 (6)	0.069 (5)	−0.047 (4)	−0.007 (4)
O11	0.098 (4)	0.231 (7)	0.104 (4)	−0.031 (4)	0.034 (3)	0.025 (4)
O12	0.211 (7)	0.131 (5)	0.139 (5)	0.040 (5)	−0.018 (4)	−0.055 (4)
O13	0.071 (2)	0.060 (2)	0.072 (2)	−0.0039 (18)	0.0140 (19)	−0.0092 (18)
N1	0.053 (2)	0.045 (2)	0.0384 (19)	−0.0008 (17)	0.0109 (17)	0.0019 (16)
N2	0.076 (3)	0.070 (3)	0.044 (2)	−0.024 (2)	0.020 (2)	−0.011 (2)
N3	0.058 (2)	0.050 (2)	0.039 (2)	0.0012 (18)	0.0133 (18)	−0.0002 (17)
N4	0.053 (2)	0.053 (2)	0.047 (2)	−0.0011 (19)	0.0056 (18)	−0.0067 (18)
N5	0.051 (2)	0.092 (3)	0.073 (3)	−0.010 (2)	0.014 (2)	−0.033 (3)
N6	0.047 (2)	0.050 (2)	0.050 (2)	−0.0041 (17)	0.0092 (18)	−0.0075 (18)
N7	0.061 (2)	0.055 (2)	0.050 (2)	0.0086 (19)	0.0152 (19)	0.0115 (19)
N8	0.062 (3)	0.075 (3)	0.061 (3)	0.018 (2)	0.019 (2)	0.021 (2)
N9	0.056 (2)	0.052 (2)	0.054 (2)	0.0006 (19)	0.0050 (19)	0.0151 (19)
N10	0.058 (3)	0.063 (3)	0.045 (2)	0.002 (2)	0.0160 (19)	−0.0011 (19)

N11	0.073 (3)	0.071 (3)	0.051 (2)	0.019 (2)	0.025 (2)	0.004 (2)
N12	0.057 (2)	0.052 (2)	0.048 (2)	−0.0028 (19)	0.0166 (19)	−0.0078 (18)
C1	0.064 (3)	0.063 (3)	0.043 (3)	−0.016 (2)	0.013 (2)	−0.007 (2)
C2	0.051 (3)	0.050 (3)	0.044 (2)	−0.004 (2)	0.010 (2)	−0.003 (2)
C3	0.071 (3)	0.065 (3)	0.034 (2)	0.005 (2)	0.010 (2)	−0.004 (2)
C4	0.059 (3)	0.046 (2)	0.034 (2)	−0.003 (2)	0.0090 (19)	−0.0033 (18)
C5	0.067 (3)	0.048 (2)	0.036 (2)	−0.002 (2)	0.002 (2)	0.0002 (19)
C6	0.070 (3)	0.072 (3)	0.044 (3)	0.016 (3)	−0.001 (2)	−0.004 (2)
C7	0.052 (3)	0.090 (4)	0.056 (3)	−0.013 (3)	0.007 (2)	−0.010 (3)
C8	0.077 (3)	0.052 (3)	0.045 (3)	−0.018 (2)	0.008 (2)	−0.005 (2)
C9	0.058 (3)	0.054 (2)	0.036 (2)	−0.002 (2)	0.005 (2)	−0.0080 (19)
C10	0.079 (3)	0.074 (3)	0.044 (3)	−0.008 (3)	0.019 (2)	−0.011 (2)
C11	0.122 (5)	0.073 (3)	0.040 (2)	−0.024 (3)	0.019 (3)	0.002 (3)
C12	0.127 (5)	0.061 (3)	0.050 (3)	0.010 (3)	−0.020 (3)	0.002 (3)
C13	0.066 (3)	0.071 (3)	0.046 (3)	0.007 (2)	−0.009 (2)	−0.007 (2)
C14	0.059 (3)	0.060 (3)	0.045 (3)	−0.006 (2)	0.000 (2)	−0.009 (2)
C15	0.053 (3)	0.051 (3)	0.046 (3)	−0.004 (2)	0.008 (2)	−0.008 (2)
C16	0.053 (3)	0.083 (4)	0.066 (3)	−0.007 (3)	0.019 (3)	−0.029 (3)
C17	0.060 (3)	0.071 (3)	0.053 (3)	0.014 (3)	0.018 (2)	0.021 (3)
C18	0.073 (3)	0.055 (3)	0.049 (3)	0.010 (2)	0.016 (2)	0.013 (2)
C19	0.065 (3)	0.061 (3)	0.060 (3)	0.000 (2)	−0.004 (3)	0.022 (2)
C20	0.064 (3)	0.061 (3)	0.050 (3)	0.009 (2)	0.013 (2)	0.023 (2)
C21	0.082 (3)	0.063 (3)	0.057 (3)	0.000 (2)	−0.003 (2)	0.017 (2)
C22	0.152 (6)	0.065 (3)	0.063 (3)	−0.002 (4)	−0.009 (4)	0.010 (3)
C23	0.175 (6)	0.081 (4)	0.056 (3)	0.039 (4)	0.040 (4)	0.019 (3)
C24	0.096 (4)	0.089 (4)	0.068 (3)	0.024 (3)	0.039 (3)	0.042 (3)
C25	0.060 (3)	0.052 (3)	0.042 (2)	0.005 (2)	0.013 (2)	0.007 (2)
C26	0.103 (4)	0.059 (3)	0.061 (3)	0.028 (3)	0.038 (3)	0.028 (2)
C27	0.086 (4)	0.130 (5)	0.094 (5)	0.053 (4)	0.045 (3)	0.072 (4)
C28	0.064 (3)	0.162 (6)	0.078 (4)	−0.017 (4)	0.002 (3)	0.059 (4)
C29	0.084 (4)	0.076 (3)	0.051 (2)	−0.014 (3)	−0.002 (3)	0.012 (2)
C30	0.065 (3)	0.077 (4)	0.042 (3)	0.003 (3)	0.015 (2)	0.002 (2)
C31	0.061 (3)	0.053 (3)	0.052 (3)	0.007 (2)	0.019 (2)	0.001 (2)
C32	0.071 (3)	0.053 (3)	0.053 (3)	0.008 (2)	0.020 (3)	0.001 (2)
C33	0.090 (4)	0.081 (4)	0.057 (3)	−0.010 (3)	−0.019 (3)	−0.001 (3)
C34	0.090 (5)	0.102 (5)	0.076 (4)	−0.026 (4)	0.009 (4)	−0.023 (4)
C35	0.285 (15)	0.122 (8)	0.153 (10)	0.075 (9)	−0.069 (10)	−0.008 (6)
C36	0.247 (10)	0.170 (7)	0.225 (9)	0.040 (8)	0.022 (8)	−0.013 (7)
C37	0.221 (14)	0.183 (9)	0.292 (14)	0.092 (11)	0.096 (13)	0.070 (13)
C38	0.264 (11)	0.275 (11)	0.245 (9)	−0.015 (9)	0.005 (8)	0.054 (8)
C39	0.198 (9)	0.259 (10)	0.160 (8)	0.003 (8)	−0.031 (6)	−0.045 (7)
C40	0.38 (3)	0.30 (2)	0.254 (17)	0.09 (2)	−0.007 (16)	−0.097 (15)

Geometric parameters (Å, °)

Co1—O13	2.093 (4)	C4—C5	1.420 (7)
Co1—O1	2.118 (3)	C4—C8	1.431 (7)
Co1—N6^{i}	2.149 (4)	C5—C6	1.407 (7)
Co1—N7	2.149 (4)	C5—H5	0.9800

