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The one-electron oxidation product of a metallocenyl-terminated cyanine

Stephen Barlow,[a]*† Michael W. Day[a] and Seth R. Marder[b]‡

[a]Beckman Institute, 139-74 California Institute of Technology, Pasadena, CA 91125, USA, and [b]Beckman Institute and Jet Propulsion Laboratory, 139-74 California Institute of Technology, Pasadena, CA 91125, USA
Correspondence e-mail: stephen.barlow@chem.ox.ac.uk

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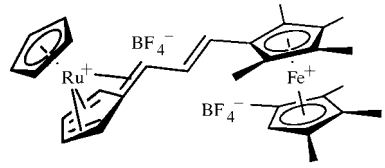
The 1-(2,3,4,5,1′,2′,3′,4′-octamethylferrocen-1-yl)-3-(ruthenocenyl)allylium cation readily undergoes one-electron oxidation to a dication in which an octamethylferrocenium moiety is bridged by a vinylene group to a [(η^6-fulvene)(η^5-cyclopentadienyl)ruthenium]$^+$ moiety. In the title compound, 1-(2,3,4,5,1′,2′,3′,4′-octamethylferrocen-1-yl)-3-(ruthenocenylidene)-prop-1-enium(2+) bis(tetrafluoroborate), [$FeRu(C_5H_5)(C_9H_{13})(C_{17}H_{19})](BF_4)_2$, the C—C bond lengths in the bridge (average for two independent molecules) are, starting from the *ipso* octamethylferrocenium carbon and ending at the *exo* carbon of the coordinated fulvene, 1.455 (6), 1.344 (3) and 1.449 (8) Å, indicating a localized electronic structure.

Comment

In the course of our work on symmetrical and unsymmetrical metallocene-terminated polymethines (Barlow *et al.*, 2000), aimed at understanding Peierls distortion effects in cyanines (Tolbert, 1992, and references therein), we attempted to isolate 1-(2,3,4,5,1′,2′,3′,4′-octamethylferrocen-1-yl)-3-(ruthenocenyl)allylium tetrafluoroborate by treating 1-(2,3,4,5,1′,2′,3′,4′-octamethylferrocen-1-yl)-3-(ruthenocenyl)prop-2-en-1-ol with anhydrous HBF_4. We found the product contained comparable amounts of the target compound and its one-electron oxidation product, (I), which is the subject of the present structure determination (Fig. 1). We did not encounter complications from oxidation in the analogous synthesis of a variety of related ferrocene and octamethylferrocene allylium salts. Significantly, electrochemistry shows 1-(2,3,4,5,1′,2′,3′,4′-octamethylferrocen-1-yl)-3-(ruthenocenyl)allylium is more easily oxidized ($E_{1/2}$ = −190 mV *versus* ferrocenium/ferrocene in tetrahydrofuran) than these other species ($E_{1/2}$ = −140 to +145 mV). Presumably the oxidant is H^+. Several cases of similar acids effecting the oxidation of organometallics with similar potentials have been reported (Connelly & Geiger, 1996, and references therein).



(I)

The octamethylferrocenyl moiety has clearly been oxidized; the average Fe—C distance of 2.098 (3) Å [range 2.065 (5)–2.120 (5) Å] may be compared with average Fe—C distances of 2.050 (2) Å for decamethylferrocene (Freyberg *et al.*, 1979) and between 2.086 (2) and 2.096 (1) Å for a variety of decamethylferrocenium salts (Miller *et al.*, 1987, and references therein). The ruthenium coordination is best described as (η^6-fulvene)(η^5-cyclopentadienyl) and is similar to that in other ruthenocenyl carbocations. The Ru—α-C distances of 2.367 (6) (molecule *A*) and 2.337 (6) Å (molecule *B*) can be compared with literature values ranging from 2.270 (3) to 2.571 (4) Å (Yanovsky *et al.*, 1989; Watanabe *et al.*, 1996*a*,*b*; Sato *et al.*, 1998; Barlow *et al.*, 1999), while the Ru—C(ring) distances fall in the range 2.082 (5) to 2.232 (5) Å. The allylium bridging group shows clear bond-length alternation [0.100 (10) Å in molecule *A* and 0.111 (11) Å in molecule *B*] between the formally single C29—C30 bond and the formally double C30—C31 bond, similar in magnitude to that in the structures of the Peierls-distorted cation 1,3-bis(ruthenocenyl)allylium [0.100 (6) Å] (Barlow *et al.*, 1999) and of 1-ferrocenyl-3-ruthenocenylallylium [0.100 (7) Å] (Barlow *et al.*, 2000), both of which can be considered as a (η^6-fulvene)(η^5-cyclopentadienyl)ruthenium cation vinylene-bridged to a 'normal' metallocene. Unfortunately, we have no direct evidence for the structure of our original target compound. However, electrochemical data suggest the structure may be similar to that of 1-(ferrocenyl)-3-(2,3,4,5,1′,2′,3′,4′-octamethylferrocen-1-yl)allylium (Barlow *et al.*, 2000), in which the cationic charge is shared, albeit

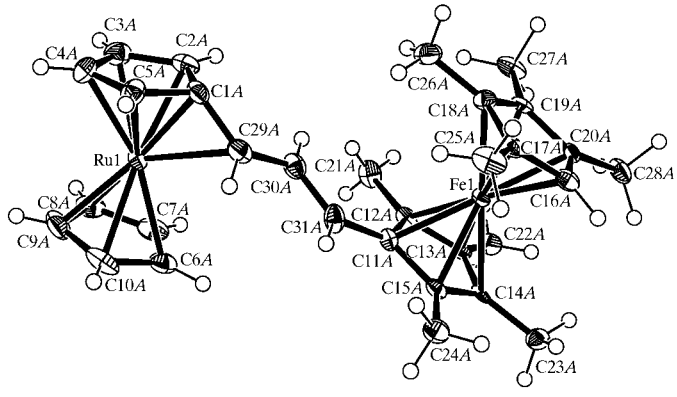


Figure 1
View of one of the two independent cations (*A*) in the asymmetric unit of (I), showing 50% displacement probability ellipsoids. The other cation is labeled in an analogous fashion and has a similar structure.

† Current address: Inorganic Chemistry Laboratory, South Parks Road, Oxford, OX1 3QR, England.
‡ Current address: Department of Chemistry, University of Arizona, Tucson, AZ 85721, USA.

unevenly, between the two metallocenes. Thus, it appears that, in this case, it is the oxidation which leads to the shift of the ruthenium to full fulvene coordination.

Experimental

Attempts were made to isolate 1-(2,3,4,5,1′,2′,3′,4′-octamethylferrocen-1-yl)-3-(ruthenocenyl)allylium tetrafluoroborate by the method we used for a range of other bis(metallocenyl)allylium salts (Barlow *et al.*, 2000). Specifically, a diethyl ether solution of 1-(2,3,4,5,1′,2′,3′,4′-octamethylferrocen-1-yl)-3-(ruthenocenyl)prop-2-en-1-ol (Barlow *et al.*, 2000) was treated with ethereal HBF_4. The resulting precipitate was washed with diethyl ether and extracted into dichloromethane solution. Layering of this solution with diethyl ether afforded a crystalline product, which was found to be a mixture of the desired compound and its one-electron oxidation product by elemental analysis (which indicated approximately half the material to be oxidized) and ^{1}H NMR (which indicated paramagnetic species present). Both compounds are reasonably stable in the solid state and in solution in deoxygenated dichloromethane, but solutions exposed to air, or in more polar solvents such as Me_2SO, slowly decompose. We were unable to separate the two compounds in bulk. However, a number of crystals were found to be the oxidation product and are the subject of the present structure determination.

Crystal data

$[FeRu(C_5H_5)(C_9H_{13})(C_{17}H_{19})](BF_4)_2$
M_r = 740.16
Monoclinic, $P2_1/c$
a = 19.178 (4) Å
b = 10.988 (3) Å
c = 28.728 (7) Å
β = 101.75 (2)°
V = 5927 (2) Å^3
Z = 8
D_x = 1.657 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 13.5–14.2°
μ = 1.071 mm^{-1}
T = 85 K
Blade, dark green–brown
0.39 × 0.33 × 0.14 mm

Data collection

CAD-4 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.666, T_{max} = 0.861
22 328 measured reflections
10 404 independent reflections
7469 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25°
$h = -22 \rightarrow 22$
$k = -13 \rightarrow 13$
$l = 0 \rightarrow 34$
3 standard reflections
frequency: 75 min
intensity decay: 0.36%

Refinement

Refinement on F^2
$R(F)$ = 0.052
$wR(F^2)$ = 0.095
S = 1.751
10 403 reflections
832 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/\sigma^2(F_o^2)$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.927 e Å^{-3}
$\Delta\rho_{min}$ = −0.851 e Å^{-3}

Refined C—H distances are in the range 0.78 (4)–1.14 (4) Å.

Data reduction: *CRYM* (Duchamp, 1964); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994).

Table 1
Selected geometric parameters (Å, °).

C1*A*—C29*A*	1.428 (7)	C1*B*—C29*B*	1.405 (7)
C11*A*—C31*A*	1.461 (7)	C11*B*—C31*B*	1.450 (7)
C29*A*—C30*A*	1.441 (7)	C29*B*—C30*B*	1.457 (8)
C30*A*—C31*A*	1.341 (7)	C30*B*—C31*B*	1.346 (8)
C1*A*—C29*A*—C30*A*	125.6 (6)	C1*B*—C29*B*—C30*B*	123.9 (6)
C31*A*—C30*A*—C29*A*	120.6 (5)	C31*B*—C30*B*—C29*B*	122.0 (6)
C30*A*—C31*A*—C11*A*	128.5 (5)	C30*B*—C31*B*—C11*B*	128.0 (5)

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD1066). Services for accessing these data are described at the back of the journal.

