

Bis(cobaltocenium) tetrachloridocobaltate(II) dichloromethane 1.2-solvate

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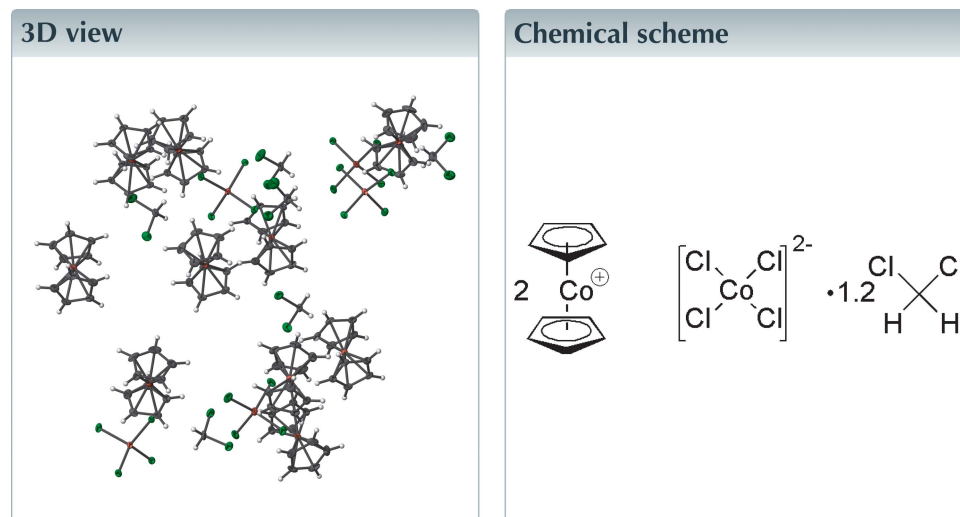
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Structural data: full structural data are available from iucrdata.iucr.org

The structure of bis(cobaltocenium) tetrachloridocobaltate(II) dichloromethane 1.2-solvate, $[\text{Co}(\text{C}_5\text{H}_5)_2]_2[\text{CoCl}_4] \cdot 1.2\text{CH}_2\text{Cl}_2$, has been determined at 100 K. The title compound crystallizes in the space group $P\bar{1}$ and is an example of an unusual $Z' = 5$ structure. The asymmetric unit contains ten cobaltocenium ions, five tetrachloridocobaltate(II) ions and six molecules of dichloromethane, *i.e.* $5\{[\text{Cp}_2\text{Co}]_2[\text{CoCl}_4]\} \cdot 6\text{CH}_2\text{Cl}_2$. All the cobaltocenium ions are determined to be in the eclipsed conformation with respect to the cyclopentadienyl rings.



Structure description

The cell parameters of $[\text{Cp}_2\text{Co}]_2[\text{CoCl}_4]$ ($\text{Cp} = \eta^5\text{-C}_5\text{H}_5$) have been previously reported (Gunter *et al.*, 1970). The molecular structure of the unsolvated compound has not been reported, but it appears to be a single-chain magnetic material [Balaji *et al.*, 2010]. A small number of cobaltocenium derivatives with the $[\text{CoCl}_4]^{2-}$ counter-ion have been reported (Herberhold *et al.*, 2000; Braga *et al.*, 2005; Ransom *et al.*, 2009; Merola *et al.*, 2013). The title compound is the dichloromethane solvate of the parent compound $[\text{Cp}_2\text{Co}]_2[\text{CoCl}_4]$.

The basic components of the compound are shown in Fig. 1. Each asymmetric unit in the unit cell contains five of the $[\text{Cp}_2\text{Co}]_2[\text{CoCl}_4] \cdot \text{CH}_2\text{Cl}_2$ groups pictured in addition to one extra molecule of CH_2Cl_2 , and is an example of a $Z' = 5$ structure. One of the five $[\text{CoCl}_4]^{2-}$ ions in the asymmetric unit is pictured in Fig. 1. Bond distances for atoms labelled $\text{Co1K}-\text{Cl1K}$, $\text{Co1K}-\text{Cl2K}$, $\text{Co1K}-\text{Cl3K}$, and $\text{Co1K}-\text{Cl4K}$ are 2.2792 (9), 2.2685, 2.2819 (9), and 2.2860 (9) Å, respectively. The bond angles in this $[\text{CoCl}_4]^{2-}$ ion vary from 106.83 (3) to 112.28 (3)°. These parameters are typical for the $[\text{CoCl}_4]^{2-}$

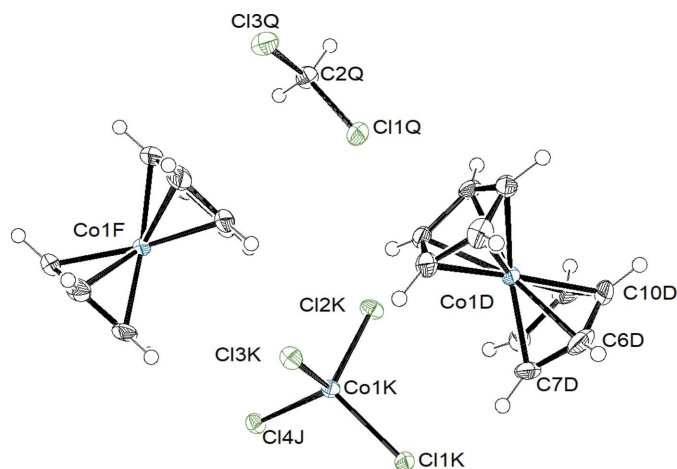


Figure 1
Portion of the unit cell (fractional coordinates x : 0.3 – 1/2, y : 0.1 – 0.5; z : 0.2 – 1/2) showing the formula $[\text{Cp}_2\text{Co}]_2[\text{CoCl}_4]\cdot\text{CH}_2\text{Cl}_2$. Displacement ellipsoids for non-hydrogen atoms are drawn at the 50% probability level.

dianion and are comparable to those found in similar compounds (Braga *et al.*, 2005; Ransom *et al.*, 2009; Merola *et al.*, 2013).

In Fig. 1, two cobaltocenium units are pictured. The distances and angles within the cyclopentadienyl rings are typical for such systems, as are the Co–C bond distances, *e.g.* Co1D–C7D is 2.029 (4) Å. Within the Cp rings, typical bond distances and angles are also observed. The cyclopentadienyl rings in each cobaltocenium ion are coplanar with an average dihedral angle between the least squares planes of 2.97 (1)°. Each cobaltocenium ion is in the eclipsed conformation with respect to the cyclopentadienyl rings, with relative rotations in the range of 0.65 (9)–6.30 (9)°, and an average value of 2.97 (9)°. The two $[\text{Cp}_2\text{Co}]^+$ ions in Fig. 1 are approximately

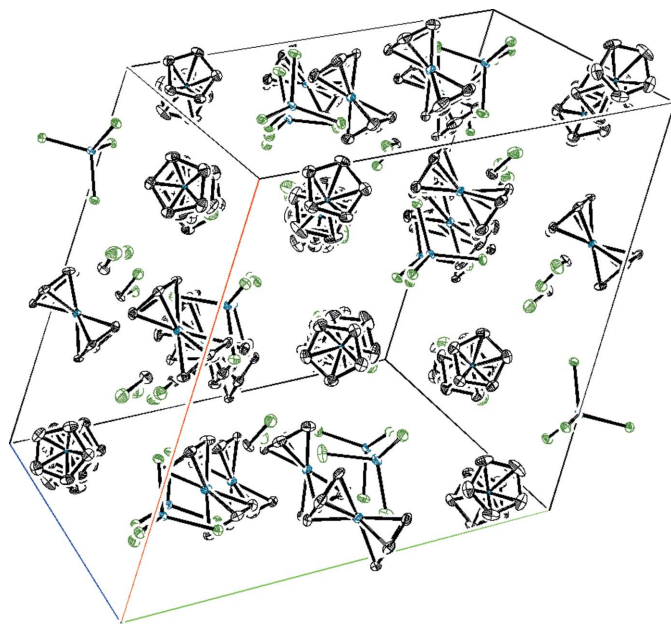


Figure 2
A view of the unit cell drawn looking down chains of cobaltocenium ions. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms have been omitted for clarity.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[\text{Co}(\text{C}_5\text{H}_5)_2]_{10}[\text{CoCl}_4]_5\cdot 6\text{CH}_2\text{Cl}_2$
M_r	3404.30
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	18.1419 (16), 19.9967 (17), 20.3048 (17)
α, β, γ (°)	79.631 (2), 78.398 (2), 63.844 (2)
V (Å ³)	6441.7 (10)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	2.58
Crystal size (mm)	0.44 × 0.28 × 0.26
Data collection	
Diffractometer	Bruker APEX CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2007)
$T_{\text{min}}, T_{\text{max}}$	0.396, 0.553
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	74645, 31791, 23455
R_{int}	0.044
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.043, 0.091, 0.99
No. of reflections	31791
No. of parameters	1378
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.62, -0.51

Computer programs: SMART (Bruker, 2007), SAINT (Bruker, 2007), SHELXTL (Sheldrick, 2008), SHELXL2018 (Sheldrick, 2015), ORTEP-3 for Windows (Farrugia, 2012).

related by an S_2 improper axis of rotation through the $[\text{CoCl}_4]^{2-}$ unit.

The packing of the ions in the title compound (Fig. 2) is more complicated than found for the related decamethylcobaltocenium derivative (Merola *et al.*, 2013), which forms a clear two-dimensional-network of $[(\eta^5\text{-C}_5(\text{CH}_3)_5)_2\text{Co}]^+$ -chains parallel to two of its unit cell axes. In the title compound, the cobaltocenium ions alternate with dichloromethane molecules in loose chains, with two sets of parallel chains aligned roughly at right angles to form layers which also include the CH_2Cl_2 and $[\text{CoCl}_4]^{2-}$ moieties. The $[\text{CoCl}_4]^{2-}$ ions are each surrounded by four $[\text{Cp}_2\text{Co}]^+$ ions in a distorted tetrahedral arrangement with Co–Co distances in the range of 5.0–5.3 Å.

Synthesis and crystallization

The title compound was obtained serendipitously as a byproduct from the reaction of orange crystals of $\text{CpRu}(\text{PPh}_3)_2\text{Cl}$ (0.2013 g, 0.277 mmol) with sublimed Cp_2Co (0.1150 g, 0.608 mmol, 2.19 equiv) in CH_2Cl_2 (5.0 ml) in a sample vial under an atmosphere of argon in an inert-atmosphere drybox. The sample vial was left undisturbed in the drybox for four months during which time green crystals of $5[\text{Cp}_2\text{Co}]_2[\text{CoCl}_4]\cdot 6\text{CH}_2\text{Cl}_2$ grew. Exposure to light, such as from a compact fluorescent light bulb, was found to be required for the isolation of the title compound.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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full crystallographic data

IUCrData (2018). 3, x180552 [https://doi.org/10.1107/S2414314618005527]

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Crystal data

$[\text{Co}(\text{C}_5\text{H}_5)_2]_{10}[\text{CoCl}_4]_5 \cdot 6\text{CH}_2\text{Cl}_2$

$M_r = 3404.30$

Triclinic, $P\bar{1}$

$a = 18.1419$ (16) Å

$b = 19.9967$ (17) Å

$c = 20.3048$ (17) Å

$\alpha = 79.631$ (2)°

$\beta = 78.398$ (2)°

$\gamma = 63.844$ (2)°

$V = 6441.7$ (10) Å³

$Z = 2$

$F(000) = 3394$

$D_x = 1.755$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 8748 reflections

$\theta = 2.3$ – 28.3 °

$\mu = 2.58$ mm⁻¹

$T = 100$ K

Prism, green

$0.44 \times 0.28 \times 0.26$ mm

Data collection

Bruker APEX CCD
diffractometer

ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2007)

$T_{\min} = 0.396$, $T_{\max} = 0.553$

74645 measured reflections

31791 independent reflections

23455 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 28.3$ °, $\theta_{\min} = 1.3$ °

$h = -24 \rightarrow 24$

$k = -23 \rightarrow 26$

$l = -27 \rightarrow 27$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.091$

$S = 0.99$

31791 reflections

1378 parameters

0 restraints

Primary atom site location: dual

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 0.930P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.62$ e Å⁻³

$\Delta\rho_{\min} = -0.51$ e Å⁻³

Special details

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

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1A	0.38674 (3)	0.01972 (2)	0.86756 (2)	0.01318 (9)
C1A	0.2712 (2)	0.05189 (19)	0.84485 (16)	0.0201 (7)
H1A	0.238848	0.023849	0.856174	0.024*
C2A	0.3279 (2)	0.05029 (18)	0.78493 (16)	0.0200 (7)
H2A	0.339838	0.021132	0.748843	0.024*
C3A	0.3634 (2)	0.09945 (18)	0.78834 (15)	0.0206 (7)
H3A	0.403500	0.109009	0.755028	0.025*
C4A	0.3289 (2)	0.13215 (18)	0.84992 (16)	0.0191 (7)
H4A	0.341765	0.167445	0.865195	0.023*
C5A	0.2719 (2)	0.10304 (18)	0.88464 (16)	0.0188 (7)
H5A	0.239587	0.115569	0.927333	0.023*
C6A	0.4168 (2)	-0.08149 (18)	0.92218 (16)	0.0217 (8)
H6A	0.382892	-0.107999	0.935272	0.026*
C7A	0.4736 (2)	-0.08716 (19)	0.86185 (16)	0.0211 (8)
H7A	0.484204	-0.117979	0.827397	0.025*
C8A	0.5115 (2)	-0.0388 (2)	0.86211 (16)	0.0224 (8)
H8A	0.552427	-0.031722	0.827910	0.027*
C9A	0.4781 (2)	-0.00272 (19)	0.92210 (16)	0.0200 (7)
H9A	0.492273	0.033011	0.935070	0.024*
C10A	0.4196 (2)	-0.02950 (18)	0.95942 (15)	0.0199 (7)
H10A	0.387947	-0.015029	1.001925	0.024*
Co1B	0.15938 (3)	0.44890 (2)	0.91288 (2)	0.01607 (10)
C1B	0.0501 (2)	0.50933 (19)	0.87546 (16)	0.0219 (8)
H1B	0.006552	0.494360	0.878160	0.026*
C2B	0.1182 (2)	0.49687 (19)	0.82341 (16)	0.0239 (8)
H2B	0.128336	0.471632	0.784903	0.029*
C3B	0.1688 (2)	0.52810 (19)	0.83806 (16)	0.0231 (8)
H3B	0.218307	0.527850	0.811221	0.028*
C4B	0.1322 (2)	0.55984 (19)	0.90014 (16)	0.0226 (8)
H4B	0.153068	0.584400	0.922425	0.027*
C5B	0.0593 (2)	0.54858 (18)	0.92303 (16)	0.0216 (7)
H5B	0.022588	0.564488	0.963344	0.026*
C6B	0.1609 (2)	0.3491 (2)	0.95657 (19)	0.0315 (9)
H6B	0.118456	0.332963	0.958342	0.038*
C7B	0.2292 (2)	0.3385 (2)	0.90497 (18)	0.0304 (9)
H7B	0.240811	0.313249	0.866171	0.036*
C8B	0.2770 (2)	0.3714 (2)	0.92050 (17)	0.0275 (8)
H8B	0.325959	0.372682	0.893997	0.033*
C9B	0.2390 (2)	0.4023 (2)	0.98298 (17)	0.0283 (9)
H9B	0.257973	0.427922	1.005931	0.034*
C10B	0.1677 (2)	0.3878 (2)	1.00463 (16)	0.0289 (9)
H10B	0.130445	0.401989	1.045066	0.035*
Co1C	0.29284 (3)	0.61378 (2)	0.57233 (2)	0.01398 (9)
C1C	0.2904 (2)	0.54019 (19)	0.51713 (16)	0.0227 (8)
H1C	0.256520	0.513545	0.528735	0.027*

C2C	0.3704 (2)	0.5157 (2)	0.53462 (16)	0.0237 (8)
H2C	0.399757	0.469841	0.560130	0.028*
C3C	0.3993 (2)	0.5714 (2)	0.50754 (16)	0.0225 (8)
H3C	0.451521	0.569530	0.511406	0.027*
C4C	0.3364 (2)	0.6307 (2)	0.47354 (15)	0.0231 (8)
H4C	0.339006	0.675649	0.450836	0.028*
C5C	0.2694 (2)	0.6113 (2)	0.47929 (15)	0.0232 (8)
H5C	0.218993	0.640720	0.461019	0.028*
C6C	0.2066 (2)	0.62170 (19)	0.65474 (15)	0.0204 (7)
H6C	0.170280	0.597477	0.664474	0.024*
C7C	0.2866 (2)	0.59296 (19)	0.67415 (15)	0.0196 (7)
H7C	0.313417	0.545921	0.699119	0.024*
C8C	0.3198 (2)	0.64633 (19)	0.64996 (15)	0.0206 (7)
H8C	0.372662	0.641422	0.655745	0.025*
C9C	0.2601 (2)	0.70837 (19)	0.61559 (16)	0.0226 (8)
H9C	0.265890	0.752558	0.594477	0.027*
C10C	0.1904 (2)	0.69302 (19)	0.61821 (16)	0.0232 (8)
H10C	0.141378	0.724941	0.598865	0.028*
Co1D	0.40315 (3)	0.22407 (2)	0.51667 (2)	0.01624 (10)
C1D	0.2834 (2)	0.2803 (2)	0.49941 (17)	0.0280 (8)
H1D	0.240370	0.264272	0.516257	0.034*
C2D	0.3367 (2)	0.2638 (2)	0.43735 (17)	0.0260 (8)
H2D	0.335187	0.235440	0.405246	0.031*
C3D	0.3927 (2)	0.29699 (19)	0.43153 (16)	0.0231 (8)
H3D	0.435563	0.294555	0.395136	0.028*
C4D	0.3730 (2)	0.33458 (19)	0.48994 (16)	0.0233 (8)
H4D	0.400417	0.361961	0.499502	0.028*
C5D	0.3051 (2)	0.32412 (19)	0.53171 (17)	0.0257 (8)
H5D	0.278995	0.343409	0.573934	0.031*
C6D	0.4151 (2)	0.1287 (2)	0.57681 (19)	0.0351 (10)
H6D	0.372319	0.112276	0.593413	0.042*
C7D	0.4696 (2)	0.11179 (19)	0.51563 (18)	0.0287 (9)
H7D	0.469669	0.081953	0.484083	0.034*
C8D	0.5238 (2)	0.1465 (2)	0.50922 (17)	0.0252 (8)
H8D	0.566709	0.144285	0.472882	0.030*
C9D	0.5026 (2)	0.1854 (2)	0.56693 (18)	0.0301 (9)
H9D	0.528925	0.214020	0.575998	0.036*
C10D	0.4352 (2)	0.1743 (2)	0.60897 (17)	0.0336 (10)
H10D	0.408539	0.194007	0.650959	0.040*
Co1E	0.12112 (3)	0.01634 (3)	0.64600 (2)	0.01757 (10)
C1E	0.0861 (2)	0.0052 (2)	0.56081 (16)	0.0272 (8)
H1E	0.032293	0.030395	0.547488	0.033*
C2E	0.1160 (2)	-0.0644 (2)	0.60140 (18)	0.0324 (9)
H2E	0.086085	-0.093828	0.620126	0.039*
C3E	0.1989 (2)	-0.0819 (2)	0.60887 (18)	0.0310 (9)
H3E	0.234606	-0.125432	0.633445	0.037*
C4E	0.2189 (2)	-0.0232 (2)	0.57323 (17)	0.0280 (9)
H4E	0.270443	-0.020346	0.569834	0.034*