Co1—N1	2.156 (3)	C6—C7	1.411 (8)
Co1—N12^{ii}	2.157 (4)	C6—H6	0.9800
Fe1—C5	2.023 (4)	C7—C8	1.399 (8)
Fe1—C9	2.030 (5)	C7—H7	0.9800
Fe1—C4	2.029 (4)	C8—H8	0.9800
Fe1—C13	2.038 (5)	C9—C13	1.421 (7)
Fe1—C10	2.037 (5)	C9—C10	1.428 (7)
Fe1—C6	2.038 (5)	C9—C14	1.487 (7)
Fe1—C11	2.043 (5)	C10—C11	1.395 (8)
Fe1—C12	2.045 (6)	C10—H10	0.9800
Fe1—C7	2.052 (5)	C11—C12	1.400 (9)
Fe1—C8	2.057 (5)	C11—H11	0.9800
Fe2—C25	2.019 (4)	C12—C13	1.412 (8)
Fe2—C21	2.024 (6)	C12—H12	0.9800
Fe2—C26	2.027 (5)	C13—H13	0.9800
Fe2—C22	2.029 (7)	C14—H14A	0.9700
Fe2—C29	2.031 (6)	C14—H14B	0.9700
Fe2—C20	2.031 (5)	C15—H15	0.9300
Fe2—C23	2.036 (6)	C16—H16	0.9300
Fe2—C24	2.039 (5)	C17—H17	0.9300
Fe2—C27	2.045 (6)	C18—H18	0.9300
Fe2—C28	2.046 (7)	C19—C20	1.497 (8)
Cl1—O8	1.320 (8)	C19—H19A	0.9700
Cl1—O7	1.329 (10)	C19—H19B	0.9700
Cl1—O6	1.349 (7)	C20—C21	1.402 (8)
Cl1—O5	1.357 (6)	C20—C24	1.443 (8)
Cl2—O9	1.389 (5)	C21—C22	1.418 (9)
Cl2—O11	1.397 (5)	C21—H21	0.9800
Cl2—O10	1.406 (6)	C22—C23	1.385 (11)
Cl2—O12	1.446 (6)	C22—H22	0.9800
O1—C33	1.428 (6)	C23—C24	1.390 (10)
O1—H1D	0.9286	C23—H23	0.9800
O2—C35	1.427 (7)	C24—H24	0.9800
O2—H2D	0.8200	C25—C29	1.407 (8)
O3—C37	1.445 (8)	C25—C26	1.421 (7)
O3—H3D	0.8545	C25—C30	1.483 (7)
O4—C39	1.437 (8)	C26—C27	1.408 (10)
O4—H4D	0.8430	C26—H26	0.9800
O13—H1W	0.8548	C27—C28	1.400 (11)
O13—H2W	0.9031	C27—H27	0.9800
N1—C2	1.329 (6)	C28—C29	1.426 (9)
N1—C1	1.357 (6)	C28—H28	0.9800
N2—C1	1.304 (6)	C29—H29	0.9800
N2—N3	1.345 (5)	C30—H30A	0.9700
N3—C2	1.317 (5)	C30—H30B	0.9700
N3—C3	1.481 (5)	C31—H31	0.9300
N4—C15	1.317 (6)	C32—H32	0.9300
N4—N5	1.357 (5)	C33—C34	1.497 (8)
N4—C14	1.470 (6)	C33—H33A	0.9700

N5—C16	1.310 (7)	C33—H33B	0.9700
N6—C15	1.329 (6)	C34—H34A	0.9600
N6—C16	1.346 (6)	C34—H34B	0.9600
N6—Co1^{iii}	2.149 (4)	C34—H34C	0.9600
N7—C18	1.333 (6)	C35—C36	1.468 (8)
N7—C17	1.363 (6)	C35—H35A	0.9700
N8—C17	1.296 (6)	C35—H35B	0.9700
N8—N9	1.357 (5)	C36—H36A	0.9600
N9—C18	1.308 (6)	C36—H36B	0.9600
N9—C19	1.469 (6)	C36—H36C	0.9600
N10—C31	1.323 (6)	C37—C38	1.480 (9)
N10—N11	1.357 (6)	C37—H37A	0.9700
N10—C30	1.473 (6)	C37—H37B	0.9700
N11—C32	1.305 (6)	C38—H38A	0.9600
N12—C31	1.314 (6)	C38—H38B	0.9600
N12—C32	1.353 (6)	C38—H38C	0.9600
N12—Co1^{iv}	2.157 (4)	C39—C40	1.446 (9)
C1—H1	0.9300	C39—H39A	0.9700
C2—H2A	0.9300	C39—H39B	0.9700
C3—C4	1.491 (7)	C40—H40A	0.9600
C3—H3A	0.9700	C40—H40B	0.9600
C3—H3B	0.9700	C40—H40C	0.9600
O13—Co1—O1	177.28 (14)	C8—C7—Fe1	70.3 (3)
O13—Co1—N6^{i}	88.06 (15)	C6—C7—Fe1	69.3 (3)
O1—Co1—N6^{i}	89.30 (15)	C8—C7—H7	125.9
O13—Co1—N7	89.14 (16)	C6—C7—H7	125.9
O1—Co1—N7	93.51 (15)	Fe1—C7—H7	125.9
N6^{i}—Co1—N7	177.00 (16)	C7—C8—C4	108.3 (5)
O13—Co1—N1	90.49 (14)	C7—C8—Fe1	69.9 (3)
O1—Co1—N1	88.92 (13)	C4—C8—Fe1	68.4 (3)
N6^{i}—Co1—N1	91.48 (14)	C7—C8—H8	125.8
N7—Co1—N1	89.63 (14)	C4—C8—H8	125.8
O13—Co1—N12^{ii}	91.36 (15)	Fe1—C8—H8	125.8
O1—Co1—N12^{ii}	89.25 (14)	C13—C9—C10	107.1 (5)
N6^{i}—Co1—N12^{ii}	89.05 (15)	C13—C9—C14	126.3 (5)
N7—Co1—N12^{ii}	89.94 (15)	C10—C9—C14	126.4 (5)
N1—Co1—N12^{ii}	178.09 (16)	C13—C9—Fe1	69.8 (3)
C5—Fe1—C9	106.20 (19)	C10—C9—Fe1	69.7 (3)
C5—Fe1—C4	41.01 (18)	C14—C9—Fe1	122.3 (3)
C9—Fe1—C4	131.56 (19)	C11—C10—C9	108.2 (5)
C5—Fe1—C13	113.0 (2)	C11—C10—Fe1	70.2 (3)
C9—Fe1—C13	40.9 (2)	C9—C10—Fe1	69.2 (3)
C4—Fe1—C13	109.0 (2)	C11—C10—H10	125.9
C5—Fe1—C10	131.3 (2)	C9—C10—H10	125.9
C9—Fe1—C10	41.1 (2)	Fe1—C10—H10	125.9
C4—Fe1—C10	171.2 (2)	C10—C11—C12	108.6 (6)