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1-(2,3,4,5,1′,2′,3′,4′-octamethylferrocenium-1-yl)- 3-(ruthenocenyl)allylium bis-tetrafluoroborate

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$c = 28.728\ (7)$ Å
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$V = 5927\ (2)$ Å^3
$Z = 8$
$F(000) = 3000$
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Cell parameters from 25 reflections
$\theta = 13.5–14.2°$
$\mu = 1.07$ mm^{-1}
$T = 85$ K
Blade, dark green-brown
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$h = -22 \rightarrow 22$
$k = -13 \rightarrow 13$
$l = 0 \rightarrow 34$
3 standard reflections every 75 min
intensity decay: decay 0.36%

Refinement

Refinement on F^2
Least-squares matrix: Full matrix
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.095$
$S = 1.75$
10403 reflections
832 parameters
3 restraints
Primary atom site location: Direct methods
Secondary atom site location: Difference Fourier map
Hydrogen site location: Geometric sites
H atoms treated by a mixture of independent and constrained refinement
Observed $w = 1/s^2(F_o^2)$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.93$ e Å^{-3}
$\Delta\rho_{min} = -0.85$ e Å^{-3}

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. The weighting scheme was based upon $1/[s^2(F_o^2)]$. The variances $[s^2(F_o^2)]$ were derived from counting statistics plus an additional term, $(0.014I)^2$, and the variances of the merged data were obtained by propagation of error plus the addition of another term, $(0.014\langle I\rangle)^2$. Disorder was modelled in one of the tetrafluoroborate anions; the populations of the two orientations were found to be approximately 84:16. Hydrogen atoms were placed geometrically; C–H bonding distances were refined, with the angles fixed. Their temperature factors were set to values 1.2 times those of the atoms to which they are bonded. The maximum and minimum residual electron density are both within 1 Å of Ru1.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
B1	0.0453 (3)	0.5147 (6)	0.2383 (2)	0.0226 (15)	
F1A	0.05756 (17)	0.5658 (3)	0.19663 (11)	0.0306 (8)	
F2A	0.04225 (19)	0.6059 (3)	0.27090 (12)	0.0368 (9)	
F3A	−0.02005 (19)	0.4541 (3)	0.22894 (12)	0.0385 (9)	
F4A	0.0992 (2)	0.4357 (4)	0.25669 (13)	0.0503 (11)	
B2	0.3808 (4)	0.1773 (6)	0.0048 (2)	0.0279 (17)	
F1B	0.3853 (3)	0.1081 (4)	0.04620 (14)	0.0643 (13)	
F2B	0.4025 (2)	0.2927 (3)	0.02012 (13)	0.0502 (11)	
F3B	0.42542 (19)	0.1262 (3)	−0.02103 (13)	0.0448 (10)	
F4B	0.3121 (2)	0.1772 (4)	−0.01776 (17)	0.0811 (16)	
B3	0.4347 (4)	0.5080 (7)	0.2466 (2)	0.0294 (17)	
F1C	0.44078 (18)	0.4080 (3)	0.21806 (12)	0.0352 (9)	
F2C	0.4385 (2)	0.4685 (4)	0.29268 (12)	0.0494 (11)	
F3C	0.36980 (18)	0.5660 (3)	0.23067 (12)	0.0343 (8)	
F4C	0.4885 (2)	0.5896 (3)	0.24421 (15)	0.0547 (12)	
B4	0.1203 (4)	0.8171 (6)	0.5014 (2)	0.0316 (18)	
F1D	0.08546 (18)	0.7114 (3)	0.48216 (11)	0.0356 (8)	
F2D	0.1147 (3)	0.9019 (4)	0.46390 (16)	0.0509 (16)	0.837 (8)
F3D	0.1919 (3)	0.7948 (4)	0.5150 (2)	0.066 (2)	0.837 (8)
F4D	0.0886 (3)	0.8673 (5)	0.5350 (2)	0.066 (2)	0.837 (8)
F2DA	0.1494 (10)	0.7813 (17)	0.5491 (5)	0.028 (6)*	0.163 (8)
F3DA	0.0744 (14)	0.916 (2)	0.5024 (12)	0.073 (10)*	0.163 (8)
F4DA	0.170 (2)	0.862 (3)	0.4844 (13)	0.087 (11)*	0.163 (8)
Ru1	0.55235 (2)	0.20543 (4)	0.396127 (14)	0.01718 (11)	
Fe1	0.70167 (4)	0.25312 (6)	0.64337 (3)	0.01469 (18)	
C1A	0.6204 (3)	0.3483 (5)	0.42313 (19)	0.0219 (13)	
C2A	0.6641 (3)	0.2551 (5)	0.4076 (2)	0.0257 (14)	
H2AA	0.701 (2)	0.214 (3)	0.4262 (12)	0.031*	
C3A	0.6394 (3)	0.2393 (5)	0.3584 (2)	0.0280 (15)	
H3AA	0.6550 (11)	0.187 (4)	0.3411 (12)	0.034*	

C4A	0.5842 (3)	0.3246 (5)	0.3422 (2)	0.0286 (15)
H4AA	0.5606 (15)	0.3330 (7)	0.3124 (19)	0.034*
C5A	0.5731 (3)	0.3929 (5)	0.38081 (19)	0.0274 (15)
H5AA	0.546 (2)	0.446 (4)	0.3798 (2)	0.033*
C6A	0.4818 (3)	0.1134 (5)	0.4366 (2)	0.0277 (14)
H6AA	0.4802 (3)	0.1330 (12)	0.4688 (19)	0.033*
C7A	0.5268 (3)	0.0252 (5)	0.4214 (2)	0.0303 (15)
H7AA	0.557 (2)	−0.021 (3)	0.4397 (13)	0.036*
C8A	0.5132 (3)	0.0272 (5)	0.3716 (2)	0.0322 (17)
H8AA	0.5320 (15)	−0.013 (3)	0.3556 (12)	0.039*
C9A	0.4598 (3)	0.1142 (6)	0.3553 (2)	0.0352 (17)
H9AA	0.4421 (12)	0.1324 (14)	0.325 (2)	0.042*
C10A	0.4397 (3)	0.1669 (6)	0.3952 (2)	0.0341 (16)
H10A	0.405 (2)	0.226 (4)	0.3947 (2)	0.041*
C11A	0.6188 (3)	0.1912 (5)	0.58880 (17)	0.0184 (12)
C12A	0.6735 (3)	0.1002 (4)	0.60060 (19)	0.0165 (12)
C13A	0.6793 (3)	0.0689 (5)	0.64934 (18)	0.0169 (12)
C14A	0.6286 (3)	0.1402 (5)	0.66832 (18)	0.0154 (12)
C15A	0.5911 (3)	0.2145 (5)	0.63077 (18)	0.0176 (12)
C16A	0.7327 (3)	0.3909 (5)	0.6921 (2)	0.0211 (13)
H16A	0.7055 (14)	0.4138 (12)	0.7181 (13)	0.025*
C17A	0.7206 (3)	0.4415 (5)	0.64486 (19)	0.0204 (13)
C18A	0.7692 (3)	0.3826 (5)	0.62048 (19)	0.0189 (12)
C19A	0.8107 (3)	0.2984 (5)	0.65262 (17)	0.0180 (12)
C20A	0.7878 (3)	0.3053 (5)	0.69657 (17)	0.0178 (11)
C21A	0.7130 (3)	0.0407 (5)	0.56697 (19)	0.0267 (15)
H21A	0.6905 (8)	−0.018 (2)	0.5547 (5)	0.032*
H21B	0.7517 (13)	0.0184 (9)	0.5814 (5)	0.032*
H21C	0.7181 (3)	0.0889 (16)	0.5466 (7)	0.032*
C22A	0.7274 (3)	−0.0265 (5)	0.67552 (19)	0.0234 (13)
H22A	0.7042 (7)	−0.100 (2)	0.6724 (2)	0.028*
H22B	0.7397 (5)	−0.0059 (7)	0.7072 (9)	0.028*
H22C	0.7679 (12)	−0.0319 (5)	0.6630 (4)	0.028*
C23A	0.6167 (3)	0.1372 (5)	0.71795 (18)	0.0236 (13)
H23A	0.5807 (10)	0.0787 (17)	0.7202 (2)	0.028*
H23B	0.6018 (5)	0.216 (2)	0.7263 (3)	0.028*
H23C	0.6600 (12)	0.1153 (8)	0.7392 (6)	0.028*
C24A	0.5311 (3)	0.2984 (5)	0.63414 (19)	0.0258 (13)
H24A	0.4872 (13)	0.2553 (12)	0.6263 (3)	0.031*
H24B	0.5307 (3)	0.3644 (19)	0.6126 (6)	0.031*
H24C	0.5373 (3)	0.3291 (10)	0.6657 (9)	0.031*
C25A	0.6678 (3)	0.5379 (5)	0.6262 (2)	0.0308 (15)
H25A	0.6902 (7)	0.616 (2)	0.6315 (3)	0.037*
H25B	0.6286 (12)	0.5337 (5)	0.6423 (5)	0.037*
H25C	0.6506 (6)	0.5259 (6)	0.5926 (10)	0.037*
C26A	0.7757 (3)	0.4083 (5)	0.5706 (2)	0.0292 (15)
H26A	0.8086 (10)	0.4679 (18)	0.5705 (2)	0.035*
H26B	0.7327 (13)	0.4331 (9)	0.5535 (6)	0.035*

