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Bis(*tert*-butyl isocyanide)-1κ^2C-di-μ-carbonyl-2:3κ^4C-octacarbonyl-1κ^2C,2κ^3C,3κ^3C-*triangulo*-diironosmium

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.021
wR factor = 0.042
Data-to-parameter ratio = 34.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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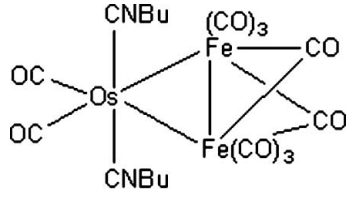
The preparation of the mixed-metal cluster, $[Fe_2Os(C_5H_9N)_2(CO)_{10}]$, and its crystal structure at 100 K are reported. This complex, along with the cluster in the preceding paper, are the first structurally characterized substitution derivatives of $Fe_2Os(CO)_{12}$. The isonitrile ligands adopt axial positions on the osmium centre and the cluster is isostructural with the Fe_2Ru analogue.

Comment

The background to this study has been set out in the preceding paper (Evans *et al.*, 2006). We report here and in that paper the synthesis and structures of $Fe_2Os(CO)_{12-n}(CNBu^t)_n$ (n = 1 and 2).

$Fe_2Os(CO)_{10}(CNBu^t)_2$, (II), was prepared by carbonyl substitution of the parent $Fe_2Os(CO)_{12}$ cluster using standard methods (Farrugia & Mertes, 2002). The compound was characterized spectroscopically, by FAB mass spectrometry, and by single-crystal X-ray structure determination. The structure was determined at room temperature and 100 K with no discernible metal atom disorder at either temperature. As the structures at different temperatures are essentially identical, only the more precise low-temperature structure will be discussed here.



(II)

The structure of (II) at 100 K is shown in Fig. 1. Both isonitrile ligands adopt axial positions on the Os atom, identical to that reported for the Fe_2Ru analogue but contrasting with $Fe_3(CO)_{10}(CNBu^t)_2$ [where one isonitrile is axial and the other equatorial (Murray *et al.*, 1990)] and $M_3(CO)_{10}(CNR)_2$ [M = Ru and Os; R = Bu^t and Me] (Dawson *et al.*, 1982; Bruce *et al.*, 1983; Farrugia *et al.*, 1998), where the two isonitrile ligands are axial but attached to different metal centres. The average Fe—Os distance [2.7590 (3) Å] and Fe—Fe distance [2.5738 (3) Å] are longer than those reported (Farrugia & Mertes, 2002) for the ruthenium analogue [Ru—Fe = 2.7527 (3) Å and Fe—Fe = 2.5678 (2) Å]. Two carbonyl ligands symmetrically bridge the Fe—Fe bond [$\delta(M-C)$ = 0.009 and 0.003 Å for C14 and C24, respectively].

Experimental

Complex (II) was prepared in the same manner as reported for the ruthenium analogue (Farrugia & Mertes, 2002) by reaction of the parent carbonyl with a 1:2 molar ratio of isonitrile. The product was purified by chromatography on Florisil using hexane/CH_2Cl_2 mixtures as eluant. Crystals were obtained from a concentrated hexane solution at 25 K. Analysis calculated for $C_{20}H_{18}Fe_2N_2O_{10}Os$: C 32.10, H 2.42, N 3.74%; found: C 32.15, H 2.20, N 3.74%. IR [ν(CN), cm^{-1}] 2200 (*vw*), 2170 (*m*); IR [ν(CO), cm^{-1}] 2053 (*w*), 2021 (*vs*), 2015 (*vs*), 1981 (*m*), 1975 (*m*), 1901 (*vw*), 1834 (*vw*), 1802 (*w*). ^{1}H NMR: δ 1.54 (*s*, CH_3). Mass spectrum, m/z = 750.2 [M^+], 694.2 [$M^+ - 2CO$], 666.2 [$M^+ - 3CO$], 638.2 [$M^+ - 4CO$], 610.2 [$M^+ - 5CO$], 582.2 [$M^+ - 6CO$], 554.3 [$M^+ - 7CO$], 526.3 [$M^+ - 8CO$], 498.3 [$M^+ - 9CO$], 470.3 [$M^+ - 10CO$].