C13—Fe1—C10	68.4 (2)	C10—C11—Fe1	69.8 (3)
C5—Fe1—C6	40.5 (2)	C12—C11—Fe1	70.0 (3)
C9—Fe1—C6	112.0 (2)	C10—C11—H11	125.7
C4—Fe1—C6	68.5 (2)	C12—C11—H11	125.7
C13—Fe1—C6	143.5 (2)	Fe1—C11—H11	125.7
C10—Fe1—C6	108.2 (2)	C11—C12—C13	108.5 (5)
C5—Fe1—C11	171.0 (2)	C11—C12—Fe1	69.9 (3)
C9—Fe1—C11	68.3 (2)	C13—C12—Fe1	69.5 (3)
C4—Fe1—C11	147.9 (2)	C11—C12—H12	125.8
C13—Fe1—C11	68.0 (3)	C13—C12—H12	125.8
C10—Fe1—C11	40.0 (2)	Fe1—C12—H12	125.8
C6—Fe1—C11	133.7 (3)	C12—C13—C9	107.6 (5)
C5—Fe1—C12	145.9 (3)	C12—C13—Fe1	70.0 (3)
C9—Fe1—C12	68.3 (2)	C9—C13—Fe1	69.3 (3)
C4—Fe1—C12	116.5 (2)	C12—C13—H13	126.2
C13—Fe1—C12	40.5 (2)	C9—C13—H13	126.2
C10—Fe1—C12	67.5 (3)	Fe1—C13—H13	126.2
C6—Fe1—C12	173.6 (3)	N4—C14—C9	113.0 (4)
C11—Fe1—C12	40.0 (3)	N4—C14—H14A	109.0
C5—Fe1—C7	68.2 (2)	C9—C14—H14A	109.0
C9—Fe1—C7	144.1 (2)	N4—C14—H14B	109.0
C4—Fe1—C7	68.4 (2)	C9—C14—H14B	109.0
C13—Fe1—C7	174.9 (2)	H14A—C14—H14B	107.8
C10—Fe1—C7	114.8 (2)	N4—C15—N6	110.9 (4)
C6—Fe1—C7	40.4 (2)	N4—C15—H15	124.6
C11—Fe1—C7	111.7 (3)	N6—C15—H15	124.6
C12—Fe1—C7	136.1 (3)	N5—C16—N6	114.8 (4)
C5—Fe1—C8	68.32 (19)	N5—C16—H16	122.6
C9—Fe1—C8	172.51 (19)	N6—C16—H16	122.6
C4—Fe1—C8	40.98 (19)	N8—C17—N7	114.6 (4)
C13—Fe1—C8	135.5 (2)	N8—C17—H17	122.7
C10—Fe1—C8	146.4 (2)	N7—C17—H17	122.7
C6—Fe1—C8	67.5 (2)	N9—C18—N7	110.6 (4)
C11—Fe1—C8	117.8 (2)	N9—C18—H18	124.7
C12—Fe1—C8	113.1 (2)	N7—C18—H18	124.7
C7—Fe1—C8	39.8 (2)	N9—C19—C20	109.7 (4)
C25—Fe2—C21	107.4 (2)	N9—C19—H19A	109.7
C25—Fe2—C26	41.13 (19)	C20—C19—H19A	109.7
C21—Fe2—C26	128.2 (3)	N9—C19—H19B	109.7
C25—Fe2—C22	117.2 (3)	C20—C19—H19B	109.7
C21—Fe2—C22	41.0 (3)	H19A—C19—H19B	108.2
C26—Fe2—C22	107.4 (3)	C21—C20—C24	106.0 (5)
C25—Fe2—C29	40.7 (2)	C21—C20—C19	126.8 (5)
C21—Fe2—C29	117.6 (3)	C24—C20—C19	127.0 (5)
C26—Fe2—C29	68.6 (2)	C21—C20—Fe2	69.5 (3)
C22—Fe2—C29	151.0 (3)	C24—C20—Fe2	69.5 (3)
C25—Fe2—C20	127.6 (2)	C19—C20—Fe2	128.1 (4)
C21—Fe2—C20	40.5 (2)	C20—C21—C22	108.8 (6)
C26—Fe2—C20	166.1 (2)	C20—C21—Fe2	70.0 (3)

C22—Fe2—C20	68.8 (2)	C22—C21—Fe2	69.7 (4)
C29—Fe2—C20	107.8 (2)	C20—C21—H21	125.6
C25—Fe2—C23	150.5 (3)	C22—C21—H21	125.6
C21—Fe2—C23	67.9 (3)	Fe2—C21—H21	125.6
C26—Fe2—C23	117.5 (3)	C23—C22—C21	107.9 (7)
C22—Fe2—C23	39.8 (3)	C23—C22—Fe2	70.3 (4)
C29—Fe2—C23	167.9 (3)	C21—C22—Fe2	69.4 (4)
C20—Fe2—C23	68.8 (2)	C23—C22—H22	126.0
C25—Fe2—C24	167.6 (2)	C21—C22—H22	126.0
C21—Fe2—C24	68.0 (3)	Fe2—C22—H22	126.0
C26—Fe2—C24	150.7 (2)	C22—C23—C24	108.9 (7)
C22—Fe2—C24	67.4 (3)	C22—C23—Fe2	69.8 (4)
C29—Fe2—C24	130.1 (3)	C24—C23—Fe2	70.2 (4)
C20—Fe2—C24	41.5 (2)	C22—C23—H23	125.5
C23—Fe2—C24	39.9 (3)	C24—C23—H23	125.5
C25—Fe2—C27	68.6 (2)	Fe2—C23—H23	125.5
C21—Fe2—C27	166.3 (3)	C23—C24—C20	108.3 (6)
C26—Fe2—C27	40.4 (3)	C23—C24—Fe2	69.9 (3)
C22—Fe2—C27	128.1 (3)	C20—C24—Fe2	68.9 (3)
C29—Fe2—C27	68.5 (3)	C23—C24—H24	125.9
C20—Fe2—C27	152.2 (3)	C20—C24—H24	125.9
C23—Fe2—C27	108.8 (3)	Fe2—C24—H24	125.9
C24—Fe2—C27	118.6 (3)	C29—C25—C26	107.9 (5)
C25—Fe2—C28	68.3 (2)	C29—C25—C30	126.7 (5)
C21—Fe2—C28	152.1 (3)	C26—C25—C30	125.3 (5)
C26—Fe2—C28	67.8 (3)	C29—C25—Fe2	70.1 (3)
C22—Fe2—C28	166.2 (4)	C26—C25—Fe2	69.8 (3)
C29—Fe2—C28	40.9 (3)	C30—C25—Fe2	124.2 (3)
C20—Fe2—C28	119.0 (3)	C27—C26—C25	108.2 (6)
C23—Fe2—C28	129.6 (4)	C27—C26—Fe2	70.5 (3)
C24—Fe2—C28	110.0 (3)	C25—C26—Fe2	69.1 (3)
C27—Fe2—C28	40.0 (3)	C27—C26—H26	125.9
O8—Cl1—O7	106.4 (8)	C25—C26—H26	125.9
O8—Cl1—O6	109.8 (8)	Fe2—C26—H26	125.9
O7—Cl1—O6	107.1 (9)	C28—C27—C26	108.0 (6)
O8—Cl1—O5	114.2 (6)	C28—C27—Fe2	70.0 (4)
O7—Cl1—O5	112.7 (7)	C26—C27—Fe2	69.1 (3)
O6—Cl1—O5	106.5 (5)	C28—C27—H27	126.0
O9—Cl2—O11	109.8 (4)	C26—C27—H27	126.0
O9—Cl2—O10	112.8 (5)	Fe2—C27—H27	126.0
O11—Cl2—O10	109.6 (4)	C27—C28—C29	108.5 (6)
O9—Cl2—O12	105.6 (4)	C27—C28—Fe2	70.0 (4)
O11—Cl2—O12	108.6 (5)	C29—C28—Fe2	69.0 (4)
O10—Cl2—O12	110.3 (4)	C27—C28—H28	125.7
C33—O1—Co1	129.8 (3)	C29—C28—H28	125.7
C33—O1—H1D	114.6	Fe2—C28—H28	125.7
Co1—O1—H1D	113.0	C25—C29—C28	107.4 (6)
C35—O2—H2D	109.5	C25—C29—Fe2	69.2 (3)
C37—O3—H3D	109.6	C28—C29—Fe2	70.1 (4)

