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Bis(4-cobaltoceniumyl-1-ferrocenyl-3-methyl-1,2,3-triazolylidene)gold(I) hexafluoridophosphate–trifluoromethanesulfonate (1.2/1.8)

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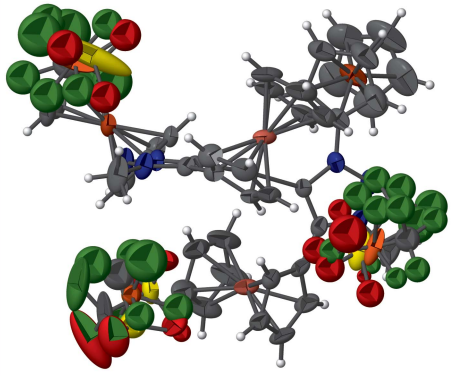
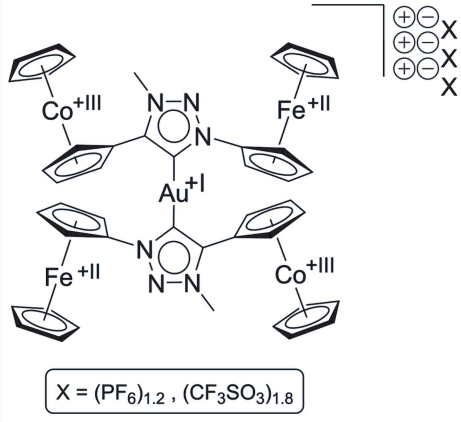
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[AuCo_2Fe_2(C_5H_5)_4(C_{13}H_{11}N_3)_2](PF_6)_{1.2}(CF_3SO_3)_{1.8}$, was synthesized by deprotonation of 4-cobaltoceniumyl-1-ferrocenyl-3-methyl-1,2,3-triazolium hexafluoridophosphate trifluoromethanesulfonate with thallium ethoxide, followed by transmetalation with chlorido(triphenylphosphine)-gold(I), crystallizing as orange prisms. It is a unique example of a homoleptic dimetallocenyl-substituted triazolylidene complex.

3D view



Chemical scheme



Structure description

The title compound (Figs. 1 and 2) is the first representative of a homoleptic dimetallocenyl substituted triazolylidene complex. As a result of the divergent electronic properties of the metallocene moieties, the ligand scaffold constitutes a *push–pull* system.

Structurally, regular ferrocene and cobaltocenium sandwich entities are observed, exhibiting coplanar cyclopentadienyl rings and displaying unexceptional carbon–iron [2.016 (4)–2.054 (14) Å], carbon–cobalt [2.014 (6)–2.048 (5) Å], as well as carbon–carbon [1.392 (15)(16)–1.433 (7)(14) Å] bond distances. The triazolylidene ring also has the anticipated bond lengths similar to its heteroleptic congeners, which have been published recently (Vanicek *et al.*, 2018). The carbene–gold distances of 2.021 (4) and 2.030 (4) Å are in line with expectations for this class of compounds.

Synthesis and crystallization

Bis(4-cobaltoceniumyl-1-ferrocenyl-3-methyltriazolylidene)gold(I)–hexafluoridophosphate–trifluoromethanesulfonate (1/1.2/1.8) was obtained by deprotonating 0.140 g (0.186 mmol, 1 equiv.) of 4-cobaltoceniumyl-1-ferrocenyl-3-methyltriazolium hexa-

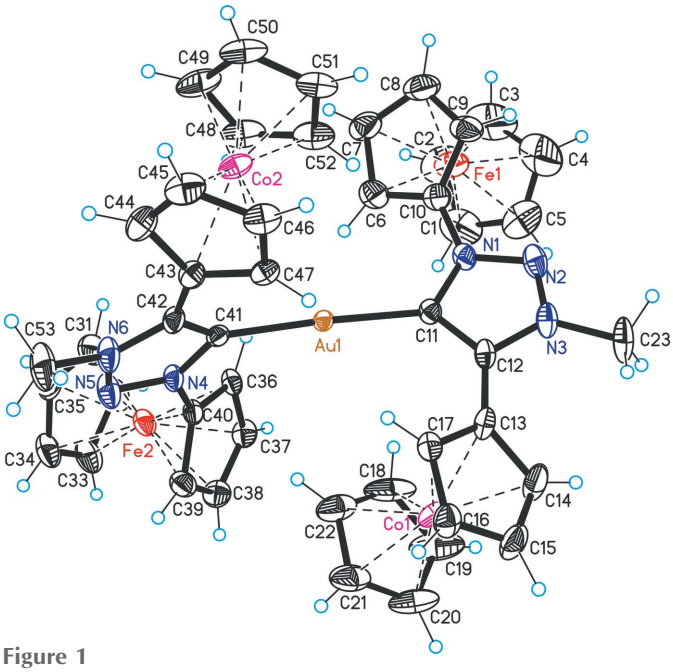


Figure 1
The structure of the title compound, with displacement ellipsoids drawn at the 30% probability level for non-H atoms (the disordered counter-ions were omitted for clarity).

fluoridophosphate trifluoromethanesulfonate (Vanicek *et al.*, 2018) with 0.37 ml of a freshly prepared 0.5 *M* thallium ethoxide THF solution (0.186 mmol, 1 equiv.) in 35 ml of THF (abs) at −80°C with the exclusion of light and under protection from air by an argon atmosphere. The reaction mixture was allowed to warm to −60°C and 0.092 g (0.186 mmol, 1 equiv.) of chlorido(triphenylphosphine)gold(I) was added. After warming to room temperature, the reaction was completed overnight. Precipitated thallium chloride was filtered off *via* syringe filtration, 300 ml of diethyl ether was added and the orange product was allowed to precipitate at −20°C for 2 h. The orange powder was filtered off through a Büchner funnel and washed thoroughly with three portions of diethyl ether. Meanwhile, the oily product was washed out of the funnel with acetone and the solvent was removed on a rotary evaporator. Drying *in vacuo* provided an orange oily foam, representing a product mixture containing various hetero- and homoleptic triazolylidene complexes from the ^{1}H, ^{13}C NMR and mass spectra. Single crystals of the title compound were obtained at 4°C *via* diffusion crystallization in acetone out of diethyl ether.

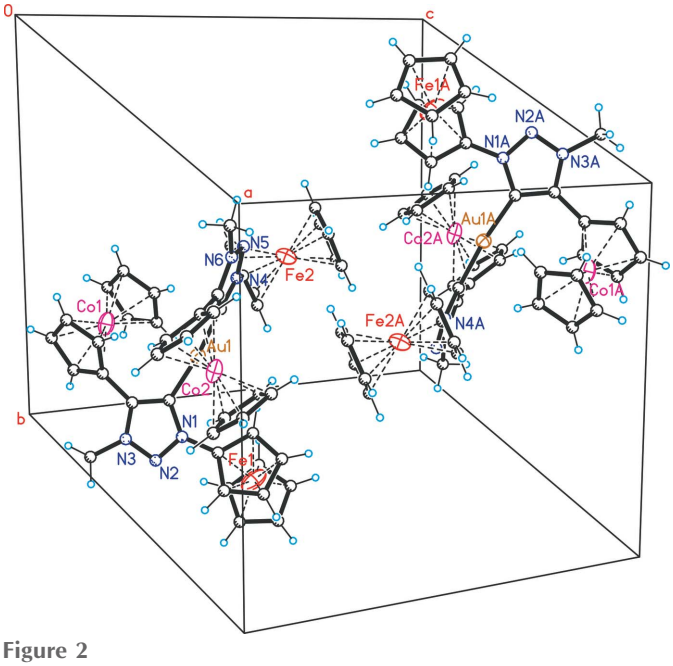


Figure 2
The arrangement of molecular entities of the tricationic title compound in the unit cell (the counter-ions were omitted for clarity). [Symmetry code: $1-x, 1-y, 1-z$.]

Table 1
Experimental details.

Crystal data	
Chemical formula	$[AuCo_2Fe_2(C_5H_5)_4(C_{13}H_{11}N_3)_2]$-$(PF_6)_{1.2}(CF_3O_3S)_{1.8}$
M_r	1547.67
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	173
a, b, c (Å)	12.1395 (6), 13.8587 (7), 17.3660 (7)
α, β, γ (°)	85.994 (1), 80.863 (1), 66.136 (1)
V (Å^3)	2637.9 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.13
Crystal size (mm)	0.17 × 0.08 × 0.06
Data collection	
Diffractometer	Bruker D8 QUEST PHOTON 100
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.697, 0.875
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	99685, 9826, 9103
R_{int}	0.036
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.080, 1.03
No. of reflections	9826
No. of parameters	796
No. of restraints	14
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.15, −0.97

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*)*Mercury* (Macrae *et al.*, 2008), and *WinGX* (Farrugia 2012).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Specifically, the structure contains a statistical mixture of hexafluoridophosphate and trifluoromethanesulfonate anions with different distributions over three positions. The overall ratio of PF_6/CF_3SO_3 is approximately 1.2/1.8, leading to many nearly overlapping positions. The PF_6^- anions seem well ordered; however, in one instance they were refined with restrained bond distances. At two of the three positions, the trifluoromethanesulfonate anions show additional positional disorder effects. Most of the C, F

and O atoms were therefore refined with isotropic displacement parameters. The P and S atoms could be refined anisotropically, except for P2 and S2*B* with occupancies of 20% and 15% respectively. EADP/EXYZ commands were used to accommodate overlapping O- and F-atom positions in the case of the trifluoromethanesulfonate S2*B*.