Crystal data

$[Fe_2Os(C_5H_9N)_2(CO)_{10}]$	D_x = 1.943 Mg m^{-3}
M_r = 748.26	Mo $K\alpha$ radiation
Monoclinic, $P2_1/a$	Cell parameters from 11369 reflections
a = 11.6903 (2) Å	θ = 2.2–35.0°
b = 12.4357 (2) Å	μ = 6.13 mm^{-1}
c = 17.6041 (3) Å	T = 100 (2) K
β = 91.753 (1)°	Prism, purple
V = 2558.03 (7) Å^3	0.3 × 0.3 × 0.2 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	9945 reflections with $I > 2\sigma(I)$
φ or ω scans	R_{int} = 0.032
Absorption correction: multi-scan (Blessing, 1995)	θ_{max} = 35.0°
T_{min} = 0.197, T_{max} = 0.294	$h = -18 \rightarrow 18$
64585 measured reflections	$k = -20 \rightarrow 20$
10967 independent reflections	$l = -27 \rightarrow 28$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0113P)^2 + 1.9594P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.021	$(\Delta/\sigma)_{max}$ = 0.002
$wR(F^2)$ = 0.042	$\Delta\rho_{max}$ = 1.28 e Å^{-3}
S = 1.1	$\Delta\rho_{min}$ = −0.94 e Å^{-3}
10967 reflections	Extinction correction: *SHELXL97*
317 parameters	Extinction coefficient: 0.00024 (4)
H-atom parameters constrained	

All H atoms were placed in calculated positions and refined using a riding model [C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C)]. The highest features in the difference map are associated with the Os atom.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

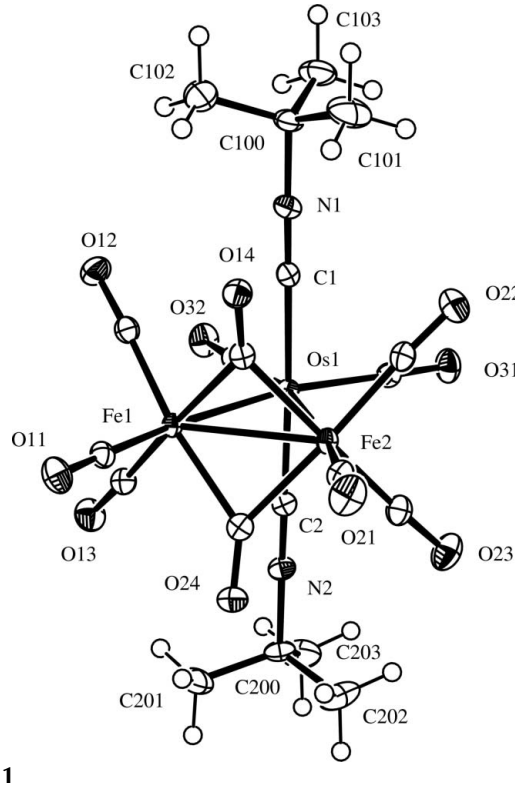


Figure 1
A view of $Fe_2Os(CO)_{10}(CNBu^t)_2$, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level, with H atoms represented by circles of arbitrary size.

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supporting information

Acta Cryst. (2006). E**62**, m478–m479 [https://doi.org/10.1107/S1600536806004247]

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KappaCCD diffractometer
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9945 reflections with $I > 2\sigma(I)$
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$\theta_{max} = 35.0°$, $\theta_{min} = 2.4°$
$h = -18 \rightarrow 18$
$k = -20 \rightarrow 20$
$l = -27 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.042$
$S = 1.1$
10967 reflections
317 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0113P)^2 + 1.9594P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.28$ e Å^{-3}
$\Delta\rho_{min} = -0.94$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00024 (4)