H26C	0.7896 (5)	0.339 (2)	0.5574 (5)	0.035*
C27A	0.8685 (3)	0.2185 (5)	0.6423 (2)	0.0283 (14)
H27A	0.9177 (13)	0.2658 (13)	0.6504 (3)	0.034*
H27B	0.8571 (4)	0.1942 (8)	0.6058 (10)	0.034*
H27C	0.8718 (3)	0.139 (2)	0.6634 (6)	0.034*
C28A	0.8184 (3)	0.2351 (5)	0.74085 (19)	0.0270 (14)
H28A	0.8603 (11)	0.2824 (13)	0.7604 (6)	0.032*
H28B	0.8357 (5)	0.152 (2)	0.7318 (3)	0.032*
H28C	0.7800 (10)	0.2233 (6)	0.7606 (6)	0.032*
C29A	0.5907 (3)	0.3283 (5)	0.4642 (2)	0.0272 (14)
H29A	0.542 (4)	0.367 (3)	0.4644 (2)	0.08 (3)*
C30A	0.6232 (3)	0.2585 (5)	0.50540 (19)	0.0233 (14)
H30A	0.666 (2)	0.214 (3)	0.50522 (19)	0.028*
C31A	0.5939 (3)	0.2555 (5)	0.54401 (19)	0.0252 (14)
H31A	0.555 (3)	0.297 (3)	0.5421 (2)	0.030*
Ru2	0.06210 (2)	0.29927 (4)	0.384733 (14)	0.01472 (11)
Fe2	0.21271 (4)	0.26160 (7)	0.62912 (3)	0.01586 (18)
C1B	0.1353 (3)	0.1638 (5)	0.41121 (19)	0.0226 (13)
C2B	0.1769 (3)	0.2656 (5)	0.3991 (2)	0.0227 (13)
H2BA	0.214 (2)	0.313 (3)	0.4215 (12)	0.027*
C3B	0.1552 (3)	0.2846 (6)	0.3494 (2)	0.0262 (13)
H3BA	0.1755 (10)	0.359 (4)	0.3281 (10)	0.031*
C4B	0.1036 (3)	0.1943 (5)	0.3305 (2)	0.0265 (13)
H4BA	0.0795 (13)	0.1869 (7)	0.2965 (19)	0.032*
C5B	0.0921 (3)	0.1177 (5)	0.3672 (2)	0.0261 (14)
H5BA	0.0618 (18)	0.049 (4)	0.3640 (3)	0.031*
C6B	−0.0188 (3)	0.3659 (5)	0.4216 (2)	0.0248 (14)
H6BA	−0.0232 (4)	0.3389 (17)	0.4503 (17)	0.030*
C7B	0.0232 (3)	0.4666 (5)	0.4132 (2)	0.0253 (14)
H7BA	0.0482 (17)	0.512 (3)	0.4341 (14)	0.030*
C8B	0.0154 (3)	0.4772 (5)	0.3634 (2)	0.0246 (14)
H8BA	0.0387 (13)	0.540 (3)	0.3464 (9)	0.029*
C9B	−0.0313 (3)	0.3829 (5)	0.3412 (2)	0.0251 (14)
H9BA	−0.0463 (8)	0.3676 (10)	0.3059 (19)	0.030*
C10B	−0.0527 (3)	0.3150 (5)	0.3778 (2)	0.0260 (14)
H10B	−0.0822 (19)	0.252 (4)	0.3738 (3)	0.031*
C11B	0.1232 (3)	0.3047 (5)	0.57612 (18)	0.0190 (12)
C12B	0.1004 (3)	0.2725 (5)	0.61872 (19)	0.0197 (13)
C13B	0.1329 (3)	0.3532 (5)	0.65516 (19)	0.0222 (13)
C14B	0.1755 (3)	0.4373 (5)	0.63547 (19)	0.0200 (13)
C15B	0.1698 (3)	0.4083 (5)	0.58632 (19)	0.0195 (12)
C16B	0.3158 (3)	0.2273 (5)	0.61973 (19)	0.0210 (13)
H16B	0.3391 (13)	0.273 (3)	0.5993 (11)	0.025*
C17B	0.2732 (3)	0.1208 (5)	0.6070 (2)	0.0197 (13)
C18B	0.2465 (3)	0.0816 (5)	0.64694 (19)	0.0205 (13)
C19B	0.2743 (3)	0.1640 (5)	0.68558 (18)	0.0191 (12)
C20B	0.3168 (3)	0.2519 (5)	0.66790 (19)	0.0212 (13)
C21B	0.0494 (3)	0.1716 (5)	0.6228 (2)	0.0305 (16)

H21D	0.0048 (14)	0.2006 (10)	0.6165 (3)	0.037*
H21E	0.0594 (4)	0.1411 (11)	0.6523 (9)	0.037*
H21F	0.0536 (3)	0.1128 (19)	0.6019 (7)	0.037*
C22B	0.1225 (3)	0.3519 (5)	0.70577 (19)	0.0285 (15)
H22D	0.0833 (12)	0.4001 (15)	0.7082 (2)	0.034*
H22E	0.1632 (12)	0.3827 (10)	0.7258 (6)	0.034*
H22F	0.1146 (4)	0.272 (2)	0.7147 (3)	0.034*
C23B	0.2173 (3)	0.5410 (5)	0.6609 (2)	0.0283 (15)
H23D	0.1899 (8)	0.607 (2)	0.6587 (2)	0.034*
H23E	0.2545 (12)	0.5561 (7)	0.6479 (4)	0.034*
H23F	0.2322 (6)	0.5217 (7)	0.6913 (9)	0.034*
C24B	0.2022 (3)	0.4816 (5)	0.5522 (2)	0.0273 (15)
H24D	0.1714 (10)	0.5389 (18)	0.5389 (5)	0.033*
H24E	0.2123 (4)	0.4329 (15)	0.5296 (7)	0.033*
H24F	0.2421 (12)	0.5169 (12)	0.5678 (5)	0.033*
C25B	0.2612 (3)	0.0639 (5)	0.5588 (2)	0.0315 (15)
H25D	0.2971 (11)	0.0007 (19)	0.5584 (2)	0.038*
H25E	0.2649 (3)	0.1262 (18)	0.5351 (7)	0.038*
H25F	0.2136 (14)	0.0273 (12)	0.5515 (3)	0.038*
C26B	0.2010 (3)	−0.0262 (5)	0.6492 (2)	0.0315 (15)
H26D	0.2319 (9)	−0.099 (2)	0.6587 (3)	0.038*
H26E	0.1696 (10)	−0.0405 (7)	0.6172 (9)	0.038*
H26F	0.1706 (9)	−0.0117 (6)	0.6733 (7)	0.038*
C27B	0.2637 (3)	0.1565 (5)	0.73517 (19)	0.0302 (14)
H27D	0.3026 (11)	0.1019 (16)	0.7548 (6)	0.036*
H27E	0.2143 (14)	0.1198 (11)	0.73534 (19)	0.036*
H27F	0.2668 (3)	0.242 (2)	0.7498 (5)	0.036*
C28B	0.3603 (3)	0.3505 (5)	0.6973 (2)	0.0307 (14)
H28D	0.4126 (14)	0.3152 (10)	0.7130 (5)	0.037*
H28E	0.3336 (7)	0.3795 (9)	0.7252 (8)	0.037*
H28F	0.3658 (3)	0.427 (2)	0.6746 (6)	0.037*
C29B	0.1020 (3)	0.1733 (5)	0.4503 (2)	0.0292 (15)
H29B	0.052 (3)	0.125 (3)	0.4487 (2)	0.05 (2)*
C30B	0.1303 (3)	0.2438 (5)	0.4929 (2)	0.0297 (15)
H30B	0.172 (2)	0.295 (3)	0.4935 (2)	0.036*
C31B	0.1007 (3)	0.2405 (5)	0.53150 (19)	0.0259 (14)
H31B	0.062 (2)	0.192 (3)	0.5293 (2)	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
B1	0.016 (3)	0.024 (4)	0.025 (4)	0.000 (3)	−0.001 (3)	−0.004 (3)
F1A	0.031 (2)	0.038 (2)	0.0230 (18)	−0.0023 (16)	0.0057 (16)	0.0029 (15)
F2A	0.044 (2)	0.039 (2)	0.034 (2)	−0.0160 (17)	0.0225 (18)	−0.0169 (16)
F3A	0.037 (2)	0.040 (2)	0.038 (2)	−0.0199 (17)	0.0046 (18)	−0.0030 (16)
F4A	0.047 (3)	0.054 (3)	0.050 (2)	0.026 (2)	0.012 (2)	0.0178 (19)
B2	0.025 (4)	0.031 (5)	0.027 (4)	−0.009 (3)	0.006 (3)	−0.009 (3)
F1B	0.104 (4)	0.041 (3)	0.057 (3)	0.018 (2)	0.039 (3)	0.006 (2)