C39—O4—H4D	107.3	C25—C29—H29	126.3
Co1—O13—H1W	115.8	C28—C29—H29	126.3
Co1—O13—H2W	128.1	Fe2—C29—H29	126.3
H1W—O13—H2W	113.2	N10—C30—C25	112.5 (4)
C2—N1—C1	102.1 (4)	N10—C30—H30A	109.1
C2—N1—Co1	130.7 (3)	C25—C30—H30A	109.1
C1—N1—Co1	127.0 (3)	N10—C30—H30B	109.1
C1—N2—N3	102.6 (4)	C25—C30—H30B	109.1
C2—N3—N2	110.5 (4)	H30A—C30—H30B	107.8
C2—N3—C3	128.7 (4)	N12—C31—N10	110.5 (4)
N2—N3—C3	120.8 (4)	N12—C31—H31	124.7
C15—N4—N5	109.2 (4)	N10—C31—H31	124.7
C15—N4—C14	129.2 (4)	N11—C32—N12	115.0 (5)
N5—N4—C14	121.5 (4)	N11—C32—H32	122.5
C16—N5—N4	102.8 (4)	N12—C32—H32	122.5
C15—N6—C16	102.2 (4)	O1—C33—C34	113.3 (5)
C15—N6—Co1^{iii}	128.0 (3)	O1—C33—H33A	108.9
C16—N6—Co1^{iii}	129.8 (3)	C34—C33—H33A	108.9
C18—N7—C17	101.9 (4)	O1—C33—H33B	108.9
C18—N7—Co1	130.2 (3)	C34—C33—H33B	108.9
C17—N7—Co1	127.7 (3)	H33A—C33—H33B	107.7
C17—N8—N9	103.0 (4)	C33—C34—H34A	109.5
C18—N9—N8	109.8 (4)	C33—C34—H34B	109.5
C18—N9—C19	128.5 (4)	H34A—C34—H34B	109.5
N8—N9—C19	121.7 (4)	C33—C34—H34C	109.5
C31—N10—N11	109.7 (4)	H34A—C34—H34C	109.5
C31—N10—C30	128.8 (5)	H34B—C34—H34C	109.5
N11—N10—C30	121.2 (4)	O2—C35—C36	117.9 (8)
C32—N11—N10	102.2 (4)	O2—C35—H35A	107.8
C31—N12—C32	102.5 (4)	C36—C35—H35A	107.8
C31—N12—Co1^{iv}	130.2 (3)	O2—C35—H35B	107.8
C32—N12—Co1^{iv}	127.2 (3)	C36—C35—H35B	107.8
N2—C1—N1	114.8 (4)	H35A—C35—H35B	107.2
N2—C1—H1	122.6	C35—C36—H36A	109.5
N1—C1—H1	122.6	C35—C36—H36B	109.5
N3—C2—N1	110.0 (4)	H36A—C36—H36B	109.5
N3—C2—H2A	125.0	C35—C36—H36C	109.5
N1—C2—H2A	125.0	H36A—C36—H36C	109.5
N3—C3—C4	112.0 (4)	H36B—C36—H36C	109.5
N3—C3—H3A	109.2	O3—C37—C38	112.9 (9)
C4—C3—H3A	109.2	O3—C37—H37A	109.0
N3—C3—H3B	109.2	C38—C37—H37A	109.0
C4—C3—H3B	109.2	O3—C37—H37B	109.0
H3A—C3—H3B	107.9	C38—C37—H37B	109.0
C5—C4—C8	107.0 (4)	H37A—C37—H37B	107.8
C5—C4—C3	126.9 (4)	C37—C38—H38A	109.5
C8—C4—C3	126.1 (5)	C37—C38—H38B	109.5
C5—C4—Fe1	69.3 (2)	H38A—C38—H38B	109.5

C8—C4—Fe1	70.6 (3)	C37—C38—H38C	109.5
C3—C4—Fe1	124.6 (3)	H38A—C38—H38C	109.5
C6—C5—C4	108.1 (4)	H38B—C38—H38C	109.5
C6—C5—Fe1	70.3 (3)	O4—C39—C40	117.5 (9)
C4—C5—Fe1	69.7 (3)	O4—C39—H39A	107.9
C6—C5—H5	125.9	C40—C39—H39A	107.9
C4—C5—H5	125.9	O4—C39—H39B	107.9
Fe1—C5—H5	125.9	C40—C39—H39B	107.9
C5—C6—C7	108.4 (5)	H39A—C39—H39B	107.2
C5—C6—Fe1	69.2 (3)	C39—C40—H40A	109.5
C7—C6—Fe1	70.4 (3)	C39—C40—H40B	109.5
C5—C6—H6	125.8	H40A—C40—H40B	109.5
C7—C6—H6	125.8	C39—C40—H40C	109.5
Fe1—C6—H6	125.8	H40A—C40—H40C	109.5
C8—C7—C6	108.2 (5)	H40B—C40—H40C	109.5
N6^{i}—Co1—O1—C33	175.9 (4)	C15—N6—C16—N5	1.4 (7)
N7—Co1—O1—C33	−3.0 (4)	Co1^{iii}—N6—C16—N5	−176.0 (4)
N1—Co1—O1—C33	−92.6 (4)	N9—N8—C17—N7	0.0 (6)
N12^{ii}—Co1—O1—C33	86.9 (4)	C18—N7—C17—N8	0.5 (7)
O13—Co1—N1—C2	9.4 (4)	Co1—N7—C17—N8	−173.9 (4)
O1—Co1—N1—C2	−167.9 (4)	N8—N9—C18—N7	0.9 (6)
N6^{i}—Co1—N1—C2	−78.7 (4)	C19—N9—C18—N7	−178.2 (5)
N7—Co1—N1—C2	98.5 (4)	C17—N7—C18—N9	−0.8 (6)
O13—Co1—N1—C1	−165.6 (4)	Co1—N7—C18—N9	173.3 (3)
O1—Co1—N1—C1	17.0 (4)	C18—N9—C19—C20	122.1 (6)
N6^{i}—Co1—N1—C1	106.3 (4)	N8—N9—C19—C20	−57.0 (6)
N7—Co1—N1—C1	−76.5 (4)	N9—C19—C20—C21	−75.0 (6)
C1—N2—N3—C2	−0.5 (6)	N9—C19—C20—C24	101.1 (6)
C1—N2—N3—C3	176.4 (4)	N9—C19—C20—Fe2	−166.9 (4)
C15—N4—N5—C16	0.8 (6)	C25—Fe2—C20—C21	−71.2 (4)
C14—N4—N5—C16	179.5 (5)	C26—Fe2—C20—C21	−39.1 (12)
O13—Co1—N7—C18	−101.5 (5)	C22—Fe2—C20—C21	37.5 (4)
O1—Co1—N7—C18	79.1 (5)	C29—Fe2—C20—C21	−111.9 (4)
N1—Co1—N7—C18	168.0 (5)	C23—Fe2—C20—C21	80.4 (4)
N12^{ii}—Co1—N7—C18	−10.1 (5)	C24—Fe2—C20—C21	117.0 (5)
O13—Co1—N7—C17	71.3 (5)	C27—Fe2—C20—C21	170.6 (6)
O1—Co1—N7—C17	−108.1 (5)	C28—Fe2—C20—C21	−155.1 (4)
N1—Co1—N7—C17	−19.2 (5)	C25—Fe2—C20—C24	171.8 (4)
N12^{ii}—Co1—N7—C17	162.7 (5)	C21—Fe2—C20—C24	−117.0 (5)
C17—N8—N9—C18	−0.6 (6)	C26—Fe2—C20—C24	−156.1 (10)
C17—N8—N9—C19	178.7 (5)	C22—Fe2—C20—C24	−79.5 (5)
C31—N10—N11—C32	−0.3 (6)	C29—Fe2—C20—C24	131.1 (4)
C30—N10—N11—C32	−175.5 (5)	C23—Fe2—C20—C24	−36.6 (5)
N3—N2—C1—N1	1.0 (6)	C27—Fe2—C20—C24	53.6 (7)
C2—N1—C1—N2	−1.2 (6)	C28—Fe2—C20—C24	87.9 (5)
Co1—N1—C1—N2	174.9 (4)	C25—Fe2—C20—C19	50.2 (6)
N2—N3—C2—N1	−0.3 (6)	C21—Fe2—C20—C19	121.4 (6)

