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trans-Bis(2,2′-bipyridine)dichloridoruthenium(II)

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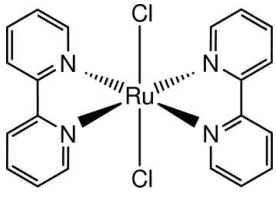
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.004 Å; R factor = 0.026; wR factor = 0.058; data-to-parameter ratio = 16.5.

In the title compound, $[RuCl_2(C_{10}H_8N_2)_2]$, the Ru atom is located on a crystallographic inversion center. The bipyridine (bpy) ligands are thus coordinated *trans*, leading to steric interactions between pairs of opposite *ortho*-H atoms. The result is a marked deviation from the expected planarity of some units; the two pyridine rings of an individual bpy ligand enclose a 23.8 (1)° angle. With the RuN_4 plane, the same pyridine rings enclose angles of 22.3 (1) and 21.0 (1)°. The octahedral environment of the Ru atom, however, is not markedly distorted, with the Ru—Cl axis enclosing a 87.32 (6)° angle with the RuN_4 plane. In the crystal structure, the most significant intermolecular interaction, besides the expected π stacking [3.424 (3) Å perpendicular distance of parallel-stacked rings, and 3.389 (3) Å closest ring–atom distance for an inclined contact], is a weak C—H···Cl hydrogen bond.

Related literature

Sullivan *et al.* (1978) describe the corresponding *cis*-coordinated complex which was used as the starting material for the synthesis of the title compound. Weathers *et al.* (1997) describe a related complex cation with the chlorido ligands of the title compound substituted by aqua ligands. For ring puckering analysis, see: Cremer & Pople (1975).



Experimental

Crystal data

$[RuCl_2(C_{10}H_8N_2)_2]$
M_r = 484.34
Monoclinic, $P2_1/c$
a = 7.0047 (3) Å
b = 14.9489 (6) Å
c = 8.7301 (3) Å
β = 99.692 (2)°
V = 901.10 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 200 (2) K
0.15 × 0.10 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.763, T_{max} = 0.932
10312 measured reflections
2067 independent reflections
1719 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.058
S = 1.06
2067 reflections
125 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···Cl1^{i}	0.95	2.72	3.573 (3)	150

Symmetry code: (i) $-x-1, y-\frac{1}{2}, -z-\frac{1}{2}$.

Data collection: *COLLECT* (Hooft, 2004); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2023).

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supplementary materials

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trans-Bis(2,2'-bipyridine)dichloridoruthenium(II)

P. Klüfers and A. Zangl

Comment

The title compound, $C_{20}H_{16}Cl_2N_4Ru$, was obtained accidentally on the attempted preparation of [Ru(*cis*-CptdH$_{-2}$)(bipy)$_2$] (*cis*-CptdH$_{-2}$ = twofold deprotonated *cis*-1,2-cyclopentanediol, bipy = 2,2'-bipyridine).

The molecular structure is shown in Fig. 1. The five-membered chelate ring Ru—N1—C5—C6—N2 adopts an envelope conformation on Ru (Q_2 = 0.2785 (17) Å, φ_2 = 184.3 (5)°). Ring-puckering parameters (Cremer & Pople, 1975) were calculated with *PLATON* (Spek, 2003).

Bond lengths and angles are comparable to similar compounds (Weathers *et al.*, 1997).

The molecular packing is shown in Fig. 2 which shows a layer of molecules of (I) in the *bc* plane. Hydrogen bonds of the C–H···Cl type connect these layers along [100]. [100]-stacking is supported by π stacking of aromatic rings that enclose a 23.8 (1)° angle, the closest ring···atom contact being 3.389 (3) Å.

π stacking is also observed for adjacent molecules along [001] between aromatic rings that are connected by an inversion center. The perpendicular ring distance is 3.424 (3) Å for this interaction.

Experimental

The title compound was obtained accidentally on the attempted preparation of [Ru(*cis*-CptdH$_{-2}$)(bipy)$_2$] by refluxing 58 mg (0.12 mmol) *cis*-[RuCl$_2$(bipy)$_2$] (Sullivan *et al.*, 1978), 27 mg (0.26 mmol) *cis*-1,2-cyclopentanediol and 15 mg (0.27 mmol) KOH for 4 h in a solution of 1.4 ml H_2O and 4 ml 2-propanol under an inert gas atmosphere (N_2). When the closed reaction flask was left standing at room temperature in bright daylight, violet-black crystals were obtained after several months.

Refinement

All H atoms were included in calculated positions and refined as riding on their parent atoms with one common isotropic displacement parameter.

Figures

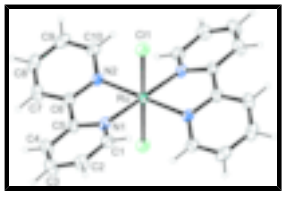

Fig. 1. The molecular structure of (I), with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

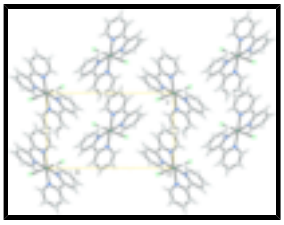

Fig. 2. A layer of molecules of (I) in the *bc* plane.

i>trans-Bis(2,2'-bipyridine)dichloridoruthenium(II)

Crystal data

$[RuCl_2(C_{10}H_8N_2)_2]$	F_{000} = 484
M_r = 484.34	D_x = 1.785 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6762 reflections
a = 7.0047 (3) Å	θ = 3.1–27.5º
b = 14.9489 (6) Å	μ = 1.18 mm^{-1}
c = 8.7301 (3) Å	T = 200 (2) K
β = 99.692 (2)º	Platelet, black-violet
V = 901.10 (6) Å^3	0.15 × 0.10 × 0.06 mm
Z = 2	