F2B	0.055 (3)	0.035 (2)	0.068 (3)	−0.020 (2)	0.032 (2)	−0.025 (2)
F3B	0.036 (2)	0.050 (3)	0.051 (2)	−0.0004 (18)	0.016 (2)	−0.0232 (19)
F4B	0.033 (2)	0.095 (4)	0.095 (3)	0.023 (2)	−0.034 (2)	−0.058 (3)
B3	0.022 (4)	0.038 (4)	0.029 (4)	−0.009 (3)	0.006 (3)	−0.006 (3)
F1C	0.034 (2)	0.029 (2)	0.047 (2)	−0.0075 (16)	0.0184 (18)	−0.0145 (16)
F2C	0.051 (3)	0.063 (3)	0.028 (2)	0.006 (2)	−0.0054 (19)	−0.0003 (18)
F3C	0.030 (2)	0.036 (2)	0.041 (2)	0.0022 (16)	0.0163 (18)	0.0053 (16)
F4C	0.034 (2)	0.054 (3)	0.080 (3)	−0.025 (2)	0.022 (2)	−0.031 (2)
B4	0.040 (5)	0.029 (5)	0.028 (4)	−0.008 (3)	0.011 (4)	0.002 (3)
F1D	0.043 (2)	0.030 (2)	0.0348 (19)	−0.0165 (17)	0.0097 (17)	−0.0098 (16)
F2D	0.076 (4)	0.030 (3)	0.046 (3)	0.000 (3)	0.010 (3)	0.012 (2)
F3D	0.042 (3)	0.033 (3)	0.100 (5)	0.015 (2)	−0.042 (3)	−0.027 (3)
F4D	0.099 (5)	0.050 (3)	0.067 (4)	−0.035 (3)	0.061 (4)	−0.031 (3)
Ru1	0.0164 (2)	0.0153 (2)	0.0182 (2)	−0.0003 (2)	−0.00032 (19)	0.00000 (19)
Fe1	0.0129 (4)	0.0142 (4)	0.0159 (4)	0.0008 (3)	0.0006 (3)	0.0027 (3)
C1A	0.020 (3)	0.020 (3)	0.024 (3)	−0.006 (2)	−0.002 (3)	0.002 (2)
C2A	0.016 (3)	0.024 (3)	0.037 (4)	−0.002 (2)	0.005 (3)	0.005 (3)
C3A	0.029 (4)	0.027 (3)	0.031 (3)	−0.005 (3)	0.013 (3)	−0.007 (3)
C4A	0.033 (4)	0.032 (4)	0.021 (3)	−0.002 (3)	0.006 (3)	0.008 (3)
C5A	0.038 (4)	0.022 (3)	0.022 (3)	−0.003 (3)	0.007 (3)	0.003 (2)
C6A	0.023 (3)	0.026 (4)	0.035 (4)	−0.009 (3)	0.008 (3)	−0.001 (3)
C7A	0.028 (4)	0.015 (3)	0.048 (4)	−0.007 (3)	0.009 (3)	0.003 (3)
C8A	0.031 (4)	0.024 (4)	0.044 (4)	−0.012 (3)	0.016 (3)	−0.014 (3)
C9A	0.028 (4)	0.037 (4)	0.035 (4)	−0.012 (3)	−0.007 (3)	−0.003 (3)
C10A	0.016 (3)	0.025 (4)	0.058 (5)	−0.003 (3)	0.000 (3)	−0.003 (3)
C11A	0.017 (3)	0.019 (3)	0.017 (3)	0.000 (2)	−0.001 (2)	−0.001 (2)
C12A	0.014 (3)	0.011 (3)	0.023 (3)	0.003 (2)	0.001 (2)	−0.002 (2)
C13A	0.015 (3)	0.013 (3)	0.022 (3)	−0.003 (2)	0.003 (2)	0.000 (2)
C14A	0.011 (3)	0.011 (3)	0.022 (3)	−0.008 (2)	−0.002 (2)	0.000 (2)
C15A	0.013 (3)	0.016 (3)	0.023 (3)	−0.003 (2)	0.002 (2)	−0.006 (2)
C16A	0.022 (3)	0.013 (3)	0.028 (3)	−0.006 (2)	0.004 (3)	−0.002 (2)
C17A	0.019 (3)	0.016 (3)	0.025 (3)	−0.006 (2)	0.000 (3)	0.006 (2)
C18A	0.016 (3)	0.019 (3)	0.022 (3)	0.002 (2)	0.005 (3)	0.003 (2)
C19A	0.009 (3)	0.018 (3)	0.026 (3)	−0.004 (2)	0.003 (2)	−0.003 (2)
C20A	0.017 (3)	0.020 (3)	0.014 (3)	−0.008 (2)	−0.002 (2)	0.001 (2)
C21A	0.024 (3)	0.024 (3)	0.029 (3)	0.010 (3)	−0.001 (3)	0.000 (3)
C22A	0.021 (3)	0.022 (3)	0.028 (3)	0.002 (2)	0.004 (3)	0.005 (2)
C23A	0.023 (3)	0.025 (3)	0.023 (3)	−0.002 (3)	0.006 (3)	0.004 (2)
C24A	0.017 (3)	0.031 (3)	0.029 (3)	0.006 (3)	0.004 (3)	0.001 (3)
C25A	0.025 (4)	0.018 (3)	0.049 (4)	0.003 (3)	0.006 (3)	0.006 (3)
C26A	0.028 (4)	0.030 (4)	0.031 (4)	−0.006 (3)	0.012 (3)	0.002 (3)
C27A	0.020 (3)	0.017 (3)	0.048 (4)	−0.002 (2)	0.007 (3)	−0.006 (3)
C28A	0.023 (3)	0.028 (3)	0.025 (3)	−0.007 (3)	−0.007 (3)	0.006 (2)
C29A	0.022 (3)	0.029 (4)	0.029 (3)	−0.006 (3)	0.002 (3)	−0.001 (3)
C30A	0.023 (3)	0.020 (3)	0.025 (3)	0.000 (2)	−0.001 (3)	0.001 (2)
C31A	0.024 (3)	0.028 (3)	0.021 (3)	0.008 (3)	−0.002 (3)	−0.003 (2)
Ru2	0.0122 (2)	0.0153 (2)	0.0154 (2)	0.00158 (19)	−0.00003 (18)	−0.00049 (18)
Fe2	0.0135 (4)	0.0162 (4)	0.0162 (4)	0.0020 (3)	−0.0008 (3)	−0.0011 (3)

C1B	0.022 (3)	0.022 (3)	0.023 (3)	0.009 (3)	0.003 (3)	0.000 (2)
C2B	0.012 (3)	0.024 (3)	0.033 (3)	0.006 (2)	0.005 (3)	−0.001 (3)
C3B	0.014 (3)	0.036 (4)	0.031 (3)	0.004 (3)	0.010 (3)	−0.004 (3)
C4B	0.028 (3)	0.031 (3)	0.022 (3)	0.009 (3)	0.008 (3)	−0.006 (3)
C5B	0.027 (3)	0.019 (3)	0.029 (3)	0.009 (3)	−0.002 (3)	−0.009 (3)
C6B	0.022 (3)	0.024 (3)	0.030 (3)	0.007 (3)	0.008 (3)	0.005 (3)
C7B	0.017 (3)	0.025 (3)	0.031 (4)	0.004 (3)	0.000 (3)	−0.008 (3)
C8B	0.016 (3)	0.017 (3)	0.041 (4)	0.006 (2)	0.004 (3)	0.007 (3)
C9B	0.017 (3)	0.024 (3)	0.029 (3)	0.007 (3)	−0.007 (3)	0.000 (3)
C10B	0.015 (3)	0.022 (3)	0.040 (4)	−0.002 (3)	0.002 (3)	0.006 (3)
C11B	0.012 (3)	0.020 (3)	0.022 (3)	0.000 (2)	−0.002 (2)	0.007 (2)
C12B	0.009 (3)	0.023 (3)	0.025 (3)	0.005 (2)	−0.002 (2)	0.009 (2)
C13B	0.019 (3)	0.029 (3)	0.020 (3)	0.012 (3)	0.006 (3)	0.006 (2)
C14B	0.013 (3)	0.019 (3)	0.027 (3)	0.006 (2)	0.001 (3)	0.000 (2)
C15B	0.016 (3)	0.020 (3)	0.020 (3)	0.002 (2)	−0.001 (2)	0.003 (2)
C16B	0.013 (3)	0.025 (3)	0.027 (3)	0.002 (2)	0.007 (2)	−0.001 (2)
C17B	0.012 (3)	0.016 (3)	0.031 (3)	0.006 (2)	0.002 (3)	−0.003 (2)
C18B	0.014 (3)	0.017 (3)	0.030 (3)	0.011 (2)	0.003 (3)	0.004 (2)
C19B	0.018 (3)	0.020 (3)	0.018 (3)	0.010 (2)	0.002 (2)	0.006 (2)
C20B	0.016 (3)	0.021 (3)	0.025 (3)	0.006 (2)	−0.001 (2)	0.006 (2)
C21B	0.017 (3)	0.038 (4)	0.033 (3)	−0.003 (3)	−0.001 (3)	0.013 (3)
C22B	0.023 (3)	0.031 (3)	0.030 (3)	0.011 (3)	0.002 (3)	0.004 (3)
C23B	0.024 (3)	0.028 (4)	0.031 (3)	0.007 (3)	0.001 (3)	−0.010 (3)
C24B	0.037 (4)	0.014 (3)	0.031 (3)	−0.008 (3)	0.007 (3)	0.002 (2)
C25B	0.034 (4)	0.025 (3)	0.037 (4)	0.002 (3)	0.013 (3)	−0.005 (3)
C26B	0.027 (4)	0.020 (3)	0.050 (4)	0.002 (3)	0.014 (3)	0.008 (3)
C27B	0.030 (4)	0.030 (3)	0.030 (3)	0.015 (3)	0.004 (3)	0.008 (3)
C28B	0.023 (3)	0.025 (3)	0.040 (4)	0.002 (3)	−0.002 (3)	−0.004 (3)
C29B	0.025 (3)	0.026 (4)	0.032 (4)	0.000 (3)	−0.005 (3)	0.002 (3)
C30B	0.023 (4)	0.027 (4)	0.034 (4)	−0.003 (3)	−0.005 (3)	0.005 (3)
C31B	0.019 (3)	0.035 (4)	0.020 (3)	−0.009 (3)	−0.005 (3)	0.006 (3)