Funding information

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full crystallographic data

IUCrData (2018). **3**, x180623 [https://doi.org/10.1107/S2414314618006235]

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Bis(4-cobaltoceniumyl-1-ferrocenyl-3-methyl-1,2,3-triazolylidene)gold(I) hexafluoridophosphate–triflate (1.2/1.8)

Crystal data

$[AuCo_2Fe_2(C_5H_5)_4(C_{13}H_{11}N_3)_2](PF_6)_{1.2}(CF_3O_3S)_{1.8}$
M_r = 1547.67
Triclinic, $P\overline{1}$
a = 12.1395 (6) Å
b = 13.8587 (7) Å
c = 17.3660 (7) Å
α = 85.994 (1)°
β = 80.863 (1)°
γ = 66.136 (1)°
V = 2637.9 (2) Å^3
Z = 2
$F(000)$ = 1518
D_x = 1.949 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9667 reflections
θ = 2.8–26.7°
μ = 4.13 mm^{-1}
T = 173 K
Prism, orange
0.17 × 0.08 × 0.06 mm

Data collection

Bruker D8 QUEST PHOTON 100 diffractometer
Radiation source: Incoatec Microfocus
Multi layered optics monochromator
Detector resolution: 10.4 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
T_{min} = 0.697, T_{max} = 0.875
99685 measured reflections
9826 independent reflections
9103 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 25.5°, θ_{min} = 2.1°
h = −14→14
k = −16→16
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.080
S = 1.03
9826 reflections
796 parameters
14 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0385P)^2 + 8.2499P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 1.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.97 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.

Refinement. statistical mixture of PF6/triflate anions with different distribution over three positions. The ratio PF6/triflate is around 1.2/1.8, whereas many nearly overlying positions are formed. The PF6 anions seem well ordered, but must be refined in one case with restrained bond distances. At two of the three positions the triflate anions show additional positional disordered effects. Most of the C-, F- and O-atoms were refined with isotropic displacement parameters.The P- and S-atoms could be refined anisotropically, except for P2 and S2B with occupancies of 20% and 15%. EADP/EXYZ orders were used for overlying O- and F-positions at triflate S2B.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Au1	0.29711 (2)	0.72636 (2)	0.25524 (2)	0.02587 (6)	
Co1	−0.05618 (6)	0.81395 (6)	0.20823 (4)	0.04671 (17)	
Co2	0.63689 (5)	0.57749 (6)	0.12477 (3)	0.03945 (15)	
Fe1	0.33999 (8)	1.04602 (7)	0.36457 (6)	0.0616 (2)	
Fe2	0.22712 (7)	0.52340 (5)	0.50978 (4)	0.04258 (17)	
N1	0.2489 (4)	0.9607 (3)	0.2382 (2)	0.0384 (9)	
N2	0.1862 (4)	1.0520 (3)	0.2043 (3)	0.0512 (11)	
N3	0.1094 (4)	1.0309 (3)	0.1709 (3)	0.0494 (11)	
N4	0.3356 (3)	0.5135 (3)	0.3317 (2)	0.0359 (8)	
N5	0.3851 (4)	0.4093 (3)	0.3233 (3)	0.0535 (12)	
N6	0.4595 (4)	0.3954 (3)	0.2573 (3)	0.0510 (11)	
C1	0.1979 (8)	1.0944 (7)	0.4519 (6)	0.097 (3)	
H1	0.1544	1.0535	0.4749	0.116*	
C2	0.3046 (9)	1.0986 (8)	0.4759 (5)	0.098 (3)	
H2	0.3443	1.0611	0.5184	0.118*	
C3	0.3383 (11)	1.1676 (9)	0.4255 (8)	0.126 (4)	
H3	0.4062	1.1847	0.4269	0.151*	
C4	0.2549 (11)	1.2075 (7)	0.3722 (7)	0.115 (4)	
H4	0.2560	1.2573	0.3319	0.138*	
C5	0.1714 (8)	1.1630 (7)	0.3876 (5)	0.092 (3)	
H5	0.1058	1.1764	0.3592	0.111*	
C6	0.3868 (6)	0.8924 (4)	0.3399 (4)	0.0559 (14)	
H6	0.3521	0.8475	0.3676	0.067*	
C7	0.4907 (6)	0.9074 (5)	0.3558 (5)	0.0688 (18)	
H7	0.5387	0.8735	0.3957	0.083*	
C8	0.5088 (6)	0.9821 (6)	0.3011 (5)	0.080 (2)	
H8	0.5712	1.0074	0.2988	0.096*	
C9	0.4210 (5)	1.0126 (5)	0.2512 (4)	0.0634 (17)	
H9	0.4130	1.0614	0.2090	0.076*	
C10	0.3457 (5)	0.9568 (4)	0.2756 (3)	0.0460 (12)	
C11	0.2141 (4)	0.8809 (3)	0.2264 (3)	0.0324 (9)	
C12	0.1211 (4)	0.9299 (3)	0.1827 (3)	0.0383 (10)	
C13	0.0476 (5)	0.8868 (4)	0.1491 (3)	0.0422 (11)	
C14	−0.0773 (6)	0.9399 (4)	0.1376 (4)	0.0620 (16)	

H14	−0.1286	1.0112	0.1505	0.074*
C15	−0.1107 (6)	0.8679 (5)	0.1037 (4)	0.0639 (17)
H15	−0.1883	0.8829	0.0892	0.077*
C16	−0.0092 (5)	0.7696 (4)	0.0948 (3)	0.0501 (13)
H16	−0.0067	0.7071	0.0738	0.060*
C17	0.0882 (5)	0.7814 (4)	0.1229 (3)	0.0411 (11)
H17	0.1674	0.7278	0.1241	0.049*
C18	−0.0429 (7)	0.8145 (9)	0.3229 (4)	0.091 (3)
H18	0.0009	0.8458	0.3455	0.109*
C19	−0.1668 (7)	0.8659 (8)	0.3107 (4)	0.096 (3)
H19	−0.2202	0.9367	0.3233	0.116*
C20	−0.1947 (6)	0.7897 (7)	0.2759 (4)	0.080 (2)
H20	−0.2711	0.8009	0.2612	0.096*
C21	−0.0893 (6)	0.6949 (7)	0.2670 (4)	0.073 (2)
H21	−0.0826	0.6314	0.2452	0.088*
C22	0.0041 (7)	0.7106 (8)	0.2962 (4)	0.082 (2)
H22	0.0847	0.6597	0.2974	0.099*
C23	0.0288 (7)	1.1149 (4)	0.1238 (4)	0.074 (2)
H23A	−0.0509	1.1506	0.1551	0.111*
H23B	0.0189	1.0837	0.0777	0.111*
H23C	0.0649	1.1661	0.1071	0.111*
C31	0.3660 (7)	0.4859 (6)	0.5743 (4)	0.074 (2)
H31	0.4256	0.5150	0.5683	0.089*
C32	0.2541 (7)	0.5256 (5)	0.6223 (3)	0.0680 (18)
H32	0.2241	0.5863	0.6543	0.082*
C33	0.1932 (7)	0.4596 (5)	0.6148 (4)	0.0656 (17)
H33	0.1151	0.4680	0.6412	0.079*
C34	0.2683 (6)	0.3788 (5)	0.5614 (4)	0.0657 (17)
H34	0.2498	0.3235	0.5455	0.079*
C35	0.3762 (6)	0.3950 (5)	0.5359 (4)	0.0726 (19)
H35	0.4432	0.3528	0.4997	0.087*
C36	0.2244 (4)	0.6475 (3)	0.4379 (3)	0.0365 (10)
H36	0.2784	0.6822	0.4342	0.044*
C37	0.1113 (5)	0.6749 (4)	0.4875 (3)	0.0452 (12)
H37	0.0760	0.7318	0.5233	0.054*
C38	0.0602 (5)	0.6033 (4)	0.4745 (3)	0.0506 (13)
H38	−0.0154	0.6044	0.5001	0.061*
C39	0.1406 (5)	0.5293 (4)	0.4168 (3)	0.0458 (12)
H39	0.1294	0.4721	0.3971	0.055*
C40	0.2409 (4)	0.5585 (3)	0.3950 (3)	0.0351 (10)
C41	0.3741 (4)	0.5687 (3)	0.2726 (2)	0.0295 (9)
C42	0.4578 (4)	0.4880 (3)	0.2247 (3)	0.0352 (10)
C43	0.5281 (4)	0.4953 (4)	0.1495 (3)	0.0377 (10)
C44	0.6498 (5)	0.4271 (4)	0.1185 (3)	0.0529 (14)
H44	0.7020	0.3668	0.1439	0.064*
C45	0.6785 (5)	0.4650 (5)	0.0442 (3)	0.0544 (14)
H45	0.7536	0.4343	0.0106	0.065*
C46	0.5782 (5)	0.5555 (5)	0.0277 (3)	0.0471 (12)

