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(2,2-Bipyridine-κ^2N,N')chlorido[η^6-1-methyl-4-(propan-2-yl)benzene]ruthenium(II) tetraphenylborate

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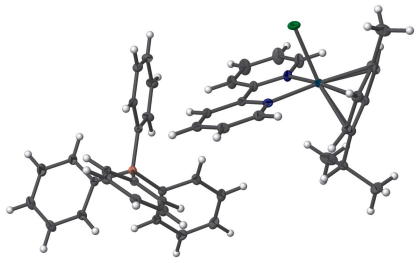
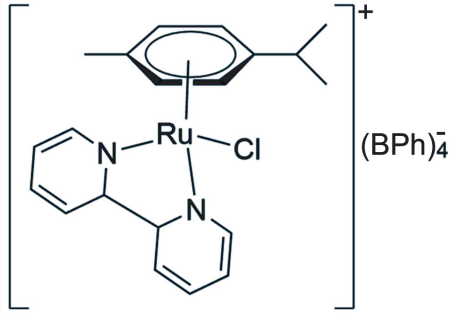
Structural data: full structural data are available from iucrdata.iucr.org

The title complex, [RuCl($C_{10}H_{14}$)($C_{10}H_8N_2$)]($C_{24}H_{20}B$), has monoclinic ($P2_1$) symmetry at 100 K. It was prepared by the reaction of the dichlorido[1-methyl-4-(propan-2-yl)benzene]ruthenium(II) dimer with 2,2′-bipyridine, followed by the addition of ammonium tetraphenylborate. The 1-methyl-4-(propan-2-yl)benzene group, the 2,2′-bipyridine unit and a chloride ion coordinate the ruthenium(II) atom, with the 1-methyl-4-(propan-2-yl)benzene ring and bipyridine moieties *trans* to each other. In the crystal, the complex cations are linked by C—H···Cl hydrogen bonds, forming chains parallel to [010]. These chains are linked by a number of C—H···π interactions, involving the phenyl rings of the tetraphenylborate anion and a pyridine ring of the bpy ligand, resulting in the formation of layers parallel to ($10\bar{1}$).

3D view



Chemical scheme



Structure description

N-Heterocyclic carbenes (NHCs) of ruthenium have been of significant interest to the organometallic community for many years, and have a number of applications in homogeneous chemical catalysis (Weskamp *et al.*, 1999; Fürstner *et al.*, 2001; Son *et al.*, 2004; Tudose *et al.*, 2006; Gandolfi *et al.*, 2009); Sanz *et al.*, 2010; Fogler *et al.*, 2011; Hackenberg *et al.*, 2013). The catalytic properties of these complexes have also been studied intensively (Fogler *et al.*, 2011; Ortega *et al.*, 2013; Day & Fogg, 2018). In an effort to access alternative synthetic starting materials for the synthesis of bipyridine-substituted complexes of ruthenium that include NHCs, the title complex was synthesized.

Complex **1** is comprised of an Ru^{II} metal atom coordinated by an η^6 1-methyl-4-(propan-2-yl)benzene (*p*-cymene) ring, a chloride ion and the bidentate ligand 2,2′-bipyridine, with a tetraphenylborate anion as counter ion (Fig. 1). The 1-methyl-4-(propan-2-yl)benzene ring and bipyridine moieties are *trans* to each other. The complex

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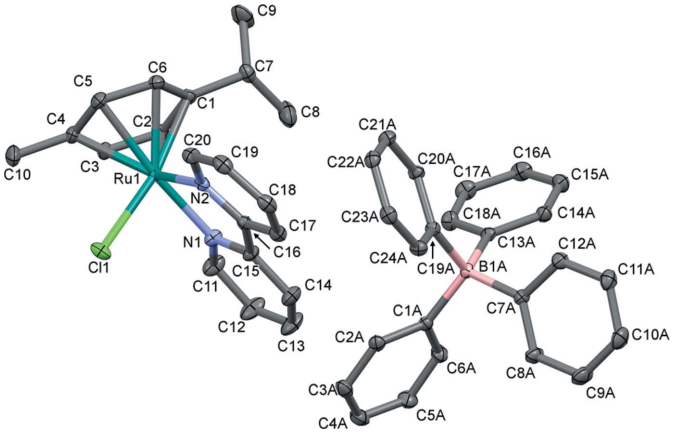

Figure 1
The molecular structure of complex **1**, with the atom labeling. Displacement ellipsoids are drawn at the 50% probability level.

crystallizes in the chiral monoclinic $P2_1$ space group with a refined absolute structure Flack parameter of −0.014 (7). The most significant bond lengths and bond angles involving atom Ru1 are given in Table 1.

In the crystal, the complex cations are linked by bifurcated C—(H,H)···Cl hydrogen bonds, forming chains propagating parallel to [010]; see Fig. 2 and Table 2. The chains are linked by a number of C—H···π interactions involving the phenyl rings of the tetraphenylborate anion and a pyridine ring of the bpy ligand, resulting in the formation of layers lying parallel to the (10$\bar{1}$) plane; see Fig. 2 and Table 2.