C3—N3—C2—N1	−176.8 (4)	C26—Fe2—C20—C19	82.3 (12)
C1—N1—C2—N3	0.8 (5)	C22—Fe2—C20—C19	158.9 (6)
Co1—N1—C2—N3	−175.1 (3)	C29—Fe2—C20—C19	9.5 (5)
C2—N3—C3—C4	−123.2 (5)	C23—Fe2—C20—C19	−158.3 (6)
N2—N3—C3—C4	60.6 (6)	C24—Fe2—C20—C19	−121.6 (7)
N3—C3—C4—C5	79.9 (6)	C27—Fe2—C20—C19	−68.1 (8)
N3—C3—C4—C8	−101.1 (5)	C28—Fe2—C20—C19	−33.7 (6)
N3—C3—C4—Fe1	168.8 (3)	C24—C20—C21—C22	1.2 (6)
C9—Fe1—C4—C5	63.2 (4)	C19—C20—C21—C22	178.0 (5)
C13—Fe1—C4—C5	103.4 (3)	Fe2—C20—C21—C22	−59.1 (4)
C6—Fe1—C4—C5	−37.7 (3)	C24—C20—C21—Fe2	60.3 (3)
C11—Fe1—C4—C5	−177.9 (4)	C19—C20—C21—Fe2	−122.9 (5)
C12—Fe1—C4—C5	146.8 (3)	C25—Fe2—C21—C20	128.2 (3)
C7—Fe1—C4—C5	−81.2 (3)	C26—Fe2—C21—C20	168.9 (3)
C8—Fe1—C4—C5	−117.7 (4)	C22—Fe2—C21—C20	−120.0 (5)
C5—Fe1—C4—C8	117.7 (4)	C29—Fe2—C21—C20	85.4 (4)
C9—Fe1—C4—C8	−179.1 (3)	C23—Fe2—C21—C20	−82.8 (4)
C13—Fe1—C4—C8	−138.8 (3)	C24—Fe2—C21—C20	−39.6 (4)
C6—Fe1—C4—C8	80.0 (3)	C27—Fe2—C21—C20	−161.1 (10)
C11—Fe1—C4—C8	−60.2 (6)	C28—Fe2—C21—C20	51.9 (7)
C12—Fe1—C4—C8	−95.5 (4)	C25—Fe2—C21—C22	−111.8 (4)
C7—Fe1—C4—C8	36.5 (3)	C26—Fe2—C21—C22	−71.1 (5)
C5—Fe1—C4—C3	−121.2 (5)	C29—Fe2—C21—C22	−154.6 (4)
C9—Fe1—C4—C3	−58.1 (5)	C20—Fe2—C21—C22	120.0 (5)
C13—Fe1—C4—C3	−17.8 (5)	C23—Fe2—C21—C22	37.2 (4)
C6—Fe1—C4—C3	−158.9 (5)	C24—Fe2—C21—C22	80.4 (5)
C11—Fe1—C4—C3	60.9 (6)	C27—Fe2—C21—C22	−41.1 (12)
C12—Fe1—C4—C3	25.6 (5)	C28—Fe2—C21—C22	171.9 (5)
C7—Fe1—C4—C3	157.5 (5)	C20—C21—C22—C23	−0.7 (7)
C8—Fe1—C4—C3	121.0 (5)	Fe2—C21—C22—C23	−60.0 (5)
C8—C4—C5—C6	−0.8 (5)	C20—C21—C22—Fe2	59.3 (4)
C3—C4—C5—C6	178.4 (4)	C25—Fe2—C22—C23	−155.7 (4)
Fe1—C4—C5—C6	60.0 (3)	C21—Fe2—C22—C23	119.0 (6)
C8—C4—C5—Fe1	−60.8 (3)	C26—Fe2—C22—C23	−112.3 (4)
C3—C4—C5—Fe1	118.4 (5)	C29—Fe2—C22—C23	170.6 (5)
C9—Fe1—C5—C6	105.1 (3)	C20—Fe2—C22—C23	81.9 (4)
C4—Fe1—C5—C6	−119.0 (4)	C24—Fe2—C22—C23	37.0 (4)
C13—Fe1—C5—C6	148.0 (3)	C27—Fe2—C22—C23	−72.4 (5)
C10—Fe1—C5—C6	67.2 (4)	C28—Fe2—C22—C23	−45.0 (14)
C12—Fe1—C5—C6	−179.9 (4)	C25—Fe2—C22—C21	85.4 (4)
C7—Fe1—C5—C6	−37.3 (3)	C26—Fe2—C22—C21	128.8 (4)
C8—Fe1—C5—C6	−80.3 (3)	C29—Fe2—C22—C21	51.6 (7)
C9—Fe1—C5—C4	−135.9 (3)	C20—Fe2—C22—C21	−37.1 (3)
C13—Fe1—C5—C4	−93.0 (3)	C23—Fe2—C22—C21	−119.0 (6)
C10—Fe1—C5—C4	−173.8 (3)	C24—Fe2—C22—C21	−82.0 (4)
C6—Fe1—C5—C4	119.0 (4)	C27—Fe2—C22—C21	168.6 (4)
C12—Fe1—C5—C4	−60.9 (5)	C28—Fe2—C22—C21	−163.9 (11)
C7—Fe1—C5—C4	81.7 (3)	C21—C22—C23—C24	−0.1 (8)
C8—Fe1—C5—C4	38.7 (3)	Fe2—C22—C23—C24	−59.5 (5)