H46	0.5736	0.5966	−0.0187	0.056*	
C47	0.4854 (4)	0.5748 (4)	0.0921 (3)	0.0354 (10)	
H47	0.4074	0.6315	0.0965	0.043*	
C48	0.6425 (5)	0.6436 (6)	0.2236 (3)	0.0625 (17)	
H48	0.6043	0.6358	0.2744	0.075*	
C49	0.7611 (5)	0.5771 (6)	0.1896 (4)	0.0701 (19)	
H49	0.8164	0.5171	0.2134	0.084*	
C50	0.7824 (5)	0.6162 (6)	0.1138 (3)	0.0650 (18)	
H50	0.8550	0.5869	0.0779	0.078*	
C51	0.6771 (6)	0.7065 (5)	0.1003 (4)	0.0611 (16)	
H51	0.6662	0.7478	0.0539	0.073*	
C52	0.5907 (6)	0.7235 (5)	0.1693 (3)	0.0592 (16)	
H52	0.5120	0.7790	0.1773	0.071*	
C53	0.5188 (7)	0.2880 (4)	0.2244 (4)	0.082 (2)	
H53A	0.4879	0.2410	0.2567	0.124*	
H53B	0.6070	0.2620	0.2236	0.124*	
H53C	0.5009	0.2898	0.1712	0.124*	
P1	0.3445 (10)	0.8760 (7)	−0.0345 (6)	0.076 (3)	0.4
F1	0.3882 (12)	0.8736 (12)	0.0659 (7)	0.092 (4)*	0.4
F2	0.3341 (8)	0.8927 (7)	−0.1145 (5)	0.0510 (19)*	0.4
F3	0.3694 (14)	0.7628 (10)	−0.0246 (8)	0.073 (3)*	0.4
F4	0.354 (2)	0.9909 (19)	−0.0235 (16)	0.154 (8)*	0.4
F5	0.5015 (12)	0.8239 (11)	−0.0462 (8)	0.094 (4)*	0.4
F6	0.2087 (7)	0.9386 (6)	0.0068 (5)	0.038 (2)*	0.4
S1	0.3163 (8)	0.8598 (6)	−0.0152 (4)	0.101 (2)	0.3
O1A	0.452 (3)	0.763 (3)	−0.047 (2)	0.163 (11)*	0.3
O2A	0.334 (2)	0.7606 (19)	−0.0398 (14)	0.094 (8)*	0.3
O3A	0.3595 (14)	0.8355 (12)	0.0636 (8)	0.060 (4)*	0.3
C53A	0.394 (2)	0.925 (2)	−0.0715 (15)	0.071 (6)*	0.3
F1A	0.3942 (15)	1.0076 (13)	−0.0505 (10)	0.077 (4)*	0.3
F2A	0.5255 (17)	0.8591 (16)	−0.0750 (12)	0.099 (5)*	0.3
F3A	0.3692 (13)	0.9259 (11)	−0.1323 (8)	0.072 (3)*	0.3
S1B	0.3163 (8)	0.8598 (6)	−0.0152 (4)	0.101 (2)	0.3
O1B	0.1899 (10)	0.9208 (9)	−0.0018 (6)	0.023 (3)*	0.3
O2B	0.3142 (17)	0.7648 (14)	0.0209 (11)	0.082 (5)*	0.3
O3B	0.2927 (17)	0.8443 (15)	−0.1044 (10)	0.084 (5)*	0.3
C53B	0.419 (2)	0.9188 (18)	−0.0009 (13)	0.059 (5)*	0.3
F1B	0.5321 (16)	0.8820 (14)	−0.0338 (11)	0.098 (5)*	0.3
F2B	0.383 (2)	1.0248 (19)	−0.0113 (16)	0.121 (7)*	0.3
F3B	0.4194 (13)	0.9153 (12)	0.0689 (8)	0.079 (4)*	0.3
P2	0.1628 (7)	0.4061 (9)	0.1531 (4)	0.0445 (19)*	0.2
F7	0.1686 (18)	0.4546 (16)	0.2361 (11)	0.119 (7)*	0.2
F8	0.216 (2)	0.363 (2)	0.0692 (12)	0.094 (7)*	0.2
F9	0.305 (2)	0.386 (3)	0.135 (2)	0.202 (16)*	0.2
F10	0.025 (2)	0.430 (3)	0.1822 (18)	0.123 (9)*	0.2
F11	0.239 (4)	0.309 (3)	0.206 (3)	0.153 (17)*	0.2
F12	0.119 (3)	0.521 (2)	0.113 (2)	0.101 (12)*	0.2
S2	0.1531 (2)	0.4602 (2)	0.15495 (14)	0.0562 (6)	0.65

O4	0.2742 (8)	0.4450 (10)	0.1396 (5)	0.086 (3)	0.65
O5	0.0910 (13)	0.4842 (9)	0.2327 (6)	0.127 (4)	0.65
O6	0.0814 (14)	0.5195 (11)	0.1027 (10)	0.104 (6)	0.65
C54	0.1445 (13)	0.3373 (8)	0.1429 (7)	0.112 (6)	0.65
F4A	0.0326 (12)	0.3493 (10)	0.1622 (8)	0.229 (7)	0.65
F5A	0.1733 (8)	0.3092 (6)	0.0690 (4)	0.130 (3)	0.65
F6A	0.2163 (13)	0.2677 (6)	0.1874 (6)	0.184 (6)	0.65
S2B	0.1136 (13)	0.4051 (12)	0.1147 (9)	0.081 (3)*	0.15
O4B	0.075 (4)	0.528 (3)	0.082 (2)	0.039 (8)*	0.15
O5B	0.1733 (8)	0.3092 (6)	0.0690 (4)	0.130 (3)	0.15
O6B	0.0326 (12)	0.3493 (10)	0.1622 (8)	0.229 (7)	0.15
C54B	0.209 (3)	0.3722 (16)	0.1826 (15)	0.11 (2)*	0.15
F4B	0.2163 (13)	0.2677 (6)	0.1874 (6)	0.184 (6)	0.15
F5B	0.1686 (18)	0.4546 (16)	0.2361 (11)	0.119 (7)*	0.15
F6B	0.305 (2)	0.386 (3)	0.135 (2)	0.202 (16)*	0.15
P3	0.7881 (5)	0.1575 (5)	0.3563 (5)	0.128 (2)	0.6
F13	0.8969 (18)	0.0396 (15)	0.3758 (12)	0.217 (8)*	0.6
F14	0.6805 (14)	0.2834 (12)	0.3404 (10)	0.179 (5)*	0.6
F15	0.750 (2)	0.1998 (19)	0.4445 (15)	0.246 (11)*	0.6
F16	0.8041 (9)	0.1167 (9)	0.2766 (6)	0.118 (3)*	0.6
F17	0.8940 (9)	0.2015 (8)	0.3482 (6)	0.104 (3)*	0.6
F18	0.6711 (10)	0.1305 (9)	0.3665 (7)	0.132 (3)*	0.6
S3	0.8416 (13)	0.1643 (19)	0.3200 (9)	0.319 (15)	0.4
O7	0.7946 (16)	0.1717 (15)	0.2465 (10)	0.110 (5)*	0.4
O8	0.8867 (18)	0.2320 (15)	0.3144 (12)	0.112 (6)*	0.4
O9	0.914 (2)	0.0664 (19)	0.3175 (14)	0.142 (7)*	0.4
C55	0.712 (3)	0.188 (3)	0.3978 (18)	0.102 (7)*	0.4
F7A	0.7831 (18)	0.1487 (17)	0.4649 (11)	0.137 (6)*	0.4
F8A	0.6929 (15)	0.0853 (13)	0.4124 (10)	0.128 (5)*	0.4
F9A	0.6562 (14)	0.2606 (13)	0.3942 (9)	0.108 (4)*	0.4

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.02331 (9)	0.02233 (9)	0.03010 (9)	−0.00691 (6)	−0.00328 (6)	−0.00339 (6)
Co1	0.0280 (3)	0.0628 (4)	0.0456 (4)	−0.0115 (3)	−0.0106 (3)	−0.0057 (3)
Co2	0.0273 (3)	0.0622 (4)	0.0283 (3)	−0.0163 (3)	−0.0031 (2)	−0.0089 (3)
Fe1	0.0478 (5)	0.0529 (5)	0.0876 (6)	−0.0211 (4)	−0.0017 (4)	−0.0362 (4)
Fe2	0.0494 (4)	0.0345 (4)	0.0410 (4)	−0.0178 (3)	0.0018 (3)	0.0057 (3)
N1	0.041 (2)	0.0247 (19)	0.045 (2)	−0.0096 (16)	0.0007 (17)	−0.0080 (16)
N2	0.064 (3)	0.025 (2)	0.057 (3)	−0.011 (2)	−0.002 (2)	−0.0044 (18)
N3	0.063 (3)	0.026 (2)	0.046 (2)	−0.005 (2)	−0.008 (2)	0.0018 (17)
N4	0.036 (2)	0.0230 (18)	0.040 (2)	−0.0055 (15)	0.0024 (16)	−0.0015 (15)
N5	0.062 (3)	0.026 (2)	0.055 (3)	−0.007 (2)	0.012 (2)	−0.0004 (18)
N6	0.056 (3)	0.025 (2)	0.051 (3)	0.0006 (19)	0.006 (2)	−0.0030 (18)
C1	0.095 (6)	0.093 (6)	0.095 (6)	−0.041 (5)	0.038 (5)	−0.047 (5)
C2	0.100 (6)	0.115 (7)	0.082 (6)	−0.039 (6)	−0.006 (5)	−0.048 (5)
C3	0.122 (9)	0.121 (8)	0.155 (10)	−0.064 (7)	0.011 (8)	−0.093 (8)