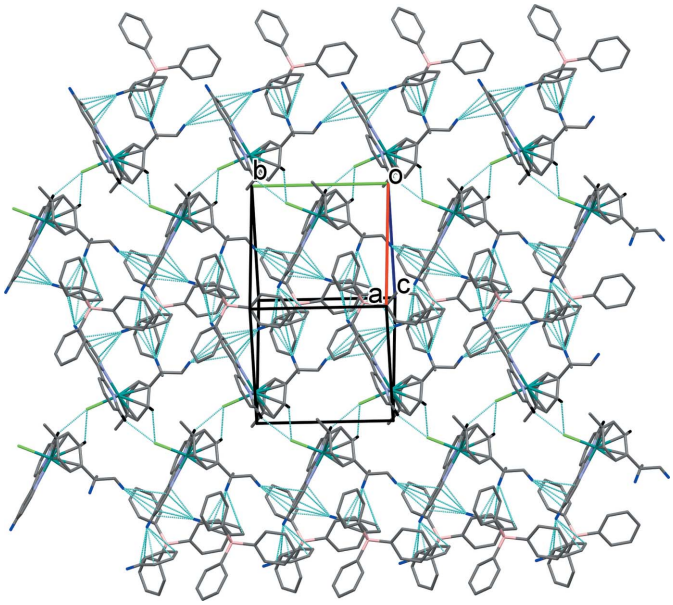

Figure 2
A view normal to plane (10$\bar{1}$) of the crystal packing of complex **1**. The C—H···Cl hydrogen bonds and C—H···π interactions (see Table 2) are shown as dashed lines. For clarity, only the hydrogen atoms involved in these interactions have been included.

Table 1
Selected geometric parameters (Å, °).

Ru1—Cl1	2.3851 (5)	Ru1—C3	2.2123 (16)
Ru1—N1	2.0892 (13)	Ru1—C4	2.2391 (16)
Ru1—N2	2.0839 (13)	Ru1—C5	2.2005 (16)
Ru1—C1	2.2234 (16)	Ru1—C6	2.1626 (16)
Ru1—C2	2.1863 (18)		
N2—Ru1—N1	76.98 (5)	C4—Ru1—Cl1	87.95 (5)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*2 are the centroids of rings C19*A*–C24*A* and N2/C16–C20, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Cl1^{i}	1.00	2.66	3.421 (2)	133
C11—H11···Cl1^{i}	0.95	2.62	3.484 (2)	151
C7—H7···*Cg*1^{ii}	1.00	2.67	3.616 (2)	158
C9—H9*B*···*Cg*2^{iii}	0.98	2.91	3.733 (2)	143
C18—H18···*Cg*1	0.95	2.73	3.431 (2)	131
C23*A*—H23*A*···*Cg*2^{iv}	0.95	2.60	3.461 (2)	151

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

Synthesis and crystallization

All chemicals were purchased from Sigma–Aldrich and used without further purification under a nitrogen atmosphere. The dichlorido(*p*-cymene)ruthenium(II) dimer was prepared following the literature protocol of Bennett *et al.* (2007). The reaction scheme is shown in Fig. 3. [Ru(*p*-cymene)Cl_2]$_2$ (100 mg, 163.29 mmol) and 2,2′-bipyridine (28 mg, 179.28 mmol) in 5 ml of methanol were refluxed for 16 h. The reaction mixture was cooled to room temperature and then filtered through celite. Ammonium tetraphenylborate (29 mg, 86 mmol) dissolved in 3 ml of MeOH was added to the filtrate. Precipitation proceeded over the next 60 min, at which point a solid yellow product was collected by filtration (110 mg, 147 mmol, 90%). Crystals suitable for X-ray crystallography were grown in CH_2Cl_2/pentane by slow vapor diffusion. HR FT–ICR MS: Calc. for $C_{20}H_{22}ClN_2Ru$ (427.0542); Found *m/z* (*M*-BPh_4) 427.0515.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Acknowledgements

Dr Doug Powell performed the data collection and the refinement of the structure. We are grateful to the University

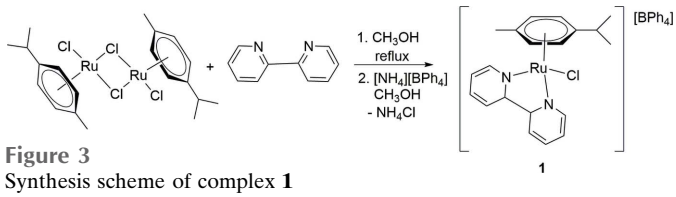

Figure 3
Synthesis scheme of complex **1**

of Arkansas for start-up funding, and for some support for the NMR Facility at the University of Arkansas provided by the Arkansas Biosciences Institute. We also thank the University of Oklahoma for funds to purchase the and computers.

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Table 3
Experimental details.

Crystal data	
Chemical formula	$[RuCl(C_{10}H_{14})(C_{10}H_8N_2)](C_{24}H_{20}B)$
M_r	746.12
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	100
a, b, c (Å)	14.1396 (15), 9.4811 (11), 14.3009 (15)
β (°)	109.013 (4)
V (Å^3)	1812.6 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.54
Crystal size (mm)	0.27 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker Photon II cpad
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.391, 0.439
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	57149, 18389, 17627
R_{int}	0.040
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.848
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.062, 1.01
No. of reflections	18389
No. of parameters	446
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.43, −0.60
Absolute structure	Flack x determined using 7947 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.014 (7)

Computer programs: *APEX3* and *SAINT* (Bruker, 2018), *SHELXT* (Sheldrick, 2015*a*), *Mercury* (Macrae *et al.*, 2008), *SHELXL2018* (Sheldrick, 2015*b*), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2019). **4**, x191006 [https://doi.org/10.1107/S2414314619010006X]

(2,2-Bipyridine-κ^2N,N')chlorido[η^6-1-methyl-4-(propan-2-yl)benzene]-ruthenium(II) tetraphenylborate

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(2,2-Bipyridine-κ^2N,N')chlorido[η^6-1-methyl-4-(propan-2-yl)benzene]ruthenium(II) tetraphenylborate

Crystal data

$[RuCl(C_{10}H_{14})(C_{10}H_8N_2)](C_{24}H_{20}B)$
M_r = 746.12
Monoclinic, $P2_1$
a = 14.1396 (15) Å
b = 9.4811 (11) Å
c = 14.3009 (15) Å
β = 109.013 (4)°
V = 1812.6 (3) Å^3
Z = 2
$F(000)$ = 772
D_x = 1.367 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9150 reflections
θ = 4.3–37.1°
μ = 0.54 mm^{-1}
T = 100 K
Block, orange
0.27 × 0.15 × 0.10 mm