C5E	0.1490 (2)	0.0307 (2)	0.54349 (16)	0.0246 (8)
H5E	0.145317	0.075974	0.516705	0.030*
C6E	0.0205 (2)	0.0912 (2)	0.70007 (17)	0.0263 (8)
H6E	-0.034355	0.116019	0.689034	0.032*
C7E	0.0538 (2)	0.0216 (2)	0.73925 (17)	0.0285 (9)
H7E	0.025006	-0.008436	0.759091	0.034*
C8E	0.1377 (2)	0.0039 (2)	0.74419 (16)	0.0272 (8)
H8E	0.174776	-0.039688	0.767749	0.033*
C9E	0.1555 (2)	0.0638 (2)	0.70706 (16)	0.0242 (8)
H9E	0.207032	0.067239	0.701405	0.029*
C10E	0.0834 (2)	0.11749 (19)	0.68004 (16)	0.0219 (8)
H10E	0.078115	0.163098	0.653211	0.026*
Co1F	0.49501 (3)	0.38504 (3)	0.11572 (2)	0.01764 (10)
C1F	0.4545 (3)	0.3857 (2)	0.21625 (17)	0.0324 (9)
H1F	0.440444	0.348714	0.244829	0.039*
C2F	0.4001 (3)	0.4496 (2)	0.18057 (18)	0.0367 (10)
H2F	0.342734	0.463415	0.181034	0.044*
C3F	0.4452 (3)	0.4895 (2)	0.14412 (19)	0.0412 (11)
H3F	0.423686	0.534901	0.115524	0.049*
C4F	0.5279 (3)	0.4504 (2)	0.15739 (19)	0.0427 (11)
H4F	0.572038	0.464653	0.139352	0.051*
C5F	0.5334 (3)	0.3860 (2)	0.20238 (18)	0.0358 (10)
H5F	0.581822	0.349485	0.220088	0.043*
C6F	0.5012 (2)	0.2898 (2)	0.08915 (17)	0.0261 (8)
H6F	0.489522	0.251798	0.118283	0.031*
C7F	0.4435 (2)	0.3535 (2)	0.05504 (17)	0.0274 (8)
H7F	0.386122	0.366049	0.057642	0.033*
C8F	0.4860 (2)	0.3954 (2)	0.01630 (16)	0.0263 (8)
H8F	0.462257	0.440639	-0.011970	0.032*
C9F	0.5699 (2)	0.35812 (19)	0.02708 (16)	0.0244 (8)
H9F	0.612454	0.374040	0.007526	0.029*
C10F	0.5795 (2)	0.2928 (2)	0.07219 (17)	0.0282 (8)
H10F	0.629525	0.257215	0.088227	0.034*
Co1G	0.07274 (3)	0.83615 (3)	0.02802 (2)	0.01593 (10)
C1G	0.0639 (2)	0.8063 (2)	-0.05954 (17)	0.0296 (9)
H1G	0.015930	0.805981	-0.071151	0.036*
C2G	0.1247 (2)	0.7466 (2)	-0.02600 (17)	0.0313 (9)
H2G	0.125075	0.698630	-0.010990	0.038*
C3G	0.1850 (2)	0.7695 (2)	-0.01828 (17)	0.0330 (10)
H3G	0.233287	0.740023	0.002809	0.040*
C4G	0.1609 (3)	0.8447 (2)	-0.04766 (18)	0.0370 (11)
H4G	0.189850	0.874857	-0.049846	0.044*
C5G	0.0859 (2)	0.8665 (2)	-0.07301 (17)	0.0320 (9)
H5G	0.055389	0.914103	-0.095497	0.038*
C6G	-0.0386 (2)	0.8582 (2)	0.08568 (16)	0.0255 (8)
H6G	-0.084429	0.854321	0.073624	0.031*
C7G	0.0252 (2)	0.8004 (2)	0.11922 (16)	0.0228 (8)
H7G	0.030099	0.750821	0.133369	0.027*

C8G	0.0804 (2)	0.82942 (19)	0.12796 (16)	0.0211 (7)
H8G	0.128794	0.802782	0.149453	0.025*
C9G	0.0514 (2)	0.9051 (2)	0.09922 (16)	0.0224 (8)
H9G	0.076867	0.938046	0.097732	0.027*
C10G	-0.0226 (2)	0.9226 (2)	0.07311 (17)	0.0244 (8)
H10G	-0.055683	0.969573	0.051006	0.029*
Co1H	0.33027 (3)	0.78813 (2)	0.19003 (2)	0.01623 (10)
C1H	0.3149 (2)	0.7987 (2)	0.09182 (16)	0.0232 (8)
H1H	0.266280	0.831337	0.072173	0.028*
C2H	0.3336 (2)	0.7244 (2)	0.12064 (15)	0.0219 (8)
H2H	0.300026	0.698183	0.123830	0.026*
C3H	0.4118 (2)	0.6956 (2)	0.14406 (16)	0.0246 (8)
H3H	0.439626	0.646827	0.165790	0.029*
C4H	0.4409 (2)	0.7523 (2)	0.12940 (16)	0.0246 (8)
H4H	0.491846	0.748161	0.139407	0.030*
C5H	0.3810 (2)	0.8166 (2)	0.09714 (15)	0.0247 (8)
H5H	0.384456	0.863035	0.081887	0.030*
C6H	0.2223 (2)	0.8580 (2)	0.23997 (16)	0.0271 (8)
H6H	0.172597	0.889006	0.221206	0.033*
C7H	0.2446 (2)	0.7833 (2)	0.27024 (16)	0.0274 (8)
H7H	0.212358	0.755571	0.275499	0.033*
C8H	0.3236 (2)	0.7573 (2)	0.29133 (15)	0.0242 (8)
H8H	0.353512	0.708966	0.313021	0.029*
C9H	0.3502 (2)	0.81647 (19)	0.27419 (16)	0.0240 (8)
H9H	0.400798	0.814618	0.282460	0.029*
C10H	0.2873 (2)	0.8785 (2)	0.24261 (16)	0.0264 (8)
H10H	0.288447	0.925610	0.226049	0.032*
Co1I	0.93084 (3)	0.47721 (3)	0.64319 (2)	0.01930 (10)
C1I	1.0483 (2)	0.4000 (2)	0.62018 (19)	0.0397 (11)
H1I	1.075078	0.385991	0.576365	0.048*
C2I	1.0017 (3)	0.3667 (2)	0.6655 (2)	0.0362 (10)
H2I	0.991459	0.326298	0.657681	0.043*
C3I	0.9730 (2)	0.4031 (2)	0.72373 (19)	0.0392 (11)
H3I	0.940027	0.391897	0.762858	0.047*
C4I	1.0016 (3)	0.4595 (2)	0.7144 (2)	0.0427 (12)
H4I	0.991026	0.493402	0.746023	0.051*
C5I	1.0485 (2)	0.4569 (2)	0.6503 (2)	0.0408 (11)
H5I	1.075602	0.488510	0.630837	0.049*
C6I	0.8784 (2)	0.5175 (2)	0.55729 (18)	0.0318 (9)
H6I	0.904611	0.503253	0.513406	0.038*
C7I	0.8334 (2)	0.4832 (2)	0.60440 (19)	0.0334 (9)
H7I	0.823663	0.442165	0.597517	0.040*
C8I	0.8056 (2)	0.5202 (2)	0.66338 (19)	0.0325 (9)
H8I	0.774019	0.508435	0.703213	0.039*
C9I	0.8329 (2)	0.5780 (2)	0.65304 (18)	0.0308 (9)
H9I	0.823075	0.611673	0.684675	0.037*
C10I	0.8775 (2)	0.5766 (2)	0.58683 (18)	0.0301 (9)
H10I	0.902402	0.609657	0.566128	0.036*

Co1J	0.13178 (3)	0.23051 (3)	0.26464 (2)	0.01871 (10)
C1J	0.0434 (2)	0.2470 (2)	0.20827 (17)	0.0259 (8)
H1J	0.036319	0.209478	0.190907	0.031*
C2J	0.0923 (2)	0.28480 (19)	0.17528 (16)	0.0230 (8)
H2J	0.124118	0.277191	0.131772	0.028*
C3J	0.0859 (2)	0.3366 (2)	0.21855 (17)	0.0256 (8)
H3J	0.112460	0.369591	0.209001	0.031*
C4J	0.0330 (2)	0.3299 (2)	0.27786 (18)	0.0283 (9)
H4J	0.017582	0.357731	0.315548	0.034*
C5J	0.0068 (2)	0.2745 (2)	0.27160 (18)	0.0296 (9)
H5J	-0.029219	0.258658	0.304405	0.036*
C6J	0.1968 (2)	0.1177 (2)	0.28138 (17)	0.0293 (9)
H6J	0.186056	0.080393	0.267251	0.035*
C7J	0.2488 (2)	0.1518 (2)	0.24448 (17)	0.0242 (8)
H7J	0.279386	0.141032	0.200925	0.029*
C8J	0.2475 (2)	0.2043 (2)	0.28325 (18)	0.0311 (9)
H8J	0.276977	0.234856	0.270360	0.037*
C9J	0.1945 (2)	0.2036 (2)	0.34471 (19)	0.0375 (10)
H9J	0.181833	0.233612	0.380267	0.045*
C10J	0.1638 (2)	0.1501 (2)	0.34352 (17)	0.0361 (10)
H10J	0.127138	0.137712	0.378600	0.043*
Co1K	0.41972 (3)	0.84722 (2)	0.70620 (2)	0.01641 (10)
C11K	0.39707 (5)	0.95645 (5)	0.63826 (4)	0.02059 (17)
C12K	0.39742 (5)	0.76861 (5)	0.65306 (4)	0.02231 (18)
C13K	0.55417 (5)	0.79583 (5)	0.72616 (4)	0.02188 (18)
C14K	0.33149 (5)	0.86497 (5)	0.80568 (4)	0.02035 (17)
Co1L	0.39327 (3)	0.36379 (2)	0.71459 (2)	0.01594 (10)
C11L	0.40434 (5)	0.43484 (5)	0.78534 (4)	0.01944 (17)
C12L	0.49545 (5)	0.34596 (5)	0.62462 (4)	0.01951 (17)
C13L	0.26600 (5)	0.42224 (5)	0.67867 (4)	0.02089 (17)
C14L	0.41064 (5)	0.25029 (5)	0.77055 (4)	0.02272 (18)
Co1M	0.98352 (3)	0.25947 (3)	0.50885 (2)	0.01685 (10)
C11M	0.98011 (5)	0.16950 (5)	0.45581 (4)	0.01978 (17)
C12M	0.90156 (5)	0.26499 (5)	0.61051 (4)	0.02182 (18)
C13M	0.93720 (5)	0.37434 (5)	0.44732 (4)	0.02347 (18)
C14M	1.11578 (5)	0.23119 (5)	0.52155 (4)	0.02580 (19)
Co1N	0.18729 (3)	0.05966 (2)	0.08754 (2)	0.01576 (10)
C11N	0.14557 (5)	0.17984 (4)	0.03778 (4)	0.01867 (17)
C12N	0.31216 (5)	0.02373 (5)	0.12280 (4)	0.01823 (17)
C13N	0.20261 (5)	-0.01769 (5)	0.01098 (4)	0.02053 (17)
C14N	0.09263 (5)	0.05050 (5)	0.17624 (4)	0.02412 (19)
Co1O	0.18728 (3)	0.56027 (3)	0.10547 (2)	0.02074 (10)
C11O	0.05686 (5)	0.61245 (5)	0.07693 (4)	0.0278 (2)
C12O	0.28416 (5)	0.55429 (5)	0.01259 (4)	0.0272 (2)
C13O	0.19824 (6)	0.63039 (5)	0.17638 (4)	0.0288 (2)
C14O	0.20884 (7)	0.44343 (5)	0.15783 (4)	0.0350 (2)
C11P	0.41792 (5)	0.19389 (5)	-0.02485 (4)	0.0269 (2)
C2P	0.3371 (2)	0.1900 (2)	0.03897 (17)	0.0264 (8)

H2P1	0.352349	0.137669	0.059603	0.032*
H2P2	0.285822	0.206471	0.018669	0.032*
Cl3P	0.31882 (6)	0.24813 (6)	0.10229 (4)	0.0322 (2)
Cl1Q	0.44608 (6)	0.44375 (5)	0.37259 (4)	0.0301 (2)
C2Q	0.4330 (2)	0.53087 (19)	0.32596 (17)	0.0232 (8)
H2Q1	0.437956	0.563235	0.354839	0.028*
H2Q2	0.477321	0.522887	0.286791	0.028*
Cl3Q	0.33543 (6)	0.57606 (5)	0.29705 (5)	0.0318 (2)
Cl1R	0.72060 (6)	0.15466 (6)	0.55293 (5)	0.0376 (2)
C2R	0.8217 (2)	0.1303 (2)	0.56974 (19)	0.0354 (10)
H2R1	0.858119	0.131021	0.526448	0.043*
H2R2	0.820077	0.168142	0.596112	0.043*
Cl3R	0.86359 (7)	0.04147 (6)	0.61483 (5)	0.0438 (3)
Cl1S	0.20679 (6)	0.22430 (6)	0.67440 (5)	0.0342 (2)
C2S	0.2016 (2)	0.2774 (2)	0.73751 (16)	0.0244 (8)
H2S1	0.257013	0.257982	0.751949	0.029*
H2S2	0.186199	0.330149	0.718315	0.029*
Cl3S	0.12907 (6)	0.27364 (6)	0.80822 (5)	0.0400 (3)
Cl1T	0.24279 (7)	0.67192 (6)	0.82826 (5)	0.0445 (3)
C2T	0.2274 (2)	0.7606 (2)	0.78589 (17)	0.0272 (8)
H2T1	0.269239	0.754803	0.745072	0.033*
H2T2	0.235613	0.790166	0.815717	0.033*
Cl3T	0.12709 (6)	0.80988 (6)	0.76181 (5)	0.0397 (2)
Cl1U	0.60295 (6)	1.02794 (6)	0.68828 (5)	0.0384 (2)
C2U	0.5892 (2)	0.9653 (2)	0.64581 (19)	0.0348 (9)
H2U1	0.530878	0.986789	0.637245	0.042*
H2U2	0.600406	0.917505	0.675001	0.042*
Cl3U	0.65574 (7)	0.94760 (6)	0.56807 (5)	0.0437 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1A	0.0139 (2)	0.0139 (2)	0.01226 (19)	-0.00582 (18)	-0.00345 (17)	-0.00074 (17)
C1A	0.0141 (17)	0.0199 (19)	0.0266 (17)	-0.0060 (15)	-0.0094 (14)	0.0009 (15)
C2A	0.0232 (18)	0.0152 (18)	0.0164 (15)	0.0001 (15)	-0.0116 (14)	-0.0009 (13)
C3A	0.0249 (19)	0.0191 (19)	0.0157 (16)	-0.0090 (16)	-0.0040 (14)	0.0037 (14)
C4A	0.0250 (19)	0.0122 (17)	0.0223 (16)	-0.0083 (15)	-0.0071 (14)	-0.0011 (14)
C5A	0.0160 (17)	0.0172 (18)	0.0174 (16)	-0.0012 (14)	-0.0046 (13)	-0.0006 (13)
C6A	0.0218 (19)	0.0163 (19)	0.0247 (17)	-0.0051 (15)	-0.0104 (15)	0.0032 (14)
C7A	0.0183 (18)	0.0177 (18)	0.0240 (17)	0.0007 (15)	-0.0102 (14)	-0.0079 (14)
C8A	0.0128 (17)	0.032 (2)	0.0204 (16)	-0.0062 (16)	-0.0053 (14)	-0.0024 (15)
C9A	0.0162 (17)	0.0233 (19)	0.0218 (16)	-0.0055 (15)	-0.0076 (14)	-0.0074 (14)
C10A	0.0186 (18)	0.0207 (19)	0.0135 (15)	-0.0019 (15)	-0.0045 (13)	0.0007 (13)
Co1B	0.0152 (2)	0.0168 (2)	0.0156 (2)	-0.00653 (19)	-0.00260 (17)	-0.00001 (18)
C1B	0.0177 (18)	0.022 (2)	0.0252 (17)	-0.0078 (15)	-0.0083 (14)	0.0030 (15)
C2B	0.027 (2)	0.022 (2)	0.0181 (16)	-0.0049 (16)	-0.0091 (15)	-0.0004 (14)
C3B	0.0226 (19)	0.021 (2)	0.0198 (17)	-0.0069 (16)	-0.0020 (14)	0.0052 (14)
C4B	0.0260 (19)	0.0182 (19)	0.0256 (18)	-0.0102 (16)	-0.0082 (15)	0.0007 (15)