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Os1	0.796803 (5)	0.078714 (5)	0.264536 (3)	0.01175 (2)
Fe1	0.715245 (19)	−0.128082 (18)	0.246561 (13)	0.01250 (4)
Fe2	0.567762 (19)	0.024601 (19)	0.256179 (14)	0.01351 (4)
N1	0.79148 (13)	0.09910 (12)	0.08484 (9)	0.0182 (3)
N2	0.79307 (13)	0.04302 (13)	0.44331 (9)	0.0176 (3)
O11	0.59757 (13)	−0.33642 (11)	0.23028 (9)	0.0249 (3)
O12	0.88483 (13)	−0.14605 (12)	0.12654 (8)	0.0261 (3)
O13	0.88504 (13)	−0.19340 (12)	0.36481 (9)	0.0270 (3)
O14	0.58792 (12)	−0.07302 (11)	0.10291 (8)	0.0207 (2)
O21	0.33447 (12)	−0.06186 (13)	0.23777 (10)	0.0294 (3)
O22	0.53743 (15)	0.20690 (13)	0.15018 (10)	0.0320 (3)
O23	0.53714 (14)	0.17035 (13)	0.38615 (9)	0.0308 (3)
O24	0.58865 (12)	−0.12054 (11)	0.39045 (8)	0.0212 (2)
O31	0.79104 (13)	0.32166 (11)	0.28107 (9)	0.0265 (3)
O32	1.05737 (12)	0.07111 (12)	0.26688 (10)	0.0273 (3)
C1	0.79257 (14)	0.09169 (13)	0.15043 (10)	0.0149 (3)
C2	0.79353 (14)	0.05589 (13)	0.37818 (10)	0.0158 (3)
C11	0.64394 (15)	−0.25598 (14)	0.23622 (10)	0.0166 (3)
C12	0.81911 (15)	−0.13642 (14)	0.17307 (10)	0.0180 (3)
C13	0.81919 (15)	−0.16485 (14)	0.31989 (10)	0.0180 (3)
C14	0.61172 (14)	−0.06415 (13)	0.16762 (10)	0.0163 (3)
C21	0.42448 (15)	−0.02751 (14)	0.24587 (10)	0.0182 (3)
C22	0.55314 (15)	0.13531 (15)	0.19031 (11)	0.0201 (3)
C23	0.55223 (15)	0.11236 (15)	0.33704 (11)	0.0202 (3)
C24	0.61162 (14)	−0.09012 (14)	0.32994 (10)	0.0168 (3)
C31	0.79279 (14)	0.22992 (14)	0.27532 (10)	0.0170 (3)
C32	0.95936 (15)	0.07170 (13)	0.26613 (10)	0.0168 (3)
C100	0.78631 (17)	0.10920 (16)	0.00192 (10)	0.0206 (3)
C101	0.6633 (2)	0.1395 (2)	−0.02095 (14)	0.0380 (6)
H11A	0.6444	0.2092	0.0015	0.057*
H11B	0.6109	0.0845	−0.0025	0.057*
H11C	0.6557	0.1443	−0.0764	0.057*
C102	0.8185 (3)	0.00110 (19)	−0.03189 (13)	0.0362 (5)
H12A	0.7626	−0.0533	−0.0175	0.054*
H12B	0.8948	−0.0199	−0.0126	0.054*