Data collection

Bruker Photon II cpad diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.391, T_{max} = 0.439
57149 measured reflections
18389 independent reflections
17627 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 37.1°, θ_{min} = 2.5°
h = −23→23
k = −16→16
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.062
S = 1.01
18389 reflections
446 parameters
1 restraint
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 0.240P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}
Extinction correction: (SHELXL2018; Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0054 (9)
Absolute structure: Flack x determined using 7947 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.014 (7)

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. Hydrogen atoms were included in calculated positions and treated as riding on the parent C atom: C—H = 0.95–1.00 Å with U_{iso}(H) = 1.5U_{eq}(*C*-methyl) and 1.2U_{eq}(C) for other H atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.18068 (2)	0.51286 (2)	0.07448 (2)	0.01075 (3)
Cl1	0.12759 (4)	0.74527 (5)	0.01726 (4)	0.01957 (8)
N1	0.09601 (10)	0.54459 (14)	0.16818 (10)	0.0145 (2)
N2	0.27945 (9)	0.61963 (14)	0.19404 (10)	0.0126 (2)
C1	0.22538 (12)	0.28724 (16)	0.09615 (11)	0.0146 (2)
C2	0.12355 (14)	0.29922 (19)	0.03465 (13)	0.0150 (3)
H2	0.070093	0.263351	0.060173	0.018*
C3	0.09526 (13)	0.38097 (18)	−0.05258 (11)	0.0166 (3)
H3	0.022771	0.401613	−0.086461	0.020*
C4	0.16818 (13)	0.45675 (19)	−0.08118 (12)	0.0182 (3)
C5	0.26946 (13)	0.45044 (19)	−0.01971 (12)	0.0181 (3)
H5	0.319034	0.518072	−0.030787	0.022*
C6	0.29636 (12)	0.36769 (18)	0.06801 (12)	0.0160 (3)
H6	0.364984	0.379252	0.116869	0.019*
C7	0.25764 (13)	0.19334 (18)	0.18562 (12)	0.0179 (3)
H7	0.321125	0.232642	0.232325	0.022*
C8	0.18197 (17)	0.1836 (3)	0.24075 (17)	0.0333 (5)
H8A	0.169370	0.278072	0.261917	0.050*
H8B	0.208624	0.122886	0.298870	0.050*
H8C	0.119277	0.143665	0.196898	0.050*
C9	0.2809 (2)	0.0474 (2)	0.15284 (17)	0.0327 (5)
H9A	0.219180	0.004466	0.109425	0.049*
H9B	0.309489	−0.012467	0.211108	0.049*
H9C	0.329040	0.056781	0.117002	0.049*
C10	0.13714 (16)	0.5463 (2)	−0.17228 (13)	0.0259 (4)
H10A	0.137720	0.489475	−0.229329	0.039*
H10B	0.183840	0.625332	−0.163962	0.039*
H10C	0.069533	0.582760	−0.183212	0.039*
C11	−0.00049 (11)	0.5078 (3)	0.14594 (12)	0.0215 (3)
H11	−0.032789	0.461693	0.084867	0.026*
C12	−0.05456 (14)	0.5350 (2)	0.20943 (15)	0.0283 (5)
H12	−0.122792	0.507808	0.191893	0.034*
C13	−0.00786 (15)	0.6023 (3)	0.29879 (16)	0.0278 (4)
H13	−0.043449	0.620928	0.343492	0.033*
C14	0.09145 (13)	0.6420 (2)	0.32182 (13)	0.0206 (3)
H14	0.124927	0.688474	0.382439	0.025*
C15	0.14161 (11)	0.61250 (17)	0.25445 (11)	0.0145 (2)

C16	0.24499 (11)	0.65497 (16)	0.26890 (11)	0.0128 (2)
C17	0.30385 (12)	0.72922 (17)	0.35107 (12)	0.0163 (3)
H17	0.278860	0.751998	0.403353	0.020*
C18	0.39957 (12)	0.76962 (17)	0.35571 (13)	0.0182 (3)
H18	0.441031	0.820014	0.411425	0.022*
C19	0.43407 (12)	0.73577 (18)	0.27837 (13)	0.0186 (3)
H19	0.499069	0.763543	0.279754	0.022*
C20	0.37197 (11)	0.66058 (17)	0.19884 (12)	0.0161 (3)
H20	0.395644	0.637128	0.145788	0.019*
C1A	0.23530 (11)	0.77267 (17)	0.60471 (11)	0.0132 (2)
C2A	0.23565 (12)	0.88711 (16)	0.54243 (11)	0.0152 (2)
H2A	0.298056	0.920629	0.539820	0.018*
C3A	0.14809 (14)	0.95384 (18)	0.48412 (13)	0.0196 (3)
H3A	0.152034	1.030055	0.442426	0.023*
C4A	0.05535 (14)	0.9094 (2)	0.48677 (13)	0.0217 (3)
H4A	−0.004269	0.954885	0.447650	0.026*
C5A	0.05165 (13)	0.7970 (2)	0.54779 (13)	0.0217 (3)
H5A	−0.010993	0.765367	0.550926	0.026*
C6A	0.13943 (12)	0.73070 (19)	0.60434 (12)	0.0181 (3)
H6A	0.134581	0.653307	0.644725	0.022*
C7A	0.36590 (11)	0.75614 (16)	0.78984 (11)	0.0129 (2)
C8A	0.30762 (13)	0.8527 (2)	0.82111 (12)	0.0197 (3)
H8AA	0.247185	0.885698	0.774408	0.024*
C9A	0.33465 (16)	0.9025 (2)	0.91823 (14)	0.0268 (4)
H9AA	0.293176	0.968914	0.935999	0.032*
C10A	0.42176 (14)	0.8554 (2)	0.98886 (13)	0.0228 (3)
H10D	0.439700	0.887490	1.055300	0.027*
C11A	0.48227 (13)	0.7604 (2)	0.96048 (12)	0.0202 (3)
H11A	0.542283	0.727121	1.007701	0.024*
C12A	0.45494 (12)	0.71423 (19)	0.86297 (12)	0.0173 (3)
H12A	0.498421	0.651443	0.844919	0.021*
C13A	0.31168 (10)	0.5213 (2)	0.67714 (9)	0.0126 (2)
C14A	0.34015 (13)	0.43489 (17)	0.76138 (12)	0.0161 (3)
H14A	0.376568	0.475869	0.823269	0.019*
C15A	0.31722 (14)	0.29086 (19)	0.75824 (14)	0.0202 (3)
H15A	0.337552	0.236845	0.817420	0.024*
C16A	0.26504 (14)	0.22670 (18)	0.66926 (14)	0.0212 (3)
H16A	0.249287	0.129060	0.666635	0.025*
C17A	0.23636 (14)	0.3084 (2)	0.58416 (14)	0.0206 (3)
H17A	0.200600	0.266322	0.522461	0.025*
C18A	0.25953 (13)	0.45161 (18)	0.58838 (12)	0.0177 (3)
H18A	0.239247	0.504547	0.528734	0.021*
C19A	0.43290 (11)	0.71807 (15)	0.63904 (11)	0.0122 (2)
C20A	0.47654 (11)	0.61317 (16)	0.59733 (11)	0.0140 (2)
H20A	0.449422	0.520595	0.590472	0.017*
C21A	0.55858 (12)	0.63956 (18)	0.56539 (12)	0.0156 (2)
H21A	0.586610	0.565195	0.538421	0.019*
C22A	0.59897 (12)	0.77414 (18)	0.57306 (11)	0.0161 (3)