C5B	0.0195 (18)	0.0177 (19)	0.0206 (16)	-0.0022 (15)	-0.0017 (14)	-0.0012 (14)
C6B	0.028 (2)	0.021 (2)	0.046 (2)	-0.0129 (18)	-0.0144 (18)	0.0140 (18)
C7B	0.035 (2)	0.019 (2)	0.030 (2)	-0.0016 (17)	-0.0133 (17)	-0.0026 (16)
C8B	0.0171 (18)	0.025 (2)	0.0291 (19)	-0.0025 (16)	-0.0053 (15)	0.0098 (16)
C9B	0.025 (2)	0.031 (2)	0.0263 (18)	-0.0080 (17)	-0.0116 (16)	0.0025 (16)
C10B	0.023 (2)	0.034 (2)	0.0154 (16)	-0.0027 (17)	-0.0004 (14)	0.0061 (16)
Co1C	0.0132 (2)	0.0142 (2)	0.0135 (2)	-0.00497 (19)	-0.00067 (17)	-0.00237 (17)
C1C	0.028 (2)	0.022 (2)	0.0184 (16)	-0.0094 (16)	0.0015 (15)	-0.0108 (15)
C2C	0.0248 (19)	0.021 (2)	0.0182 (16)	-0.0026 (16)	-0.0010 (14)	-0.0058 (14)
C3C	0.0165 (17)	0.028 (2)	0.0194 (17)	-0.0067 (16)	0.0044 (14)	-0.0099 (15)
C4C	0.0251 (19)	0.021 (2)	0.0158 (16)	-0.0067 (16)	0.0045 (14)	-0.0011 (14)
C5C	0.0203 (18)	0.029 (2)	0.0130 (15)	-0.0012 (16)	-0.0030 (14)	-0.0083 (15)
C6C	0.0180 (18)	0.029 (2)	0.0153 (15)	-0.0109 (16)	0.0033 (13)	-0.0074 (14)
C7C	0.0264 (19)	0.0166 (18)	0.0136 (15)	-0.0069 (15)	-0.0022 (14)	-0.0026 (13)
C8C	0.0211 (18)	0.0222 (19)	0.0209 (17)	-0.0086 (15)	-0.0060 (14)	-0.0059 (14)
C9C	0.032 (2)	0.0127 (18)	0.0226 (17)	-0.0086 (16)	-0.0021 (15)	-0.0059 (14)
C10C	0.0199 (18)	0.022 (2)	0.0193 (17)	0.0015 (15)	-0.0036 (14)	-0.0089 (15)
Co1D	0.0191 (2)	0.0151 (2)	0.0157 (2)	-0.0084 (2)	-0.00245 (18)	-0.00110 (18)
C1D	0.0173 (18)	0.035 (2)	0.0314 (19)	-0.0119 (17)	-0.0056 (15)	0.0030 (17)
C2D	0.030 (2)	0.027 (2)	0.0229 (18)	-0.0101 (17)	-0.0122 (16)	-0.0009 (15)
C3D	0.0245 (19)	0.0193 (19)	0.0171 (16)	-0.0041 (16)	0.0000 (14)	0.0019 (14)
C4D	0.033 (2)	0.0142 (18)	0.0260 (18)	-0.0119 (16)	-0.0082 (16)	0.0013 (14)
C5D	0.0235 (19)	0.022 (2)	0.0205 (17)	-0.0008 (16)	-0.0007 (15)	-0.0017 (15)
C6D	0.036 (2)	0.021 (2)	0.038 (2)	-0.0090 (18)	0.0007 (18)	0.0104 (17)
C7D	0.037 (2)	0.0139 (19)	0.033 (2)	-0.0066 (17)	-0.0098 (17)	-0.0040 (16)
C8D	0.024 (2)	0.024 (2)	0.0225 (17)	-0.0048 (16)	-0.0059 (15)	-0.0015 (15)
C9D	0.029 (2)	0.022 (2)	0.037 (2)	-0.0019 (17)	-0.0215 (18)	-0.0016 (17)
C10D	0.044 (3)	0.025 (2)	0.0179 (18)	-0.0021 (19)	-0.0080 (17)	0.0029 (16)
Co1E	0.0154 (2)	0.0193 (3)	0.0188 (2)	-0.0075 (2)	-0.00378 (18)	-0.00164 (19)
C1E	0.024 (2)	0.034 (2)	0.0234 (18)	-0.0083 (17)	-0.0107 (15)	-0.0056 (16)
C2E	0.044 (3)	0.033 (2)	0.0277 (19)	-0.021 (2)	-0.0054 (18)	-0.0078 (17)
C3E	0.037 (2)	0.021 (2)	0.0265 (19)	0.0003 (18)	-0.0134 (17)	-0.0048 (16)
C4E	0.0192 (19)	0.036 (2)	0.0240 (18)	-0.0047 (17)	-0.0002 (15)	-0.0128 (17)
C5E	0.027 (2)	0.026 (2)	0.0179 (16)	-0.0083 (17)	-0.0022 (15)	-0.0037 (15)
C6E	0.0165 (18)	0.030 (2)	0.0282 (19)	-0.0042 (16)	0.0002 (15)	-0.0110 (16)
C7E	0.032 (2)	0.030 (2)	0.0228 (18)	-0.0157 (18)	0.0044 (16)	-0.0032 (16)
C8E	0.037 (2)	0.024 (2)	0.0191 (17)	-0.0095 (18)	-0.0087 (16)	-0.0003 (15)
C9E	0.0237 (19)	0.028 (2)	0.0247 (18)	-0.0126 (17)	-0.0063 (15)	-0.0049 (16)
C10E	0.0262 (19)	0.0157 (18)	0.0207 (17)	-0.0046 (15)	-0.0053 (15)	-0.0033 (14)
Co1F	0.0197 (2)	0.0157 (2)	0.0175 (2)	-0.0073 (2)	-0.00261 (18)	-0.00167 (18)
C1F	0.049 (3)	0.027 (2)	0.0167 (17)	-0.014 (2)	0.0009 (17)	-0.0034 (16)
C2F	0.032 (2)	0.036 (2)	0.026 (2)	0.0011 (19)	0.0027 (17)	-0.0122 (18)
C3F	0.072 (3)	0.019 (2)	0.025 (2)	-0.012 (2)	-0.006 (2)	-0.0049 (17)
C4F	0.068 (3)	0.053 (3)	0.031 (2)	-0.047 (3)	0.004 (2)	-0.017 (2)
C5F	0.041 (3)	0.042 (3)	0.027 (2)	-0.014 (2)	-0.0129 (18)	-0.0109 (19)
C6F	0.037 (2)	0.019 (2)	0.0297 (19)	-0.0159 (17)	-0.0035 (17)	-0.0085 (16)
C7F	0.027 (2)	0.028 (2)	0.033 (2)	-0.0114 (17)	-0.0102 (16)	-0.0084 (17)
C8F	0.034 (2)	0.026 (2)	0.0183 (17)	-0.0110 (18)	-0.0038 (15)	-0.0055 (15)

C9F	0.027 (2)	0.025 (2)	0.0207 (17)	-0.0117 (17)	0.0030 (15)	-0.0068 (15)
C10F	0.025 (2)	0.022 (2)	0.031 (2)	-0.0018 (17)	-0.0043 (16)	-0.0082 (16)
Co1G	0.0130 (2)	0.0171 (2)	0.0180 (2)	-0.00594 (19)	-0.00098 (17)	-0.00493 (18)
C1G	0.022 (2)	0.049 (3)	0.0214 (18)	-0.0135 (19)	0.0002 (15)	-0.0209 (18)
C2G	0.045 (3)	0.023 (2)	0.0253 (19)	-0.0163 (19)	0.0066 (17)	-0.0097 (16)
C3G	0.0145 (18)	0.047 (3)	0.0246 (19)	0.0017 (18)	-0.0018 (15)	-0.0137 (18)
C4G	0.045 (3)	0.056 (3)	0.029 (2)	-0.040 (2)	0.0201 (18)	-0.027 (2)
C5G	0.042 (2)	0.022 (2)	0.0174 (17)	-0.0017 (18)	0.0010 (16)	-0.0036 (15)
C6G	0.0179 (18)	0.036 (2)	0.0258 (18)	-0.0143 (17)	0.0050 (15)	-0.0128 (17)
C7G	0.0249 (19)	0.026 (2)	0.0181 (16)	-0.0124 (16)	0.0039 (14)	-0.0061 (15)
C8G	0.0167 (17)	0.026 (2)	0.0189 (16)	-0.0063 (15)	-0.0016 (14)	-0.0063 (15)
C9G	0.0225 (19)	0.027 (2)	0.0230 (17)	-0.0138 (16)	0.0021 (14)	-0.0110 (15)
C10G	0.0188 (18)	0.020 (2)	0.0267 (18)	-0.0016 (15)	0.0029 (15)	-0.0086 (15)
Co1H	0.0166 (2)	0.0168 (2)	0.0135 (2)	-0.0067 (2)	-0.00061 (17)	0.00022 (18)
C1H	0.0214 (19)	0.025 (2)	0.0179 (16)	-0.0042 (16)	-0.0040 (14)	-0.0019 (15)
C2H	0.0231 (19)	0.025 (2)	0.0185 (16)	-0.0110 (16)	0.0004 (14)	-0.0069 (15)
C3H	0.027 (2)	0.023 (2)	0.0168 (16)	-0.0052 (16)	-0.0011 (14)	-0.0028 (15)
C4H	0.0158 (18)	0.038 (2)	0.0179 (16)	-0.0105 (17)	0.0024 (14)	-0.0057 (16)
C5H	0.033 (2)	0.029 (2)	0.0130 (15)	-0.0168 (18)	0.0037 (14)	-0.0021 (15)
C6H	0.0225 (19)	0.027 (2)	0.0199 (17)	-0.0008 (17)	0.0015 (15)	-0.0030 (15)
C7H	0.027 (2)	0.033 (2)	0.0204 (17)	-0.0154 (18)	0.0067 (15)	-0.0005 (16)
C8H	0.032 (2)	0.025 (2)	0.0134 (15)	-0.0117 (17)	0.0003 (14)	0.0010 (14)
C9H	0.031 (2)	0.025 (2)	0.0168 (16)	-0.0118 (17)	-0.0013 (15)	-0.0057 (15)
C10H	0.043 (2)	0.0174 (19)	0.0163 (16)	-0.0120 (17)	0.0044 (16)	-0.0058 (14)
Co1I	0.0216 (3)	0.0190 (3)	0.0192 (2)	-0.0095 (2)	-0.00516 (19)	-0.00133 (19)
C1I	0.028 (2)	0.042 (3)	0.025 (2)	0.005 (2)	0.0004 (17)	-0.0028 (19)
C2I	0.044 (3)	0.014 (2)	0.053 (3)	-0.0080 (19)	-0.025 (2)	0.0020 (18)
C3I	0.029 (2)	0.047 (3)	0.026 (2)	-0.008 (2)	-0.0059 (17)	0.0145 (19)
C4I	0.048 (3)	0.030 (2)	0.047 (3)	0.001 (2)	-0.033 (2)	-0.015 (2)
C5I	0.025 (2)	0.027 (2)	0.072 (3)	-0.0161 (19)	-0.022 (2)	0.023 (2)
C6I	0.036 (2)	0.036 (2)	0.0219 (18)	-0.0114 (19)	-0.0138 (17)	0.0014 (17)
C7I	0.030 (2)	0.032 (2)	0.046 (2)	-0.0160 (19)	-0.0188 (19)	-0.0011 (19)
C8I	0.021 (2)	0.040 (3)	0.036 (2)	-0.0110 (18)	-0.0049 (17)	-0.0046 (19)
C9I	0.026 (2)	0.029 (2)	0.034 (2)	-0.0019 (18)	-0.0135 (17)	-0.0092 (17)
C10I	0.031 (2)	0.022 (2)	0.039 (2)	-0.0108 (18)	-0.0178 (18)	0.0074 (17)
Co1J	0.0146 (2)	0.0219 (3)	0.0168 (2)	-0.0057 (2)	0.00055 (18)	-0.00346 (19)
C1J	0.0214 (19)	0.022 (2)	0.034 (2)	-0.0058 (16)	-0.0091 (16)	-0.0047 (16)
C2J	0.0179 (18)	0.025 (2)	0.0206 (17)	-0.0029 (16)	-0.0052 (14)	-0.0034 (15)
C3J	0.027 (2)	0.022 (2)	0.0287 (19)	-0.0112 (17)	-0.0077 (16)	0.0017 (16)
C4J	0.025 (2)	0.023 (2)	0.0268 (19)	0.0014 (16)	-0.0028 (16)	-0.0080 (16)
C5J	0.0127 (18)	0.033 (2)	0.033 (2)	-0.0037 (16)	0.0020 (15)	-0.0009 (17)
C6J	0.027 (2)	0.024 (2)	0.0294 (19)	-0.0076 (17)	-0.0012 (16)	0.0040 (16)
C7J	0.0171 (18)	0.025 (2)	0.0209 (17)	-0.0014 (16)	-0.0001 (14)	-0.0030 (15)
C8J	0.0192 (19)	0.039 (2)	0.034 (2)	-0.0082 (18)	-0.0078 (16)	-0.0075 (18)
C9J	0.030 (2)	0.043 (3)	0.028 (2)	0.001 (2)	-0.0107 (17)	-0.0104 (19)
C10J	0.025 (2)	0.044 (3)	0.0195 (18)	-0.0032 (19)	0.0023 (16)	0.0089 (17)
Co1K	0.0171 (2)	0.0165 (2)	0.0182 (2)	-0.0090 (2)	-0.00285 (18)	-0.00249 (18)
C11K	0.0258 (4)	0.0189 (4)	0.0190 (4)	-0.0111 (4)	-0.0041 (3)	-0.0008 (3)

Cl2K	0.0223 (4)	0.0239 (5)	0.0267 (4)	-0.0144 (4)	0.0001 (3)	-0.0082 (4)
Cl3K	0.0177 (4)	0.0254 (5)	0.0234 (4)	-0.0085 (4)	-0.0037 (3)	-0.0051 (3)
Cl4K	0.0218 (4)	0.0233 (5)	0.0194 (4)	-0.0127 (4)	-0.0009 (3)	-0.0042 (3)
Co1L	0.0177 (2)	0.0162 (2)	0.0159 (2)	-0.0099 (2)	-0.00141 (18)	-0.00018 (18)
Cl1L	0.0215 (4)	0.0218 (4)	0.0182 (4)	-0.0115 (4)	-0.0031 (3)	-0.0029 (3)
Cl2L	0.0193 (4)	0.0194 (4)	0.0189 (4)	-0.0086 (4)	0.0009 (3)	-0.0023 (3)
Cl3L	0.0191 (4)	0.0208 (4)	0.0242 (4)	-0.0095 (4)	-0.0044 (3)	-0.0013 (3)
Cl4L	0.0272 (5)	0.0207 (5)	0.0245 (4)	-0.0153 (4)	-0.0068 (4)	0.0052 (3)
Co1M	0.0165 (2)	0.0200 (3)	0.0164 (2)	-0.0101 (2)	-0.00189 (18)	-0.00152 (18)
Cl1M	0.0180 (4)	0.0202 (4)	0.0229 (4)	-0.0085 (4)	-0.0047 (3)	-0.0031 (3)
Cl2M	0.0190 (4)	0.0261 (5)	0.0179 (4)	-0.0090 (4)	-0.0009 (3)	0.0005 (3)
Cl3M	0.0271 (5)	0.0221 (5)	0.0229 (4)	-0.0134 (4)	-0.0032 (3)	0.0017 (3)
Cl4M	0.0198 (4)	0.0380 (5)	0.0259 (4)	-0.0173 (4)	-0.0048 (3)	-0.0026 (4)
Co1N	0.0135 (2)	0.0168 (2)	0.0180 (2)	-0.00804 (19)	-0.00157 (17)	-0.00057 (18)
Cl1N	0.0185 (4)	0.0166 (4)	0.0208 (4)	-0.0075 (3)	-0.0029 (3)	-0.0011 (3)
Cl2N	0.0160 (4)	0.0227 (4)	0.0182 (4)	-0.0104 (3)	-0.0036 (3)	0.0001 (3)
Cl3N	0.0219 (4)	0.0200 (4)	0.0234 (4)	-0.0116 (4)	-0.0039 (3)	-0.0029 (3)
Cl4N	0.0182 (4)	0.0259 (5)	0.0266 (4)	-0.0113 (4)	0.0036 (3)	-0.0006 (4)
Co1O	0.0212 (3)	0.0207 (3)	0.0232 (2)	-0.0123 (2)	-0.00141 (19)	-0.0017 (2)
Cl1O	0.0202 (4)	0.0375 (6)	0.0319 (5)	-0.0158 (4)	-0.0016 (4)	-0.0105 (4)
Cl2O	0.0198 (4)	0.0281 (5)	0.0296 (4)	-0.0103 (4)	0.0009 (4)	0.0028 (4)
Cl3O	0.0338 (5)	0.0245 (5)	0.0354 (5)	-0.0156 (4)	-0.0139 (4)	-0.0017 (4)
Cl4O	0.0555 (7)	0.0251 (5)	0.0274 (5)	-0.0238 (5)	0.0029 (4)	-0.0013 (4)
Cl1P	0.0236 (5)	0.0266 (5)	0.0265 (4)	-0.0092 (4)	0.0005 (4)	-0.0004 (4)
C2P	0.024 (2)	0.028 (2)	0.0334 (19)	-0.0195 (17)	-0.0006 (16)	0.0010 (16)
Cl3P	0.0349 (5)	0.0382 (6)	0.0260 (4)	-0.0209 (5)	0.0037 (4)	-0.0030 (4)
Cl1Q	0.0414 (6)	0.0239 (5)	0.0252 (4)	-0.0150 (4)	-0.0064 (4)	0.0025 (4)
C2Q	0.027 (2)	0.023 (2)	0.0251 (18)	-0.0171 (17)	-0.0013 (15)	-0.0005 (15)
Cl3Q	0.0309 (5)	0.0245 (5)	0.0405 (5)	-0.0101 (4)	-0.0105 (4)	-0.0026 (4)
Cl1R	0.0347 (6)	0.0449 (6)	0.0335 (5)	-0.0163 (5)	0.0000 (4)	-0.0107 (5)
C2R	0.035 (2)	0.046 (3)	0.034 (2)	-0.027 (2)	0.0044 (18)	-0.0096 (19)
Cl3R	0.0351 (6)	0.0430 (7)	0.0440 (6)	-0.0099 (5)	0.0011 (5)	-0.0067 (5)
Cl1S	0.0372 (6)	0.0333 (6)	0.0359 (5)	-0.0160 (5)	-0.0062 (4)	-0.0079 (4)
C2S	0.0223 (19)	0.028 (2)	0.0279 (18)	-0.0151 (17)	-0.0031 (15)	-0.0020 (16)
Cl3S	0.0255 (5)	0.0607 (7)	0.0267 (5)	-0.0158 (5)	-0.0020 (4)	0.0045 (5)
Cl1T	0.0616 (7)	0.0297 (6)	0.0354 (5)	-0.0214 (5)	0.0154 (5)	-0.0057 (4)
C2T	0.030 (2)	0.030 (2)	0.0308 (19)	-0.0229 (18)	0.0028 (16)	-0.0063 (17)
Cl3T	0.0321 (6)	0.0567 (7)	0.0339 (5)	-0.0216 (5)	-0.0028 (4)	-0.0073 (5)
Cl1U	0.0416 (6)	0.0335 (6)	0.0420 (5)	-0.0156 (5)	-0.0150 (5)	0.0012 (5)
C2U	0.033 (2)	0.036 (2)	0.040 (2)	-0.020 (2)	-0.0084 (18)	0.0031 (19)
Cl3U	0.0413 (6)	0.0529 (7)	0.0367 (5)	-0.0181 (6)	-0.0113 (5)	-0.0016 (5)