H12C	0.819	0.0069	−0.0874	0.054*
C103	0.8706 (2)	0.19684 (19)	−0.01871 (13)	0.0317 (5)
H13A	0.8473	0.2651	0.0039	0.048*
H13B	0.8716	0.2044	−0.0741	0.048*
H13C	0.9473	0.1775	0.0008	0.048*
C200	0.78282 (16)	0.02367 (16)	0.52508 (10)	0.0203 (3)
C201	0.8067 (2)	−0.09521 (18)	0.53928 (12)	0.0321 (5)
H21A	0.7491	−0.1386	0.5117	0.048*
H21B	0.8035	−0.1102	0.5938	0.048*
H21C	0.8829	−0.1132	0.5214	0.048*
C202	0.6608 (2)	0.0530 (2)	0.54526 (13)	0.0358 (5)
H22A	0.6068	0.0062	0.5174	0.054*
H22B	0.6457	0.1281	0.5314	0.054*
H22C	0.6515	0.0437	0.6	0.054*
C203	0.8706 (2)	0.0943 (2)	0.56696 (12)	0.0328 (5)
H23A	0.9478	0.073	0.5529	0.049*
H23B	0.8629	0.0857	0.6219	0.049*
H23C	0.8576	0.1697	0.553	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Os1	0.01157 (3)	0.01227 (3)	0.01136 (3)	−0.00138 (2)	−0.00030 (2)	0.00027 (2)
Fe1	0.01141 (9)	0.01120 (9)	0.01485 (10)	0.00009 (7)	−0.00012 (7)	−0.00092 (7)
Fe2	0.01043 (9)	0.01270 (9)	0.01735 (10)	0.00028 (7)	−0.00046 (8)	−0.00107 (8)
N1	0.0176 (6)	0.0210 (7)	0.0161 (6)	−0.0007 (5)	0.0000 (5)	0.0036 (5)
N2	0.0175 (6)	0.0206 (7)	0.0148 (6)	−0.0028 (5)	−0.0002 (5)	−0.0020 (5)
O11	0.0254 (7)	0.0174 (6)	0.0317 (8)	−0.0042 (5)	−0.0045 (6)	0.0005 (5)
O12	0.0241 (7)	0.0309 (7)	0.0237 (7)	0.0057 (6)	0.0058 (5)	−0.0002 (6)
O13	0.0269 (7)	0.0290 (7)	0.0246 (7)	0.0034 (6)	−0.0082 (6)	0.0002 (6)
O14	0.0216 (6)	0.0230 (6)	0.0173 (6)	0.0020 (5)	−0.0034 (5)	−0.0020 (5)
O21	0.0170 (6)	0.0325 (8)	0.0388 (9)	−0.0052 (5)	0.0000 (6)	−0.0067 (6)
O22	0.0361 (8)	0.0272 (7)	0.0329 (8)	0.0083 (6)	0.0025 (7)	0.0084 (6)
O23	0.0309 (8)	0.0314 (8)	0.0300 (8)	0.0043 (6)	−0.0008 (6)	−0.0121 (6)
O24	0.0224 (6)	0.0236 (6)	0.0179 (6)	−0.0021 (5)	0.0028 (5)	0.0013 (5)
O31	0.0250 (7)	0.0162 (6)	0.0383 (8)	−0.0008 (5)	0.0025 (6)	−0.0014 (5)
O32	0.0152 (6)	0.0293 (7)	0.0375 (8)	0.0000 (5)	−0.0006 (5)	0.0005 (6)
C1	0.0122 (6)	0.0147 (7)	0.0177 (7)	−0.0004 (5)	−0.0001 (5)	0.0012 (5)
C2	0.0146 (7)	0.0162 (7)	0.0165 (7)	−0.0022 (5)	−0.0001 (5)	−0.0010 (5)
C11	0.0181 (7)	0.0160 (7)	0.0156 (7)	0.0018 (5)	−0.0028 (5)	0.0003 (5)
C12	0.0168 (7)	0.0183 (7)	0.0188 (7)	0.0023 (6)	−0.0011 (6)	0.0013 (6)
C13	0.0177 (7)	0.0177 (7)	0.0186 (7)	−0.0006 (6)	−0.0004 (6)	−0.0008 (6)
C14	0.0135 (7)	0.0159 (7)	0.0195 (7)	−0.0010 (5)	−0.0002 (5)	0.0002 (5)
C21	0.0165 (7)	0.0188 (7)	0.0194 (8)	0.0006 (6)	0.0007 (6)	−0.0022 (6)
C22	0.0179 (7)	0.0200 (8)	0.0226 (8)	0.0033 (6)	0.0013 (6)	−0.0012 (6)
C23	0.0167 (7)	0.0207 (8)	0.0232 (8)	0.0015 (6)	−0.0014 (6)	−0.0017 (6)
C24	0.0147 (7)	0.0173 (7)	0.0184 (7)	−0.0026 (5)	−0.0010 (5)	−0.0019 (6)
C31	0.0142 (7)	0.0182 (7)	0.0188 (8)	−0.0014 (5)	0.0013 (6)	−0.0003 (6)