H22A	0.653725	0.793064	0.550248	0.019*
C23A	0.55809 (12)	0.88118 (17)	0.61471 (12)	0.0158 (3)
H23A	0.584916	0.973856	0.620306	0.019*
C24A	0.47790 (12)	0.85237 (16)	0.64813 (12)	0.0146 (2)
H24A	0.452554	0.926073	0.678224	0.018*
B1A	0.33633 (12)	0.69173 (18)	0.67724 (12)	0.0124 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01025 (4)	0.01104 (4)	0.01128 (4)	0.00032 (4)	0.00393 (3)	0.00047 (4)
Cl1	0.01740 (17)	0.01448 (16)	0.02383 (19)	0.00399 (13)	0.00261 (14)	0.00439 (14)
N1	0.0140 (5)	0.0145 (5)	0.0164 (5)	−0.0034 (4)	0.0068 (4)	−0.0035 (4)
N2	0.0110 (5)	0.0118 (5)	0.0148 (5)	0.0004 (4)	0.0038 (4)	0.0013 (4)
C1	0.0170 (6)	0.0115 (5)	0.0142 (6)	0.0018 (5)	0.0038 (5)	−0.0009 (4)
C2	0.0173 (7)	0.0132 (6)	0.0130 (6)	−0.0003 (5)	0.0028 (5)	−0.0014 (5)
C3	0.0181 (6)	0.0178 (6)	0.0124 (6)	0.0009 (5)	0.0030 (5)	−0.0014 (5)
C4	0.0217 (7)	0.0216 (7)	0.0125 (6)	0.0042 (6)	0.0074 (5)	0.0011 (5)
C5	0.0191 (7)	0.0217 (7)	0.0166 (6)	0.0028 (5)	0.0099 (6)	0.0014 (5)
C6	0.0154 (6)	0.0169 (6)	0.0162 (6)	0.0035 (5)	0.0057 (5)	−0.0009 (5)
C7	0.0206 (7)	0.0150 (6)	0.0147 (6)	−0.0003 (5)	0.0010 (5)	0.0018 (5)
C8	0.0301 (10)	0.0434 (13)	0.0271 (9)	0.0023 (9)	0.0103 (8)	0.0167 (9)
C9	0.0478 (13)	0.0140 (7)	0.0293 (9)	0.0052 (7)	0.0030 (9)	0.0013 (6)
C10	0.0283 (8)	0.0346 (10)	0.0167 (7)	0.0058 (7)	0.0102 (6)	0.0087 (6)
C11	0.0166 (5)	0.0260 (7)	0.0241 (6)	−0.0095 (8)	0.0097 (5)	−0.0094 (9)
C12	0.0196 (7)	0.0391 (14)	0.0321 (8)	−0.0112 (7)	0.0167 (7)	−0.0118 (8)
C13	0.0237 (8)	0.0388 (11)	0.0277 (9)	−0.0077 (8)	0.0178 (7)	−0.0091 (8)
C14	0.0210 (7)	0.0255 (8)	0.0186 (7)	−0.0030 (6)	0.0109 (6)	−0.0058 (6)
C15	0.0141 (6)	0.0152 (6)	0.0149 (6)	−0.0020 (5)	0.0058 (5)	−0.0028 (5)
C16	0.0127 (5)	0.0110 (5)	0.0140 (5)	−0.0001 (4)	0.0036 (5)	0.0000 (4)
C17	0.0174 (6)	0.0135 (6)	0.0156 (6)	−0.0001 (5)	0.0019 (5)	−0.0016 (5)
C18	0.0158 (6)	0.0135 (6)	0.0199 (7)	−0.0013 (5)	−0.0015 (5)	−0.0008 (5)
C19	0.0129 (6)	0.0165 (6)	0.0233 (7)	−0.0027 (5)	0.0018 (5)	0.0024 (5)
C20	0.0115 (6)	0.0163 (6)	0.0206 (7)	−0.0011 (5)	0.0053 (5)	0.0018 (5)
C1A	0.0143 (6)	0.0127 (6)	0.0125 (5)	0.0005 (5)	0.0043 (5)	−0.0012 (4)
C2A	0.0180 (6)	0.0122 (6)	0.0148 (6)	−0.0001 (5)	0.0047 (5)	−0.0008 (4)
C3A	0.0240 (7)	0.0140 (7)	0.0179 (7)	0.0032 (5)	0.0032 (6)	0.0009 (5)
C4A	0.0194 (7)	0.0208 (7)	0.0208 (7)	0.0063 (6)	0.0009 (6)	−0.0001 (6)
C5A	0.0140 (6)	0.0276 (8)	0.0221 (7)	0.0028 (6)	0.0040 (6)	0.0014 (6)
C6A	0.0139 (6)	0.0224 (7)	0.0177 (6)	0.0010 (5)	0.0046 (5)	0.0043 (5)
C7A	0.0127 (6)	0.0132 (6)	0.0133 (5)	−0.0013 (4)	0.0049 (5)	−0.0014 (4)
C8A	0.0189 (7)	0.0225 (7)	0.0160 (6)	0.0040 (6)	0.0034 (5)	−0.0057 (5)
C9A	0.0266 (8)	0.0325 (10)	0.0205 (8)	0.0056 (7)	0.0067 (7)	−0.0106 (7)
C10A	0.0239 (8)	0.0290 (9)	0.0146 (6)	−0.0043 (7)	0.0052 (6)	−0.0060 (6)
C11A	0.0166 (6)	0.0271 (8)	0.0146 (6)	−0.0033 (6)	0.0021 (5)	−0.0016 (5)
C12A	0.0139 (6)	0.0212 (7)	0.0156 (6)	0.0003 (5)	0.0032 (5)	−0.0017 (5)
C13A	0.0123 (4)	0.0129 (5)	0.0139 (4)	−0.0005 (6)	0.0059 (4)	−0.0006 (6)
C14A	0.0193 (6)	0.0147 (6)	0.0147 (6)	0.0003 (5)	0.0064 (5)	0.0000 (5)