Geometric parameters (Å, °)

Co1A—C3A	2.016 (3)	C6F—H6F	0.9500
Co1A—C4A	2.016 (3)	C7F—C8F	1.415 (5)
Co1A—C10A	2.018 (3)	C7F—H7F	0.9500
Co1A—C9A	2.020 (3)	C8F—C9F	1.413 (5)

Co1A—C6A	2.021 (3)	C8F—H8F	0.9500
Co1A—C5A	2.023 (3)	C9F—C10F	1.418 (5)
Co1A—C2A	2.026 (3)	C9F—H9F	0.9500
Co1A—C7A	2.028 (3)	C10F—H10F	0.9500
Co1A—C1A	2.027 (3)	Co1G—C6G	2.023 (3)
Co1A—C8A	2.029 (3)	Co1G—C3G	2.024 (3)
C1A—C5A	1.418 (4)	Co1G—C2G	2.025 (4)
C1A—C2A	1.422 (4)	Co1G—C4G	2.026 (4)
C1A—H1A	0.9500	Co1G—C7G	2.027 (3)
C2A—C3A	1.409 (5)	Co1G—C5G	2.029 (3)
C2A—H2A	0.9500	Co1G—C10G	2.029 (3)
C3A—C4A	1.415 (4)	Co1G—C1G	2.030 (3)
C3A—H3A	0.9500	Co1G—C8G	2.038 (3)
C4A—C5A	1.412 (4)	Co1G—C9G	2.041 (3)
C4A—H4A	0.9500	C1G—C5G	1.392 (5)
C5A—H5A	0.9500	C1G—C2G	1.398 (5)
C6A—C10A	1.414 (4)	C1G—H1G	0.9500
C6A—C7A	1.419 (5)	C2G—C3G	1.404 (5)
C6A—H6A	0.9500	C2G—H2G	0.9500
C7A—C8A	1.414 (5)	C3G—C4G	1.418 (5)
C7A—H7A	0.9500	C3G—H3G	0.9500
C8A—C9A	1.416 (4)	C4G—C5G	1.409 (5)
C8A—H8A	0.9500	C4G—H4G	0.9500
C9A—C10A	1.421 (4)	C5G—H5G	0.9500
C9A—H9A	0.9500	C6G—C10G	1.411 (5)
C10A—H10A	0.9500	C6G—C7G	1.412 (5)
Co1B—C2B	2.016 (3)	C6G—H6G	0.9500
Co1B—C7B	2.021 (4)	C7G—C8G	1.412 (5)
Co1B—C6B	2.024 (3)	C7G—H7G	0.9500
Co1B—C8B	2.028 (3)	C8G—C9G	1.419 (5)
Co1B—C4B	2.028 (3)	C8G—H8G	0.9500
Co1B—C3B	2.028 (3)	C9G—C10G	1.419 (5)
Co1B—C10B	2.029 (3)	C9G—H9G	0.9500
Co1B—C5B	2.029 (3)	C10G—H10G	0.9500
Co1B—C1B	2.032 (3)	Co1H—C5H	2.026 (3)
Co1B—C9B	2.036 (3)	Co1H—C4H	2.029 (3)
C1B—C2B	1.416 (5)	Co1H—C6H	2.029 (3)
C1B—C5B	1.425 (4)	Co1H—C1H	2.030 (3)
C1B—H1B	0.9500	Co1H—C10H	2.032 (3)
C2B—C3B	1.416 (5)	Co1H—C3H	2.033 (3)
C2B—H2B	0.9500	Co1H—C7H	2.033 (3)
C3B—C4B	1.419 (5)	Co1H—C8H	2.033 (3)
C3B—H3B	0.9500	Co1H—C9H	2.037 (3)
C4B—C5B	1.412 (5)	Co1H—C2H	2.039 (3)
C4B—H4B	0.9500	C1H—C2H	1.410 (5)
C5B—H5B	0.9500	C1H—C5H	1.423 (5)
C6B—C10B	1.404 (5)	C1H—H1H	0.9500
C6B—C7B	1.416 (5)	C2H—C3H	1.423 (5)

C6B—H6B	0.9500	C2H—H2H	0.9500
C7B—C8B	1.403 (5)	C3H—C4H	1.413 (5)
C7B—H7B	0.9500	C3H—H3H	0.9500
C8B—C9B	1.422 (5)	C4H—C5H	1.419 (5)
C8B—H8B	0.9500	C4H—H4H	0.9500
C9B—C10B	1.418 (5)	C5H—H5H	0.9500
C9B—H9B	0.9500	C6H—C7H	1.417 (5)
C10B—H10B	0.9500	C6H—C10H	1.421 (5)
Co1C—C10C	2.018 (3)	C6H—H6H	0.9500
Co1C—C2C	2.021 (3)	C7H—C8H	1.420 (5)
Co1C—C1C	2.024 (3)	C7H—H7H	0.9500
Co1C—C6C	2.024 (3)	C8H—C9H	1.429 (5)
Co1C—C7C	2.024 (3)	C8H—H8H	0.9500
Co1C—C9C	2.025 (3)	C9H—C10H	1.418 (5)
Co1C—C8C	2.026 (3)	C9H—H9H	0.9500
Co1C—C3C	2.028 (3)	C10H—H10H	0.9500
Co1C—C4C	2.029 (3)	Co1I—C4I	2.006 (4)
Co1C—C5C	2.032 (3)	Co1I—C5I	2.020 (4)
C1C—C2C	1.412 (5)	Co1I—C6I	2.020 (3)
C1C—C5C	1.416 (5)	Co1I—C3I	2.022 (4)
C1C—H1C	0.9500	Co1I—C8I	2.024 (4)
C2C—C3C	1.412 (5)	Co1I—C7I	2.024 (3)
C2C—H2C	0.9500	Co1I—C1I	2.025 (4)
C3C—C4C	1.419 (5)	Co1I—C9I	2.026 (4)
C3C—H3C	0.9500	Co1I—C2I	2.027 (4)
C4C—C5C	1.409 (5)	Co1I—C10I	2.032 (3)
C4C—H4C	0.9500	C1I—C5I	1.387 (6)
C5C—H5C	0.9500	C1I—C2I	1.403 (5)
C6C—C7C	1.416 (4)	C1I—H1I	0.9500
C6C—C10C	1.417 (5)	C2I—C3I	1.388 (5)
C6C—H6C	0.9500	C2I—H2I	0.9500
C7C—C8C	1.414 (4)	C3I—C4I	1.406 (6)
C7C—H7C	0.9500	C3I—H3I	0.9500
C8C—C9C	1.416 (4)	C4I—C5I	1.400 (6)
C8C—H8C	0.9500	C4I—H4I	0.9500
C9C—C10C	1.417 (5)	C5I—H5I	0.9500
C9C—H9C	0.9500	C6I—C7I	1.412 (5)
C10C—H10C	0.9500	C6I—C10I	1.413 (5)
Co1D—C6D	2.020 (4)	C6I—H6I	0.9500
Co1D—C10D	2.024 (3)	C7I—C8I	1.409 (5)
Co1D—C4D	2.024 (3)	C7I—H7I	0.9500
Co1D—C7D	2.029 (3)	C8I—C9I	1.413 (5)
Co1D—C1D	2.029 (3)	C8I—H8I	0.9500
Co1D—C9D	2.030 (3)	C9I—C10I	1.422 (5)
Co1D—C5D	2.031 (3)	C9I—H9I	0.9500
Co1D—C3D	2.033 (3)	C10I—H10I	0.9500
Co1D—C2D	2.038 (3)	Co1J—C7J	2.022 (3)
Co1D—C8D	2.044 (3)	Co1J—C5J	2.023 (3)

C1D—C5D	1.403 (5)	Co1J—C4J	2.023 (3)
C1D—C2D	1.418 (5)	Co1J—C8J	2.025 (3)
C1D—H1D	0.9500	Co1J—C2J	2.028 (3)
C2D—C3D	1.414 (5)	Co1J—C3J	2.028 (3)
C2D—H2D	0.9500	Co1J—C10J	2.028 (4)
C3D—C4D	1.419 (4)	Co1J—C9J	2.029 (4)
C3D—H3D	0.9500	Co1J—C1J	2.031 (3)
C4D—C5D	1.423 (5)	Co1J—C6J	2.034 (4)
C4D—H4D	0.9500	C1J—C2J	1.406 (5)
C5D—H5D	0.9500	C1J—C5J	1.409 (5)
C6D—C10D	1.412 (5)	C1J—H1J	0.9500
C6D—C7D	1.414 (5)	C2J—C3J	1.427 (5)
C6D—H6D	0.9500	C2J—H2J	0.9500
C7D—C8D	1.409 (5)	C3J—C4J	1.406 (5)
C7D—H7D	0.9500	C3J—H3J	0.9500
C8D—C9D	1.417 (5)	C4J—C5J	1.418 (5)
C8D—H8D	0.9500	C4J—H4J	0.9500
C9D—C10D	1.424 (5)	C5J—H5J	0.9500
C9D—H9D	0.9500	C6J—C7J	1.420 (5)
C10D—H10D	0.9500	C6J—C10J	1.421 (5)
Co1E—C3E	2.020 (4)	C6J—H6J	0.9500
Co1E—C4E	2.021 (3)	C7J—C8J	1.411 (5)
Co1E—C9E	2.021 (3)	C7J—H7J	0.9500
Co1E—C7E	2.029 (3)	C8J—C9J	1.416 (5)
Co1E—C8E	2.031 (3)	C8J—H8J	0.9500
Co1E—C2E	2.032 (4)	C9J—C10J	1.412 (6)
Co1E—C10E	2.032 (3)	C9J—H9J	0.9500
Co1E—C6E	2.038 (3)	C10J—H10J	0.9500
Co1E—C1E	2.038 (3)	Co1K—C12K	2.2685 (9)
Co1E—C5E	2.040 (3)	Co1K—C11K	2.2792 (9)
C1E—C5E	1.406 (5)	Co1K—C13K	2.2819 (9)
C1E—C2E	1.418 (5)	Co1K—C14K	2.2860 (9)
C1E—H1E	0.9500	Co1L—C14L	2.2642 (9)
C2E—C3E	1.420 (5)	Co1L—C12L	2.2782 (9)
C2E—H2E	0.9500	Co1L—C13L	2.2847 (9)
C3E—C4E	1.414 (5)	Co1L—C11L	2.2858 (9)
C3E—H3E	0.9500	Co1M—C14M	2.2680 (9)
C4E—C5E	1.415 (5)	Co1M—C12M	2.2775 (9)
C4E—H4E	0.9500	Co1M—C11M	2.2853 (9)
C5E—H5E	0.9500	Co1M—C13M	2.2871 (9)
C6E—C7E	1.409 (5)	Co1N—C14N	2.2674 (9)
C6E—C10E	1.418 (5)	Co1N—C12N	2.2787 (9)
C6E—H6E	0.9500	Co1N—C11N	2.2802 (9)
C7E—C8E	1.423 (5)	Co1N—C13N	2.2803 (9)
C7E—H7E	0.9500	Co1O—C13O	2.2731 (10)
C8E—C9E	1.424 (5)	Co1O—C11O	2.2761 (10)
C8E—H8E	0.9500	Co1O—C14O	2.2824 (10)
C9E—C10E	1.415 (5)	Co1O—C12O	2.2853 (9)

C9E—H9E	0.9500	C11P—C2P	1.770 (3)
C10E—H10E	0.9500	C2P—C13P	1.772 (4)
Co1F—C7F	2.013 (3)	C2P—H2P1	0.9900
Co1F—C4F	2.017 (4)	C2P—H2P2	0.9900
Co1F—C3F	2.018 (4)	C11Q—C2Q	1.766 (3)
Co1F—C10F	2.021 (4)	C2Q—C13Q	1.764 (3)
Co1F—C6F	2.022 (3)	C2Q—H2Q1	0.9900
Co1F—C5F	2.024 (3)	C2Q—H2Q2	0.9900
Co1F—C9F	2.024 (3)	C11R—C2R	1.767 (4)
Co1F—C8F	2.024 (3)	C2R—C13R	1.754 (4)
Co1F—C1F	2.026 (3)	C2R—H2R1	0.9900
Co1F—C2F	2.026 (4)	C2R—H2R2	0.9900
C1F—C5F	1.403 (5)	C11S—C2S	1.769 (3)
C1F—C2F	1.405 (5)	C2S—C13S	1.757 (3)
C1F—H1F	0.9500	C2S—H2S1	0.9900
C2F—C3F	1.404 (6)	C2S—H2S2	0.9900
C2F—H2F	0.9500	C11T—C2T	1.754 (4)
C3F—C4F	1.411 (6)	C2T—C13T	1.768 (4)
C3F—H3F	0.9500	C2T—H2T1	0.9900
C4F—C5F	1.414 (5)	C2T—H2T2	0.9900
C4F—H4F	0.9500	C11U—C2U	1.768 (4)
C5F—H5F	0.9500	C2U—C13U	1.770 (4)
C6F—C7F	1.412 (5)	C2U—H2U1	0.9900
C6F—C10F	1.418 (5)	C2U—H2U2	0.9900
C3A—Co1A—C4A	41.07 (12)	C5F—Co1F—C1F	40.54 (15)
C3A—Co1A—C10A	157.22 (14)	C9F—Co1F—C1F	160.93 (15)
C4A—Co1A—C10A	120.73 (13)	C8F—Co1F—C1F	156.61 (16)
C3A—Co1A—C9A	121.61 (14)	C7F—Co1F—C2F	106.19 (16)
C4A—Co1A—C9A	106.72 (13)	C4F—Co1F—C2F	68.59 (18)
C10A—Co1A—C9A	41.20 (13)	C3F—Co1F—C2F	40.64 (16)
C3A—Co1A—C6A	160.75 (13)	C10F—Co1F—C2F	159.80 (16)
C4A—Co1A—C6A	156.49 (13)	C6F—Co1F—C2F	122.68 (16)
C10A—Co1A—C6A	40.98 (13)	C5F—Co1F—C2F	68.34 (16)
C9A—Co1A—C6A	69.15 (14)	C9F—Co1F—C2F	157.38 (15)
C3A—Co1A—C5A	68.90 (13)	C8F—Co1F—C2F	121.18 (15)
C4A—Co1A—C5A	40.91 (13)	C1F—Co1F—C2F	40.59 (15)
C10A—Co1A—C5A	106.15 (13)	C5F—C1F—C2F	108.2 (4)
C9A—Co1A—C5A	123.10 (13)	C5F—C1F—Co1F	69.7 (2)
C6A—Co1A—C5A	120.67 (14)	C2F—C1F—Co1F	69.7 (2)
C3A—Co1A—C2A	40.79 (13)	C5F—C1F—H1F	125.9
C4A—Co1A—C2A	68.94 (13)	C2F—C1F—H1F	125.9
C10A—Co1A—C2A	160.07 (14)	Co1F—C1F—H1F	126.3
C9A—Co1A—C2A	157.62 (14)	C3F—C2F—C1F	108.1 (4)
C6A—Co1A—C2A	123.68 (13)	C3F—C2F—Co1F	69.4 (2)
C5A—Co1A—C2A	68.86 (13)	C1F—C2F—Co1F	69.7 (2)
C3A—Co1A—C7A	124.19 (14)	C3F—C2F—H2F	125.9
C4A—Co1A—C7A	160.99 (14)	C1F—C2F—H2F	125.9