Geometric parameters (Å, º)

B1—F4A	1.371 (7)	C26A—H26B	0.9109
B1—F2A	1.380 (7)	C26A—H26C	0.9109
B1—F1A	1.386 (7)	C27A—H27A	1.0608
B1—F3A	1.396 (7)	C27A—H27B	1.0609
B2—F4B	1.346 (8)	C27A—H27C	1.0608
B2—F3B	1.362 (7)	C28A—H28A	1.0242
B2—F2B	1.379 (7)	C28A—H28B	1.0242
B2—F1B	1.399 (8)	C28A—H28C	1.0242
B3—F2C	1.380 (8)	C29A—C30A	1.441 (7)
B3—F4C	1.379 (7)	C29A—H29A	1.0275
B3—F1C	1.390 (7)	C30A—C31A	1.341 (7)
B3—F3C	1.390 (8)	C30A—H30A	0.9502
B4—F3DA	1.403 (11)	C31A—H31A	0.8647
B4—F4DA	1.26 (3)	Ru2—C1B	2.082 (5)

B4—F4D	1.358 (8)	Ru2—C5B	2.163 (5)
B4—F3D	1.372 (9)	Ru2—C9B	2.170 (5)
B4—F2D	1.412 (7)	Ru2—C10B	2.176 (5)
B4—F1D	1.396 (8)	Ru2—C6B	2.177 (5)
B4—F2DA	1.426 (10)	Ru2—C8B	2.186 (5)
F2D—F3DA	1.48 (3)	Ru2—C2B	2.186 (5)
F2D—F4DA	1.20 (4)	Ru2—C7B	2.204 (5)
F3D—F4DA	1.15 (4)	Ru2—C4B	2.212 (5)
F3D—F2DA	1.402 (18)	Ru2—C3B	2.232 (5)
F4D—F3DA	1.06 (3)	Ru2—C29B	2.337 (6)
F4D—F2DA	1.493 (18)	Fe2—C14B	2.079 (5)
F3DA—F4DA	2.10 (4)	Fe2—C20B	2.082 (5)
Ru1—C1A	2.088 (5)	Fe2—C16B	2.083 (5)
Ru1—C5A	2.160 (6)	Fe2—C15B	2.092 (5)
Ru1—C8A	2.163 (6)	Fe2—C13B	2.093 (5)
Ru1—C9A	2.164 (6)	Fe2—C19B	2.097 (5)
Ru1—C2A	2.170 (6)	Fe2—C11B	2.103 (5)
Ru1—C10A	2.196 (6)	Fe2—C17B	2.108 (5)
Ru1—C7A	2.199 (6)	Fe2—C18B	2.111 (5)
Ru1—C3A	2.200 (6)	Fe2—C12B	2.117 (5)
Ru1—C6A	2.200 (6)	C1B—C29B	1.405 (7)
Ru1—C4A	2.207 (5)	C1B—C2B	1.456 (8)
Ru1—C29A	2.367 (6)	C1B—C5B	1.453 (8)
Fe1—C16A	2.065 (5)	C2B—C3B	1.418 (8)
Fe1—C12A	2.087 (5)	C2B—H2BA	0.9974
Fe1—C13A	2.083 (5)	C3B—C4B	1.428 (8)
Fe1—C20A	2.089 (5)	C3B—H3BA	1.1394
Fe1—C17A	2.101 (5)	C4B—C5B	1.401 (8)
Fe1—C11A	2.105 (5)	C4B—H4BA	0.9966
Fe1—C14A	2.104 (5)	C5B—H5BA	0.9471
Fe1—C19A	2.114 (5)	C6B—C10B	1.410 (8)
Fe1—C18A	2.117 (5)	C6B—C7B	1.418 (8)
Fe1—C15A	2.120 (5)	C6B—H6BA	0.8948
C1A—C29A	1.428 (7)	C7B—C8B	1.414 (8)
C1A—C5A	1.447 (7)	C7B—H7BA	0.8495
C1A—C2A	1.450 (8)	C8B—C9B	1.432 (8)
C2A—C3A	1.407 (8)	C8B—H8BA	1.0020
C2A—H2AA	0.9081	C9B—C10B	1.416 (8)
C3A—C4A	1.420 (8)	C9B—H9BA	1.0103
C3A—H3AA	0.8508	C10B—H10B	0.8897
C4A—C5A	1.390 (8)	C11B—C12B	1.426 (7)
C4A—H4AA	0.8882	C11B—C15B	1.440 (7)
C5A—H5AA	0.7784	C11B—C31B	1.450 (7)
C6A—C7A	1.422 (8)	C12B—C13B	1.416 (8)
C6A—C10A	1.420 (8)	C12B—C21B	1.497 (7)
C6A—H6AA	0.9576	C13B—C14B	1.425 (8)
C7A—C8A	1.400 (8)	C13B—C22B	1.507 (7)
C7A—H7AA	0.8695	C14B—C15B	1.430 (7)

C8A—C9A	1.409 (8)	C14B—C23B	1.496 (7)
C8A—H8AA	0.7782	C15B—C24B	1.496 (7)
C9A—C10A	1.406 (8)	C16B—C20B	1.406 (7)
C9A—H9AA	0.8817	C16B—C17B	1.432 (7)
C10A—H10A	0.9256	C16B—H16B	0.9521
C11A—C15A	1.437 (7)	C17B—C18B	1.416 (7)
C11A—C12A	1.439 (7)	C17B—C25B	1.492 (7)
C11A—C31A	1.461 (7)	C18B—C19B	1.448 (7)
C12A—C13A	1.424 (7)	C18B—C26B	1.480 (7)
C12A—C21A	1.493 (7)	C19B—C20B	1.423 (7)
C13A—C14A	1.439 (7)	C19B—C27B	1.482 (7)
C13A—C22A	1.494 (7)	C20B—C28B	1.515 (8)
C14A—C15A	1.425 (7)	C21B—H21D	0.8967
C14A—C23A	1.489 (7)	C21B—H21E	0.8967
C15A—C24A	1.492 (7)	C21B—H21F	0.8967
C16A—C20A	1.401 (7)	C22B—H22D	0.9338
C16A—C17A	1.440 (7)	C22B—H22E	0.9338
C16A—H16A	1.0274	C22B—H22F	0.9338
C17A—C18A	1.429 (7)	C23B—H23D	0.8870
C17A—C25A	1.488 (7)	C23B—H23E	0.8870
C18A—C19A	1.429 (7)	C23B—H23F	0.8870
C18A—C26A	1.490 (7)	C24B—H24D	0.8938
C19A—C20A	1.421 (7)	C24B—H24E	0.8938
C19A—C27A	1.490 (7)	C24B—H24F	0.8938
C20A—C28A	1.501 (7)	C25B—H25D	0.9800
C21A—H21A	0.8104	C25B—H25E	0.9800
C21A—H21B	0.8104	C25B—H25F	0.9800
C21A—H21C	0.8104	C26B—H26D	1.0042
C22A—H22A	0.9217	C26B—H26E	1.0042
C22A—H22B	0.9217	C26B—H26F	1.0042
C22A—H22C	0.9217	C27B—H27D	1.0310
C23A—H23A	0.9560	C27B—H27E	1.0310
C23A—H23B	0.9560	C27B—H27F	1.0310
C23A—H23C	0.9560	C28B—H28D	1.0849
C24A—H24A	0.9531	C28B—H28E	1.0849
C24A—H24B	0.9531	C28B—H28F	1.0849
C24A—H24C	0.9531	C29B—C30B	1.457 (8)
C25A—H25A	0.9619	C29B—H29B	1.0833
C25A—H25B	0.9619	C30B—C31B	1.346 (8)
C25A—H25C	0.9619	C30B—H30B	0.9719
C26A—H26A	0.9109	C31B—H31B	0.9065

F4A—B1—F2A	109.4 (5)	H25B—C25A—H25C	109.5
F4A—B1—F1A	109.9 (5)	C18A—C26A—H26A	109.5
F2A—B1—F1A	109.3 (5)	C18A—C26A—H26B	109.5
F4A—B1—F3A	110.4 (5)	H26A—C26A—H26B	109.5
F2A—B1—F3A	108.5 (5)	C18A—C26A—H26C	109.5
F1A—B1—F3A	109.2 (5)	H26A—C26A—H26C	109.5