C4—C5—C6—C7	0.0 (6)	C21—C22—C23—Fe2	59.4 (4)
Fe1—C5—C6—C7	59.6 (4)	C25—Fe2—C23—C22	48.0 (7)
C4—C5—C6—Fe1	−59.7 (3)	C21—Fe2—C23—C22	−38.3 (4)
C9—Fe1—C6—C5	−89.5 (3)	C26—Fe2—C23—C22	84.5 (5)
C4—Fe1—C6—C5	38.1 (3)	C29—Fe2—C23—C22	−157.7 (12)
C13—Fe1—C6—C5	−55.1 (5)	C20—Fe2—C23—C22	−81.9 (4)
C10—Fe1—C6—C5	−133.2 (3)	C24—Fe2—C23—C22	−120.0 (6)
C11—Fe1—C6—C5	−169.9 (3)	C27—Fe2—C23—C22	127.6 (5)
C7—Fe1—C6—C5	119.6 (4)	C28—Fe2—C23—C22	167.4 (5)
C8—Fe1—C6—C5	82.4 (3)	C25—Fe2—C23—C24	168.0 (4)
C5—Fe1—C6—C7	−119.6 (4)	C21—Fe2—C23—C24	81.7 (4)
C9—Fe1—C6—C7	150.9 (3)	C26—Fe2—C23—C24	−155.5 (4)
C4—Fe1—C6—C7	−81.5 (3)	C22—Fe2—C23—C24	120.0 (6)
C13—Fe1—C6—C7	−174.7 (3)	C29—Fe2—C23—C24	−37.7 (15)
C10—Fe1—C6—C7	107.2 (3)	C20—Fe2—C23—C24	38.1 (4)
C11—Fe1—C6—C7	70.5 (4)	C27—Fe2—C23—C24	−112.4 (5)
C8—Fe1—C6—C7	−37.2 (3)	C28—Fe2—C23—C24	−72.6 (6)
C5—C6—C7—C8	0.9 (6)	C22—C23—C24—C20	0.8 (7)
Fe1—C6—C7—C8	59.7 (4)	Fe2—C23—C24—C20	−58.4 (4)
C5—C6—C7—Fe1	−58.9 (3)	C22—C23—C24—Fe2	59.2 (5)
C5—Fe1—C7—C8	−81.8 (3)	C21—C20—C24—C23	−1.3 (6)
C9—Fe1—C7—C8	−169.6 (3)	C19—C20—C24—C23	−178.1 (5)
C4—Fe1—C7—C8	−37.5 (3)	Fe2—C20—C24—C23	59.0 (4)
C10—Fe1—C7—C8	151.4 (3)	C21—C20—C24—Fe2	−60.3 (4)
C6—Fe1—C7—C8	−119.3 (4)	C19—C20—C24—Fe2	122.9 (5)
C11—Fe1—C7—C8	107.9 (4)	C25—Fe2—C24—C23	−151.7 (11)
C12—Fe1—C7—C8	68.7 (5)	C21—Fe2—C24—C23	−81.3 (5)
C5—Fe1—C7—C6	37.5 (3)	C26—Fe2—C24—C23	48.6 (8)
C9—Fe1—C7—C6	−50.2 (5)	C22—Fe2—C24—C23	−36.9 (5)
C4—Fe1—C7—C6	81.8 (3)	C29—Fe2—C24—C23	170.4 (5)
C10—Fe1—C7—C6	−89.2 (3)	C20—Fe2—C24—C23	−119.9 (6)
C11—Fe1—C7—C6	−132.8 (3)	C27—Fe2—C24—C23	85.4 (6)
C12—Fe1—C7—C6	−172.0 (4)	C28—Fe2—C24—C23	128.5 (5)
C8—Fe1—C7—C6	119.3 (4)	C25—Fe2—C24—C20	−31.7 (14)
C6—C7—C8—C4	−1.3 (6)	C21—Fe2—C24—C20	38.6 (4)
Fe1—C7—C8—C4	57.8 (3)	C26—Fe2—C24—C20	168.5 (5)
C6—C7—C8—Fe1	−59.1 (4)	C22—Fe2—C24—C20	83.0 (4)
C5—C4—C8—C7	1.3 (5)	C29—Fe2—C24—C20	−69.7 (5)
C3—C4—C8—C7	−177.9 (4)	C23—Fe2—C24—C20	119.9 (6)
Fe1—C4—C8—C7	−58.7 (4)	C27—Fe2—C24—C20	−154.7 (4)
C5—C4—C8—Fe1	60.0 (3)	C28—Fe2—C24—C20	−111.6 (4)
C3—C4—C8—Fe1	−119.2 (5)	C21—Fe2—C25—C29	−112.4 (4)
C5—Fe1—C8—C7	81.6 (3)	C26—Fe2—C25—C29	118.8 (5)
C4—Fe1—C8—C7	120.3 (5)	C22—Fe2—C25—C29	−155.6 (4)
C13—Fe1—C8—C7	−177.2 (3)	C20—Fe2—C25—C29	−72.3 (4)
C10—Fe1—C8—C7	−51.6 (5)	C23—Fe2—C25—C29	172.0 (6)
C6—Fe1—C8—C7	37.7 (3)	C24—Fe2—C25—C29	−46.2 (13)
C11—Fe1—C8—C7	−91.1 (4)	C27—Fe2—C25—C29	81.4 (4)
C12—Fe1—C8—C7	−135.4 (4)	C28—Fe2—C25—C29	38.3 (4)

C5—Fe1—C8—C4	−38.7 (3)	C21—Fe2—C25—C26	128.8 (4)
C13—Fe1—C8—C4	62.5 (4)	C22—Fe2—C25—C26	85.6 (4)
C10—Fe1—C8—C4	−171.9 (4)	C29—Fe2—C25—C26	−118.8 (5)
C6—Fe1—C8—C4	−82.6 (3)	C20—Fe2—C25—C26	168.8 (4)
C11—Fe1—C8—C4	148.6 (3)	C23—Fe2—C25—C26	53.2 (7)
C12—Fe1—C8—C4	104.3 (4)	C24—Fe2—C25—C26	−165.1 (11)
C7—Fe1—C8—C4	−120.3 (5)	C27—Fe2—C25—C26	−37.4 (5)
C5—Fe1—C9—C13	106.5 (3)	C28—Fe2—C25—C26	−80.5 (5)
C4—Fe1—C9—C13	69.0 (4)	C21—Fe2—C25—C30	9.1 (5)
C10—Fe1—C9—C13	−118.0 (4)	C26—Fe2—C25—C30	−119.6 (6)
C6—Fe1—C9—C13	149.1 (3)	C22—Fe2—C25—C30	−34.1 (5)
C11—Fe1—C9—C13	−81.0 (4)	C29—Fe2—C25—C30	121.5 (6)
C12—Fe1—C9—C13	−37.8 (3)	C20—Fe2—C25—C30	49.2 (5)
C7—Fe1—C9—C13	−178.4 (4)	C23—Fe2—C25—C30	−66.5 (7)
C5—Fe1—C9—C10	−135.4 (3)	C24—Fe2—C25—C30	75.3 (13)
C4—Fe1—C9—C10	−173.0 (3)	C27—Fe2—C25—C30	−157.0 (6)
C13—Fe1—C9—C10	118.0 (4)	C28—Fe2—C25—C30	159.8 (6)
C6—Fe1—C9—C10	−92.8 (4)	C29—C25—C26—C27	−0.1 (6)
C11—Fe1—C9—C10	37.0 (4)	C30—C25—C26—C27	178.1 (5)
C12—Fe1—C9—C10	80.3 (4)	Fe2—C25—C26—C27	59.9 (4)
C7—Fe1—C9—C10	−60.3 (5)	C29—C25—C26—Fe2	−60.0 (4)
C5—Fe1—C9—C14	−14.4 (5)	C30—C25—C26—Fe2	118.2 (5)
C4—Fe1—C9—C14	−52.0 (5)	C25—Fe2—C26—C27	−119.3 (6)
C13—Fe1—C9—C14	−121.0 (5)	C21—Fe2—C26—C27	169.5 (5)
C10—Fe1—C9—C14	121.0 (6)	C22—Fe2—C26—C27	129.0 (5)
C6—Fe1—C9—C14	28.2 (5)	C29—Fe2—C26—C27	−81.5 (5)
C11—Fe1—C9—C14	158.0 (5)	C20—Fe2—C26—C27	−159.1 (10)
C12—Fe1—C9—C14	−158.7 (5)	C23—Fe2—C26—C27	87.0 (6)
C7—Fe1—C9—C14	60.6 (6)	C24—Fe2—C26—C27	54.2 (8)
C13—C9—C10—C11	0.5 (6)	C28—Fe2—C26—C27	−37.3 (5)
C14—C9—C10—C11	−175.5 (5)	C21—Fe2—C26—C25	−71.2 (5)
Fe1—C9—C10—C11	−59.6 (4)	C22—Fe2—C26—C25	−111.7 (4)
C13—C9—C10—Fe1	60.1 (3)	C29—Fe2—C26—C25	37.8 (3)
C14—C9—C10—Fe1	−115.8 (5)	C20—Fe2—C26—C25	−39.8 (12)
C5—Fe1—C10—C11	−176.8 (4)	C23—Fe2—C26—C25	−153.6 (4)
C9—Fe1—C10—C11	119.4 (5)	C24—Fe2—C26—C25	173.5 (5)
C13—Fe1—C10—C11	81.0 (4)	C27—Fe2—C26—C25	119.3 (6)
C6—Fe1—C10—C11	−137.7 (4)	C28—Fe2—C26—C25	82.1 (4)
C12—Fe1—C10—C11	37.2 (4)	C25—C26—C27—C28	0.4 (7)
C7—Fe1—C10—C11	−94.7 (4)	Fe2—C26—C27—C28	59.5 (4)
C8—Fe1—C10—C11	−61.1 (6)	C25—C26—C27—Fe2	−59.0 (4)
C5—Fe1—C10—C9	63.8 (4)	C25—Fe2—C27—C28	−81.3 (4)
C13—Fe1—C10—C9	−38.4 (3)	C21—Fe2—C27—C28	−156.7 (10)
C6—Fe1—C10—C9	102.9 (3)	C26—Fe2—C27—C28	−119.3 (6)
C11—Fe1—C10—C9	−119.4 (5)	C22—Fe2—C27—C28	170.2 (4)
C12—Fe1—C10—C9	−82.2 (4)	C29—Fe2—C27—C28	−37.5 (4)
C7—Fe1—C10—C9	145.8 (3)	C20—Fe2—C27—C28	50.1 (7)
C8—Fe1—C10—C9	179.4 (4)	C23—Fe2—C27—C28	130.0 (5)
C9—C10—C11—C12	−0.5 (6)	C24—Fe2—C27—C28	87.5 (5)