C4	0.124 (8)	0.060 (5)	0.152 (10)	−0.034 (5)	0.022 (7)	−0.057 (6)
C5	0.072 (5)	0.074 (5)	0.100 (6)	0.003 (4)	0.008 (4)	−0.054 (5)
C6	0.064 (4)	0.043 (3)	0.067 (4)	−0.025 (3)	−0.012 (3)	−0.011 (3)
C7	0.048 (3)	0.053 (4)	0.106 (5)	−0.012 (3)	−0.023 (3)	−0.022 (4)
C8	0.046 (4)	0.061 (4)	0.137 (7)	−0.024 (3)	−0.004 (4)	−0.024 (4)
C9	0.043 (3)	0.046 (3)	0.095 (5)	−0.019 (3)	0.015 (3)	−0.017 (3)
C10	0.040 (3)	0.031 (2)	0.063 (3)	−0.011 (2)	0.000 (2)	−0.017 (2)
C11	0.033 (2)	0.025 (2)	0.034 (2)	−0.0079 (18)	0.0008 (18)	−0.0062 (17)
C12	0.045 (3)	0.023 (2)	0.038 (2)	−0.0051 (19)	−0.004 (2)	−0.0018 (18)
C13	0.047 (3)	0.031 (2)	0.039 (3)	−0.003 (2)	−0.017 (2)	0.0025 (19)
C14	0.060 (4)	0.041 (3)	0.075 (4)	0.000 (3)	−0.038 (3)	0.001 (3)
C15	0.064 (4)	0.058 (4)	0.066 (4)	−0.010 (3)	−0.044 (3)	0.008 (3)
C16	0.066 (4)	0.047 (3)	0.040 (3)	−0.021 (3)	−0.020 (2)	0.001 (2)
C17	0.043 (3)	0.037 (3)	0.038 (3)	−0.011 (2)	−0.005 (2)	0.002 (2)
C18	0.084 (5)	0.197 (10)	0.036 (3)	−0.104 (6)	−0.002 (3)	−0.003 (4)
C19	0.065 (4)	0.165 (8)	0.077 (5)	−0.068 (5)	0.025 (4)	−0.062 (5)
C20	0.046 (4)	0.135 (7)	0.072 (4)	−0.050 (4)	0.009 (3)	−0.034 (4)
C21	0.061 (4)	0.119 (6)	0.059 (4)	−0.057 (4)	−0.006 (3)	0.015 (4)
C22	0.071 (4)	0.148 (8)	0.052 (4)	−0.069 (5)	−0.027 (3)	0.044 (5)
C23	0.097 (5)	0.032 (3)	0.075 (4)	−0.004 (3)	−0.028 (4)	0.017 (3)
C31	0.083 (5)	0.081 (5)	0.071 (4)	−0.044 (4)	−0.029 (4)	0.034 (4)
C32	0.108 (6)	0.057 (4)	0.043 (3)	−0.040 (4)	−0.014 (3)	0.017 (3)
C33	0.083 (4)	0.056 (4)	0.053 (3)	−0.030 (3)	0.001 (3)	0.019 (3)
C34	0.086 (5)	0.042 (3)	0.068 (4)	−0.028 (3)	−0.010 (3)	0.018 (3)
C35	0.069 (4)	0.055 (4)	0.072 (4)	−0.006 (3)	−0.011 (3)	0.025 (3)
C36	0.041 (3)	0.028 (2)	0.035 (2)	−0.0117 (19)	0.0022 (19)	0.0032 (18)
C37	0.047 (3)	0.037 (3)	0.039 (3)	−0.008 (2)	0.006 (2)	−0.002 (2)
C38	0.039 (3)	0.058 (3)	0.048 (3)	−0.018 (2)	0.009 (2)	0.003 (2)
C39	0.046 (3)	0.044 (3)	0.049 (3)	−0.023 (2)	−0.001 (2)	0.001 (2)
C40	0.036 (2)	0.028 (2)	0.036 (2)	−0.0107 (19)	0.0014 (19)	0.0015 (18)
C41	0.023 (2)	0.029 (2)	0.035 (2)	−0.0087 (17)	−0.0050 (17)	−0.0006 (17)
C42	0.030 (2)	0.027 (2)	0.039 (2)	−0.0018 (18)	−0.0017 (18)	−0.0031 (18)
C43	0.032 (2)	0.037 (2)	0.038 (2)	−0.0072 (19)	−0.0015 (19)	−0.0084 (19)
C44	0.039 (3)	0.048 (3)	0.052 (3)	0.000 (2)	0.004 (2)	−0.013 (2)
C45	0.046 (3)	0.067 (4)	0.043 (3)	−0.018 (3)	0.013 (2)	−0.022 (3)
C46	0.051 (3)	0.068 (3)	0.029 (2)	−0.029 (3)	−0.007 (2)	−0.010 (2)
C47	0.033 (2)	0.044 (3)	0.031 (2)	−0.015 (2)	−0.0095 (18)	−0.0068 (19)
C48	0.055 (3)	0.111 (5)	0.038 (3)	−0.049 (4)	−0.001 (3)	−0.021 (3)
C49	0.046 (3)	0.124 (6)	0.051 (3)	−0.040 (4)	−0.019 (3)	−0.006 (4)
C50	0.044 (3)	0.118 (6)	0.047 (3)	−0.047 (4)	0.005 (2)	−0.021 (3)
C51	0.060 (4)	0.086 (5)	0.053 (3)	−0.047 (4)	0.001 (3)	−0.011 (3)
C52	0.055 (3)	0.081 (4)	0.054 (3)	−0.041 (3)	0.006 (3)	−0.028 (3)
C53	0.107 (6)	0.024 (3)	0.077 (4)	0.002 (3)	0.021 (4)	−0.009 (3)
P1	0.089 (5)	0.035 (3)	0.048 (4)	0.016 (3)	0.030 (3)	0.011 (2)
S1	0.122 (5)	0.057 (3)	0.078 (5)	−0.005 (3)	0.026 (3)	0.008 (3)
S1B	0.122 (5)	0.057 (3)	0.078 (5)	−0.005 (3)	0.026 (3)	0.008 (3)
S2	0.0739 (17)	0.0406 (13)	0.0530 (14)	−0.0293 (12)	0.0118 (11)	−0.0005 (10)
O4	0.077 (5)	0.134 (9)	0.069 (5)	−0.062 (6)	−0.025 (4)	0.014 (5)

O5	0.159 (11)	0.118 (8)	0.082 (6)	−0.055 (8)	0.066 (7)	−0.052 (6)
O6	0.093 (8)	0.062 (6)	0.162 (15)	−0.021 (5)	−0.079 (10)	0.041 (7)
C54	0.189 (17)	0.039 (6)	0.099 (10)	−0.059 (9)	0.044 (10)	−0.010 (7)
F4A	0.239 (13)	0.198 (11)	0.284 (14)	−0.170 (11)	0.147 (11)	−0.125 (10)
F5A	0.181 (8)	0.096 (5)	0.107 (5)	−0.062 (5)	0.028 (5)	−0.038 (4)
F6A	0.301 (16)	0.062 (4)	0.148 (8)	−0.050 (7)	0.009 (8)	0.031 (5)
O5B	0.181 (8)	0.096 (5)	0.107 (5)	−0.062 (5)	0.028 (5)	−0.038 (4)
O6B	0.239 (13)	0.198 (11)	0.284 (14)	−0.170 (11)	0.147 (11)	−0.125 (10)
F4B	0.301 (16)	0.062 (4)	0.148 (8)	−0.050 (7)	0.009 (8)	0.031 (5)
P3	0.084 (3)	0.150 (5)	0.165 (5)	−0.049 (3)	−0.013 (3)	−0.093 (4)
S3	0.182 (11)	0.64 (4)	0.252 (14)	−0.287 (18)	0.144 (11)	−0.35 (2)

Geometric parameters (Å, º)

Au1—C41	2.021 (4)	C31—C32	1.394 (10)
Au1—C11	2.030 (4)	C31—C35	1.419 (10)
Co1—C14	2.014 (6)	C31—H31	0.9500
Co1—C15	2.021 (5)	C32—C33	1.413 (9)
Co1—C18	2.023 (6)	C32—H32	0.9500
Co1—C20	2.024 (6)	C33—C34	1.413 (9)
Co1—C17	2.025 (5)	C33—H33	0.9500
Co1—C21	2.025 (7)	C34—C35	1.415 (10)
Co1—C16	2.028 (5)	C34—H34	0.9500
Co1—C22	2.030 (7)	C35—H35	0.9500
Co1—C19	2.032 (6)	C36—C40	1.413 (6)
Co1—C13	2.033 (5)	C36—C37	1.422 (7)
Co2—C46	2.018 (5)	C36—H36	0.9500
Co2—C49	2.018 (5)	C37—C38	1.411 (8)
Co2—C50	2.022 (5)	C37—H37	0.9500
Co2—C45	2.022 (5)	C38—C39	1.425 (7)
Co2—C47	2.024 (4)	C38—H38	0.9500
Co2—C48	2.025 (5)	C39—C40	1.423 (7)
Co2—C44	2.035 (6)	C39—H39	0.9500
Co2—C51	2.037 (6)	C41—C42	1.384 (6)
Co2—C52	2.042 (6)	C42—C43	1.464 (6)
Co2—C43	2.048 (5)	C43—C47	1.423 (7)
Fe1—C10	2.021 (5)	C43—C44	1.433 (7)
Fe1—C1	2.025 (7)	C44—C45	1.405 (8)
Fe1—C6	2.027 (5)	C44—H44	0.9500
Fe1—C5	2.031 (7)	C45—C46	1.401 (8)
Fe1—C2	2.033 (8)	C45—H45	0.9500
Fe1—C8	2.037 (7)	C46—C47	1.411 (7)
Fe1—C7	2.041 (6)	C46—H46	0.9500
Fe1—C3	2.043 (8)	C47—H47	0.9500
Fe1—C9	2.050 (7)	C48—C52	1.411 (9)
Fe1—C4	2.054 (8)	C48—C49	1.415 (9)
Fe2—C40	2.016 (4)	C48—H48	0.9500
Fe2—C33	2.027 (5)	C49—C50	1.413 (9)