C15A	0.0251 (8)	0.0154 (6)	0.0218 (7)	−0.0001 (6)	0.0100 (6)	0.0023 (5)
C16A	0.0237 (8)	0.0148 (6)	0.0285 (8)	−0.0044 (6)	0.0130 (7)	−0.0023 (6)
C17A	0.0200 (7)	0.0184 (7)	0.0235 (7)	−0.0057 (6)	0.0071 (6)	−0.0061 (6)
C18A	0.0186 (7)	0.0169 (7)	0.0165 (6)	−0.0038 (5)	0.0041 (5)	−0.0015 (5)
C19A	0.0120 (5)	0.0117 (5)	0.0125 (5)	−0.0003 (4)	0.0035 (4)	−0.0004 (4)
C20A	0.0151 (6)	0.0117 (5)	0.0156 (6)	−0.0002 (4)	0.0056 (5)	−0.0005 (4)
C21A	0.0144 (6)	0.0167 (6)	0.0170 (6)	0.0003 (5)	0.0069 (5)	−0.0019 (5)
C22A	0.0130 (6)	0.0203 (7)	0.0156 (6)	−0.0015 (5)	0.0054 (5)	0.0016 (5)
C23A	0.0147 (6)	0.0143 (6)	0.0173 (6)	−0.0035 (5)	0.0035 (5)	0.0012 (5)
C24A	0.0142 (6)	0.0125 (6)	0.0171 (6)	−0.0012 (5)	0.0050 (5)	−0.0015 (5)
B1A	0.0125 (6)	0.0128 (6)	0.0116 (6)	−0.0009 (5)	0.0036 (5)	−0.0010 (5)

Geometric parameters (Å, º)

Ru1—Cl1	2.3851 (5)	C19—C20	1.386 (2)
Ru1—N1	2.0892 (13)	C19—H19	0.9500
Ru1—N2	2.0839 (13)	C20—H20	0.9500
Ru1—C1	2.2234 (16)	C1A—C2A	1.405 (2)
Ru1—C2	2.1863 (18)	C1A—C6A	1.411 (2)
Ru1—C3	2.2123 (16)	C1A—B1A	1.655 (2)
Ru1—C4	2.2391 (16)	C2A—C3A	1.399 (2)
Ru1—C5	2.2005 (16)	C2A—H2A	0.9500
Ru1—C6	2.1626 (16)	C3A—C4A	1.390 (3)
N1—C11	1.3423 (19)	C3A—H3A	0.9500
N1—C15	1.354 (2)	C4A—C5A	1.389 (3)
N2—C20	1.345 (2)	C4A—H4A	0.9500
N2—C16	1.355 (2)	C5A—C6A	1.391 (2)
C1—C6	1.419 (2)	C5A—H5A	0.9500
C1—C2	1.426 (3)	C6A—H6A	0.9500
C1—C7	1.502 (2)	C7A—C8A	1.399 (2)
C2—C3	1.411 (2)	C7A—C12A	1.407 (2)
C2—H2	1.0000	C7A—B1A	1.644 (2)
C3—C4	1.422 (2)	C8A—C9A	1.397 (2)
C3—H3	1.0000	C8A—H8AA	0.9500
C4—C5	1.417 (2)	C9A—C10A	1.388 (3)
C4—C10	1.496 (2)	C9A—H9AA	0.9500
C5—C6	1.422 (2)	C10A—C11A	1.391 (3)
C5—H5	1.0000	C10A—H10D	0.9500
C6—H6	1.0000	C11A—C12A	1.391 (2)
C7—C8	1.525 (3)	C11A—H11A	0.9500
C7—C9	1.531 (3)	C12A—H12A	0.9500
C7—H7	1.0000	C13A—C14A	1.403 (2)
C8—H8A	0.9800	C13A—C18A	1.408 (2)
C8—H8B	0.9800	C13A—B1A	1.653 (3)
C8—H8C	0.9800	C14A—C15A	1.401 (2)
C9—H9A	0.9800	C14A—H14A	0.9500
C9—H9B	0.9800	C15A—C16A	1.386 (3)
C9—H9C	0.9800	C15A—H15A	0.9500