C10A—Co1A—C7A	69.07 (13)	Co1F—C2F—H2F	126.6
C9A—Co1A—C7A	69.05 (13)	C2F—C3F—C4F	108.1 (4)
C6A—Co1A—C7A	41.03 (13)	C2F—C3F—Co1F	70.0 (2)
C5A—Co1A—C7A	156.90 (14)	C4F—C3F—Co1F	69.5 (2)
C2A—Co1A—C7A	107.53 (13)	C2F—C3F—H3F	126.0
C3A—Co1A—C1A	69.04 (13)	C4F—C3F—H3F	126.0
C4A—Co1A—C1A	69.12 (13)	Co1F—C3F—H3F	126.1
C10A—Co1A—C1A	122.67 (13)	C3F—C4F—C5F	107.7 (4)
C9A—Co1A—C1A	159.80 (13)	C3F—C4F—Co1F	69.6 (2)
C6A—Co1A—C1A	106.37 (14)	C5F—C4F—Co1F	69.8 (2)
C5A—Co1A—C1A	40.99 (12)	C3F—C4F—H4F	126.2
C2A—Co1A—C1A	41.06 (13)	C5F—C4F—H4F	126.2
C7A—Co1A—C1A	121.29 (13)	Co1F—C4F—H4F	126.0
C3A—Co1A—C8A	107.85 (14)	C1F—C5F—C4F	107.9 (4)
C4A—Co1A—C8A	124.07 (14)	C1F—C5F—Co1F	69.8 (2)
C10A—Co1A—C8A	68.99 (13)	C4F—C5F—Co1F	69.2 (2)
C9A—Co1A—C8A	40.95 (12)	C1F—C5F—H5F	126.0
C6A—Co1A—C8A	68.85 (14)	C4F—C5F—H5F	126.0
C5A—Co1A—C8A	160.47 (14)	Co1F—C5F—H5F	126.5
C2A—Co1A—C8A	122.09 (13)	C7F—C6F—C10F	107.9 (3)
C7A—Co1A—C8A	40.80 (13)	C7F—C6F—Co1F	69.2 (2)
C1A—Co1A—C8A	157.53 (13)	C10F—C6F—Co1F	69.4 (2)
C5A—C1A—C2A	107.4 (3)	C7F—C6F—H6F	126.1
C5A—C1A—Co1A	69.34 (18)	C10F—C6F—H6F	126.1
C2A—C1A—Co1A	69.40 (18)	Co1F—C6F—H6F	126.9
C5A—C1A—H1A	126.3	C6F—C7F—C8F	108.2 (3)
C2A—C1A—H1A	126.3	C6F—C7F—Co1F	69.85 (19)
Co1A—C1A—H1A	126.5	C8F—C7F—Co1F	69.92 (19)
C3A—C2A—C1A	108.1 (3)	C6F—C7F—H7F	125.9
C3A—C2A—Co1A	69.23 (18)	C8F—C7F—H7F	125.9
C1A—C2A—Co1A	69.54 (17)	Co1F—C7F—H7F	125.9
C3A—C2A—H2A	125.9	C9F—C8F—C7F	108.0 (3)
C1A—C2A—H2A	125.9	C9F—C8F—Co1F	69.56 (19)
Co1A—C2A—H2A	126.9	C7F—C8F—Co1F	69.05 (19)
C2A—C3A—C4A	108.2 (3)	C9F—C8F—H8F	126.0
C2A—C3A—Co1A	69.98 (18)	C7F—C8F—H8F	126.0
C4A—C3A—Co1A	69.47 (18)	Co1F—C8F—H8F	126.9
C2A—C3A—H3A	125.9	C8F—C9F—C10F	108.0 (3)
C4A—C3A—H3A	125.9	C8F—C9F—Co1F	69.58 (19)
Co1A—C3A—H3A	126.3	C10F—C9F—Co1F	69.36 (19)
C5A—C4A—C3A	107.9 (3)	C8F—C9F—H9F	126.0
C5A—C4A—Co1A	69.80 (18)	C10F—C9F—H9F	126.0
C3A—C4A—Co1A	69.45 (18)	Co1F—C9F—H9F	126.6
C5A—C4A—H4A	126.1	C9F—C10F—C6F	107.9 (3)
C3A—C4A—H4A	126.1	C9F—C10F—Co1F	69.6 (2)
Co1A—C4A—H4A	126.3	C6F—C10F—Co1F	69.5 (2)
C4A—C5A—C1A	108.3 (3)	C9F—C10F—H10F	126.0
C4A—C5A—Co1A	69.28 (19)	C6F—C10F—H10F	126.0

C1A—C5A—Co1A	69.67 (18)	Co1F—C10F—H10F	126.4
C4A—C5A—H5A	125.9	C6G—Co1G—C3G	155.07 (16)
C1A—C5A—H5A	125.9	C6G—Co1G—C2G	119.14 (15)
Co1A—C5A—H5A	126.8	C3G—Co1G—C2G	40.57 (15)
C10A—C6A—C7A	108.1 (3)	C6G—Co1G—C4G	161.15 (17)
C10A—C6A—Co1A	69.39 (18)	C3G—Co1G—C4G	40.98 (16)
C7A—C6A—Co1A	69.73 (19)	C2G—Co1G—C4G	68.38 (15)
C10A—C6A—H6A	125.9	C6G—Co1G—C7G	40.80 (13)
C7A—C6A—H6A	125.9	C3G—Co1G—C7G	120.49 (15)
Co1A—C6A—H6A	126.5	C2G—Co1G—C7G	105.45 (14)
C8A—C7A—C6A	107.9 (3)	C4G—Co1G—C7G	157.68 (16)
C8A—C7A—Co1A	69.66 (19)	C6G—Co1G—C5G	123.31 (15)
C6A—C7A—Co1A	69.25 (19)	C3G—Co1G—C5G	68.36 (15)
C8A—C7A—H7A	126.1	C2G—Co1G—C5G	67.79 (15)
C6A—C7A—H7A	126.1	C4G—Co1G—C5G	40.67 (15)
Co1A—C7A—H7A	126.6	C7G—Co1G—C5G	158.73 (15)
C7A—C8A—C9A	108.3 (3)	C6G—Co1G—C10G	40.76 (14)
C7A—C8A—Co1A	69.54 (19)	C3G—Co1G—C10G	163.13 (16)
C9A—C8A—Co1A	69.17 (18)	C2G—Co1G—C10G	155.15 (15)
C7A—C8A—H8A	125.9	C4G—Co1G—C10G	125.88 (16)
C9A—C8A—H8A	125.9	C7G—Co1G—C10G	68.71 (14)
Co1A—C8A—H8A	127.0	C5G—Co1G—C10G	108.46 (15)
C8A—C9A—C10A	107.8 (3)	C6G—Co1G—C1G	105.58 (14)
C8A—C9A—Co1A	69.88 (18)	C3G—Co1G—C1G	68.18 (14)
C10A—C9A—Co1A	69.34 (18)	C2G—Co1G—C1G	40.33 (15)
C8A—C9A—H9A	126.1	C4G—Co1G—C1G	68.16 (14)
C10A—C9A—H9A	126.1	C7G—Co1G—C1G	121.85 (15)
Co1A—C9A—H9A	126.2	C5G—Co1G—C1G	40.11 (15)
C6A—C10A—C9A	108.0 (3)	C10G—Co1G—C1G	120.84 (15)
C6A—C10A—Co1A	69.63 (18)	C6G—Co1G—C8G	68.33 (13)
C9A—C10A—Co1A	69.46 (17)	C3G—Co1G—C8G	108.46 (14)
C6A—C10A—H10A	126.0	C2G—Co1G—C8G	123.75 (15)
C9A—C10A—H10A	126.0	C4G—Co1G—C8G	123.74 (15)
Co1A—C10A—H10A	126.5	C7G—Co1G—C8G	40.65 (13)
C2B—Co1B—C7B	107.93 (14)	C5G—Co1G—C8G	159.68 (15)
C2B—Co1B—C6B	122.90 (15)	C10G—Co1G—C8G	68.40 (14)
C7B—Co1B—C6B	40.97 (15)	C1G—Co1G—C8G	159.14 (15)
C2B—Co1B—C8B	122.86 (14)	C6G—Co1G—C9G	68.62 (13)
C7B—Co1B—C8B	40.56 (14)	C3G—Co1G—C9G	126.10 (14)
C6B—Co1B—C8B	68.94 (15)	C2G—Co1G—C9G	161.57 (15)
C2B—Co1B—C4B	68.83 (14)	C4G—Co1G—C9G	109.99 (14)
C7B—Co1B—C4B	157.04 (15)	C7G—Co1G—C9G	68.74 (14)
C6B—Co1B—C4B	159.85 (15)	C5G—Co1G—C9G	123.80 (15)
C8B—Co1B—C4B	120.74 (15)	C10G—Co1G—C9G	40.80 (13)
C2B—Co1B—C3B	40.97 (13)	C1G—Co1G—C9G	157.61 (15)
C7B—Co1B—C3B	121.67 (15)	C8G—Co1G—C9G	40.70 (13)
C6B—Co1B—C3B	158.33 (15)	C5G—C1G—C2G	108.2 (3)
C8B—Co1B—C3B	105.96 (14)	C5G—C1G—Co1G	69.9 (2)

C4B—Co1B—C3B	40.95 (13)	C2G—C1G—Co1G	69.6 (2)
C2B—Co1B—C10B	158.89 (15)	C5G—C1G—H1G	125.9
C7B—Co1B—C10B	68.17 (15)	C2G—C1G—H1G	125.9
C6B—Co1B—C10B	40.52 (15)	Co1G—C1G—H1G	126.2
C8B—Co1B—C10B	68.60 (14)	C1G—C2G—C3G	108.4 (3)
C4B—Co1B—C10B	123.08 (15)	C1G—C2G—Co1G	70.0 (2)
C3B—Co1B—C10B	159.04 (15)	C3G—C2G—Co1G	69.7 (2)
C2B—Co1B—C5B	68.71 (13)	C1G—C2G—H2G	125.8
C7B—Co1B—C5B	161.16 (15)	C3G—C2G—H2G	125.8
C6B—Co1B—C5B	124.11 (15)	Co1G—C2G—H2G	126.1
C8B—Co1B—C5B	156.98 (15)	C2G—C3G—C4G	107.6 (3)
C4B—Co1B—C5B	40.72 (13)	C2G—C3G—Co1G	69.8 (2)
C3B—Co1B—C5B	68.77 (13)	C4G—C3G—Co1G	69.6 (2)
C10B—Co1B—C5B	107.89 (14)	C2G—C3G—H3G	126.2
C2B—Co1B—C1B	40.93 (13)	C4G—C3G—H3G	126.2
C7B—Co1B—C1B	124.32 (14)	Co1G—C3G—H3G	126.0
C6B—Co1B—C1B	108.05 (14)	C5G—C4G—C3G	107.3 (3)
C8B—Co1B—C1B	159.98 (14)	C5G—C4G—Co1G	69.8 (2)
C4B—Co1B—C1B	69.06 (14)	C3G—C4G—Co1G	69.4 (2)
C3B—Co1B—C1B	69.14 (13)	C5G—C4G—H4G	126.3
C10B—Co1B—C1B	122.82 (14)	C3G—C4G—H4G	126.3
C5B—Co1B—C1B	41.07 (13)	Co1G—C4G—H4G	126.0
C2B—Co1B—C9B	158.99 (15)	C1G—C5G—C4G	108.5 (3)
C7B—Co1B—C9B	68.48 (15)	C1G—C5G—Co1G	70.0 (2)
C6B—Co1B—C9B	68.87 (15)	C4G—C5G—Co1G	69.6 (2)
C8B—Co1B—C9B	40.97 (14)	C1G—C5G—H5G	125.8
C4B—Co1B—C9B	105.98 (14)	C4G—C5G—H5G	125.8
C3B—Co1B—C9B	121.91 (15)	Co1G—C5G—H5G	126.2
C10B—Co1B—C9B	40.83 (14)	C10G—C6G—C7G	108.3 (3)
C5B—Co1B—C9B	121.44 (14)	C10G—C6G—Co1G	69.83 (19)
C1B—Co1B—C9B	158.10 (14)	C7G—C6G—Co1G	69.75 (19)
C2B—C1B—C5B	107.0 (3)	C10G—C6G—H6G	125.8
C2B—C1B—Co1B	68.91 (18)	C7G—C6G—H6G	125.8
C5B—C1B—Co1B	69.36 (18)	Co1G—C6G—H6G	126.2
C2B—C1B—H1B	126.5	C6G—C7G—C8G	107.7 (3)
C5B—C1B—H1B	126.5	C6G—C7G—Co1G	69.46 (19)
Co1B—C1B—H1B	126.8	C8G—C7G—Co1G	70.10 (19)
C1B—C2B—C3B	109.0 (3)	C6G—C7G—H7G	126.1
C1B—C2B—Co1B	70.15 (18)	C8G—C7G—H7G	126.1
C3B—C2B—Co1B	69.98 (18)	Co1G—C7G—H7G	125.9
C1B—C2B—H2B	125.5	C7G—C8G—C9G	108.4 (3)
C3B—C2B—H2B	125.5	C7G—C8G—Co1G	69.25 (18)
Co1B—C2B—H2B	125.9	C9G—C8G—Co1G	69.74 (18)
C2B—C3B—C4B	107.5 (3)	C7G—C8G—H8G	125.8
C2B—C3B—Co1B	69.04 (19)	C9G—C8G—H8G	125.8
C4B—C3B—Co1B	69.50 (19)	Co1G—C8G—H8G	126.8
C2B—C3B—H3B	126.3	C10G—C9G—C8G	107.4 (3)
C4B—C3B—H3B	126.3	C10G—C9G—Co1G	69.15 (18)

Co1B—C3B—H3B	126.8	C8G—C9G—Co1G	69.55 (19)
C5B—C4B—C3B	108.1 (3)	C10G—C9G—H9G	126.3
C5B—C4B—Co1B	69.71 (19)	C8G—C9G—H9G	126.3
C3B—C4B—Co1B	69.55 (19)	Co1G—C9G—H9G	126.5
C5B—C4B—H4B	125.9	C6G—C10G—C9G	108.1 (3)
C3B—C4B—H4B	125.9	C6G—C10G—Co1G	69.40 (19)
Co1B—C4B—H4B	126.4	C9G—C10G—Co1G	70.05 (19)
C4B—C5B—C1B	108.5 (3)	C6G—C10G—H10G	125.9
C4B—C5B—Co1B	69.57 (19)	C9G—C10G—H10G	125.9
C1B—C5B—Co1B	69.57 (19)	Co1G—C10G—H10G	126.2
C4B—C5B—H5B	125.8	C5H—Co1H—C4H	40.96 (13)
C1B—C5B—H5B	125.8	C5H—Co1H—C6H	123.76 (14)
Co1B—C5B—H5B	126.7	C4H—Co1H—C6H	160.19 (15)
C10B—C6B—C7B	107.3 (3)	C5H—Co1H—C1H	41.07 (13)
C10B—C6B—Co1B	69.9 (2)	C4H—Co1H—C1H	68.76 (13)
C7B—C6B—Co1B	69.4 (2)	C6H—Co1H—C1H	107.94 (14)
C10B—C6B—H6B	126.4	C5H—Co1H—C10H	106.60 (14)
C7B—C6B—H6B	126.4	C4H—Co1H—C10H	122.94 (15)
Co1B—C6B—H6B	125.8	C6H—Co1H—C10H	40.96 (14)
C8B—C7B—C6B	108.9 (3)	C1H—Co1H—C10H	121.90 (14)
C8B—C7B—Co1B	70.0 (2)	C5H—Co1H—C3H	68.81 (14)
C6B—C7B—Co1B	69.6 (2)	C4H—Co1H—C3H	40.71 (14)
C8B—C7B—H7B	125.6	C6H—Co1H—C3H	157.98 (15)
C6B—C7B—H7B	125.6	C1H—Co1H—C3H	68.54 (13)
Co1B—C7B—H7B	126.4	C10H—Co1H—C3H	159.58 (15)
C7B—C8B—C9B	107.8 (3)	C5H—Co1H—C7H	161.01 (14)
C7B—C8B—Co1B	69.5 (2)	C4H—Co1H—C7H	157.03 (15)
C9B—C8B—Co1B	69.8 (2)	C6H—Co1H—C7H	40.85 (14)
C7B—C8B—H8B	126.1	C1H—Co1H—C7H	124.53 (14)
C9B—C8B—H8B	126.1	C10H—Co1H—C7H	68.78 (15)
Co1B—C8B—H8B	126.2	C3H—Co1H—C7H	121.95 (15)
C10B—C9B—C8B	107.2 (3)	C5H—Co1H—C8H	156.40 (14)
C10B—C9B—Co1B	69.31 (19)	C4H—Co1H—C8H	120.75 (14)
C8B—C9B—Co1B	69.19 (19)	C6H—Co1H—C8H	68.85 (14)
C10B—C9B—H9B	126.4	C1H—Co1H—C8H	160.94 (14)
C8B—C9B—H9B	126.4	C10H—Co1H—C8H	68.81 (14)
Co1B—C9B—H9B	126.6	C3H—Co1H—C8H	106.99 (14)
C6B—C10B—C9B	108.9 (3)	C7H—Co1H—C8H	40.87 (14)
C6B—C10B—Co1B	69.53 (19)	C5H—Co1H—C9H	120.34 (14)
C9B—C10B—Co1B	69.85 (19)	C4H—Co1H—C9H	106.03 (14)
C6B—C10B—H10B	125.6	C6H—Co1H—C9H	68.95 (14)
C9B—C10B—H10B	125.6	C1H—Co1H—C9H	156.94 (14)
Co1B—C10B—H10B	126.6	C10H—Co1H—C9H	40.79 (13)
C10C—Co1C—C2C	160.47 (15)	C3H—Co1H—C9H	123.02 (14)
C10C—Co1C—C1C	123.86 (14)	C7H—Co1H—C9H	68.98 (14)
C2C—Co1C—C1C	40.85 (13)	C8H—Co1H—C9H	41.11 (13)
C10C—Co1C—C6C	41.05 (13)	C5H—Co1H—C2H	68.86 (14)
C2C—Co1C—C6C	123.22 (14)	C4H—Co1H—C2H	68.73 (14)