Fe2—C32	2.036 (6)	C49—H49	0.9500
Fe2—C34	2.038 (5)	C50—C51	1.419 (9)
Fe2—C39	2.041 (5)	C50—H50	0.9500
Fe2—C31	2.043 (7)	C51—C52	1.425 (8)
Fe2—C36	2.046 (4)	C51—H51	0.9500
Fe2—C35	2.047 (6)	C52—H52	0.9500
Fe2—C38	2.047 (6)	C53—H53A	0.9800
Fe2—C37	2.051 (5)	C53—H53B	0.9800
N1—N2	1.337 (6)	C53—H53C	0.9800
N1—C11	1.371 (6)	P1—F2	1.409 (14)
N1—C10	1.412 (7)	P1—F3	1.476 (16)
N2—N3	1.307 (7)	P1—F6	1.594 (12)
N3—C12	1.354 (6)	P1—F4	1.67 (3)
N3—C23	1.476 (7)	P1—F5	1.726 (17)
N4—N5	1.330 (5)	P1—F1	1.896 (19)
N4—C41	1.372 (6)	S1—O2A	1.39 (3)
N4—C40	1.426 (6)	S1—O3A	1.510 (18)
N5—N6	1.315 (6)	S1—O1A	1.69 (4)
N6—C42	1.360 (6)	S1—C53A	1.72 (3)
N6—C53	1.476 (6)	O1A—O2A	1.43 (4)
C1—C5	1.405 (12)	C53A—F3A	1.14 (3)
C1—C2	1.446 (12)	C53A—F1A	1.22 (3)
C1—H1	0.9500	C53A—F2A	1.48 (3)
C2—C3	1.392 (15)	S1B—O1B	1.411 (14)
C2—H2	0.9500	S1B—O2B	1.43 (2)
C3—C4	1.400 (15)	S1B—O3B	1.66 (2)
C3—H3	0.9500	S1B—C53B	1.80 (2)
C4—C5	1.369 (13)	C53B—F3B	1.21 (2)
C4—H4	0.9500	C53B—F1B	1.30 (3)
C5—H5	0.9500	C53B—F2B	1.36 (3)
C6—C10	1.404 (8)	P2—F8	1.55 (2)
C6—C7	1.428 (8)	P2—F10	1.57 (2)
C6—H6	0.9500	P2—F12	1.61 (3)
C7—C8	1.414 (11)	P2—F9	1.61 (2)
C7—H7	0.9500	P2—F11	1.62 (3)
C8—C9	1.395 (10)	P2—F7	1.655 (18)
C8—H8	0.9500	S2—O6	1.351 (12)
C9—C10	1.420 (8)	S2—O4	1.382 (8)
C9—H9	0.9500	S2—O5	1.427 (8)
C11—C12	1.375 (6)	S2—C54	1.777 (10)
C12—C13	1.463 (7)	C54—F4A	1.290 (14)
C13—C17	1.421 (7)	C54—F6A	1.309 (14)
C13—C14	1.432 (7)	C54—F5A	1.319 (12)
C14—C15	1.412 (9)	S2B—O5B	1.452 (16)
C14—H14	0.9500	S2B—O6B	1.585 (17)
C15—C16	1.418 (8)	S2B—O4B	1.66 (5)
C15—H15	0.9500	S2B—C54B	1.69 (2)
C16—C17	1.419 (7)	C54B—F6B	1.389 (19)

C16—H16	0.9500	C54B—F5B	1.399 (18)
C17—H17	0.9500	C54B—F4B	1.412 (18)
C18—C22	1.400 (12)	P3—F16	1.486 (12)
C18—C19	1.423 (11)	P3—F18	1.590 (13)
C18—H18	0.9500	P3—F15	1.61 (3)
C19—C20	1.428 (10)	P3—F17	1.615 (11)
C19—H19	0.9500	P3—F13	1.69 (2)
C20—C21	1.412 (11)	P3—F14	1.740 (16)
C20—H20	0.9500	S3—O8	1.26 (2)
C21—C22	1.410 (9)	S3—O9	1.28 (3)
C21—H21	0.9500	S3—O7	1.46 (2)
C22—H22	0.9500	S3—C55	1.84 (3)
C23—H23A	0.9800	C55—F9A	0.96 (3)
C23—H23B	0.9800	C55—F7A	1.50 (4)
C23—H23C	0.9800	C55—F8A	1.54 (3)

C41—Au1—C11	173.35 (17)	C17—C16—H16	126.2
C14—Co1—C15	41.0 (2)	Co1—C16—H16	126.7
C14—Co1—C18	123.1 (4)	C16—C17—C13	108.7 (4)
C15—Co1—C18	159.1 (4)	C16—C17—Co1	69.6 (3)
C14—Co1—C20	124.3 (3)	C13—C17—Co1	69.8 (3)
C15—Co1—C20	107.4 (3)	C16—C17—H17	125.7
C18—Co1—C20	68.6 (3)	C13—C17—H17	125.7
C14—Co1—C17	69.3 (2)	Co1—C17—H17	126.5
C15—Co1—C17	68.9 (2)	C22—C18—C19	109.2 (6)
C18—Co1—C17	123.2 (2)	C22—C18—Co1	70.0 (4)
C20—Co1—C17	156.2 (3)	C19—C18—Co1	69.8 (4)
C14—Co1—C21	160.4 (3)	C22—C18—H18	125.4
C15—Co1—C21	123.0 (3)	C19—C18—H18	125.4
C18—Co1—C21	68.3 (3)	Co1—C18—H18	126.4
C20—Co1—C21	40.8 (3)	C18—C19—C20	106.3 (8)
C17—Co1—C21	120.1 (3)	C18—C19—Co1	69.1 (4)
C14—Co1—C16	69.3 (2)	C20—C19—Co1	69.1 (4)
C15—Co1—C16	41.0 (2)	C18—C19—H19	126.8
C18—Co1—C16	158.9 (3)	C20—C19—H19	126.8
C20—Co1—C16	120.8 (3)	Co1—C19—H19	126.5
C17—Co1—C16	41.0 (2)	C21—C20—C19	108.3 (6)
C21—Co1—C16	105.6 (3)	C21—C20—Co1	69.6 (4)
C14—Co1—C22	158.0 (3)	C19—C20—Co1	69.7 (4)
C15—Co1—C22	159.1 (3)	C21—C20—H20	125.8
C18—Co1—C22	40.4 (3)	C19—C20—H20	125.8
C20—Co1—C22	68.6 (3)	Co1—C20—H20	126.4
C17—Co1—C22	106.0 (3)	C22—C21—C20	108.2 (8)
C21—Co1—C22	40.7 (3)	C22—C21—Co1	69.8 (4)
C16—Co1—C22	122.0 (3)	C20—C21—Co1	69.6 (4)
C14—Co1—C19	108.0 (4)	C22—C21—H21	125.9
C15—Co1—C19	122.4 (3)	C20—C21—H21	125.9
C18—Co1—C19	41.1 (3)	Co1—C21—H21	126.3

C20—Co1—C19	41.2 (3)	C18—C22—C21	107.9 (7)
C17—Co1—C19	160.5 (2)	C18—C22—Co1	69.6 (4)
C21—Co1—C19	69.1 (4)	C21—C22—Co1	69.5 (4)
C16—Co1—C19	157.6 (3)	C18—C22—H22	126.0
C22—Co1—C19	69.0 (4)	C21—C22—H22	126.0
C14—Co1—C13	41.5 (2)	Co1—C22—H22	126.5
C15—Co1—C13	69.2 (2)	N3—C23—H23A	109.5
C18—Co1—C13	107.7 (2)	N3—C23—H23B	109.5
C20—Co1—C13	161.7 (3)	H23A—C23—H23B	109.5
C17—Co1—C13	41.01 (19)	N3—C23—H23C	109.5
C21—Co1—C13	156.2 (2)	H23A—C23—H23C	109.5
C16—Co1—C13	69.3 (2)	H23B—C23—H23C	109.5
C22—Co1—C13	121.0 (2)	C32—C31—C35	108.8 (6)
C19—Co1—C13	124.3 (3)	C32—C31—Fe2	69.7 (4)
C46—Co2—C49	155.6 (2)	C35—C31—Fe2	69.8 (4)
C46—Co2—C50	119.1 (2)	C32—C31—H31	125.6
C49—Co2—C50	41.0 (3)	C35—C31—H31	125.6
C46—Co2—C45	40.6 (2)	Fe2—C31—H31	126.4
C49—Co2—C45	121.4 (3)	C31—C32—C33	107.8 (6)
C50—Co2—C45	105.9 (2)	C31—C32—Fe2	70.3 (4)
C46—Co2—C47	40.87 (19)	C33—C32—Fe2	69.3 (4)
C49—Co2—C47	162.6 (2)	C31—C32—H32	126.1
C50—Co2—C47	155.1 (2)	C33—C32—H32	126.1
C45—Co2—C47	68.4 (2)	Fe2—C32—H32	125.8
C46—Co2—C48	160.5 (3)	C32—C33—C34	108.3 (6)
C49—Co2—C48	41.0 (3)	C32—C33—Fe2	70.0 (3)
C50—Co2—C48	68.7 (2)	C34—C33—Fe2	70.1 (3)
C45—Co2—C48	158.4 (3)	C32—C33—H33	125.8
C47—Co2—C48	125.2 (2)	C34—C33—H33	125.8
C46—Co2—C44	68.5 (2)	Fe2—C33—H33	125.7
C49—Co2—C44	108.6 (3)	C33—C34—C35	107.7 (6)
C50—Co2—C44	123.7 (3)	C33—C34—Fe2	69.3 (3)
C45—Co2—C44	40.5 (2)	C35—C34—Fe2	70.1 (3)
C47—Co2—C44	68.7 (2)	C33—C34—H34	126.2
C48—Co2—C44	123.9 (3)	C35—C34—H34	126.2
C46—Co2—C51	104.6 (2)	Fe2—C34—H34	126.1
C49—Co2—C51	69.1 (3)	C34—C35—C31	107.4 (6)
C50—Co2—C51	40.9 (3)	C34—C35—Fe2	69.4 (4)
C45—Co2—C51	121.6 (2)	C31—C35—Fe2	69.6 (4)
C47—Co2—C51	119.8 (2)	C34—C35—H35	126.3
C48—Co2—C51	68.8 (3)	C31—C35—H35	126.3
C44—Co2—C51	159.1 (2)	Fe2—C35—H35	126.3
C46—Co2—C52	122.7 (3)	C40—C36—C37	106.6 (4)
C49—Co2—C52	68.7 (3)	C40—C36—Fe2	68.5 (3)
C50—Co2—C52	68.6 (3)	C37—C36—Fe2	69.9 (3)
C45—Co2—C52	158.8 (3)	C40—C36—H36	126.7
C47—Co2—C52	107.4 (2)	C37—C36—H36	126.7
C48—Co2—C52	40.6 (3)	Fe2—C36—H36	126.5