Fe1—C10—C11—C12	−59.5 (4)	C25—Fe2—C27—C26	38.0 (4)
C9—C10—C11—Fe1	59.0 (4)	C21—Fe2—C27—C26	−37.3 (13)
C9—Fe1—C11—C10	−38.0 (4)	C22—Fe2—C27—C26	−70.5 (5)
C4—Fe1—C11—C10	−173.2 (4)	C29—Fe2—C27—C26	81.8 (4)
C13—Fe1—C11—C10	−82.3 (4)	C20—Fe2—C27—C26	169.4 (4)
C6—Fe1—C11—C10	62.2 (5)	C23—Fe2—C27—C26	−110.7 (5)
C12—Fe1—C11—C10	−119.7 (6)	C24—Fe2—C27—C26	−153.1 (4)
C7—Fe1—C11—C10	103.2 (4)	C28—Fe2—C27—C26	119.3 (6)
C8—Fe1—C11—C10	146.8 (4)	C26—C27—C28—C29	−0.6 (7)
C9—Fe1—C11—C12	81.6 (4)	Fe2—C27—C28—C29	58.3 (4)
C4—Fe1—C11—C12	−53.5 (6)	C26—C27—C28—Fe2	−58.9 (4)
C13—Fe1—C11—C12	37.4 (4)	C25—Fe2—C28—C27	82.2 (4)
C10—Fe1—C11—C12	119.7 (6)	C21—Fe2—C28—C27	168.5 (5)
C6—Fe1—C11—C12	−178.2 (4)	C26—Fe2—C28—C27	37.7 (4)
C7—Fe1—C11—C12	−137.1 (4)	C22—Fe2—C28—C27	−34.4 (13)
C8—Fe1—C11—C12	−93.6 (4)	C29—Fe2—C28—C27	120.2 (5)
C10—C11—C12—C13	0.4 (7)	C20—Fe2—C28—C27	−155.8 (4)
Fe1—C11—C12—C13	−59.0 (4)	C23—Fe2—C28—C27	−70.3 (5)
C10—C11—C12—Fe1	59.3 (4)	C24—Fe2—C28—C27	−111.0 (4)
C5—Fe1—C12—C11	−168.7 (4)	C25—Fe2—C28—C29	−38.0 (3)
C9—Fe1—C12—C11	−81.7 (4)	C21—Fe2—C28—C29	48.3 (7)
C4—Fe1—C12—C11	151.5 (3)	C26—Fe2—C28—C29	−82.5 (4)
C13—Fe1—C12—C11	−119.8 (5)	C22—Fe2—C28—C29	−154.5 (11)
C10—Fe1—C12—C11	−37.2 (4)	C20—Fe2—C28—C29	84.0 (4)
C7—Fe1—C12—C11	65.9 (5)	C23—Fe2—C28—C29	169.5 (4)
C8—Fe1—C12—C11	106.3 (4)	C24—Fe2—C28—C29	128.8 (4)
C5—Fe1—C12—C13	−48.8 (5)	C27—Fe2—C28—C29	−120.2 (5)
C9—Fe1—C12—C13	38.1 (3)	C26—C25—C29—C28	−0.2 (6)
C4—Fe1—C12—C13	−88.7 (4)	C30—C25—C29—C28	−178.4 (5)
C10—Fe1—C12—C13	82.6 (4)	Fe2—C25—C29—C28	−60.0 (4)
C11—Fe1—C12—C13	119.8 (5)	C26—C25—C29—Fe2	59.8 (3)
C7—Fe1—C12—C13	−174.3 (3)	C30—C25—C29—Fe2	−118.4 (5)
C8—Fe1—C12—C13	−133.9 (3)	C27—C28—C29—C25	0.5 (7)
C11—C12—C13—C9	−0.1 (6)	Fe2—C28—C29—C25	59.4 (4)
Fe1—C12—C13—C9	−59.3 (3)	C27—C28—C29—Fe2	−58.9 (5)
C11—C12—C13—Fe1	59.2 (4)	C21—Fe2—C29—C25	84.7 (4)
C10—C9—C13—C12	−0.2 (5)	C26—Fe2—C29—C25	−38.2 (3)
C14—C9—C13—C12	175.7 (5)	C22—Fe2—C29—C25	49.3 (7)
Fe1—C9—C13—C12	59.8 (4)	C20—Fe2—C29—C25	127.5 (3)
C10—C9—C13—Fe1	−60.0 (3)	C23—Fe2—C29—C25	−160.9 (12)
C14—C9—C13—Fe1	115.9 (5)	C24—Fe2—C29—C25	168.3 (3)
C5—Fe1—C13—C12	152.7 (4)	C27—Fe2—C29—C25	−81.8 (4)
C9—Fe1—C13—C12	−118.8 (5)	C28—Fe2—C29—C25	−118.5 (6)
C4—Fe1—C13—C12	108.8 (4)	C25—Fe2—C29—C28	118.5 (6)
C10—Fe1—C13—C12	−80.2 (4)	C21—Fe2—C29—C28	−156.8 (4)
C6—Fe1—C13—C12	−171.9 (4)	C26—Fe2—C29—C28	80.3 (5)
C11—Fe1—C13—C12	−37.0 (4)	C22—Fe2—C29—C28	167.8 (6)
C8—Fe1—C13—C12	70.8 (5)	C20—Fe2—C29—C28	−114.0 (4)
C5—Fe1—C13—C9	−88.5 (3)	C23—Fe2—C29—C28	−42.4 (14)

C4—Fe1—C13—C9	−132.4 (3)	C24—Fe2—C29—C28	−73.2 (5)
C10—Fe1—C13—C9	38.6 (3)	C27—Fe2—C29—C28	36.7 (4)
C6—Fe1—C13—C9	−53.1 (5)	C31—N10—C30—C25	129.5 (6)
C11—Fe1—C13—C9	81.8 (3)	N11—N10—C30—C25	−56.3 (7)
C12—Fe1—C13—C9	118.8 (5)	C29—C25—C30—N10	−87.9 (6)
C8—Fe1—C13—C9	−170.4 (3)	C26—C25—C30—N10	94.2 (6)
C15—N4—C14—C9	−108.1 (6)	Fe2—C25—C30—N10	−177.6 (3)
N5—N4—C14—C9	73.5 (6)	C32—N12—C31—N10	−1.0 (6)
C13—C9—C14—N4	91.0 (6)	Co1^{iv}—N12—C31—N10	177.3 (3)
C10—C9—C14—N4	−93.9 (6)	N11—N10—C31—N12	0.8 (6)
Fe1—C9—C14—N4	178.6 (3)	C30—N10—C31—N12	175.6 (5)
N5—N4—C15—N6	0.0 (6)	N10—N11—C32—N12	−0.3 (6)
C14—N4—C15—N6	−178.5 (4)	C31—N12—C32—N11	0.8 (6)
C16—N6—C15—N4	−0.8 (6)	Co1^{iv}—N12—C32—N11	−177.5 (4)
Co1^{iii}—N6—C15—N4	176.7 (3)	Co1—O1—C33—C34	158.2 (4)
N4—N5—C16—N6	−1.4 (7)		