F4B—B2—F3B	113.5 (5)	H26B—C26A—H26C	109.5
F4B—B2—F2B	110.8 (6)	C19A—C27A—H27A	109.5
F3B—B2—F2B	111.8 (5)	C19A—C27A—H27B	109.5
F4B—B2—F1B	107.1 (6)	H27A—C27A—H27B	109.5
F3B—B2—F1B	107.6 (6)	C19A—C27A—H27C	109.5
F2B—B2—F1B	105.4 (5)	H27A—C27A—H27C	109.5
F2C—B3—F4C	111.0 (5)	H27B—C27A—H27C	109.5
F2C—B3—F1C	108.9 (6)	C20A—C28A—H28A	109.5
F4C—B3—F1C	109.3 (5)	C20A—C28A—H28B	109.5
F2C—B3—F3C	109.2 (5)	H28A—C28A—H28B	109.5
F4C—B3—F3C	108.3 (6)	C20A—C28A—H28C	109.5
F1C—B3—F3C	110.2 (5)	H28A—C28A—H28C	109.5
F3DA—B4—F4DA	104 (2)	H28B—C28A—H28C	109.5
F3DA—B4—F4D	45.3 (13)	C1A—C29A—C30A	125.6 (6)
F4DA—B4—F4D	127.1 (17)	C1A—C29A—Ru1	61.0 (3)
F3DA—B4—F3D	136.7 (14)	C30A—C29A—Ru1	112.6 (4)
F4DA—B4—F3D	51.8 (18)	C1A—C29A—H29A	117.2
F4D—B4—F3D	115.9 (6)	C30A—C29A—H29A	117.2
F3DA—B4—F2D	63.5 (14)	Ru1—C29A—H29A	96.3
F4DA—B4—F2D	52.8 (18)	C31A—C30A—C29A	120.6 (5)
F4D—B4—F2D	107.3 (6)	C31A—C30A—H30A	119.7
F3D—B4—F2D	104.6 (6)	C29A—C30A—H30A	119.7
F3DA—B4—F1D	113.7 (14)	C30A—C31A—C11A	128.5 (5)
F4DA—B4—F1D	120.7 (16)	C30A—C31A—H31A	115.7
F4D—B4—F1D	111.9 (5)	C11A—C31A—H31A	115.7
F3D—B4—F1D	109.6 (6)	C1B—Ru2—C5B	40.0 (2)
F2D—B4—F1D	107.0 (5)	C1B—Ru2—C9B	158.5 (2)
F3DA—B4—F2DA	108.6 (17)	C5B—Ru2—C9B	118.9 (2)
F4DA—B4—F2DA	107 (2)	C1B—Ru2—C10B	133.2 (2)
F4D—B4—F2DA	64.8 (9)	C5B—Ru2—C10B	111.3 (2)
F3D—B4—F2DA	60.1 (9)	C9B—Ru2—C10B	38.0 (2)
F2D—B4—F2DA	150.3 (10)	C1B—Ru2—C6B	123.9 (2)
F1D—B4—F2DA	102.3 (9)	C5B—Ru2—C6B	132.3 (2)
F3DA—F2D—F4DA	102.8 (19)	C9B—Ru2—C6B	63.4 (2)
F3DA—F2D—B4	58.0 (8)	C10B—Ru2—C6B	37.8 (2)
F4DA—F2D—B4	57.2 (17)	C1B—Ru2—C8B	161.8 (2)
F4DA—F3D—B4	59.2 (18)	C5B—Ru2—C8B	150.8 (2)
F4DA—F3D—F2DA	115.5 (19)	C9B—Ru2—C8B	38.4 (2)
B4—F3D—F2DA	61.8 (6)	C10B—Ru2—C8B	63.5 (2)
F3DA—F4D—B4	69.6 (9)	C6B—Ru2—C8B	62.9 (2)
F3DA—F4D—F2DA	127.1 (13)	C1B—Ru2—C2B	39.8 (2)
B4—F4D—F2DA	59.8 (6)	C5B—Ru2—C2B	65.3 (2)
F3D—F2DA—F4D	106.1 (9)	C9B—Ru2—C2B	149.5 (2)
F3D—F2DA—B4	58.1 (7)	C10B—Ru2—C2B	172.4 (2)
F4D—F2DA—B4	55.4 (6)	C6B—Ru2—C2B	139.0 (2)
B4—F3DA—F4D	65.1 (10)	C8B—Ru2—C2B	122.9 (2)
B4—F3DA—F2D	58.6 (8)	C1B—Ru2—C7B	135.7 (2)
F4D—F3DA—F2D	121.7 (12)	C5B—Ru2—C7B	169.0 (2)

B4—F3DA—F4DA	35.8 (12)	C9B—Ru2—C7B	63.8 (2)
F4D—F3DA—F4DA	89.6 (15)	C10B—Ru2—C7B	63.6 (2)
F2D—F3DA—F4DA	33.8 (11)	C6B—Ru2—C7B	37.8 (2)
F3D—F4DA—F2D	139 (3)	C8B—Ru2—C7B	37.6 (2)
F3D—F4DA—B4	69.0 (19)	C2B—Ru2—C7B	118.4 (2)
F2D—F4DA—B4	70 (2)	C1B—Ru2—C4B	64.6 (2)
F3D—F4DA—F3DA	101 (2)	C5B—Ru2—C4B	37.3 (2)
F2D—F4DA—F3DA	43.5 (15)	C9B—Ru2—C4B	100.8 (2)
B4—F4DA—F3DA	40.5 (14)	C10B—Ru2—C4B	118.6 (2)
C1A—Ru1—C5A	39.8 (2)	C6B—Ru2—C4B	155.9 (2)
C1A—Ru1—C8A	162.0 (2)	C8B—Ru2—C4B	117.0 (2)
C5A—Ru1—C8A	149.7 (2)	C2B—Ru2—C4B	63.4 (2)
C1A—Ru1—C9A	158.7 (2)	C7B—Ru2—C4B	153.4 (2)
C5A—Ru1—C9A	119.7 (2)	C1B—Ru2—C3B	64.6 (2)
C8A—Ru1—C9A	38.0 (2)	C5B—Ru2—C3B	63.4 (2)
C1A—Ru1—C2A	39.8 (2)	C9B—Ru2—C3B	114.3 (2)
C5A—Ru1—C2A	64.8 (2)	C10B—Ru2—C3B	148.4 (2)
C8A—Ru1—C2A	122.9 (2)	C6B—Ru2—C3B	164.0 (2)
C9A—Ru1—C2A	151.0 (2)	C8B—Ru2—C3B	104.9 (2)
C1A—Ru1—C10A	133.5 (2)	C2B—Ru2—C3B	37.4 (2)
C5A—Ru1—C10A	113.7 (2)	C7B—Ru2—C3B	126.3 (2)
C8A—Ru1—C10A	63.0 (2)	C4B—Ru2—C3B	37.5 (2)
C9A—Ru1—C10A	37.6 (2)	C1B—Ru2—C29B	36.5 (2)
C2A—Ru1—C10A	171.3 (2)	C5B—Ru2—C29B	65.3 (2)
C1A—Ru1—C7A	136.0 (2)	C9B—Ru2—C29B	144.3 (2)
C5A—Ru1—C7A	171.4 (2)	C10B—Ru2—C29B	106.3 (2)
C8A—Ru1—C7A	37.4 (2)	C6B—Ru2—C29B	87.4 (2)
C9A—Ru1—C7A	63.1 (2)	C8B—Ru2—C29B	143.5 (2)
C2A—Ru1—C7A	117.1 (2)	C2B—Ru2—C29B	66.2 (2)
C10A—Ru1—C7A	62.9 (2)	C7B—Ru2—C29B	105.9 (2)
C1A—Ru1—C3A	64.9 (2)	C4B—Ru2—C29B	98.8 (2)
C5A—Ru1—C3A	63.2 (2)	C3B—Ru2—C29B	99.4 (2)
C8A—Ru1—C3A	103.9 (2)	C14B—Fe2—C20B	108.0 (2)
C9A—Ru1—C3A	115.6 (2)	C14B—Fe2—C16B	122.1 (2)
C2A—Ru1—C3A	37.6 (2)	C20B—Fe2—C16B	39.5 (2)
C10A—Ru1—C3A	150.5 (2)	C14B—Fe2—C15B	40.1 (2)
C7A—Ru1—C3A	123.9 (2)	C20B—Fe2—C15B	125.0 (2)
C1A—Ru1—C6A	123.7 (2)	C16B—Fe2—C15B	109.5 (2)
C5A—Ru1—C6A	134.8 (2)	C14B—Fe2—C13B	39.9 (2)
C8A—Ru1—C6A	62.9 (2)	C20B—Fe2—C13B	121.7 (2)
C9A—Ru1—C6A	63.1 (2)	C16B—Fe2—C13B	156.3 (2)
C2A—Ru1—C6A	136.9 (2)	C15B—Fe2—C13B	67.1 (2)
C10A—Ru1—C6A	37.7 (2)	C14B—Fe2—C19B	123.8 (2)
C7A—Ru1—C6A	37.7 (2)	C20B—Fe2—C19B	39.8 (2)
C3A—Ru1—C6A	161.4 (2)	C16B—Fe2—C19B	66.9 (2)
C1A—Ru1—C4A	64.7 (2)	C15B—Fe2—C19B	160.2 (2)
C5A—Ru1—C4A	37.1 (2)	C13B—Fe2—C19B	107.9 (2)
C8A—Ru1—C4A	115.9 (2)	C14B—Fe2—C11B	67.1 (2)