C44—Co2—C52	159.3 (2)	C38—C37—C36	108.4 (4)
C51—Co2—C52	40.9 (2)	C38—C37—Fe2	69.7 (3)
C46—Co2—C43	68.9 (2)	C36—C37—Fe2	69.5 (3)
C49—Co2—C43	125.8 (2)	C38—C37—H37	125.8
C50—Co2—C43	161.8 (3)	C36—C37—H37	125.8
C45—Co2—C43	68.7 (2)	Fe2—C37—H37	126.6
C47—Co2—C43	40.89 (19)	C37—C38—C39	109.0 (4)
C48—Co2—C43	109.5 (2)	C37—C38—Fe2	70.0 (3)
C44—Co2—C43	41.10 (19)	C39—C38—Fe2	69.4 (3)
C51—Co2—C43	156.8 (2)	C37—C38—H38	125.5
C52—Co2—C43	122.7 (2)	C39—C38—H38	125.5
C10—Fe1—C1	122.1 (3)	Fe2—C38—H38	126.7
C10—Fe1—C6	40.6 (2)	C40—C39—C38	105.8 (5)
C1—Fe1—C6	110.1 (3)	C40—C39—Fe2	68.5 (3)
C10—Fe1—C5	109.9 (3)	C38—C39—Fe2	69.8 (3)
C1—Fe1—C5	40.5 (4)	C40—C39—H39	127.1
C6—Fe1—C5	128.9 (3)	C38—C39—H39	127.1
C10—Fe1—C2	157.7 (4)	Fe2—C39—H39	126.1
C1—Fe1—C2	41.7 (4)	C36—C40—C39	110.1 (4)
C6—Fe1—C2	122.1 (4)	C36—C40—N4	124.8 (4)
C5—Fe1—C2	68.2 (4)	C39—C40—N4	124.5 (4)
C10—Fe1—C8	67.6 (3)	C36—C40—Fe2	70.8 (3)
C1—Fe1—C8	164.6 (4)	C39—C40—Fe2	70.4 (3)
C6—Fe1—C8	68.6 (3)	N4—C40—Fe2	132.0 (3)
C5—Fe1—C8	152.1 (4)	N4—C41—C42	101.7 (4)
C2—Fe1—C8	124.9 (4)	N4—C41—Au1	125.9 (3)
C10—Fe1—C7	68.1 (2)	C42—C41—Au1	131.4 (3)
C1—Fe1—C7	128.4 (4)	N6—C42—C41	107.6 (4)
C6—Fe1—C7	41.1 (2)	N6—C42—C43	123.5 (4)
C5—Fe1—C7	166.7 (4)	C41—C42—C43	128.8 (4)
C2—Fe1—C7	108.3 (4)	C47—C43—C44	106.6 (4)
C8—Fe1—C7	40.6 (3)	C47—C43—C42	125.0 (4)
C10—Fe1—C3	161.6 (5)	C44—C43—C42	128.5 (5)
C1—Fe1—C3	68.4 (4)	C47—C43—Co2	68.6 (3)
C6—Fe1—C3	155.1 (5)	C44—C43—Co2	69.0 (3)
C5—Fe1—C3	67.2 (4)	C42—C43—Co2	127.1 (3)
C2—Fe1—C3	39.9 (4)	C45—C44—C43	108.1 (5)
C8—Fe1—C3	106.0 (4)	C45—C44—Co2	69.2 (3)
C7—Fe1—C3	119.0 (4)	C43—C44—Co2	69.9 (3)
C10—Fe1—C9	40.8 (2)	C45—C44—H44	126.0
C1—Fe1—C9	155.2 (4)	C43—C44—H44	126.0
C6—Fe1—C9	68.9 (2)	Co2—C44—H44	126.5
C5—Fe1—C9	119.6 (3)	C46—C45—C44	108.7 (4)
C2—Fe1—C9	160.3 (4)	C46—C45—Co2	69.5 (3)
C8—Fe1—C9	39.9 (3)	C44—C45—Co2	70.2 (3)
C7—Fe1—C9	68.2 (3)	C46—C45—H45	125.6
C3—Fe1—C9	123.4 (4)	C44—C45—H45	125.6
C10—Fe1—C4	126.4 (4)	Co2—C45—H45	126.2

C1—Fe1—C4	67.4 (4)	C45—C46—C47	108.0 (5)
C6—Fe1—C4	164.2 (4)	C45—C46—Co2	69.9 (3)
C5—Fe1—C4	39.2 (4)	C47—C46—Co2	69.8 (3)
C2—Fe1—C4	67.2 (5)	C45—C46—H46	126.0
C8—Fe1—C4	118.2 (4)	C47—C46—H46	126.0
C7—Fe1—C4	152.7 (4)	Co2—C46—H46	125.9
C3—Fe1—C4	40.0 (4)	C46—C47—C43	108.6 (4)
C9—Fe1—C4	106.5 (4)	C46—C47—Co2	69.3 (3)
C40—Fe2—C33	163.2 (2)	C43—C47—Co2	70.5 (3)
C40—Fe2—C32	156.0 (2)	C46—C47—H47	125.7
C33—Fe2—C32	40.7 (3)	C43—C47—H47	125.7
C40—Fe2—C34	128.2 (2)	Co2—C47—H47	126.0
C33—Fe2—C34	40.7 (3)	C52—C48—C49	108.4 (5)
C32—Fe2—C34	68.4 (3)	C52—C48—Co2	70.4 (3)
C40—Fe2—C39	41.05 (19)	C49—C48—Co2	69.3 (3)
C33—Fe2—C39	123.9 (3)	C52—C48—H48	125.8
C32—Fe2—C39	159.8 (3)	C49—C48—H48	125.8
C34—Fe2—C39	108.4 (3)	Co2—C48—H48	126.2
C40—Fe2—C31	123.9 (2)	C50—C49—C48	107.7 (6)
C33—Fe2—C31	67.7 (3)	C50—C49—Co2	69.7 (3)
C32—Fe2—C31	40.0 (3)	C48—C49—Co2	69.8 (3)
C34—Fe2—C31	68.1 (3)	C50—C49—H49	126.2
C39—Fe2—C31	159.2 (3)	C48—C49—H49	126.2
C40—Fe2—C36	40.72 (18)	Co2—C49—H49	126.0
C33—Fe2—C36	152.9 (2)	C49—C50—C51	108.6 (5)
C32—Fe2—C36	118.9 (2)	C49—C50—Co2	69.4 (3)
C34—Fe2—C36	165.2 (2)	C51—C50—Co2	70.1 (3)
C39—Fe2—C36	69.3 (2)	C49—C50—H50	125.7
C31—Fe2—C36	108.5 (2)	C51—C50—H50	125.7
C40—Fe2—C35	111.7 (2)	Co2—C50—H50	126.4
C33—Fe2—C35	68.2 (3)	C50—C51—C52	107.2 (6)
C32—Fe2—C35	68.1 (3)	C50—C51—Co2	69.0 (4)
C34—Fe2—C35	40.5 (3)	C52—C51—Co2	69.8 (3)
C39—Fe2—C35	123.4 (3)	C50—C51—H51	126.4
C31—Fe2—C35	40.6 (3)	C52—C51—H51	126.4
C36—Fe2—C35	127.6 (2)	Co2—C51—H51	126.4
C40—Fe2—C38	67.98 (19)	C48—C52—C51	108.1 (6)
C33—Fe2—C38	105.2 (3)	C48—C52—Co2	69.0 (4)
C32—Fe2—C38	122.1 (3)	C51—C52—Co2	69.3 (3)
C34—Fe2—C38	120.2 (3)	C48—C52—H52	125.9
C39—Fe2—C38	40.8 (2)	C51—C52—H52	125.9
C31—Fe2—C38	159.2 (3)	Co2—C52—H52	127.2
C36—Fe2—C38	68.3 (2)	N6—C53—H53A	109.5
C35—Fe2—C38	157.0 (3)	N6—C53—H53B	109.5
C40—Fe2—C37	67.96 (18)	H53A—C53—H53B	109.5
C33—Fe2—C37	117.5 (2)	N6—C53—H53C	109.5
C32—Fe2—C37	104.7 (2)	H53A—C53—H53C	109.5
C34—Fe2—C37	153.5 (2)	H53B—C53—H53C	109.5