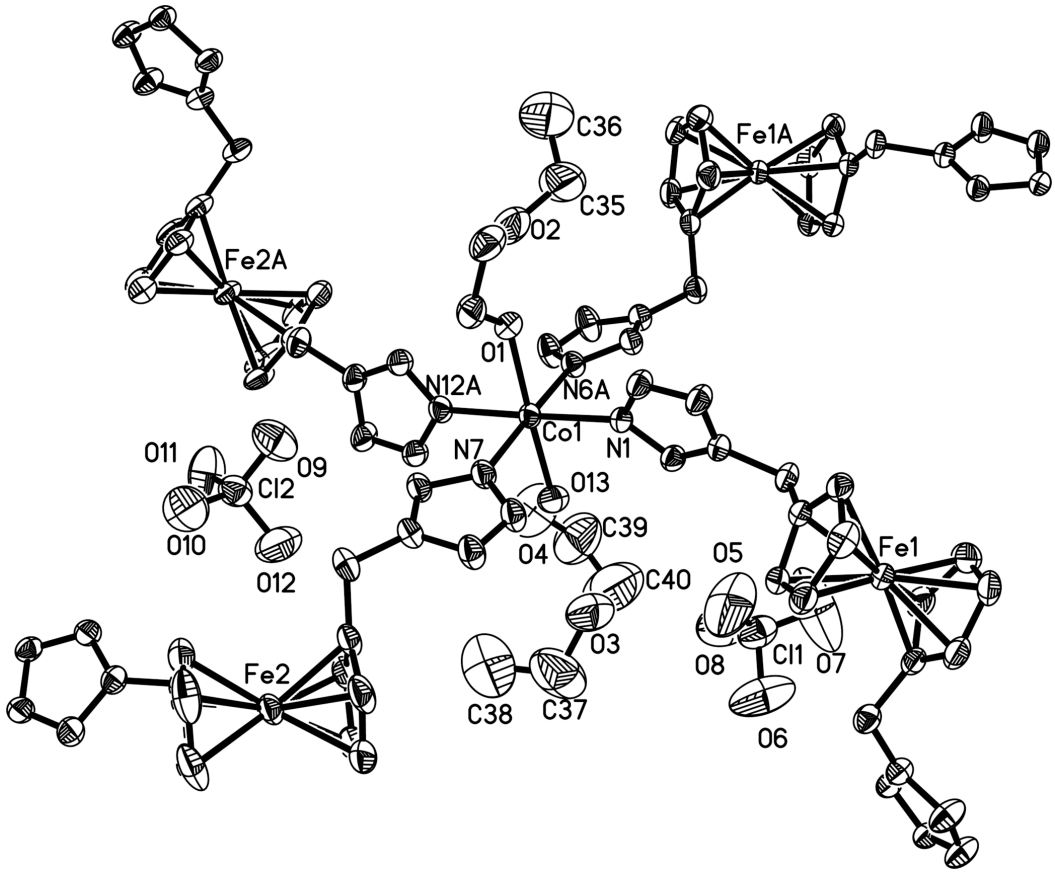
Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+1/2; (ii) −*x*+3/2, *y*+1/2, −*z*+3/2; (iii) −*x*+3/2, *y*−1/2, −*z*+1/2; (iv) −*x*+3/2, *y*−1/2, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1D···O2	0.93	1.74	2.665 (6)	174
O2—H2D···Cl2^{ii}	0.82	2.87	3.620 (6)	153
O3—H3D···O8	0.85	2.08	2.906 (12)	162
O3—H3D···Cl1	0.85	2.90	3.687 (8)	153
O4—H4D···N5^{v}	0.84	2.05	2.871 (8)	164
O13—H1W···O3	0.85	1.92	2.677 (7)	148
O13—H2W···O4	0.90	2.06	2.622 (7)	119

Symmetry codes: (ii) −*x*+3/2, *y*+1/2, −*z*+3/2; (v) *x*−1/2, −*y*+1/2, *z*+1/2.

Fig. 1


C36
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C35
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Fe2A
O1
N12A
N6A
Co1
N1
N7
O13
O11
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C39
O10
O4
O5
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C40
O12
O3
O8
Cl1
O7
Fe2
C38
C37
O6

Fig. 2

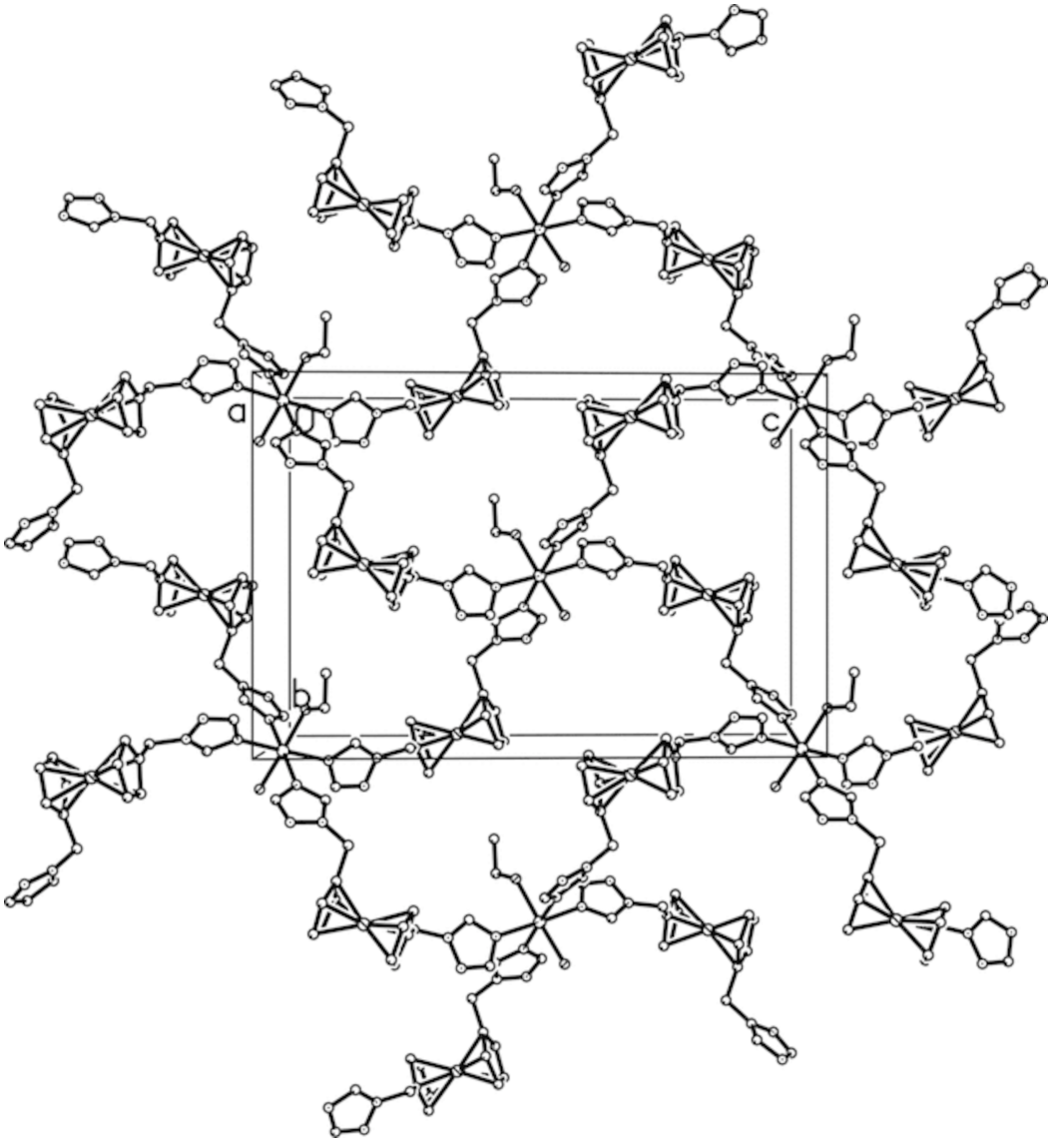

Fig. 3