C1C—Co1C—C6C	106.52 (14)	C6H—Co1H—C2H	122.30 (14)
C10C—Co1C—C7C	68.99 (13)	C1H—Co1H—C2H	40.56 (13)
C2C—Co1C—C7C	106.41 (13)	C10H—Co1H—C2H	157.84 (14)
C1C—Co1C—C7C	120.43 (14)	C3H—Co1H—C2H	40.90 (13)
C6C—Co1C—C7C	40.95 (13)	C7H—Co1H—C2H	108.06 (14)
C10C—Co1C—C9C	41.03 (13)	C8H—Co1H—C2H	124.08 (14)
C2C—Co1C—C9C	156.74 (14)	C9H—Co1H—C2H	160.42 (14)
C1C—Co1C—C9C	161.34 (14)	C2H—C1H—C5H	108.5 (3)
C6C—Co1C—C9C	68.97 (14)	C2H—C1H—Co1H	70.09 (18)
C7C—Co1C—C9C	68.81 (13)	C5H—C1H—Co1H	69.34 (18)
C10C—Co1C—C8C	69.06 (13)	C2H—C1H—H1H	125.8
C2C—Co1C—C8C	120.66 (14)	C5H—C1H—H1H	125.8
C1C—Co1C—C8C	156.09 (14)	Co1H—C1H—H1H	126.4
C6C—Co1C—C8C	68.98 (13)	C1H—C2H—C3H	107.7 (3)
C7C—Co1C—C8C	40.87 (13)	C1H—C2H—Co1H	69.35 (19)
C9C—Co1C—C8C	40.91 (13)	C3H—C2H—Co1H	69.32 (19)
C10C—Co1C—C3C	157.37 (15)	C1H—C2H—H2H	126.1
C2C—Co1C—C3C	40.81 (13)	C3H—C2H—H2H	126.1
C1C—Co1C—C3C	68.64 (14)	Co1H—C2H—H2H	126.7
C6C—Co1C—C3C	160.34 (14)	C4H—C3H—C2H	108.1 (3)
C7C—Co1C—C3C	123.74 (14)	C4H—C3H—Co1H	69.5 (2)
C9C—Co1C—C3C	121.65 (14)	C2H—C3H—Co1H	69.79 (19)
C8C—Co1C—C3C	107.28 (14)	C4H—C3H—H3H	125.9
C10C—Co1C—C4C	121.58 (14)	C2H—C3H—H3H	125.9
C2C—Co1C—C4C	68.79 (14)	Co1H—C3H—H3H	126.4
C1C—Co1C—C4C	68.58 (14)	C3H—C4H—C5H	108.2 (3)
C6C—Co1C—C4C	156.83 (13)	C3H—C4H—Co1H	69.82 (19)
C7C—Co1C—C4C	161.24 (14)	C5H—C4H—Co1H	69.43 (19)
C9C—Co1C—C4C	108.03 (14)	C3H—C4H—H4H	125.9
C8C—Co1C—C4C	124.73 (14)	C5H—C4H—H4H	125.9
C3C—Co1C—C4C	40.95 (13)	Co1H—C4H—H4H	126.4
C10C—Co1C—C5C	107.38 (13)	C4H—C5H—C1H	107.5 (3)
C2C—Co1C—C5C	68.80 (13)	C4H—C5H—Co1H	69.61 (18)
C1C—Co1C—C5C	40.86 (13)	C1H—C5H—Co1H	69.59 (18)
C6C—Co1C—C5C	120.96 (14)	C4H—C5H—H5H	126.3
C7C—Co1C—C5C	156.33 (14)	C1H—C5H—H5H	126.3
C9C—Co1C—C5C	124.72 (14)	Co1H—C5H—H5H	126.1
C8C—Co1C—C5C	161.60 (14)	C7H—C6H—C10H	108.0 (3)
C3C—Co1C—C5C	68.66 (13)	C7H—C6H—Co1H	69.7 (2)
C4C—Co1C—C5C	40.60 (13)	C10H—C6H—Co1H	69.6 (2)
C2C—C1C—C5C	108.2 (3)	C7H—C6H—H6H	126.0
C2C—C1C—Co1C	69.49 (19)	C10H—C6H—H6H	126.0
C5C—C1C—Co1C	69.89 (19)	Co1H—C6H—H6H	126.2
C2C—C1C—H1C	125.9	C6H—C7H—C8H	108.1 (3)
C5C—C1C—H1C	125.9	C6H—C7H—Co1H	69.42 (19)
Co1C—C1C—H1C	126.3	C8H—C7H—Co1H	69.58 (19)
C1C—C2C—C3C	108.0 (3)	C6H—C7H—H7H	126.0
C1C—C2C—Co1C	69.66 (19)	C8H—C7H—H7H	126.0

C3C—C2C—Co1C	69.86 (19)	Co1H—C7H—H7H	126.6
C1C—C2C—H2C	126.0	C7H—C8H—C9H	108.0 (3)
C3C—C2C—H2C	126.0	C7H—C8H—Co1H	69.55 (18)
Co1C—C2C—H2C	126.1	C9H—C8H—Co1H	69.58 (18)
C2C—C3C—C4C	107.8 (3)	C7H—C8H—H8H	126.0
C2C—C3C—Co1C	69.32 (19)	C9H—C8H—H8H	126.0
C4C—C3C—Co1C	69.54 (18)	Co1H—C8H—H8H	126.4
C2C—C3C—H3C	126.1	C10H—C9H—C8H	107.6 (3)
C4C—C3C—H3C	126.1	C10H—C9H—Co1H	69.41 (19)
Co1C—C3C—H3C	126.6	C8H—C9H—Co1H	69.31 (18)
C5C—C4C—C3C	108.1 (3)	C10H—C9H—H9H	126.2
C5C—C4C—Co1C	69.82 (18)	C8H—C9H—H9H	126.2
C3C—C4C—Co1C	69.51 (18)	Co1H—C9H—H9H	126.6
C5C—C4C—H4C	125.9	C9H—C10H—C6H	108.3 (3)
C3C—C4C—H4C	125.9	C9H—C10H—Co1H	69.80 (19)
Co1C—C4C—H4C	126.3	C6H—C10H—Co1H	69.4 (2)
C4C—C5C—C1C	107.9 (3)	C9H—C10H—H10H	125.8
C4C—C5C—Co1C	69.58 (18)	C6H—C10H—H10H	125.8
C1C—C5C—Co1C	69.25 (18)	Co1H—C10H—H10H	126.5
C4C—C5C—H5C	126.1	C4I—Co1I—C5I	40.70 (17)
C1C—C5C—H5C	126.1	C4I—Co1I—C6I	160.90 (18)
Co1C—C5C—H5C	126.7	C5I—Co1I—C6I	124.45 (17)
C7C—C6C—C10C	107.8 (3)	C4I—Co1I—C3I	40.85 (17)
C7C—C6C—Co1C	69.54 (18)	C5I—Co1I—C3I	68.38 (16)
C10C—C6C—Co1C	69.24 (18)	C6I—Co1I—C3I	156.97 (17)
C7C—C6C—H6C	126.1	C4I—Co1I—C8I	121.87 (17)
C10C—C6C—H6C	126.1	C5I—Co1I—C8I	159.12 (18)
Co1C—C6C—H6C	126.7	C6I—Co1I—C8I	68.79 (15)
C8C—C7C—C6C	108.3 (3)	C3I—Co1I—C8I	105.71 (16)
C8C—C7C—Co1C	69.64 (18)	C4I—Co1I—C7I	157.14 (18)
C6C—C7C—Co1C	69.51 (17)	C5I—Co1I—C7I	159.65 (18)
C8C—C7C—H7C	125.9	C6I—Co1I—C7I	40.87 (15)
C6C—C7C—H7C	125.9	C3I—Co1I—C7I	120.53 (17)
Co1C—C7C—H7C	126.5	C8I—Co1I—C7I	40.73 (15)
C7C—C8C—C9C	107.9 (3)	C4I—Co1I—C1I	67.90 (16)
C7C—C8C—Co1C	69.49 (18)	C5I—Co1I—C1I	40.10 (16)
C9C—C8C—Co1C	69.49 (18)	C6I—Co1I—C1I	108.42 (16)
C7C—C8C—H8C	126.1	C3I—Co1I—C1I	67.89 (16)
C9C—C8C—H8C	126.1	C8I—Co1I—C1I	158.08 (18)
Co1C—C8C—H8C	126.5	C7I—Co1I—C1I	122.94 (17)
C8C—C9C—C10C	108.1 (3)	C4I—Co1I—C9I	107.81 (15)
C8C—C9C—Co1C	69.60 (19)	C5I—Co1I—C9I	124.15 (16)
C10C—C9C—Co1C	69.21 (19)	C6I—Co1I—C9I	68.95 (15)
C8C—C9C—H9C	126.0	C3I—Co1I—C9I	122.36 (16)
C10C—C9C—H9C	126.0	C8I—Co1I—C9I	40.83 (15)
Co1C—C9C—H9C	126.8	C7I—Co1I—C9I	68.71 (15)
C9C—C10C—C6C	108.0 (3)	C1I—Co1I—C9I	160.28 (17)
C9C—C10C—Co1C	69.76 (19)	C4I—Co1I—C2I	68.00 (16)

C6C—C10C—Co1C	69.72 (19)	C5I—Co1I—C2I	67.96 (16)
C9C—C10C—H10C	126.0	C6I—Co1I—C2I	122.27 (16)
C6C—C10C—H10C	126.0	C3I—Co1I—C2I	40.09 (15)
Co1C—C10C—H10C	126.1	C8I—Co1I—C2I	121.23 (17)
C6D—Co1D—C10D	40.89 (15)	C7I—Co1I—C2I	106.17 (16)
C6D—Co1D—C4D	158.73 (15)	C1I—Co1I—C2I	40.51 (16)
C10D—Co1D—C4D	121.72 (15)	C9I—Co1I—C2I	157.66 (17)
C6D—Co1D—C7D	40.88 (14)	C4I—Co1I—C10I	124.53 (16)
C10D—Co1D—C7D	68.75 (15)	C5I—Co1I—C10I	109.58 (15)
C4D—Co1D—C7D	158.15 (15)	C6I—Co1I—C10I	40.80 (14)
C6D—Co1D—C1D	108.32 (16)	C3I—Co1I—C10I	159.96 (17)
C10D—Co1D—C1D	122.62 (15)	C8I—Co1I—C10I	68.72 (16)
C4D—Co1D—C1D	68.57 (14)	C7I—Co1I—C10I	68.60 (15)
C7D—Co1D—C1D	124.39 (15)	C1I—Co1I—C10I	124.30 (16)
C6D—Co1D—C9D	68.74 (16)	C9I—Co1I—C10I	41.01 (14)
C10D—Co1D—C9D	41.11 (15)	C2I—Co1I—C10I	159.28 (16)
C4D—Co1D—C9D	105.99 (15)	C5I—C1I—C2I	108.4 (4)
C7D—Co1D—C9D	68.31 (15)	C5I—C1I—Co1I	69.8 (2)
C1D—Co1D—C9D	158.39 (15)	C2I—C1I—Co1I	69.8 (2)
C6D—Co1D—C5D	122.91 (15)	C5I—C1I—H1I	125.8
C10D—Co1D—C5D	106.59 (14)	C2I—C1I—H1I	125.8
C4D—Co1D—C5D	41.08 (13)	Co1I—C1I—H1I	126.2
C7D—Co1D—C5D	159.86 (15)	C3I—C2I—C1I	108.1 (4)
C1D—Co1D—C5D	40.43 (14)	C3I—C2I—Co1I	69.8 (2)
C9D—Co1D—C5D	121.88 (14)	C1I—C2I—Co1I	69.6 (2)
C6D—Co1D—C3D	159.37 (15)	C3I—C2I—H2I	125.9
C10D—Co1D—C3D	158.08 (16)	C1I—C2I—H2I	125.9
C4D—Co1D—C3D	40.94 (13)	Co1I—C2I—H2I	126.2
C7D—Co1D—C3D	122.72 (14)	C2I—C3I—C4I	107.7 (4)
C1D—Co1D—C3D	68.76 (14)	C2I—C3I—Co1I	70.2 (2)
C9D—Co1D—C3D	121.69 (15)	C4I—C3I—Co1I	69.0 (2)
C5D—Co1D—C3D	68.98 (13)	C2I—C3I—H3I	126.2
C6D—Co1D—C2D	123.85 (16)	C4I—C3I—H3I	126.2
C10D—Co1D—C2D	159.48 (16)	Co1I—C3I—H3I	126.3
C4D—Co1D—C2D	68.46 (14)	C5I—C4I—C3I	108.1 (4)
C7D—Co1D—C2D	108.70 (15)	C5I—C4I—Co1I	70.2 (2)
C1D—Co1D—C2D	40.81 (14)	C3I—C4I—Co1I	70.2 (2)
C9D—Co1D—C2D	158.55 (15)	C5I—C4I—H4I	126.0
C5D—Co1D—C2D	68.42 (14)	C3I—C4I—H4I	126.0
C3D—Co1D—C2D	40.66 (13)	Co1I—C4I—H4I	125.3
C6D—Co1D—C8D	68.70 (15)	C1I—C5I—C4I	107.8 (4)
C10D—Co1D—C8D	68.97 (15)	C1I—C5I—Co1I	70.1 (2)
C4D—Co1D—C8D	121.58 (15)	C4I—C5I—Co1I	69.1 (2)
C7D—Co1D—C8D	40.48 (14)	C1I—C5I—H5I	126.1
C1D—Co1D—C8D	159.97 (14)	C4I—C5I—H5I	126.1
C9D—Co1D—C8D	40.72 (13)	Co1I—C5I—H5I	126.2
C5D—Co1D—C8D	157.97 (15)	C7I—C6I—C10I	108.0 (3)
C3D—Co1D—C8D	106.67 (14)	C7I—C6I—Co1I	69.7 (2)

C2D—Co1D—C8D	123.19 (14)	C10I—C6I—Co1I	70.0 (2)
C5D—C1D—C2D	108.4 (3)	C7I—C6I—H6I	126.0
C5D—C1D—Co1D	69.9 (2)	C10I—C6I—H6I	126.0
C2D—C1D—Co1D	69.9 (2)	Co1I—C6I—H6I	125.9
C5D—C1D—H1D	125.8	C8I—C7I—C6I	108.2 (3)
C2D—C1D—H1D	125.8	C8I—C7I—Co1I	69.6 (2)
Co1D—C1D—H1D	126.0	C6I—C7I—Co1I	69.4 (2)
C3D—C2D—C1D	108.2 (3)	C8I—C7I—H7I	125.9
C3D—C2D—Co1D	69.48 (19)	C6I—C7I—H7I	125.9
C1D—C2D—Co1D	69.25 (19)	Co1I—C7I—H7I	126.6
C3D—C2D—H2D	125.9	C7I—C8I—C9I	108.2 (3)
C1D—C2D—H2D	125.9	C7I—C8I—Co1I	69.6 (2)
Co1D—C2D—H2D	126.9	C9I—C8I—Co1I	69.6 (2)
C2D—C3D—C4D	107.5 (3)	C7I—C8I—H8I	125.9
C2D—C3D—Co1D	69.87 (19)	C9I—C8I—H8I	125.9
C4D—C3D—Co1D	69.22 (18)	Co1I—C8I—H8I	126.4
C2D—C3D—H3D	126.2	C8I—C9I—C10I	107.8 (3)
C4D—C3D—H3D	126.2	C8I—C9I—Co1I	69.5 (2)
Co1D—C3D—H3D	126.2	C10I—C9I—Co1I	69.7 (2)
C3D—C4D—C5D	108.1 (3)	C8I—C9I—H9I	126.1
C3D—C4D—Co1D	69.84 (19)	C10I—C9I—H9I	126.1
C5D—C4D—Co1D	69.71 (19)	Co1I—C9I—H9I	126.2
C3D—C4D—H4D	125.9	C6I—C10I—C9I	107.8 (3)
C5D—C4D—H4D	125.9	C6I—C10I—Co1I	69.2 (2)
Co1D—C4D—H4D	126.1	C9I—C10I—Co1I	69.3 (2)
C1D—C5D—C4D	107.8 (3)	C6I—C10I—H10I	126.1
C1D—C5D—Co1D	69.7 (2)	C9I—C10I—H10I	126.1
C4D—C5D—Co1D	69.2 (2)	Co1I—C10I—H10I	127.0
C1D—C5D—H5D	126.1	C7J—Co1J—C5J	155.34 (15)
C4D—C5D—H5D	126.1	C7J—Co1J—C4J	162.42 (15)
Co1D—C5D—H5D	126.6	C5J—Co1J—C4J	41.04 (14)
C10D—C6D—C7D	108.1 (3)	C7J—Co1J—C8J	40.82 (14)
C10D—C6D—Co1D	69.7 (2)	C5J—Co1J—C8J	161.95 (15)
C7D—C6D—Co1D	69.9 (2)	C4J—Co1J—C8J	125.17 (15)
C10D—C6D—H6D	125.9	C7J—Co1J—C2J	107.83 (14)
C7D—C6D—H6D	125.9	C5J—Co1J—C2J	68.45 (14)
Co1D—C6D—H6D	126.0	C4J—Co1J—C2J	68.74 (14)
C8D—C7D—C6D	108.6 (3)	C8J—Co1J—C2J	121.78 (15)
C8D—C7D—Co1D	70.3 (2)	C7J—Co1J—C3J	125.55 (14)
C6D—C7D—Co1D	69.2 (2)	C5J—Co1J—C3J	68.73 (15)
C8D—C7D—H7D	125.7	C4J—Co1J—C3J	40.63 (14)
C6D—C7D—H7D	125.7	C8J—Co1J—C3J	108.22 (15)
Co1D—C7D—H7D	126.3	C2J—Co1J—C3J	41.22 (13)
C7D—C8D—C9D	107.5 (3)	C7J—Co1J—C10J	68.50 (14)
C7D—C8D—Co1D	69.2 (2)	C5J—Co1J—C10J	106.64 (15)
C9D—C8D—Co1D	69.1 (2)	C4J—Co1J—C10J	120.46 (15)
C7D—C8D—H8D	126.3	C8J—Co1J—C10J	68.49 (16)
C9D—C8D—H8D	126.3	C2J—Co1J—C10J	160.95 (16)