C10—H10A	0.9800	C16A—C17A	1.387 (3)
C10—H10B	0.9800	C16A—H16A	0.9500
C10—H10C	0.9800	C17A—C18A	1.394 (3)
C11—C12	1.388 (2)	C17A—H17A	0.9500
C11—H11	0.9500	C18A—H18A	0.9500
C12—C13	1.388 (3)	C19A—C20A	1.402 (2)
C12—H12	0.9500	C19A—C24A	1.410 (2)
C13—C14	1.386 (3)	C19A—B1A	1.647 (2)
C13—H13	0.9500	C20A—C21A	1.401 (2)
C14—C15	1.398 (2)	C20A—H20A	0.9500
C14—H14	0.9500	C21A—C22A	1.388 (2)
C15—C16	1.465 (2)	C21A—H21A	0.9500
C16—C17	1.390 (2)	C22A—C23A	1.394 (2)
C17—C18	1.387 (2)	C22A—H22A	0.9500
C17—H17	0.9500	C23A—C24A	1.393 (2)
C18—C19	1.384 (3)	C23A—H23A	0.9500
C18—H18	0.9500	C24A—H24A	0.9500

N2—Ru1—N1	76.98 (5)	C13—C12—C11	119.30 (16)
N2—Ru1—C6	91.73 (6)	C13—C12—H12	120.3
N1—Ru1—C6	135.94 (6)	C11—C12—H12	120.3
N2—Ru1—C2	139.09 (6)	C14—C13—C12	119.00 (17)
N1—Ru1—C2	93.45 (6)	C14—C13—H13	120.5
C6—Ru1—C2	67.64 (7)	C12—C13—H13	120.5
N2—Ru1—C5	105.63 (6)	C13—C14—C15	118.96 (16)
N1—Ru1—C5	172.63 (6)	C13—C14—H14	120.5
C6—Ru1—C5	38.04 (6)	C15—C14—H14	120.5
C2—Ru1—C5	80.06 (7)	N1—C15—C14	121.67 (14)
N2—Ru1—C3	171.53 (6)	N1—C15—C16	114.60 (13)
N1—Ru1—C3	109.54 (6)	C14—C15—C16	123.70 (14)
C6—Ru1—C3	79.82 (6)	N2—C16—C17	121.53 (14)
C2—Ru1—C3	37.42 (6)	N2—C16—C15	114.82 (13)
C5—Ru1—C3	67.23 (7)	C17—C16—C15	123.62 (14)
N2—Ru1—C1	105.60 (5)	C18—C17—C16	119.10 (15)
N1—Ru1—C1	104.21 (6)	C18—C17—H17	120.5
C6—Ru1—C1	37.73 (6)	C16—C17—H17	120.5
C2—Ru1—C1	37.73 (7)	C19—C18—C17	119.35 (15)
C5—Ru1—C1	68.51 (6)	C19—C18—H18	120.3
C3—Ru1—C1	67.98 (6)	C17—C18—H18	120.3
N2—Ru1—C4	138.24 (6)	C18—C19—C20	118.74 (15)
N1—Ru1—C4	142.73 (6)	C18—C19—H19	120.6
C6—Ru1—C4	67.79 (6)	C20—C19—H19	120.6
C2—Ru1—C4	67.55 (7)	N2—C20—C19	122.40 (16)
C5—Ru1—C4	37.20 (6)	N2—C20—H20	118.8
C3—Ru1—C4	37.25 (6)	C19—C20—H20	118.8
C1—Ru1—C4	80.61 (6)	C2A—C1A—C6A	114.66 (14)
N2—Ru1—Cl1	83.37 (4)	C2A—C1A—B1A	125.09 (14)
N1—Ru1—Cl1	84.55 (4)	C6A—C1A—B1A	120.23 (14)