C32	0.0164 (7)	0.0157 (7)	0.0182 (7)	−0.0002 (5)	−0.0007 (5)	0.0007 (6)
C100	0.0243 (8)	0.0244 (8)	0.0130 (7)	0.0007 (6)	−0.0001 (6)	0.0042 (6)
C101	0.0302 (11)	0.0592 (16)	0.0241 (10)	0.0038 (10)	−0.0075 (8)	0.0130 (10)
C102	0.0589 (16)	0.0281 (10)	0.0214 (10)	0.0033 (10)	−0.0012 (10)	−0.0045 (8)
C103	0.0414 (12)	0.0319 (11)	0.0222 (9)	−0.0078 (9)	0.0072 (8)	0.0065 (8)
C200	0.0223 (8)	0.0285 (9)	0.0102 (7)	−0.0030 (7)	0.0013 (6)	−0.0010 (6)
C201	0.0475 (13)	0.0293 (10)	0.0194 (9)	−0.0012 (9)	0.0018 (9)	0.0061 (7)
C202	0.0257 (10)	0.0606 (16)	0.0214 (10)	0.0030 (10)	0.0062 (8)	−0.0039 (9)
C203	0.0390 (12)	0.0418 (12)	0.0171 (8)	−0.0133 (10)	−0.0059 (8)	−0.0048 (8)

Geometric parameters (Å, º)

Os1—C31	1.8906 (18)	O24—C24	1.169 (2)
Os1—C32	1.9017 (17)	O31—C31	1.146 (2)
Os1—C1	2.0143 (17)	O32—C32	1.145 (2)
Os1—C2	2.0221 (17)	C100—C103	1.521 (3)
Os1—Fe1	2.7576 (2)	C100—C102	1.522 (3)
Os1—Fe2	2.7604 (2)	C100—C101	1.528 (3)
Fe1—C11	1.8023 (17)	C101—H11A	0.98
Fe1—C13	1.8044 (18)	C101—H11B	0.98
Fe1—C12	1.8041 (18)	C101—H11C	0.98
Fe1—C14	1.9812 (17)	C102—H12A	0.98
Fe1—C24	1.9884 (18)	C102—H12B	0.98
Fe1—Fe2	2.5738 (3)	C102—H12C	0.98
Fe2—C21	1.8000 (18)	C103—H13A	0.98
Fe2—C22	1.8047 (19)	C103—H13B	0.98
Fe2—C23	1.8073 (19)	C103—H13C	0.98
Fe2—C24	1.9858 (18)	C200—C202	1.525 (3)
Fe2—C14	1.9904 (18)	C200—C203	1.524 (3)
N1—C1	1.158 (2)	C200—C201	1.524 (3)
N1—C100	1.465 (2)	C201—H21A	0.98
N2—C2	1.158 (2)	C201—H21B	0.98
N2—C200	1.468 (2)	C201—H21C	0.98
O11—C11	1.141 (2)	C202—H22A	0.98
O12—C12	1.146 (2)	C202—H22B	0.98
O13—C13	1.143 (2)	C202—H22C	0.98
O14—C14	1.169 (2)	C203—H23A	0.98
O21—C21	1.141 (2)	C203—H23B	0.98
O22—C22	1.148 (2)	C203—H23C	0.98
O23—C23	1.144 (2)		

C31—Os1—C32	94.13 (7)	O12—C12—Fe1	177.30 (17)
C31—Os1—C1	91.18 (7)	O13—C13—Fe1	176.45 (16)
C32—Os1—C1	90.71 (7)	O14—C14—Fe1	140.12 (14)
C31—Os1—C2	92.23 (7)	O14—C14—Fe2	139.09 (14)
C32—Os1—C2	91.61 (7)	Fe1—C14—Fe2	80.79 (7)
C1—Os1—C2	175.73 (7)	O21—C21—Fe2	178.31 (17)
C31—Os1—Fe1	158.36 (5)	O22—C22—Fe2	175.85 (17)