Co1D—C8D—H8D	127.0	C3J—Co1J—C10J	155.99 (15)
C8D—C9D—C10D	108.3 (3)	C7J—Co1J—C9J	68.81 (14)
C8D—C9D—Co1D	70.2 (2)	C5J—Co1J—C9J	124.23 (15)
C10D—C9D—Co1D	69.2 (2)	C4J—Co1J—C9J	107.27 (15)
C8D—C9D—H9D	125.8	C8J—Co1J—C9J	40.89 (15)
C10D—C9D—H9D	125.8	C2J—Co1J—C9J	157.13 (16)
Co1D—C9D—H9D	126.4	C3J—Co1J—C9J	121.10 (16)
C6D—C10D—C9D	107.5 (3)	C10J—Co1J—C9J	40.74 (16)
C6D—C10D—Co1D	69.4 (2)	C7J—Co1J—C1J	120.58 (14)
C9D—C10D—Co1D	69.68 (19)	C5J—Co1J—C1J	40.69 (14)
C6D—C10D—H10D	126.3	C4J—Co1J—C1J	68.78 (14)
C9D—C10D—H10D	126.3	C8J—Co1J—C1J	156.42 (14)
Co1D—C10D—H10D	126.2	C2J—Co1J—C1J	40.54 (13)
C3E—Co1E—C4E	40.98 (15)	C3J—Co1J—C1J	68.84 (14)
C3E—Co1E—C9E	122.29 (15)	C10J—Co1J—C1J	123.92 (16)
C4E—Co1E—C9E	105.97 (14)	C9J—Co1J—C1J	160.95 (16)
C3E—Co1E—C7E	122.40 (15)	C7J—Co1J—C6J	40.99 (14)
C4E—Co1E—C7E	157.89 (15)	C5J—Co1J—C6J	119.45 (15)
C9E—Co1E—C7E	68.76 (14)	C4J—Co1J—C6J	155.29 (15)
C3E—Co1E—C8E	106.36 (14)	C8J—Co1J—C6J	69.06 (16)
C4E—Co1E—C8E	120.95 (15)	C2J—Co1J—C6J	124.07 (14)
C9E—Co1E—C8E	41.16 (13)	C3J—Co1J—C6J	162.13 (14)
C7E—Co1E—C8E	41.03 (14)	C10J—Co1J—C6J	40.94 (14)
C3E—Co1E—C2E	41.02 (15)	C9J—Co1J—C6J	69.17 (16)
C4E—Co1E—C2E	68.86 (15)	C1J—Co1J—C6J	106.21 (15)
C9E—Co1E—C2E	159.60 (15)	C2J—C1J—C5J	108.0 (3)
C7E—Co1E—C2E	108.20 (15)	C2J—C1J—Co1J	69.61 (19)
C8E—Co1E—C2E	123.30 (15)	C5J—C1J—Co1J	69.4 (2)
C3E—Co1E—C10E	158.86 (15)	C2J—C1J—H1J	126.0
C4E—Co1E—C10E	122.37 (15)	C5J—C1J—H1J	126.0
C9E—Co1E—C10E	40.85 (13)	Co1J—C1J—H1J	126.6
C7E—Co1E—C10E	68.52 (14)	C1J—C2J—C3J	108.1 (3)
C8E—Co1E—C10E	69.08 (14)	C1J—C2J—Co1J	69.85 (19)
C2E—Co1E—C10E	158.54 (15)	C3J—C2J—Co1J	69.39 (19)
C3E—Co1E—C6E	158.65 (16)	C1J—C2J—H2J	125.9
C4E—Co1E—C6E	159.43 (15)	C3J—C2J—H2J	125.9
C9E—Co1E—C6E	68.69 (14)	Co1J—C2J—H2J	126.4
C7E—Co1E—C6E	40.55 (14)	C4J—C3J—C2J	107.6 (3)
C8E—Co1E—C6E	68.92 (14)	C4J—C3J—Co1J	69.5 (2)
C2E—Co1E—C6E	122.98 (15)	C2J—C3J—Co1J	69.39 (19)
C10E—Co1E—C6E	40.77 (13)	C4J—C3J—H3J	126.2
C3E—Co1E—C1E	68.55 (14)	C2J—C3J—H3J	126.2
C4E—Co1E—C1E	68.21 (14)	Co1J—C3J—H3J	126.5
C9E—Co1E—C1E	157.37 (15)	C3J—C4J—C5J	108.1 (3)
C7E—Co1E—C1E	124.78 (15)	C3J—C4J—Co1J	69.9 (2)
C8E—Co1E—C1E	160.71 (15)	C5J—C4J—Co1J	69.5 (2)
C2E—Co1E—C1E	40.79 (14)	C3J—C4J—H4J	126.0
C10E—Co1E—C1E	122.41 (14)	C5J—C4J—H4J	126.0

C6E—Co1E—C1E	108.66 (14)	Co1J—C4J—H4J	126.3
C3E—Co1E—C5E	68.84 (14)	C1J—C5J—C4J	108.2 (3)
C4E—Co1E—C5E	40.78 (13)	C1J—C5J—Co1J	70.0 (2)
C9E—Co1E—C5E	121.06 (14)	C4J—C5J—Co1J	69.5 (2)
C7E—Co1E—C5E	160.38 (14)	C1J—C5J—H5J	125.9
C8E—Co1E—C5E	157.01 (15)	C4J—C5J—H5J	125.9
C2E—Co1E—C5E	68.71 (15)	Co1J—C5J—H5J	126.2
C10E—Co1E—C5E	106.87 (14)	C7J—C6J—C10J	106.7 (3)
C6E—Co1E—C5E	123.66 (14)	C7J—C6J—Co1J	69.0 (2)
C1E—Co1E—C5E	40.36 (14)	C10J—C6J—Co1J	69.3 (2)
C5E—C1E—C2E	108.9 (3)	C7J—C6J—H6J	126.6
C5E—C1E—Co1E	69.89 (19)	C10J—C6J—H6J	126.6
C2E—C1E—Co1E	69.38 (19)	Co1J—C6J—H6J	126.6
C5E—C1E—H1E	125.6	C8J—C7J—C6J	108.7 (3)
C2E—C1E—H1E	125.6	C8J—C7J—Co1J	69.7 (2)
Co1E—C1E—H1E	126.7	C6J—C7J—Co1J	70.0 (2)
C1E—C2E—C3E	107.3 (3)	C8J—C7J—H7J	125.7
C1E—C2E—Co1E	69.8 (2)	C6J—C7J—H7J	125.7
C3E—C2E—Co1E	69.0 (2)	Co1J—C7J—H7J	126.3
C1E—C2E—H2E	126.4	C7J—C8J—C9J	108.1 (4)
C3E—C2E—H2E	126.4	C7J—C8J—Co1J	69.5 (2)
Co1E—C2E—H2E	126.3	C9J—C8J—Co1J	69.7 (2)
C4E—C3E—C2E	107.9 (3)	C7J—C8J—H8J	126.0
C4E—C3E—Co1E	69.5 (2)	C9J—C8J—H8J	126.0
C2E—C3E—Co1E	69.9 (2)	Co1J—C8J—H8J	126.4
C4E—C3E—H3E	126.1	C10J—C9J—C8J	107.5 (3)
C2E—C3E—H3E	126.1	C10J—C9J—Co1J	69.6 (2)
Co1E—C3E—H3E	126.1	C8J—C9J—Co1J	69.4 (2)
C5E—C4E—C3E	108.4 (3)	C10J—C9J—H9J	126.2
C5E—C4E—Co1E	70.3 (2)	C8J—C9J—H9J	126.2
C3E—C4E—Co1E	69.5 (2)	Co1J—C9J—H9J	126.3
C5E—C4E—H4E	125.8	C9J—C10J—C6J	109.0 (3)
C3E—C4E—H4E	125.8	C9J—C10J—Co1J	69.7 (2)
Co1E—C4E—H4E	126.0	C6J—C10J—Co1J	69.7 (2)
C1E—C5E—C4E	107.5 (3)	C9J—C10J—H10J	125.5
C1E—C5E—Co1E	69.76 (19)	C6J—C10J—H10J	125.5
C4E—C5E—Co1E	68.89 (19)	Co1J—C10J—H10J	126.7
C1E—C5E—H5E	126.2	Cl2K—Co1K—Cl1K	109.39 (3)
C4E—C5E—H5E	126.2	Cl2K—Co1K—Cl3K	110.27 (4)
Co1E—C5E—H5E	126.7	Cl1K—Co1K—Cl3K	107.54 (3)
C7E—C6E—C10E	107.9 (3)	Cl2K—Co1K—Cl4K	106.83 (3)
C7E—C6E—Co1E	69.4 (2)	Cl1K—Co1K—Cl4K	112.28 (3)
C10E—C6E—Co1E	69.41 (19)	Cl3K—Co1K—Cl4K	110.55 (3)
C7E—C6E—H6E	126.0	Cl4L—Co1L—Cl2L	108.13 (4)
C10E—C6E—H6E	126.0	Cl4L—Co1L—Cl3L	110.05 (3)
Co1E—C6E—H6E	126.8	Cl2L—Co1L—Cl3L	110.32 (3)
C6E—C7E—C8E	108.8 (3)	Cl4L—Co1L—Cl1L	109.08 (3)
C6E—C7E—Co1E	70.08 (19)	Cl2L—Co1L—Cl1L	109.36 (3)

C8E—C7E—Co1E	69.57 (19)	Cl3L—Co1L—Cl1L	109.86 (3)
C6E—C7E—H7E	125.6	Cl4M—Co1M—Cl2M	111.54 (3)
C8E—C7E—H7E	125.6	Cl4M—Co1M—Cl1M	110.24 (4)
Co1E—C7E—H7E	126.3	Cl2M—Co1M—Cl1M	107.29 (3)
C7E—C8E—C9E	106.9 (3)	Cl4M—Co1M—Cl3M	105.78 (4)
C7E—C8E—Co1E	69.40 (19)	Cl2M—Co1M—Cl3M	109.85 (4)
C9E—C8E—Co1E	69.06 (18)	Cl1M—Co1M—Cl3M	112.20 (3)
C7E—C8E—H8E	126.6	Cl4N—Co1N—Cl2N	110.29 (3)
C9E—C8E—H8E	126.6	Cl4N—Co1N—Cl1N	110.74 (3)
Co1E—C8E—H8E	126.5	Cl2N—Co1N—Cl1N	108.56 (3)
C10E—C9E—C8E	108.5 (3)	Cl4N—Co1N—Cl3N	108.70 (3)
C10E—C9E—Co1E	70.00 (19)	Cl2N—Co1N—Cl3N	108.76 (3)
C8E—C9E—Co1E	69.78 (19)	Cl1N—Co1N—Cl3N	109.75 (3)
C10E—C9E—H9E	125.8	Cl3O—Co1O—Cl1O	110.32 (4)
C8E—C9E—H9E	125.8	Cl3O—Co1O—Cl4O	110.44 (4)
Co1E—C9E—H9E	126.0	Cl1O—Co1O—Cl4O	106.45 (4)
C9E—C10E—C6E	107.9 (3)	Cl3O—Co1O—Cl2O	107.14 (4)
C9E—C10E—Co1E	69.15 (19)	Cl1O—Co1O—Cl2O	111.50 (4)
C6E—C10E—Co1E	69.8 (2)	Cl4O—Co1O—Cl2O	111.03 (4)
C9E—C10E—H10E	126.0	Cl1P—C2P—Cl3P	110.72 (18)
C6E—C10E—H10E	126.0	Cl1P—C2P—H2P1	109.5
Co1E—C10E—H10E	126.6	Cl3P—C2P—H2P1	109.5
C7F—Co1F—C4F	160.26 (17)	Cl1P—C2P—H2P2	109.5
C7F—Co1F—C3F	122.88 (17)	Cl3P—C2P—H2P2	109.5
C4F—Co1F—C3F	40.93 (17)	H2P1—C2P—H2P2	108.1
C7F—Co1F—C10F	69.09 (15)	Cl3Q—C2Q—Cl1Q	111.14 (18)
C4F—Co1F—C10F	122.36 (17)	Cl3Q—C2Q—H2Q1	109.4
C3F—Co1F—C10F	158.29 (17)	Cl1Q—C2Q—H2Q1	109.4
C7F—Co1F—C6F	40.98 (14)	Cl3Q—C2Q—H2Q2	109.4
C4F—Co1F—C6F	157.87 (17)	Cl1Q—C2Q—H2Q2	109.4
C3F—Co1F—C6F	159.32 (17)	H2Q1—C2Q—H2Q2	108.0
C10F—Co1F—C6F	41.06 (14)	Cl3R—C2R—Cl1R	112.2 (2)
C7F—Co1F—C5F	156.61 (16)	Cl3R—C2R—H2R1	109.2
C4F—Co1F—C5F	40.98 (16)	Cl1R—C2R—H2R1	109.2
C3F—Co1F—C5F	68.70 (16)	Cl3R—C2R—H2R2	109.2
C10F—Co1F—C5F	107.76 (16)	Cl1R—C2R—H2R2	109.2
C6F—Co1F—C5F	121.42 (16)	H2R1—C2R—H2R2	107.9
C7F—Co1F—C9F	69.04 (15)	Cl3S—C2S—Cl1S	111.97 (18)
C4F—Co1F—C9F	108.05 (16)	Cl3S—C2S—H2S1	109.2
C3F—Co1F—C9F	122.15 (15)	Cl1S—C2S—H2S1	109.2
C10F—Co1F—C9F	41.04 (14)	Cl3S—C2S—H2S2	109.2
C6F—Co1F—C9F	69.06 (14)	Cl1S—C2S—H2S2	109.2
C5F—Co1F—C9F	124.73 (15)	H2S1—C2S—H2S2	107.9
C7F—Co1F—C8F	41.04 (14)	Cl1T—C2T—Cl3T	112.06 (18)
C4F—Co1F—C8F	124.09 (16)	Cl1T—C2T—H2T1	109.2
C3F—Co1F—C8F	107.17 (15)	Cl3T—C2T—H2T1	109.2
C10F—Co1F—C8F	68.95 (14)	Cl1T—C2T—H2T2	109.2
C6F—Co1F—C8F	68.97 (14)	Cl3T—C2T—H2T2	109.2