C6—Ru1—Cl1	136.99 (5)	C3A—C2A—C1A	122.83 (16)
C2—Ru1—Cl1	135.91 (4)	C3A—C2A—H2A	118.6
C5—Ru1—Cl1	102.53 (5)	C1A—C2A—H2A	118.6
C3—Ru1—Cl1	102.34 (5)	C4A—C3A—C2A	120.43 (16)
C1—Ru1—Cl1	168.54 (4)	C4A—C3A—H3A	119.8
C4—Ru1—Cl1	87.95 (5)	C2A—C3A—H3A	119.8
C11—N1—C15	119.01 (14)	C5A—C4A—C3A	118.61 (16)
C11—N1—Ru1	124.14 (11)	C5A—C4A—H4A	120.7
C15—N1—Ru1	116.78 (10)	C3A—C4A—H4A	120.7
C20—N2—C16	118.85 (14)	C4A—C5A—C6A	120.18 (17)
C20—N2—Ru1	124.25 (11)	C4A—C5A—H5A	119.9
C16—N2—Ru1	116.82 (10)	C6A—C5A—H5A	119.9
C6—C1—C2	116.57 (14)	C5A—C6A—C1A	123.28 (16)
C6—C1—C7	120.89 (14)	C5A—C6A—H6A	118.4
C2—C1—C7	122.53 (15)	C1A—C6A—H6A	118.4
C6—C1—Ru1	68.81 (9)	C8A—C7A—C12A	115.15 (14)
C2—C1—Ru1	69.72 (9)	C8A—C7A—B1A	124.60 (14)
C7—C1—Ru1	133.03 (11)	C12A—C7A—B1A	120.25 (13)
C3—C2—C1	121.83 (17)	C9A—C8A—C7A	122.68 (16)
C3—C2—Ru1	72.29 (10)	C9A—C8A—H8AA	118.7
C1—C2—Ru1	72.55 (9)	C7A—C8A—H8AA	118.7
C3—C2—H2	118.6	C10A—C9A—C8A	120.37 (18)
C1—C2—H2	118.6	C10A—C9A—H9AA	119.8
Ru1—C2—H2	118.6	C8A—C9A—H9AA	119.8
C2—C3—C4	120.56 (15)	C9A—C10A—C11A	118.70 (16)
C2—C3—Ru1	70.29 (9)	C9A—C10A—H10D	120.6
C4—C3—Ru1	72.40 (9)	C11A—C10A—H10D	120.6
C2—C3—H3	119.1	C10A—C11A—C12A	120.01 (16)
C4—C3—H3	119.1	C10A—C11A—H11A	120.0
Ru1—C3—H3	119.1	C12A—C11A—H11A	120.0
C5—C4—C3	118.77 (15)	C11A—C12A—C7A	123.05 (16)
C5—C4—C10	120.99 (16)	C11A—C12A—H12A	118.5
C3—C4—C10	120.19 (16)	C7A—C12A—H12A	118.5
C5—C4—Ru1	69.92 (9)	C14A—C13A—C18A	114.82 (17)
C3—C4—Ru1	70.35 (9)	C14A—C13A—B1A	124.65 (13)
C10—C4—Ru1	129.54 (13)	C18A—C13A—B1A	120.52 (14)
C4—C5—C6	119.77 (15)	C15A—C14A—C13A	122.89 (16)
C4—C5—Ru1	72.88 (9)	C15A—C14A—H14A	118.6
C6—C5—Ru1	69.54 (9)	C13A—C14A—H14A	118.6
C4—C5—H5	119.6	C16A—C15A—C14A	120.36 (16)
C6—C5—H5	119.6	C16A—C15A—H15A	119.8
Ru1—C5—H5	119.6	C14A—C15A—H15A	119.8
C1—C6—C5	122.41 (15)	C15A—C16A—C17A	118.46 (16)
C1—C6—Ru1	73.46 (9)	C15A—C16A—H16A	120.8
C5—C6—Ru1	72.43 (9)	C17A—C16A—H16A	120.8
C1—C6—H6	118.4	C16A—C17A—C18A	120.57 (17)
C5—C6—H6	118.4	C16A—C17A—H17A	119.7
Ru1—C6—H6	118.4	C18A—C17A—H17A	119.7

C1—C7—C8	113.99 (15)	C17A—C18A—C13A	122.89 (17)
C1—C7—C9	108.11 (15)	C17A—C18A—H18A	118.6
C8—C7—C9	111.16 (18)	C13A—C18A—H18A	118.6
C1—C7—H7	107.8	C20A—C19A—C24A	115.58 (13)
C8—C7—H7	107.8	C20A—C19A—B1A	124.13 (13)
C9—C7—H7	107.8	C24A—C19A—B1A	120.29 (13)
C7—C8—H8A	109.5	C21A—C20A—C19A	122.55 (14)
C7—C8—H8B	109.5	C21A—C20A—H20A	118.7
H8A—C8—H8B	109.5	C19A—C20A—H20A	118.7
C7—C8—H8C	109.5	C22A—C21A—C20A	120.11 (15)
H8A—C8—H8C	109.5	C22A—C21A—H21A	119.9
H8B—C8—H8C	109.5	C20A—C21A—H21A	119.9
C7—C9—H9A	109.5	C21A—C22A—C23A	119.07 (14)
C7—C9—H9B	109.5	C21A—C22A—H22A	120.5
H9A—C9—H9B	109.5	C23A—C22A—H22A	120.5
C7—C9—H9C	109.5	C24A—C23A—C22A	120.06 (14)
H9A—C9—H9C	109.5	C24A—C23A—H23A	120.0
H9B—C9—H9C	109.5	C22A—C23A—H23A	120.0
C4—C10—H10A	109.5	C23A—C24A—C19A	122.58 (14)
C4—C10—H10B	109.5	C23A—C24A—H24A	118.7
H10A—C10—H10B	109.5	C19A—C24A—H24A	118.7
C4—C10—H10C	109.5	C7A—B1A—C19A	107.15 (12)
H10A—C10—H10C	109.5	C7A—B1A—C13A	110.50 (12)
H10B—C10—H10C	109.5	C19A—B1A—C13A	110.20 (12)
N1—C11—C12	122.04 (16)	C7A—B1A—C1A	109.50 (12)
N1—C11—H11	119.0	C19A—B1A—C1A	111.19 (12)
C12—C11—H11	119.0	C13A—B1A—C1A	108.31 (12)

C6—C1—C2—C3	3.2 (2)	C18—C19—C20—N2	0.1 (3)
C7—C1—C2—C3	−175.93 (15)	C6A—C1A—C2A—C3A	−0.4 (2)
Ru1—C1—C2—C3	55.22 (15)	B1A—C1A—C2A—C3A	−178.56 (15)
C6—C1—C2—Ru1	−52.00 (13)	C1A—C2A—C3A—C4A	0.9 (3)
C7—C1—C2—Ru1	128.85 (15)	C2A—C3A—C4A—C5A	−0.5 (3)
C1—C2—C3—C4	−1.1 (3)	C3A—C4A—C5A—C6A	−0.3 (3)
Ru1—C2—C3—C4	54.22 (14)	C4A—C5A—C6A—C1A	0.9 (3)
C1—C2—C3—Ru1	−55.33 (14)	C2A—C1A—C6A—C5A	−0.5 (2)
C2—C3—C4—C5	−1.0 (2)	B1A—C1A—C6A—C5A	177.80 (16)
Ru1—C3—C4—C5	52.27 (14)	C12A—C7A—C8A—C9A	−1.0 (3)
C2—C3—C4—C10	−178.31 (16)	B1A—C7A—C8A—C9A	178.62 (18)
Ru1—C3—C4—C10	−125.06 (16)	C7A—C8A—C9A—C10A	−0.8 (3)
C2—C3—C4—Ru1	−53.25 (14)	C8A—C9A—C10A—C11A	1.3 (3)
C3—C4—C5—C6	0.8 (2)	C9A—C10A—C11A—C12A	−0.1 (3)
C10—C4—C5—C6	178.13 (16)	C10A—C11A—C12A—C7A	−1.8 (3)
Ru1—C4—C5—C6	53.30 (14)	C8A—C7A—C12A—C11A	2.3 (3)
C3—C4—C5—Ru1	−52.47 (14)	B1A—C7A—C12A—C11A	−177.37 (16)
C10—C4—C5—Ru1	124.83 (16)	C18A—C13A—C14A—C15A	−1.0 (2)
C2—C1—C6—C5	−3.4 (2)	B1A—C13A—C14A—C15A	179.59 (15)
C7—C1—C6—C5	175.78 (15)	C13A—C14A—C15A—C16A	0.6 (3)