C39—Fe2—C37	68.7 (2)	F2—P1—F3	102.4 (10)
C31—Fe2—C37	124.0 (3)	F2—P1—F6	103.1 (8)
C36—Fe2—C37	40.61 (19)	F3—P1—F6	106.3 (9)
C35—Fe2—C37	162.6 (3)	F2—P1—F4	94.0 (11)
C38—Fe2—C37	40.3 (2)	F3—P1—F4	158.9 (14)
N2—N1—C11	113.9 (4)	F6—P1—F4	82.3 (10)
N2—N1—C10	117.0 (4)	F2—P1—F5	96.1 (7)
C11—N1—C10	129.0 (4)	F3—P1—F5	80.3 (8)
N3—N2—N1	103.6 (4)	F6—P1—F5	157.6 (11)
N2—N3—C12	112.5 (4)	F4—P1—F5	85.0 (11)
N2—N3—C23	117.9 (5)	F2—P1—F1	163.8 (10)
C12—N3—C23	129.5 (5)	F3—P1—F1	88.3 (8)
N5—N4—C41	115.1 (4)	F6—P1—F1	85.0 (7)
N5—N4—C40	118.8 (4)	F4—P1—F1	73.0 (11)
C41—N4—C40	125.8 (4)	F5—P1—F1	73.6 (8)
N6—N5—N4	103.2 (4)	O2A—S1—O3A	102.1 (13)
N5—N6—C42	112.4 (4)	O2A—S1—O1A	54.4 (16)
N5—N6—C53	117.8 (5)	O3A—S1—O1A	84.4 (13)
C42—N6—C53	129.3 (5)	O2A—S1—C53A	117.5 (14)
C5—C1—C2	106.2 (9)	O3A—S1—C53A	109.2 (13)
C5—C1—Fe1	69.9 (4)	O1A—S1—C53A	76.2 (16)
C2—C1—Fe1	69.4 (5)	O2A—O1A—S1	52.0 (16)
C5—C1—H1	126.9	S1—O2A—O1A	73.6 (19)
C2—C1—H1	126.9	F3A—C53A—F1A	116 (2)
Fe1—C1—H1	125.3	F3A—C53A—F2A	107 (2)
C3—C2—C1	107.4 (10)	F1A—C53A—F2A	98 (2)
C3—C2—Fe1	70.4 (5)	F3A—C53A—S1	103.9 (19)
C1—C2—Fe1	68.8 (4)	F1A—C53A—S1	122 (2)
C3—C2—H2	126.3	F2A—C53A—S1	107.7 (17)
C1—C2—H2	126.3	O1B—S1B—O2B	97.3 (10)
Fe1—C2—H2	126.0	O1B—S1B—O3B	85.0 (10)
C2—C3—C4	108.2 (10)	O2B—S1B—O3B	100.1 (12)
C2—C3—Fe1	69.7 (5)	O1B—S1B—C53B	119.1 (10)
C4—C3—Fe1	70.4 (5)	O2B—S1B—C53B	125.5 (12)
C2—C3—H3	125.9	O3B—S1B—C53B	120.8 (10)
C4—C3—H3	125.9	F3B—C53B—F1B	107 (2)
Fe1—C3—H3	125.6	F3B—C53B—F2B	98 (2)
C5—C4—C3	108.9 (11)	F1B—C53B—F2B	103 (2)
C5—C4—Fe1	69.5 (5)	F3B—C53B—S1B	104.7 (16)
C3—C4—Fe1	69.6 (6)	F1B—C53B—S1B	122.3 (17)
C5—C4—H4	125.5	F2B—C53B—S1B	118.6 (19)
C3—C4—H4	125.5	F8—P2—F10	117.8 (16)
Fe1—C4—H4	127.0	F8—P2—F12	85.8 (18)
C4—C5—C1	109.3 (10)	F10—P2—F12	87.5 (18)
C4—C5—Fe1	71.3 (5)	F8—P2—F9	70.3 (15)
C1—C5—Fe1	69.5 (5)	F10—P2—F9	171.9 (18)
C4—C5—H5	125.4	F12—P2—F9	93.5 (18)
C1—C5—H5	125.4	F8—P2—F11	102 (2)

Fe1—C5—H5	125.4	F10—P2—F11	106 (2)
C10—C6—C7	106.8 (6)	F12—P2—F11	158 (2)
C10—C6—Fe1	69.5 (3)	F9—P2—F11	71 (2)
C7—C6—Fe1	70.0 (3)	F8—P2—F7	153.4 (13)
C10—C6—H6	126.6	F10—P2—F7	88.4 (14)
C7—C6—H6	126.6	F12—P2—F7	91.5 (17)
Fe1—C6—H6	125.5	F9—P2—F7	83.5 (15)
C8—C7—C6	107.4 (6)	F11—P2—F7	72.0 (18)
C8—C7—Fe1	69.5 (4)	O6—S2—O4	116.2 (9)
C6—C7—Fe1	68.9 (3)	O6—S2—O5	110.8 (10)
C8—C7—H7	126.3	O4—S2—O5	118.9 (8)
C6—C7—H7	126.3	O6—S2—C54	100.0 (8)
Fe1—C7—H7	126.8	O4—S2—C54	107.8 (7)
C9—C8—C7	109.5 (6)	O5—S2—C54	99.7 (6)
C9—C8—Fe1	70.6 (4)	F4A—C54—F6A	112.0 (12)
C7—C8—Fe1	69.9 (4)	F4A—C54—F5A	105.7 (12)
C9—C8—H8	125.3	F6A—C54—F5A	112.3 (11)
C7—C8—H8	125.3	F4A—C54—S2	108.2 (8)
Fe1—C8—H8	125.9	F6A—C54—S2	107.8 (9)
C8—C9—C10	106.7 (6)	F5A—C54—S2	110.9 (7)
C8—C9—Fe1	69.5 (4)	O5B—S2B—O6B	86.3 (10)
C10—C9—Fe1	68.5 (3)	O5B—S2B—O4B	126.8 (16)
C8—C9—H9	126.7	O6B—S2B—O4B	130.5 (18)
C10—C9—H9	126.7	O5B—S2B—C54B	98.0 (12)
Fe1—C9—H9	126.8	O6B—S2B—C54B	92.5 (13)
C6—C10—N1	125.1 (5)	O4B—S2B—C54B	114.0 (19)
C6—C10—C9	109.6 (5)	F6B—C54B—F5B	103 (2)
N1—C10—C9	125.2 (5)	F6B—C54B—F4B	115 (2)
C6—C10—Fe1	69.9 (3)	F5B—C54B—F4B	134 (2)
N1—C10—Fe1	128.5 (3)	F6B—C54B—S2B	96.7 (19)
C9—C10—Fe1	70.7 (3)	F5B—C54B—S2B	109.1 (18)
N1—C11—C12	102.5 (4)	F4B—C54B—S2B	91.8 (14)
N1—C11—Au1	127.2 (3)	F16—P3—F18	81.9 (6)
C12—C11—Au1	129.9 (3)	F16—P3—F15	170.7 (11)
N3—C12—C11	107.5 (4)	F18—P3—F15	88.8 (11)
N3—C12—C13	122.6 (4)	F16—P3—F17	101.7 (7)
C11—C12—C13	129.9 (4)	F18—P3—F17	172.1 (7)
C17—C13—C14	107.1 (5)	F15—P3—F17	87.3 (10)
C17—C13—C12	125.3 (4)	F16—P3—F13	86.7 (8)
C14—C13—C12	127.5 (4)	F18—P3—F13	101.5 (9)
C17—C13—Co1	69.2 (3)	F15—P3—F13	96.2 (12)
C14—C13—Co1	68.6 (3)	F17—P3—F13	85.8 (8)
C12—C13—Co1	126.4 (3)	F16—P3—F14	96.7 (8)
C15—C14—C13	108.1 (5)	F18—P3—F14	81.6 (7)
C15—C14—Co1	69.8 (3)	F15—P3—F14	80.8 (11)
C13—C14—Co1	70.0 (3)	F17—P3—F14	91.0 (7)
C15—C14—H14	126.0	F13—P3—F14	175.7 (8)
C13—C14—H14	126.0	O8—S3—O9	118.5 (17)

Co1—C14—H14	125.9	O8—S3—O7	105 (2)
C14—C15—C16	108.6 (5)	O9—S3—O7	98.8 (13)
C14—C15—Co1	69.3 (3)	O8—S3—C55	115.0 (15)
C16—C15—Co1	69.7 (3)	O9—S3—C55	111 (2)
C14—C15—H15	125.7	O7—S3—C55	106.6 (14)
C16—C15—H15	125.7	F9A—C55—F7A	122 (3)
Co1—C15—H15	126.9	F9A—C55—F8A	132 (3)
C15—C16—C17	107.5 (5)	F7A—C55—F8A	82.6 (18)
C15—C16—Co1	69.3 (3)	F9A—C55—S3	108 (3)
C17—C16—Co1	69.4 (3)	F7A—C55—S3	97.8 (19)
C15—C16—H16	126.2	F8A—C55—S3	108 (2)

C11—N1—N2—N3	0.5 (5)	C37—C38—C39—C40	−0.4 (6)
C10—N1—N2—N3	176.1 (4)	Fe2—C38—C39—C40	−59.3 (3)
N1—N2—N3—C12	0.3 (6)	C37—C38—C39—Fe2	58.9 (4)
N1—N2—N3—C23	−176.8 (5)	C37—C36—C40—C39	−0.2 (5)
C41—N4—N5—N6	0.8 (6)	Fe2—C36—C40—C39	59.6 (3)
C40—N4—N5—N6	174.7 (4)	C37—C36—C40—N4	171.9 (4)
N4—N5—N6—C42	0.2 (6)	Fe2—C36—C40—N4	−128.3 (5)
N4—N5—N6—C53	−172.1 (6)	C37—C36—C40—Fe2	−59.8 (3)
C5—C1—C2—C3	−0.5 (9)	C38—C39—C40—C36	0.4 (6)
Fe1—C1—C2—C3	60.1 (6)	Fe2—C39—C40—C36	−59.8 (3)
C5—C1—C2—Fe1	−60.7 (5)	C38—C39—C40—N4	−171.7 (4)
C1—C2—C3—C4	1.1 (10)	Fe2—C39—C40—N4	128.1 (4)
Fe1—C2—C3—C4	60.2 (6)	C38—C39—C40—Fe2	60.2 (4)
C1—C2—C3—Fe1	−59.1 (5)	N5—N4—C40—C36	143.7 (5)
C2—C3—C4—C5	−1.2 (10)	C41—N4—C40—C36	−43.1 (7)
Fe1—C3—C4—C5	58.5 (6)	N5—N4—C40—C39	−45.4 (7)
C2—C3—C4—Fe1	−59.7 (6)	C41—N4—C40—C39	127.8 (5)
C3—C4—C5—C1	0.8 (9)	N5—N4—C40—Fe2	48.7 (6)
Fe1—C4—C5—C1	59.4 (5)	C41—N4—C40—Fe2	−138.1 (4)
C3—C4—C5—Fe1	−58.5 (6)	N5—N4—C41—C42	−1.4 (5)
C2—C1—C5—C4	−0.2 (8)	C40—N4—C41—C42	−174.9 (4)
Fe1—C1—C5—C4	−60.5 (5)	N5—N4—C41—Au1	167.8 (4)
C2—C1—C5—Fe1	60.3 (5)	C40—N4—C41—Au1	−5.6 (6)
C10—C6—C7—C8	0.9 (7)	N5—N6—C42—C41	−1.1 (6)
Fe1—C6—C7—C8	−59.1 (5)	C53—N6—C42—C41	170.1 (6)
C10—C6—C7—Fe1	60.0 (4)	N5—N6—C42—C43	−177.2 (5)
C6—C7—C8—C9	−0.9 (8)	C53—N6—C42—C43	−6.0 (9)
Fe1—C7—C8—C9	−59.6 (5)	N4—C41—C42—N6	1.4 (5)
C6—C7—C8—Fe1	58.7 (4)	Au1—C41—C42—N6	−166.9 (4)
C7—C8—C9—C10	0.6 (7)	N4—C41—C42—C43	177.3 (5)
Fe1—C8—C9—C10	−58.7 (4)	Au1—C41—C42—C43	9.0 (8)
C7—C8—C9—Fe1	59.2 (5)	N6—C42—C43—C47	140.2 (5)
C7—C6—C10—N1	176.1 (5)	C41—C42—C43—C47	−35.1 (8)
Fe1—C6—C10—N1	−123.6 (5)	N6—C42—C43—C44	−39.9 (8)
C7—C6—C10—C9	−0.6 (6)	C41—C42—C43—C44	144.8 (5)
Fe1—C6—C10—C9	59.8 (4)	N6—C42—C43—Co2	−131.4 (5)