C9A—Ru1—C4A	102.0 (2)	C20B—Fe2—C11B	162.0 (2)
C2A—Ru1—C4A	63.4 (2)	C16B—Fe2—C11B	127.1 (2)
C10A—Ru1—C4A	121.2 (2)	C15B—Fe2—C11B	40.2 (2)
C7A—Ru1—C4A	151.5 (2)	C13B—Fe2—C11B	66.6 (2)
C3A—Ru1—C4A	37.6 (2)	C19B—Fe2—C11B	157.4 (2)
C6A—Ru1—C4A	158.5 (2)	C14B—Fe2—C17B	158.1 (2)
C1A—Ru1—C29A	36.7 (2)	C20B—Fe2—C17B	66.3 (2)
C5A—Ru1—C29A	65.5 (2)	C16B—Fe2—C17B	40.0 (2)
C8A—Ru1—C29A	144.5 (2)	C15B—Fe2—C17B	124.3 (2)
C9A—Ru1—C29A	142.6 (2)	C13B—Fe2—C17B	161.4 (2)
C2A—Ru1—C29A	66.5 (2)	C19B—Fe2—C17B	66.4 (2)
C10A—Ru1—C29A	105.0 (2)	C11B—Fe2—C17B	111.4 (2)
C7A—Ru1—C29A	107.1 (2)	C14B—Fe2—C18B	160.4 (2)
C3A—Ru1—C29A	99.9 (2)	C20B—Fe2—C18B	67.0 (2)
C6A—Ru1—C29A	87.0 (2)	C16B—Fe2—C18B	67.0 (2)
C4A—Ru1—C29A	99.1 (2)	C15B—Fe2—C18B	158.3 (2)
C16A—Fe1—C12A	173.5 (2)	C13B—Fe2—C18B	125.0 (2)
C16A—Fe1—C13A	133.8 (2)	C19B—Fe2—C18B	40.2 (2)
C12A—Fe1—C13A	39.94 (19)	C11B—Fe2—C18B	123.5 (2)
C16A—Fe1—C20A	39.4 (2)	C17B—Fe2—C18B	39.2 (2)
C12A—Fe1—C20A	136.3 (2)	C14B—Fe2—C12B	66.6 (2)
C13A—Fe1—C20A	110.6 (2)	C20B—Fe2—C12B	156.3 (2)
C16A—Fe1—C17A	40.4 (2)	C16B—Fe2—C12B	163.2 (2)
C12A—Fe1—C17A	145.9 (2)	C15B—Fe2—C12B	66.8 (2)
C13A—Fe1—C17A	173.4 (2)	C13B—Fe2—C12B	39.3 (2)
C20A—Fe1—C17A	66.9 (2)	C19B—Fe2—C12B	122.4 (2)
C16A—Fe1—C11A	144.2 (2)	C11B—Fe2—C12B	39.50 (19)
C12A—Fe1—C11A	40.1 (2)	C17B—Fe2—C12B	127.2 (2)
C13A—Fe1—C11A	67.1 (2)	C18B—Fe2—C12B	109.9 (2)
C20A—Fe1—C11A	176.3 (2)	C29B—C1B—C2B	119.6 (5)
C17A—Fe1—C11A	115.8 (2)	C29B—C1B—C5B	116.7 (5)
C16A—Fe1—C14A	108.8 (2)	C2B—C1B—C5B	107.6 (5)
C12A—Fe1—C14A	67.4 (2)	C29B—C1B—Ru2	81.7 (3)
C13A—Fe1—C14A	40.19 (19)	C2B—C1B—Ru2	74.0 (3)
C20A—Fe1—C14A	113.3 (2)	C5B—C1B—Ru2	73.0 (3)
C17A—Fe1—C14A	134.3 (2)	C3B—C2B—C1B	106.9 (5)
C11A—Fe1—C14A	67.0 (2)	C3B—C2B—Ru2	73.0 (3)
C16A—Fe1—C19A	66.5 (2)	C1B—C2B—Ru2	66.2 (3)
C12A—Fe1—C19A	113.2 (2)	C3B—C2B—H2BA	126.5
C13A—Fe1—C19A	115.7 (2)	C1B—C2B—H2BA	126.5
C20A—Fe1—C19A	39.52 (18)	Ru2—C2B—H2BA	125.7
C17A—Fe1—C19A	66.6 (2)	C2B—C3B—C4B	108.6 (5)
C11A—Fe1—C19A	138.36 (19)	C2B—C3B—Ru2	69.5 (3)
C14A—Fe1—C19A	143.8 (2)	C4B—C3B—Ru2	70.5 (3)
C16A—Fe1—C18A	66.9 (2)	C2B—C3B—H3BA	125.7
C12A—Fe1—C18A	117.4 (2)	C4B—C3B—H3BA	125.7
C13A—Fe1—C18A	145.9 (2)	Ru2—C3B—H3BA	125.8
C20A—Fe1—C18A	66.4 (2)	C5B—C4B—C3B	109.5 (5)

C17A—Fe1—C18A	39.6 (2)	C5B—C4B—Ru2	69.4 (3)
C11A—Fe1—C18A	113.7 (2)	C3B—C4B—Ru2	72.0 (3)
C14A—Fe1—C18A	173.9 (2)	C5B—C4B—H4BA	125.2
C19A—Fe1—C18A	39.5 (2)	C3B—C4B—H4BA	125.2
C16A—Fe1—C15A	113.8 (2)	Ru2—C4B—H4BA	124.9
C12A—Fe1—C15A	67.0 (2)	C4B—C5B—C1B	107.2 (5)
C13A—Fe1—C15A	66.6 (2)	C4B—C5B—Ru2	73.2 (3)
C20A—Fe1—C15A	142.6 (2)	C1B—C5B—Ru2	67.0 (3)
C17A—Fe1—C15A	111.3 (2)	C4B—C5B—H5BA	126.4
C11A—Fe1—C15A	39.75 (19)	C1B—C5B—H5BA	126.4
C14A—Fe1—C15A	39.44 (19)	Ru2—C5B—H5BA	124.9
C19A—Fe1—C15A	176.8 (2)	C10B—C6B—C7B	109.4 (5)
C18A—Fe1—C15A	137.4 (2)	C10B—C6B—Ru2	71.1 (3)
C29A—C1A—C5A	117.3 (5)	C7B—C6B—Ru2	72.2 (3)
C29A—C1A—C2A	119.9 (5)	C10B—C6B—H6BA	125.3
C5A—C1A—C2A	106.4 (5)	C7B—C6B—H6BA	125.3
C29A—C1A—Ru1	82.3 (3)	Ru2—C6B—H6BA	123.1
C5A—C1A—Ru1	72.8 (3)	C8B—C7B—C6B	106.9 (5)
C2A—C1A—Ru1	73.2 (3)	C8B—C7B—Ru2	70.5 (3)
C3A—C2A—C1A	107.4 (5)	C6B—C7B—Ru2	70.1 (3)
C3A—C2A—Ru1	72.4 (3)	C8B—C7B—H7BA	126.5
C1A—C2A—Ru1	67.1 (3)	C6B—C7B—H7BA	126.5
C3A—C2A—H2AA	126.3	Ru2—C7B—H7BA	124.5
C1A—C2A—H2AA	126.3	C7B—C8B—C9B	108.6 (5)
Ru1—C2A—H2AA	125.8	C7B—C8B—Ru2	71.9 (3)
C2A—C3A—C4A	108.8 (5)	C9B—C8B—Ru2	70.2 (3)
C2A—C3A—Ru1	70.1 (3)	C7B—C8B—H8BA	125.7
C4A—C3A—Ru1	71.5 (3)	C9B—C8B—H8BA	125.7
C2A—C3A—H3AA	125.6	Ru2—C8B—H8BA	123.8
C4A—C3A—H3AA	125.6	C10B—C9B—C8B	107.4 (5)
Ru1—C3A—H3AA	124.4	C10B—C9B—Ru2	71.2 (3)
C5A—C4A—C3A	108.7 (5)	C8B—C9B—Ru2	71.4 (3)
C5A—C4A—Ru1	69.6 (3)	C10B—C9B—H9BA	126.3
C3A—C4A—Ru1	70.9 (3)	C8B—C9B—H9BA	126.3
C5A—C4A—H4AA	125.6	Ru2—C9B—H9BA	122.8
C3A—C4A—H4AA	125.6	C6B—C10B—C9B	107.7 (5)
Ru1—C4A—H4AA	125.4	C6B—C10B—Ru2	71.1 (3)
C4A—C5A—C1A	108.4 (5)	C9B—C10B—Ru2	70.7 (3)
C4A—C5A—Ru1	73.3 (3)	C6B—C10B—H10B	126.1
C1A—C5A—Ru1	67.4 (3)	C9B—C10B—H10B	126.1
C4A—C5A—H5AA	125.8	Ru2—C10B—H10B	123.7
C1A—C5A—H5AA	125.8	C12B—C11B—C15B	107.9 (5)
Ru1—C5A—H5AA	125.0	C12B—C11B—C31B	123.3 (5)
C7A—C6A—C10A	107.7 (6)	C15B—C11B—C31B	128.7 (5)
C7A—C6A—Ru1	71.1 (3)	C12B—C11B—Fe2	70.8 (3)
C10A—C6A—Ru1	71.0 (3)	C15B—C11B—Fe2	69.5 (3)
C7A—C6A—H6AA	126.2	C31B—C11B—Fe2	125.7 (4)
C10A—C6A—H6AA	126.2	C13B—C12B—C11B	108.2 (5)