Ru1—C1—C6—C5	−55.84 (14)	C14A—C15A—C16A—C17A	0.0 (3)
C2—C1—C6—Ru1	52.45 (13)	C15A—C16A—C17A—C18A	−0.1 (3)
C7—C1—C6—Ru1	−128.39 (14)	C16A—C17A—C18A—C13A	−0.4 (3)
C4—C5—C6—C1	1.4 (2)	C14A—C13A—C18A—C17A	0.9 (2)
Ru1—C5—C6—C1	56.31 (14)	B1A—C13A—C18A—C17A	−179.66 (15)
C4—C5—C6—Ru1	−54.87 (14)	C24A—C19A—C20A—C21A	−0.8 (2)
C6—C1—C7—C8	146.08 (18)	B1A—C19A—C20A—C21A	179.82 (14)
C2—C1—C7—C8	−34.8 (2)	C19A—C20A—C21A—C22A	−0.9 (2)
Ru1—C1—C7—C8	57.1 (2)	C20A—C21A—C22A—C23A	1.3 (2)
C6—C1—C7—C9	−89.8 (2)	C21A—C22A—C23A—C24A	0.1 (2)
C2—C1—C7—C9	89.3 (2)	C22A—C23A—C24A—C19A	−2.0 (2)
Ru1—C1—C7—C9	−178.77 (14)	C20A—C19A—C24A—C23A	2.3 (2)
C15—N1—C11—C12	−1.1 (3)	B1A—C19A—C24A—C23A	−178.31 (14)
Ru1—N1—C11—C12	−177.98 (18)	C8A—C7A—B1A—C19A	127.43 (16)
N1—C11—C12—C13	0.0 (4)	C12A—C7A—B1A—C19A	−52.97 (18)
C11—C12—C13—C14	0.7 (4)	C8A—C7A—B1A—C13A	−112.49 (17)
C12—C13—C14—C15	−0.2 (3)	C12A—C7A—B1A—C13A	67.11 (18)
C11—N1—C15—C14	1.6 (3)	C8A—C7A—B1A—C1A	6.7 (2)
Ru1—N1—C15—C14	178.68 (14)	C12A—C7A—B1A—C1A	−173.66 (14)
C11—N1—C15—C16	−176.66 (17)	C20A—C19A—B1A—C7A	129.97 (15)
Ru1—N1—C15—C16	0.40 (18)	C24A—C19A—B1A—C7A	−49.35 (18)
C13—C14—C15—N1	−0.9 (3)	C20A—C19A—B1A—C13A	9.70 (19)
C13—C14—C15—C16	177.17 (18)	C24A—C19A—B1A—C13A	−169.62 (13)
C20—N2—C16—C17	−1.6 (2)	C20A—C19A—B1A—C1A	−110.41 (16)
Ru1—N2—C16—C17	−178.47 (11)	C24A—C19A—B1A—C1A	70.27 (17)
C20—N2—C16—C15	176.78 (14)	C14A—C13A—B1A—C7A	−17.8 (2)
Ru1—N2—C16—C15	−0.12 (17)	C18A—C13A—B1A—C7A	162.90 (13)
N1—C15—C16—N2	−0.2 (2)	C14A—C13A—B1A—C19A	100.45 (16)
C14—C15—C16—N2	−178.42 (16)	C18A—C13A—B1A—C19A	−78.87 (17)
N1—C15—C16—C17	178.13 (14)	C14A—C13A—B1A—C1A	−137.72 (14)
C14—C15—C16—C17	−0.1 (3)	C18A—C13A—B1A—C1A	42.96 (18)
N2—C16—C17—C18	0.9 (2)	C2A—C1A—B1A—C7A	96.69 (17)
C15—C16—C17—C18	−177.30 (15)	C6A—C1A—B1A—C7A	−81.38 (18)
C16—C17—C18—C19	0.3 (2)	C2A—C1A—B1A—C19A	−21.5 (2)
C17—C18—C19—C20	−0.8 (2)	C6A—C1A—B1A—C19A	160.42 (14)
C16—N2—C20—C19	1.1 (2)	C2A—C1A—B1A—C13A	−142.74 (15)
Ru1—N2—C20—C19	177.71 (12)	C6A—C1A—B1A—C13A	39.19 (19)

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of rings C19*A*–C24*A* and N2/C16–C20, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Cl1^{i}	1.00	2.66	3.421 (2)	133
C11—H11···Cl1^{i}	0.95	2.62	3.484 (2)	151
C7—H7···*Cg*1^{ii}	1.00	2.67	3.616 (2)	158
C9—H9*B*···*Cg*2^{iii}	0.98	2.91	3.733 (2)	143

C18—H18···*Cg*1	0.95	2.73	3.431 (2)	131
C23*A*—H23*A*···*Cg*2^{iv}	0.95	2.60	3.461 (2)	151

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