C7—C6—C10—Fe1	−60.3 (4)	C41—C42—C43—Co2	53.3 (7)
N2—N1—C10—C6	150.7 (5)	C47—C43—C44—C45	−0.4 (6)
C11—N1—C10—C6	−34.5 (8)	C42—C43—C44—C45	179.7 (5)
N2—N1—C10—C9	−33.2 (7)	Co2—C43—C44—C45	−58.9 (4)
C11—N1—C10—C9	141.6 (5)	C47—C43—C44—Co2	58.6 (3)
N2—N1—C10—Fe1	59.3 (6)	C42—C43—C44—Co2	−121.4 (5)
C11—N1—C10—Fe1	−125.8 (5)	C43—C44—C45—C46	0.3 (7)
C8—C9—C10—C6	0.0 (6)	Co2—C44—C45—C46	−59.1 (4)
Fe1—C9—C10—C6	−59.3 (4)	C43—C44—C45—Co2	59.3 (4)
C8—C9—C10—N1	−176.6 (5)	C44—C45—C46—C47	−0.1 (6)
Fe1—C9—C10—N1	124.1 (5)	Co2—C45—C46—C47	−59.6 (3)
C8—C9—C10—Fe1	59.3 (4)	C44—C45—C46—Co2	59.5 (4)
N2—N1—C11—C12	−1.0 (5)	C45—C46—C47—C43	−0.1 (6)
C10—N1—C11—C12	−176.0 (5)	Co2—C46—C47—C43	−59.8 (3)
N2—N1—C11—Au1	171.9 (3)	C45—C46—C47—Co2	59.6 (4)
C10—N1—C11—Au1	−3.1 (7)	C44—C43—C47—C46	0.3 (5)
N2—N3—C12—C11	−0.9 (6)	C42—C43—C47—C46	−179.8 (4)
C23—N3—C12—C11	175.7 (5)	Co2—C43—C47—C46	59.1 (3)
N2—N3—C12—C13	−178.1 (4)	C44—C43—C47—Co2	−58.8 (4)
C23—N3—C12—C13	−1.5 (9)	C42—C43—C47—Co2	121.1 (5)
N1—C11—C12—N3	1.1 (5)	C52—C48—C49—C50	−0.1 (7)
Au1—C11—C12—N3	−171.5 (3)	Co2—C48—C49—C50	59.6 (4)
N1—C11—C12—C13	178.1 (5)	C52—C48—C49—Co2	−59.7 (4)
Au1—C11—C12—C13	5.4 (8)	C48—C49—C50—C51	−0.3 (7)
N3—C12—C13—C17	145.3 (5)	Co2—C49—C50—C51	59.3 (4)
C11—C12—C13—C17	−31.2 (8)	C48—C49—C50—Co2	−59.6 (4)
N3—C12—C13—C14	−36.0 (8)	C49—C50—C51—C52	0.7 (7)
C11—C12—C13—C14	147.5 (6)	Co2—C50—C51—C52	59.5 (4)
N3—C12—C13—Co1	−125.7 (4)	C49—C50—C51—Co2	−58.9 (4)
C11—C12—C13—Co1	57.8 (7)	C49—C48—C52—C51	0.5 (7)
C17—C13—C14—C15	−0.9 (7)	Co2—C48—C52—C51	−58.5 (4)
C12—C13—C14—C15	−179.9 (5)	C49—C48—C52—Co2	59.0 (4)
Co1—C13—C14—C15	−59.6 (5)	C50—C51—C52—C48	−0.7 (6)
C17—C13—C14—Co1	58.7 (4)	Co2—C51—C52—C48	58.3 (4)
C12—C13—C14—Co1	−120.2 (5)	C50—C51—C52—Co2	−59.0 (4)
C13—C14—C15—C16	0.9 (7)	O3A—S1—O1A—O2A	109.2 (17)
Co1—C14—C15—C16	−58.8 (4)	C53A—S1—O1A—O2A	−139.5 (19)
C13—C14—C15—Co1	59.7 (4)	O3A—S1—O2A—O1A	−74.0 (18)
C14—C15—C16—C17	−0.5 (7)	C53A—S1—O2A—O1A	45 (2)
Co1—C15—C16—C17	−59.0 (4)	O2A—S1—C53A—F3A	54 (2)
C14—C15—C16—Co1	58.5 (5)	O3A—S1—C53A—F3A	169.5 (16)
C15—C16—C17—C13	−0.1 (6)	O1A—S1—C53A—F3A	91 (2)
Co1—C16—C17—C13	−59.0 (3)	O2A—S1—C53A—F1A	−172 (2)
C15—C16—C17—Co1	58.9 (4)	O3A—S1—C53A—F1A	−57 (2)
C14—C13—C17—C16	0.6 (6)	O1A—S1—C53A—F1A	−136 (3)
C12—C13—C17—C16	179.6 (5)	O2A—S1—C53A—F2A	−60 (2)
Co1—C13—C17—C16	58.9 (4)	O3A—S1—C53A—F2A	55.8 (19)
C14—C13—C17—Co1	−58.3 (4)	O1A—S1—C53A—F2A	−23.2 (19)

C12—C13—C17—Co1	120.7 (5)	O1B—S1B—C53B—F3B	79.9 (17)
C22—C18—C19—C20	0.3 (8)	O2B—S1B—C53B—F3B	−45 (2)
Co1—C18—C19—C20	59.4 (5)	O3B—S1B—C53B—F3B	−177.7 (14)
C22—C18—C19—Co1	−59.1 (5)	O1B—S1B—C53B—F1B	−158.3 (17)
C18—C19—C20—C21	−0.3 (9)	O2B—S1B—C53B—F1B	77 (2)
Co1—C19—C20—C21	59.1 (5)	O3B—S1B—C53B—F1B	−56 (2)
C18—C19—C20—Co1	−59.4 (5)	O1B—S1B—C53B—F2B	−28 (2)
C19—C20—C21—C22	0.2 (8)	O2B—S1B—C53B—F2B	−154 (2)
Co1—C20—C21—C22	59.3 (4)	O3B—S1B—C53B—F2B	74 (2)
C19—C20—C21—Co1	−59.1 (5)	O6—S2—C54—F4A	−62.3 (13)
C19—C18—C22—C21	−0.2 (8)	O4—S2—C54—F4A	175.8 (10)
Co1—C18—C22—C21	−59.1 (4)	O5—S2—C54—F4A	51.0 (13)
C19—C18—C22—Co1	58.9 (5)	O6—S2—C54—F6A	176.4 (11)
C20—C21—C22—C18	0.0 (8)	O4—S2—C54—F6A	54.6 (10)
Co1—C21—C22—C18	59.1 (5)	O5—S2—C54—F6A	−70.2 (11)
C20—C21—C22—Co1	−59.2 (5)	O6—S2—C54—F5A	53.2 (13)
C35—C31—C32—C33	0.3 (7)	O4—S2—C54—F5A	−68.7 (11)
Fe2—C31—C32—C33	59.4 (4)	O5—S2—C54—F5A	166.5 (12)
C35—C31—C32—Fe2	−59.1 (4)	O5B—S2B—C54B—F6B	74.6 (18)
C31—C32—C33—C34	−0.3 (7)	O6B—S2B—C54B—F6B	161.3 (18)
Fe2—C32—C33—C34	59.8 (4)	O4B—S2B—C54B—F6B	−62 (2)
C31—C32—C33—Fe2	−60.0 (4)	O5B—S2B—C54B—F5B	−179.4 (18)
C32—C33—C34—C35	0.1 (7)	O6B—S2B—C54B—F5B	−92.7 (19)
Fe2—C33—C34—C35	59.8 (4)	O4B—S2B—C54B—F5B	44 (3)
C32—C33—C34—Fe2	−59.7 (4)	O5B—S2B—C54B—F4B	−41.1 (16)
C33—C34—C35—C31	0.1 (7)	O6B—S2B—C54B—F4B	45.6 (15)
Fe2—C34—C35—C31	59.4 (4)	O4B—S2B—C54B—F4B	−177.5 (18)
C33—C34—C35—Fe2	−59.3 (4)	O8—S3—C55—F9A	48 (4)
C32—C31—C35—C34	−0.3 (7)	O9—S3—C55—F9A	−174 (3)
Fe2—C31—C35—C34	−59.3 (4)	O7—S3—C55—F9A	−67 (3)
C32—C31—C35—Fe2	59.0 (4)	O8—S3—C55—F7A	−79 (3)
C40—C36—C37—C38	−0.1 (6)	O9—S3—C55—F7A	59 (2)
Fe2—C36—C37—C38	−59.0 (4)	O7—S3—C55—F7A	165 (2)
C40—C36—C37—Fe2	58.9 (3)	O8—S3—C55—F8A	−164 (2)
C36—C37—C38—C39	0.3 (6)	O9—S3—C55—F8A	−26 (3)
Fe2—C37—C38—C39	−58.6 (4)	O7—S3—C55—F8A	81 (2)
C36—C37—C38—Fe2	58.9 (3)		