C32—Os1—Fe1	107.50 (5)	O23—C23—Fe2	176.16 (17)
C1—Os1—Fe1	87.85 (5)	O24—C24—Fe2	140.02 (15)
C2—Os1—Fe1	88.03 (5)	O24—C24—Fe1	139.26 (15)
C31—Os1—Fe2	102.76 (5)	Fe2—C24—Fe1	80.73 (7)
C32—Os1—Fe2	163.11 (5)	O31—C31—Os1	179.18 (17)
C1—Os1—Fe2	88.41 (5)	O32—C32—Os1	177.73 (16)
C2—Os1—Fe2	88.33 (5)	N1—C100—C103	106.99 (16)
Fe1—Os1—Fe2	55.606 (7)	N1—C100—C102	108.10 (16)
C11—Fe1—C13	98.51 (8)	C103—C100—C102	111.69 (19)
C11—Fe1—C12	101.31 (8)	N1—C100—C101	107.07 (16)
C13—Fe1—C12	92.59 (8)	C103—C100—C101	111.83 (18)
C11—Fe1—C14	90.72 (7)	C102—C100—C101	110.9 (2)
C13—Fe1—C14	170.76 (7)	C100—C101—H11A	109.5
C12—Fe1—C14	85.99 (7)	C100—C101—H11B	109.5
C11—Fe1—C24	89.64 (7)	H11A—C101—H11B	109.5
C13—Fe1—C24	86.80 (8)	C100—C101—H11C	109.5
C12—Fe1—C24	168.99 (8)	H11A—C101—H11C	109.5
C14—Fe1—C24	92.84 (7)	H11B—C101—H11C	109.5
C11—Fe1—Fe2	110.43 (6)	C100—C102—H12A	109.5
C13—Fe1—Fe2	125.29 (6)	C100—C102—H12B	109.5
C12—Fe1—Fe2	123.81 (6)	H12A—C102—H12B	109.5
C14—Fe1—Fe2	49.76 (5)	C100—C102—H12C	109.5
C24—Fe1—Fe2	49.59 (5)	H12A—C102—H12C	109.5
C11—Fe1—Os1	172.65 (6)	H12B—C102—H12C	109.5
C13—Fe1—Os1	86.06 (6)	C100—C103—H13A	109.5
C12—Fe1—Os1	84.14 (6)	C100—C103—H13B	109.5
C14—Fe1—Os1	84.72 (5)	H13A—C103—H13B	109.5
C24—Fe1—Os1	84.85 (5)	C100—C103—H13C	109.5
Fe2—Fe1—Os1	62.253 (7)	H13A—C103—H13C	109.5
C21—Fe2—C22	98.07 (8)	H13B—C103—H13C	109.5
C21—Fe2—C23	100.44 (8)	N2—C200—C202	107.11 (16)
C22—Fe2—C23	92.04 (9)	N2—C200—C203	107.81 (16)
C21—Fe2—C24	91.61 (8)	C202—C200—C203	111.72 (18)
C22—Fe2—C24	170.28 (8)	N2—C200—C201	107.45 (15)
C23—Fe2—C24	87.07 (8)	C202—C200—C201	111.25 (19)
C21—Fe2—C14	89.04 (7)	C203—C200—C201	111.26 (18)
C22—Fe2—C14	86.64 (8)	C200—C201—H21A	109.5
C23—Fe2—C14	170.53 (8)	C200—C201—H21B	109.5
C24—Fe2—C14	92.64 (7)	H21A—C201—H21B	109.5
C21—Fe2—Fe1	110.55 (6)	C200—C201—H21C	109.5
C22—Fe2—Fe1	124.82 (6)	H21A—C201—H21C	109.5
C23—Fe2—Fe1	125.52 (6)	H21B—C201—H21C	109.5
C24—Fe2—Fe1	49.68 (5)	C200—C202—H22A	109.5
C14—Fe2—Fe1	49.45 (5)	C200—C202—H22B	109.5
C21—Fe2—Os1	172.43 (6)	H22A—C202—H22B	109.5
C22—Fe2—Os1	85.46 (6)	C200—C202—H22C	109.5
C23—Fe2—Os1	86.07 (6)	H22A—C202—H22C	109.5
C24—Fe2—Os1	84.82 (5)	H22B—C202—H22C	109.5