Ru1—C6A—H6AA	123.4	C13B—C12B—C21B	127.0 (5)
C8A—C7A—C6A	107.6 (6)	C11B—C12B—C21B	124.7 (5)
C8A—C7A—Ru1	69.9 (3)	C13B—C12B—Fe2	69.4 (3)
C6A—C7A—Ru1	71.2 (3)	C11B—C12B—Fe2	69.7 (3)
C8A—C7A—H7AA	126.2	C21B—C12B—Fe2	127.5 (4)
C6A—C7A—H7AA	126.2	C12B—C13B—C14B	108.3 (5)
Ru1—C7A—H7AA	124.3	C12B—C13B—C22B	125.7 (5)
C7A—C8A—C9A	108.8 (6)	C14B—C13B—C22B	126.0 (5)
C7A—C8A—Ru1	72.7 (3)	C12B—C13B—Fe2	71.3 (3)
C9A—C8A—Ru1	71.0 (3)	C14B—C13B—Fe2	69.5 (3)
C7A—C8A—H8AA	125.6	C22B—C13B—Fe2	126.2 (4)
C9A—C8A—H8AA	125.6	C13B—C14B—C15B	108.3 (5)
Ru1—C8A—H8AA	122.4	C13B—C14B—C23B	126.4 (5)
C10A—C9A—C8A	108.0 (6)	C15B—C14B—C23B	125.3 (5)
C10A—C9A—Ru1	72.4 (3)	C13B—C14B—Fe2	70.6 (3)
C8A—C9A—Ru1	71.0 (4)	C15B—C14B—Fe2	70.4 (3)
C10A—C9A—H9AA	126.0	C23B—C14B—Fe2	126.2 (4)
C8A—C9A—H9AA	126.0	C14B—C15B—C11B	107.2 (5)
Ru1—C9A—H9AA	122.3	C14B—C15B—C24B	124.6 (5)
C9A—C10A—C6A	107.9 (6)	C11B—C15B—C24B	127.9 (5)
C9A—C10A—Ru1	69.9 (3)	C14B—C15B—Fe2	69.5 (3)
C6A—C10A—Ru1	71.3 (3)	C11B—C15B—Fe2	70.4 (3)
C9A—C10A—H10A	126.0	C24B—C15B—Fe2	129.3 (4)
C6A—C10A—H10A	126.0	C20B—C16B—C17B	107.6 (5)
Ru1—C10A—H10A	124.3	C20B—C16B—Fe2	70.2 (3)
C15A—C11A—C12A	107.6 (4)	C17B—C16B—Fe2	71.0 (3)
C15A—C11A—C31A	122.8 (5)	C20B—C16B—H16B	126.2
C12A—C11A—C31A	129.5 (5)	C17B—C16B—H16B	126.2
C15A—C11A—Fe1	70.7 (3)	Fe2—C16B—H16B	124.2
C12A—C11A—Fe1	69.2 (3)	C18B—C17B—C16B	108.8 (5)
C31A—C11A—Fe1	124.2 (4)	C18B—C17B—C25B	127.7 (5)
C13A—C12A—C11A	107.8 (4)	C16B—C17B—C25B	123.5 (5)
C13A—C12A—C21A	125.6 (5)	C18B—C17B—Fe2	70.5 (3)
C11A—C12A—C21A	126.3 (5)	C16B—C17B—Fe2	69.1 (3)
C13A—C12A—Fe1	69.9 (3)	C25B—C17B—Fe2	126.7 (4)
C11A—C12A—Fe1	70.6 (3)	C17B—C18B—C19B	107.1 (5)
C21A—C12A—Fe1	129.0 (4)	C17B—C18B—C26B	126.3 (5)
C12A—C13A—C14A	108.6 (5)	C19B—C18B—C26B	126.6 (5)
C12A—C13A—C22A	125.5 (5)	C17B—C18B—Fe2	70.3 (3)
C14A—C13A—C22A	125.9 (5)	C19B—C18B—Fe2	69.4 (3)
C12A—C13A—Fe1	70.1 (3)	C26B—C18B—Fe2	127.3 (4)
C14A—C13A—Fe1	70.7 (3)	C20B—C19B—C18B	107.4 (5)
C22A—C13A—Fe1	127.3 (4)	C20B—C19B—C27B	125.6 (5)
C15A—C14A—C13A	107.5 (4)	C18B—C19B—C27B	126.9 (5)
C15A—C14A—C23A	125.8 (5)	C20B—C19B—Fe2	69.5 (3)
C13A—C14A—C23A	126.7 (5)	C18B—C19B—Fe2	70.4 (3)
C15A—C14A—Fe1	70.9 (3)	C27B—C19B—Fe2	127.3 (4)
C13A—C14A—Fe1	69.2 (3)	C16B—C20B—C19B	109.0 (5)

C23A—C14A—Fe1	125.6 (4)	C16B—C20B—C28B	125.6 (5)
C14A—C15A—C11A	108.5 (4)	C19B—C20B—C28B	125.2 (5)
C14A—C15A—C24A	125.6 (5)	C16B—C20B—Fe2	70.3 (3)
C11A—C15A—C24A	125.9 (5)	C19B—C20B—Fe2	70.7 (3)
C14A—C15A—Fe1	69.7 (3)	C28B—C20B—Fe2	128.4 (4)
C11A—C15A—Fe1	69.5 (3)	C12B—C21B—H21D	109.5
C24A—C15A—Fe1	128.5 (4)	C12B—C21B—H21E	109.5
C20A—C16A—C17A	108.7 (5)	H21D—C21B—H21E	109.5
C20A—C16A—Fe1	71.2 (3)	C12B—C21B—H21F	109.5
C17A—C16A—Fe1	71.1 (3)	H21D—C21B—H21F	109.5
C20A—C16A—H16A	125.7	H21E—C21B—H21F	109.5
C17A—C16A—H16A	125.7	C13B—C22B—H22D	109.5
Fe1—C16A—H16A	123.6	C13B—C22B—H22E	109.5
C18A—C17A—C16A	106.9 (5)	H22D—C22B—H22E	109.5
C18A—C17A—C25A	127.5 (5)	C13B—C22B—H22F	109.5
C16A—C17A—C25A	125.6 (5)	H22D—C22B—H22F	109.5
C18A—C17A—Fe1	70.8 (3)	H22E—C22B—H22F	109.5
C16A—C17A—Fe1	68.5 (3)	C14B—C23B—H23D	109.5
C25A—C17A—Fe1	126.3 (4)	C14B—C23B—H23E	109.5
C17A—C18A—C19A	108.0 (5)	H23D—C23B—H23E	109.5
C17A—C18A—C26A	125.1 (5)	C14B—C23B—H23F	109.5
C19A—C18A—C26A	126.8 (5)	H23D—C23B—H23F	109.5
C17A—C18A—Fe1	69.6 (3)	H23E—C23B—H23F	109.5
C19A—C18A—Fe1	70.1 (3)	C15B—C24B—H24D	109.5
C26A—C18A—Fe1	127.0 (4)	C15B—C24B—H24E	109.5
C20A—C19A—C18A	107.9 (5)	H24D—C24B—H24E	109.5
C20A—C19A—C27A	125.8 (5)	C15B—C24B—H24F	109.5
C18A—C19A—C27A	126.3 (5)	H24D—C24B—H24F	109.5
C20A—C19A—Fe1	69.3 (3)	H24E—C24B—H24F	109.5
C18A—C19A—Fe1	70.4 (3)	C17B—C25B—H25D	109.5
C27A—C19A—Fe1	126.4 (4)	C17B—C25B—H25E	109.5
C16A—C20A—C19A	108.5 (5)	H25D—C25B—H25E	109.5
C16A—C20A—C28A	125.5 (5)	C17B—C25B—H25F	109.5
C19A—C20A—C28A	126.0 (5)	H25D—C25B—H25F	109.5
C16A—C20A—Fe1	69.4 (3)	H25E—C25B—H25F	109.5
C19A—C20A—Fe1	71.2 (3)	C18B—C26B—H26D	109.5
C28A—C20A—Fe1	126.4 (4)	C18B—C26B—H26E	109.5
C12A—C21A—H21A	109.5	H26D—C26B—H26E	109.5
C12A—C21A—H21B	109.5	C18B—C26B—H26F	109.5
H21A—C21A—H21B	109.5	H26D—C26B—H26F	109.5
C12A—C21A—H21C	109.5	H26E—C26B—H26F	109.5
H21A—C21A—H21C	109.5	C19B—C27B—H27D	109.5
H21B—C21A—H21C	109.5	C19B—C27B—H27E	109.5
C13A—C22A—H22A	109.5	H27D—C27B—H27E	109.5
C13A—C22A—H22B	109.5	C19B—C27B—H27F	109.5
H22A—C22A—H22B	109.5	H27D—C27B—H27F	109.5
C13A—C22A—H22C	109.5	H27E—C27B—H27F	109.5
H22A—C22A—H22C	109.5	C20B—C28B—H28D	109.5

H22B—C22A—H22C	109.5	C20B—C28B—H28E	109.5
C14A—C23A—H23A	109.5	H28D—C28B—H28E	109.5
C14A—C23A—H23B	109.5	C20B—C28B—H28F	109.5
H23A—C23A—H23B	109.5	H28D—C28B—H28F	109.5
C14A—C23A—H23C	109.5	H28E—C28B—H28F	109.5
H23A—C23A—H23C	109.5	C1B—C29B—C30B	123.9 (6)
H23B—C23A—H23C	109.5	C1B—C29B—Ru2	61.8 (3)
C15A—C24A—H24A	109.5	C30B—C29B—Ru2	111.5 (4)
C15A—C24A—H24B	109.5	C1B—C29B—H29B	118.0
H24A—C24A—H24B	109.5	C30B—C29B—H29B	118.0
C15A—C24A—H24C	109.5	Ru2—C29B—H29B	96.5
H24A—C24A—H24C	109.5	C31B—C30B—C29B	122.0 (6)
H24B—C24A—H24C	109.5	C31B—C30B—H30B	119.0
C17A—C25A—H25A	109.5	C29B—C30B—H30B	119.0
C17A—C25A—H25B	109.5	C30B—C31B—C11B	128.0 (5)
H25A—C25A—H25B	109.5	C30B—C31B—H31B	116.0
C17A—C25A—H25C	109.5	C11B—C31B—H31B	116.0
H25A—C25A—H25C	109.5		