C5F—Co1F—C8F	161.32 (16)	H2T1—C2T—H2T2	107.9
C9F—Co1F—C8F	40.85 (13)	C11U—C2U—C13U	111.7 (2)
C7F—Co1F—C1F	120.61 (16)	C11U—C2U—H2U1	109.3
C4F—Co1F—C1F	68.62 (16)	C13U—C2U—H2U1	109.3
C3F—Co1F—C1F	68.47 (15)	C11U—C2U—H2U2	109.3
C10F—Co1F—C1F	123.65 (15)	C13U—C2U—H2U2	109.3
C6F—Co1F—C1F	106.57 (15)	H2U1—C2U—H2U2	107.9
C5A—C1A—C2A—C3A	0.5 (4)	C5F—C1F—C2F—C3F	0.4 (4)
Co1A—C1A—C2A—C3A	-58.6 (2)	Co1F—C1F—C2F—C3F	-58.9 (3)
C5A—C1A—C2A—Co1A	59.1 (2)	C5F—C1F—C2F—Co1F	59.2 (3)
C1A—C2A—C3A—C4A	-0.3 (4)	C1F—C2F—C3F—C4F	-0.2 (4)
Co1A—C2A—C3A—C4A	-59.1 (2)	Co1F—C2F—C3F—C4F	-59.3 (3)
C1A—C2A—C3A—Co1A	58.8 (2)	C1F—C2F—C3F—Co1F	59.1 (3)
C2A—C3A—C4A—C5A	0.0 (4)	C2F—C3F—C4F—C5F	0.0 (4)
Co1A—C3A—C4A—C5A	-59.4 (2)	Co1F—C3F—C4F—C5F	-59.6 (3)
C2A—C3A—C4A—Co1A	59.4 (2)	C2F—C3F—C4F—Co1F	59.6 (3)
C3A—C4A—C5A—C1A	0.3 (4)	C2F—C1F—C5F—C4F	-0.4 (4)
Co1A—C4A—C5A—C1A	-58.9 (2)	Co1F—C1F—C5F—C4F	58.9 (3)
C3A—C4A—C5A—Co1A	59.2 (2)	C2F—C1F—C5F—Co1F	-59.3 (3)
C2A—C1A—C5A—C4A	-0.5 (4)	C3F—C4F—C5F—C1F	0.3 (4)
Co1A—C1A—C5A—C4A	58.7 (2)	Co1F—C4F—C5F—C1F	-59.3 (3)
C2A—C1A—C5A—Co1A	-59.2 (2)	C3F—C4F—C5F—Co1F	59.5 (3)
C10A—C6A—C7A—C8A	0.2 (4)	C10F—C6F—C7F—C8F	0.7 (4)
Co1A—C6A—C7A—C8A	59.2 (2)	Co1F—C6F—C7F—C8F	59.6 (2)
C10A—C6A—C7A—Co1A	-59.0 (2)	C10F—C6F—C7F—Co1F	-58.9 (2)
C6A—C7A—C8A—C9A	-0.4 (4)	C6F—C7F—C8F—C9F	-0.7 (4)
Co1A—C7A—C8A—C9A	58.5 (2)	Co1F—C7F—C8F—C9F	58.8 (2)
C6A—C7A—C8A—Co1A	-58.9 (2)	C6F—C7F—C8F—Co1F	-59.6 (2)
C7A—C8A—C9A—C10A	0.5 (4)	C7F—C8F—C9F—C10F	0.4 (4)
Co1A—C8A—C9A—C10A	59.2 (2)	Co1F—C8F—C9F—C10F	58.9 (2)
C7A—C8A—C9A—Co1A	-58.7 (2)	C7F—C8F—C9F—Co1F	-58.5 (2)
C7A—C6A—C10A—C9A	0.1 (4)	C8F—C9F—C10F—C6F	0.1 (4)
Co1A—C6A—C10A—C9A	-59.1 (2)	Co1F—C9F—C10F—C6F	59.1 (2)
C7A—C6A—C10A—Co1A	59.2 (2)	C8F—C9F—C10F—Co1F	-59.1 (2)
C8A—C9A—C10A—C6A	-0.4 (4)	C7F—C6F—C10F—C9F	-0.5 (4)
Co1A—C9A—C10A—C6A	59.2 (2)	Co1F—C6F—C10F—C9F	-59.2 (2)
C8A—C9A—C10A—Co1A	-59.5 (2)	C7F—C6F—C10F—Co1F	58.7 (2)
C5B—C1B—C2B—C3B	-0.3 (4)	C5G—C1G—C2G—C3G	0.1 (4)
Co1B—C1B—C2B—C3B	-59.4 (2)	Co1G—C1G—C2G—C3G	-59.3 (2)
C5B—C1B—C2B—Co1B	59.1 (2)	C5G—C1G—C2G—Co1G	59.4 (2)
C1B—C2B—C3B—C4B	0.4 (4)	C1G—C2G—C3G—C4G	0.0 (4)
Co1B—C2B—C3B—C4B	-59.1 (2)	Co1G—C2G—C3G—C4G	-59.6 (2)
C1B—C2B—C3B—Co1B	59.5 (2)	C1G—C2G—C3G—Co1G	59.5 (2)
C2B—C3B—C4B—C5B	-0.4 (4)	C2G—C3G—C4G—C5G	-0.1 (4)
Co1B—C3B—C4B—C5B	-59.2 (2)	Co1G—C3G—C4G—C5G	-59.7 (2)
C2B—C3B—C4B—Co1B	58.8 (2)	C2G—C3G—C4G—Co1G	59.7 (2)
C3B—C4B—C5B—C1B	0.3 (4)	C2G—C1G—C5G—C4G	-0.2 (4)

Co1B—C4B—C5B—C1B	-58.9 (2)	Co1G—C1G—C5G—C4G	59.1 (2)
C3B—C4B—C5B—Co1B	59.1 (2)	C2G—C1G—C5G—Co1G	-59.3 (2)
C2B—C1B—C5B—C4B	0.0 (4)	C3G—C4G—C5G—C1G	0.1 (4)
Co1B—C1B—C5B—C4B	58.9 (2)	Co1G—C4G—C5G—C1G	-59.4 (2)
C2B—C1B—C5B—Co1B	-58.9 (2)	C3G—C4G—C5G—Co1G	59.5 (2)
C10B—C6B—C7B—C8B	-0.9 (4)	C10G—C6G—C7G—C8G	0.5 (4)
Co1B—C6B—C7B—C8B	59.1 (2)	Co1G—C6G—C7G—C8G	59.9 (2)
C10B—C6B—C7B—Co1B	-60.0 (2)	C10G—C6G—C7G—Co1G	-59.4 (2)
C6B—C7B—C8B—C9B	0.7 (4)	C6G—C7G—C8G—C9G	-0.6 (4)
Co1B—C7B—C8B—C9B	59.6 (2)	Co1G—C7G—C8G—C9G	58.9 (2)
C6B—C7B—C8B—Co1B	-58.9 (2)	C6G—C7G—C8G—Co1G	-59.5 (2)
C7B—C8B—C9B—C10B	-0.2 (4)	C7G—C8G—C9G—C10G	0.4 (4)
Co1B—C8B—C9B—C10B	59.1 (2)	Co1G—C8G—C9G—C10G	59.0 (2)
C7B—C8B—C9B—Co1B	-59.3 (2)	C7G—C8G—C9G—Co1G	-58.6 (2)
C7B—C6B—C10B—C9B	0.7 (4)	C7G—C6G—C10G—C9G	-0.3 (4)
Co1B—C6B—C10B—C9B	-58.9 (2)	Co1G—C6G—C10G—C9G	-59.6 (2)
C7B—C6B—C10B—Co1B	59.7 (2)	C7G—C6G—C10G—Co1G	59.3 (2)
C8B—C9B—C10B—C6B	-0.3 (4)	C8G—C9G—C10G—C6G	-0.1 (4)
Co1B—C9B—C10B—C6B	58.7 (2)	Co1G—C9G—C10G—C6G	59.2 (2)
C8B—C9B—C10B—Co1B	-59.1 (2)	C8G—C9G—C10G—Co1G	-59.3 (2)
C5C—C1C—C2C—C3C	-0.2 (4)	C5H—C1H—C2H—C3H	0.0 (4)
Co1C—C1C—C2C—C3C	-59.6 (2)	Co1H—C1H—C2H—C3H	-58.9 (2)
C5C—C1C—C2C—Co1C	59.4 (2)	C5H—C1H—C2H—Co1H	58.9 (2)
C1C—C2C—C3C—C4C	0.3 (4)	C1H—C2H—C3H—C4H	-0.2 (4)
Co1C—C2C—C3C—C4C	-59.1 (2)	Co1H—C2H—C3H—C4H	-59.1 (2)
C1C—C2C—C3C—Co1C	59.4 (2)	C1H—C2H—C3H—Co1H	58.9 (2)
C2C—C3C—C4C—C5C	-0.4 (4)	C2H—C3H—C4H—C5H	0.3 (4)
Co1C—C3C—C4C—C5C	-59.3 (2)	Co1H—C3H—C4H—C5H	-59.0 (2)
C2C—C3C—C4C—Co1C	58.9 (2)	C2H—C3H—C4H—Co1H	59.3 (2)
C3C—C4C—C5C—C1C	0.3 (4)	C3H—C4H—C5H—C1H	-0.3 (4)
Co1C—C4C—C5C—C1C	-58.9 (2)	Co1H—C4H—C5H—C1H	-59.5 (2)
C3C—C4C—C5C—Co1C	59.2 (2)	C3H—C4H—C5H—Co1H	59.3 (2)
C2C—C1C—C5C—C4C	-0.1 (4)	C2H—C1H—C5H—C4H	0.2 (4)
Co1C—C1C—C5C—C4C	59.1 (2)	Co1H—C1H—C5H—C4H	59.5 (2)
C2C—C1C—C5C—Co1C	-59.1 (2)	C2H—C1H—C5H—Co1H	-59.4 (2)
C10C—C6C—C7C—C8C	0.2 (4)	C10H—C6H—C7H—C8H	-0.3 (4)
Co1C—C6C—C7C—C8C	59.0 (2)	Co1H—C6H—C7H—C8H	59.0 (2)
C10C—C6C—C7C—Co1C	-58.9 (2)	C10H—C6H—C7H—Co1H	-59.3 (2)
C6C—C7C—C8C—C9C	0.1 (4)	C6H—C7H—C8H—C9H	0.2 (4)
Co1C—C7C—C8C—C9C	59.1 (2)	Co1H—C7H—C8H—C9H	59.2 (2)
C6C—C7C—C8C—Co1C	-59.0 (2)	C6H—C7H—C8H—Co1H	-58.9 (2)
C7C—C8C—C9C—C10C	-0.4 (4)	C7H—C8H—C9H—C10H	-0.1 (4)
Co1C—C8C—C9C—C10C	58.7 (2)	Co1H—C8H—C9H—C10H	59.1 (2)
C7C—C8C—C9C—Co1C	-59.1 (2)	C7H—C8H—C9H—Co1H	-59.1 (2)
C8C—C9C—C10C—C6C	0.5 (4)	C8H—C9H—C10H—C6H	-0.1 (4)
Co1C—C9C—C10C—C6C	59.4 (2)	Co1H—C9H—C10H—C6H	58.9 (2)
C8C—C9C—C10C—Co1C	-58.9 (2)	C8H—C9H—C10H—Co1H	-59.0 (2)
C7C—C6C—C10C—C9C	-0.4 (4)	C7H—C6H—C10H—C9H	0.3 (4)

Co1C—C6C—C10C—C9C	-59.5 (2)	Co1H—C6H—C10H—C9H	-59.1 (2)
C7C—C6C—C10C—Co1C	59.0 (2)	C7H—C6H—C10H—Co1H	59.4 (2)
C5D—C1D—C2D—C3D	0.8 (4)	C5I—C1I—C2I—C3I	0.0 (4)
Co1D—C1D—C2D—C3D	-58.8 (2)	Co1I—C1I—C2I—C3I	-59.3 (3)
C5D—C1D—C2D—Co1D	59.5 (2)	C5I—C1I—C2I—Co1I	59.3 (3)
C1D—C2D—C3D—C4D	-0.6 (4)	C1I—C2I—C3I—C4I	0.3 (4)
Co1D—C2D—C3D—C4D	-59.2 (2)	Co1I—C2I—C3I—C4I	-59.0 (3)
C1D—C2D—C3D—Co1D	58.6 (2)	C1I—C2I—C3I—Co1I	59.3 (3)
C2D—C3D—C4D—C5D	0.2 (4)	C2I—C3I—C4I—C5I	-0.5 (4)
Co1D—C3D—C4D—C5D	-59.4 (2)	Co1I—C3I—C4I—C5I	-60.2 (3)
C2D—C3D—C4D—Co1D	59.6 (2)	C2I—C3I—C4I—Co1I	59.7 (3)
C2D—C1D—C5D—C4D	-0.6 (4)	C2I—C1I—C5I—C4I	-0.3 (4)
Co1D—C1D—C5D—C4D	58.9 (2)	Co1I—C1I—C5I—C4I	59.1 (3)
C2D—C1D—C5D—Co1D	-59.5 (2)	C2I—C1I—C5I—Co1I	-59.4 (3)
C3D—C4D—C5D—C1D	0.3 (4)	C3I—C4I—C5I—C1I	0.5 (4)
Co1D—C4D—C5D—C1D	-59.2 (2)	Co1I—C4I—C5I—C1I	-59.7 (3)
C3D—C4D—C5D—Co1D	59.5 (2)	C3I—C4I—C5I—Co1I	60.2 (3)
C10D—C6D—C7D—C8D	0.0 (4)	C10I—C6I—C7I—C8I	-0.7 (4)
Co1D—C6D—C7D—C8D	59.5 (3)	Co1I—C6I—C7I—C8I	59.0 (3)
C10D—C6D—C7D—Co1D	-59.5 (3)	C10I—C6I—C7I—Co1I	-59.8 (2)
C6D—C7D—C8D—C9D	-0.1 (4)	C6I—C7I—C8I—C9I	0.3 (4)
Co1D—C7D—C8D—C9D	58.7 (2)	Co1I—C7I—C8I—C9I	59.2 (3)
C6D—C7D—C8D—Co1D	-58.8 (3)	C6I—C7I—C8I—Co1I	-58.9 (3)
C7D—C8D—C9D—C10D	0.1 (4)	C7I—C8I—C9I—C10I	0.3 (4)
Co1D—C8D—C9D—C10D	58.9 (2)	Co1I—C8I—C9I—C10I	59.5 (2)
C7D—C8D—C9D—Co1D	-58.7 (2)	C7I—C8I—C9I—Co1I	-59.2 (3)
C7D—C6D—C10D—C9D	0.1 (4)	C7I—C6I—C10I—C9I	0.9 (4)
Co1D—C6D—C10D—C9D	-59.5 (2)	Co1I—C6I—C10I—C9I	-58.6 (2)
C7D—C6D—C10D—Co1D	59.6 (3)	C7I—C6I—C10I—Co1I	59.6 (3)
C8D—C9D—C10D—C6D	-0.1 (4)	C8I—C9I—C10I—C6I	-0.8 (4)
Co1D—C9D—C10D—C6D	59.3 (2)	Co1I—C9I—C10I—C6I	58.6 (2)
C8D—C9D—C10D—Co1D	-59.5 (2)	C8I—C9I—C10I—Co1I	-59.3 (3)
C5E—C1E—C2E—C3E	-0.2 (4)	C5J—C1J—C2J—C3J	-0.1 (4)
Co1E—C1E—C2E—C3E	-59.1 (2)	Co1J—C1J—C2J—C3J	-59.0 (2)
C5E—C1E—C2E—Co1E	58.9 (2)	C5J—C1J—C2J—Co1J	58.9 (2)
C1E—C2E—C3E—C4E	0.2 (4)	C1J—C2J—C3J—C4J	0.1 (4)
Co1E—C2E—C3E—C4E	-59.4 (2)	Co1J—C2J—C3J—C4J	-59.2 (2)
C1E—C2E—C3E—Co1E	59.6 (2)	C1J—C2J—C3J—Co1J	59.3 (2)
C2E—C3E—C4E—C5E	-0.1 (4)	C2J—C3J—C4J—C5J	0.0 (4)
Co1E—C3E—C4E—C5E	-59.8 (2)	Co1J—C3J—C4J—C5J	-59.2 (2)
C2E—C3E—C4E—Co1E	59.6 (2)	C2J—C3J—C4J—Co1J	59.2 (2)
C2E—C1E—C5E—C4E	0.1 (4)	C2J—C1J—C5J—C4J	0.1 (4)
Co1E—C1E—C5E—C4E	58.7 (2)	Co1J—C1J—C5J—C4J	59.2 (2)
C2E—C1E—C5E—Co1E	-58.6 (2)	C2J—C1J—C5J—Co1J	-59.0 (2)
C3E—C4E—C5E—C1E	0.0 (4)	C3J—C4J—C5J—C1J	-0.1 (4)
Co1E—C4E—C5E—C1E	-59.3 (2)	Co1J—C4J—C5J—C1J	-59.5 (2)
C3E—C4E—C5E—Co1E	59.3 (2)	C3J—C4J—C5J—Co1J	59.4 (2)
C10E—C6E—C7E—C8E	0.1 (4)	C10J—C6J—C7J—C8J	-0.2 (4)

Co1E—C6E—C7E—C8E	59.0 (2)	Co1J—C6J—C7J—C8J	59.1 (2)
C10E—C6E—C7E—Co1E	-58.9 (2)	C10J—C6J—C7J—Co1J	-59.3 (2)
C6E—C7E—C8E—C9E	-0.2 (4)	C6J—C7J—C8J—C9J	-0.1 (4)
Co1E—C7E—C8E—C9E	59.1 (2)	Co1J—C7J—C8J—C9J	59.2 (3)
C6E—C7E—C8E—Co1E	-59.3 (2)	C6J—C7J—C8J—Co1J	-59.3 (2)
C7E—C8E—C9E—C10E	0.2 (4)	C7J—C8J—C9J—C10J	0.4 (4)
Co1E—C8E—C9E—C10E	59.5 (2)	Co1J—C8J—C9J—C10J	59.4 (3)
C7E—C8E—C9E—Co1E	-59.3 (2)	C7J—C8J—C9J—Co1J	-59.1 (2)
C8E—C9E—C10E—C6E	-0.1 (4)	C8J—C9J—C10J—C6J	-0.5 (4)
Co1E—C9E—C10E—C6E	59.3 (2)	Co1J—C9J—C10J—C6J	58.8 (3)
C8E—C9E—C10E—Co1E	-59.4 (2)	C8J—C9J—C10J—Co1J	-59.3 (3)
C7E—C6E—C10E—C9E	0.0 (4)	C7J—C6J—C10J—C9J	0.4 (4)
Co1E—C6E—C10E—C9E	-58.9 (2)	Co1J—C6J—C10J—C9J	-58.7 (3)
C7E—C6E—C10E—Co1E	58.9 (2)	C7J—C6J—C10J—Co1J	59.2 (2)

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C2P—H2P1...C12N	0.99	2.72	3.624 (3)	152
C2P—H2P2...C11N	0.99	2.76	3.574 (3)	140
C2Q—H2Q1...C12L ⁱ	0.99	2.71	3.604 (3)	151
C2Q—H2Q2...C11L ⁱ	0.99	2.71	3.582 (3)	147
C2R—H2R1...C11M	0.99	2.72	3.590 (4)	147
C2R—H2R2...C12M	0.99	2.99	3.842 (4)	145
C2S—H2S1...C14L	0.99	2.82	3.769 (3)	161
C2S—H2S2...C13L	0.99	2.74	3.516 (3)	136
C2T—H2T1...C12K	0.99	2.76	3.707 (4)	161
C2T—H2T2...C14K	0.99	2.71	3.487 (3)	136
C2U—H2U1...C11K	0.99	2.75	3.602 (4)	145
C2U—H2U2...C13K	0.99	2.87	3.747 (4)	148

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