C14—Fe2—Os1	84.47 (5)	C200—C203—H23A	109.5
Fe1—Fe2—Os1	62.141 (7)	C200—C203—H23B	109.5
C1—N1—C100	178.22 (18)	H23A—C203—H23B	109.5
C2—N2—C200	175.33 (17)	C200—C203—H23C	109.5
N1—C1—Os1	179.22 (15)	H23A—C203—H23C	109.5
N2—C2—Os1	179.17 (15)	H23B—C203—H23C	109.5
O11—C11—Fe1	179.03 (17)		

C31—Os1—Fe1—C13	−135.44 (15)	C2—Os1—Fe2—C22	137.62 (8)
C32—Os1—Fe1—C13	46.72 (8)	Fe1—Os1—Fe2—C22	−133.62 (6)
C1—Os1—Fe1—C13	136.79 (7)	C31—Os1—Fe2—C23	−46.65 (8)
C2—Os1—Fe1—C13	−44.35 (7)	C32—Os1—Fe2—C23	135.29 (19)
Fe2—Os1—Fe1—C13	−133.67 (6)	C1—Os1—Fe2—C23	−137.49 (8)
C31—Os1—Fe1—C12	131.54 (15)	C2—Os1—Fe2—C23	45.26 (8)
C32—Os1—Fe1—C12	−46.30 (8)	Fe1—Os1—Fe2—C23	134.03 (6)
C1—Os1—Fe1—C12	43.77 (7)	C31—Os1—Fe2—C24	−134.06 (7)
C2—Os1—Fe1—C12	−137.36 (7)	C32—Os1—Fe2—C24	47.88 (19)
Fe2—Os1—Fe1—C12	133.32 (6)	C1—Os1—Fe2—C24	135.09 (7)
C31—Os1—Fe1—C14	45.04 (15)	C2—Os1—Fe2—C24	−42.15 (7)
C32—Os1—Fe1—C14	−132.80 (8)	Fe1—Os1—Fe2—C24	46.61 (5)
C1—Os1—Fe1—C14	−42.73 (7)	C31—Os1—Fe2—C14	132.77 (7)
C2—Os1—Fe1—C14	136.14 (7)	C32—Os1—Fe2—C14	−45.29 (19)
Fe2—Os1—Fe1—C14	46.82 (5)	C1—Os1—Fe2—C14	41.92 (7)
C31—Os1—Fe1—C24	−48.31 (15)	C2—Os1—Fe2—C14	−135.32 (7)
C32—Os1—Fe1—C24	133.86 (8)	Fe1—Os1—Fe2—C14	−46.56 (5)
C1—Os1—Fe1—C24	−136.07 (7)	C31—Os1—Fe2—Fe1	179.33 (5)
C2—Os1—Fe1—C24	42.79 (7)	C32—Os1—Fe2—Fe1	1.27 (18)
Fe2—Os1—Fe1—C24	−46.53 (5)	C1—Os1—Fe2—Fe1	88.48 (5)
C31—Os1—Fe1—Fe2	−1.77 (14)	C2—Os1—Fe2—Fe1	−88.76 (5)
C32—Os1—Fe1—Fe2	−179.61 (6)	C11—Fe1—C14—O14	−63.4 (2)
C1—Os1—Fe1—Fe2	−89.54 (5)	C12—Fe1—C14—O14	37.9 (2)
C2—Os1—Fe1—Fe2	89.32 (5)	C24—Fe1—C14—O14	−153.1 (2)
C11—Fe1—Fe2—C21	−2.83 (9)	Fe2—Fe1—C14—O14	−180.0 (2)
C13—Fe1—Fe2—C21	−120.02 (9)	Os1—Fe1—C14—O14	122.3 (2)
C12—Fe1—Fe2—C21	117.26 (9)	C11—Fe1—C14—Fe2	116.52 (7)
C14—Fe1—Fe2—C21	69.86 (9)	C12—Fe1—C14—Fe2	−142.18 (7)
C24—Fe1—Fe2—C21	−73.82 (9)	C24—Fe1—C14—Fe2	26.85 (6)
Os1—Fe1—Fe2—C21	177.85 (6)	Os1—Fe1—C14—Fe2	−57.71 (4)
C11—Fe1—Fe2—C22	−119.14 (9)	C21—Fe2—C14—O14	61.5 (2)
C13—Fe1—Fe2—C22	123.67 (10)	C22—Fe2—C14—O14	−36.6 (2)
C12—Fe1—Fe2—C22	0.95 (10)	C24—Fe2—C14—O14	153.1 (2)
C14—Fe1—Fe2—C22	−46.45 (10)	Fe1—Fe2—C14—O14	180.0 (2)
C24—Fe1—Fe2—C22	169.87 (10)	Os1—Fe2—C14—O14	−122.4 (2)
Os1—Fe1—Fe2—C22	61.54 (7)	C21—Fe2—C14—Fe1	−118.45 (7)
C11—Fe1—Fe2—C23	117.52 (10)	C22—Fe2—C14—Fe1	143.41 (7)
C13—Fe1—Fe2—C23	0.33 (10)	C24—Fe2—C14—Fe1	−26.88 (6)
C12—Fe1—Fe2—C23	−122.39 (10)	Os1—Fe2—C14—Fe1	57.65 (4)
C14—Fe1—Fe2—C23	−169.79 (10)	C21—Fe2—C24—O24	−63.6 (2)

C24—Fe1—Fe2—C23	46.53 (10)	C23—Fe2—C24—O24	36.7 (2)
Os1—Fe1—Fe2—C23	−61.80 (8)	C14—Fe2—C24—O24	−152.8 (2)
C11—Fe1—Fe2—C24	70.99 (9)	Fe1—Fe2—C24—O24	−179.5 (2)
C13—Fe1—Fe2—C24	−46.20 (9)	Os1—Fe2—C24—O24	123.0 (2)
C12—Fe1—Fe2—C24	−168.92 (9)	C21—Fe2—C24—Fe1	115.89 (7)
C14—Fe1—Fe2—C24	143.68 (9)	C23—Fe2—C24—Fe1	−143.74 (7)
Os1—Fe1—Fe2—C24	−108.33 (6)	C14—Fe2—C24—Fe1	26.78 (6)
C11—Fe1—Fe2—C14	−72.69 (9)	Os1—Fe2—C24—Fe1	−57.42 (4)
C13—Fe1—Fe2—C14	170.12 (9)	C11—Fe1—C24—O24	61.9 (2)
C12—Fe1—Fe2—C14	47.40 (9)	C13—Fe1—C24—O24	−36.6 (2)
C24—Fe1—Fe2—C14	−143.68 (9)	C12—Fe1—C24—O24	−123.7 (4)
Os1—Fe1—Fe2—C14	107.99 (6)	C14—Fe1—C24—O24	152.6 (2)
C11—Fe1—Fe2—Os1	179.32 (6)	Fe2—Fe1—C24—O24	179.5 (2)
C13—Fe1—Fe2—Os1	62.14 (7)	Os1—Fe1—C24—O24	−122.9 (2)
C12—Fe1—Fe2—Os1	−60.59 (7)	C11—Fe1—C24—Fe2	−117.62 (7)
C14—Fe1—Fe2—Os1	−107.99 (6)	C13—Fe1—C24—Fe2	143.84 (7)
C24—Fe1—Fe2—Os1	108.33 (6)	C12—Fe1—C24—Fe2	56.7 (4)
C31—Os1—Fe2—C22	45.71 (8)	C14—Fe1—C24—Fe2	−26.92 (6)
C32—Os1—Fe2—C22	−132.35 (19)	Os1—Fe1—C24—Fe2	57.51 (4)
C1—Os1—Fe2—C22	−45.13 (7)		