Data collection

Nonius KappaCCD diffractometer	2067 independent reflections
Radiation source: rotating anode	1719 reflections with $I > 2\sigma(I)$
Monochromator: MONTEL, graded multilayered X-ray optics	R_{int} = 0.041
T = 200(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 3.3º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)	h = −9→8
T_{min} = 0.763, T_{max} = 0.932	k = −19→19
10312 measured reflections	l = −11→11

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.026	H-atom parameters constrained
$wR(F^2)$ = 0.058	$w = 1/[\sigma^2(F_o^2) + (0.015P)^2 + 0.9494P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
2067 reflections	$\Delta\rho_{max}$ = 0.53 e Å^{-3}

125 parameters	$\Delta\rho_{min} = -0.56$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. $\mu \times r = 0.116$, $T_{min}/T_{max} = 0.899$

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru	0.0000	0.0000	0.0000	0.01748 (9)
Cl1	−0.18499 (9)	0.12549 (4)	−0.11057 (7)	0.02946 (15)
N1	−0.1977 (3)	−0.09044 (12)	−0.1129 (2)	0.0204 (4)
N2	0.1001 (3)	−0.02145 (12)	−0.2052 (2)	0.0206 (4)
C1	−0.3740 (3)	−0.11069 (15)	−0.0811 (3)	0.0243 (5)
H1	−0.4268	−0.0741	−0.0097	0.033 (3)*
C2	−0.4811 (3)	−0.18208 (16)	−0.1476 (3)	0.0290 (6)
H2	−0.6049	−0.1944	−0.1218	0.033 (3)*
C3	−0.4071 (4)	−0.23546 (17)	−0.2521 (3)	0.0339 (6)
H3	−0.4755	−0.2869	−0.2954	0.033 (3)*
C4	−0.2302 (4)	−0.21242 (16)	−0.2925 (3)	0.0319 (6)
H4	−0.1772	−0.2473	−0.3661	0.033 (3)*
C5	−0.1312 (3)	−0.13828 (15)	−0.2249 (3)	0.0223 (5)
C6	0.0355 (3)	−0.09807 (15)	−0.2809 (3)	0.0231 (5)
C7	0.1040 (4)	−0.12659 (18)	−0.4124 (3)	0.0307 (6)
H7	0.0631	−0.1823	−0.4589	0.033 (3)*
C8	0.2319 (4)	−0.07363 (19)	−0.4754 (3)	0.0344 (6)
H8	0.2803	−0.0920	−0.5658	0.033 (3)*
C9	0.2882 (4)	0.00714 (18)	−0.4039 (3)	0.0333 (6)
H9	0.3730	0.0460	−0.4465	0.033 (3)*
C10	0.2200 (4)	0.03048 (17)	−0.2706 (3)	0.0273 (5)
H10	0.2598	0.0860	−0.2226	0.033 (3)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru	0.02017 (14)	0.01732 (13)	0.01542 (13)	0.00075 (10)	0.00439 (9)	−0.00161 (10)
Cl1	0.0339 (3)	0.0278 (3)	0.0268 (3)	0.0094 (3)	0.0055 (3)	0.0018 (3)
N1	0.0196 (10)	0.0255 (10)	0.0163 (9)	0.0011 (8)	0.0032 (8)	−0.0005 (8)
N2	0.0226 (10)	0.0228 (10)	0.0167 (9)	0.0017 (8)	0.0045 (8)	−0.0008 (7)
C1	0.0246 (12)	0.0245 (12)	0.0242 (13)	0.0042 (10)	0.0053 (10)	0.0006 (9)
C2	0.0206 (12)	0.0333 (13)	0.0328 (14)	−0.0006 (10)	0.0036 (11)	0.0009 (11)
C3	0.0306 (14)	0.0311 (13)	0.0395 (16)	−0.0061 (11)	0.0038 (12)	−0.0120 (12)
C4	0.0314 (14)	0.0300 (13)	0.0348 (15)	−0.0028 (11)	0.0074 (12)	−0.0133 (11)
C5	0.0233 (12)	0.0233 (11)	0.0203 (12)	0.0022 (9)	0.0036 (9)	−0.0036 (9)
C6	0.0244 (12)	0.0253 (12)	0.0191 (12)	0.0043 (9)	0.0022 (10)	−0.0030 (9)
C7	0.0288 (13)	0.0358 (14)	0.0275 (13)	0.0033 (11)	0.0048 (11)	−0.0110 (11)

C8	0.0322 (14)	0.0505 (16)	0.0224 (13)	0.0041 (13)	0.0097 (11)	−0.0054 (12)
C9	0.0319 (14)	0.0431 (15)	0.0279 (13)	0.0002 (12)	0.0136 (11)	0.0069 (12)
C10	0.0308 (13)	0.0275 (12)	0.0247 (13)	−0.0014 (10)	0.0084 (11)	0.0015 (10)

Geometric parameters (Å, °)

Ru—N2	2.0560 (19)	C3—C4	1.388 (4)
Ru—N2^{i}	2.0560 (19)	C3—H3	0.9500
Ru—N1	2.0632 (18)	C4—C5	1.385 (3)
Ru—N1^{i}	2.0632 (18)	C4—H4	0.9500
Ru—Cl1^{i}	2.3893 (6)	C5—C6	1.468 (3)
Ru—Cl1	2.3893 (6)	C6—C7	1.384 (3)
N1—C1	1.345 (3)	C7—C8	1.378 (4)
N1—C5	1.356 (3)	C7—H7	0.9500
N2—C10	1.340 (3)	C8—C9	1.386 (4)
N2—C6	1.361 (3)	C8—H8	0.9500
C1—C2	1.376 (3)	C9—C10	1.375 (4)
C1—H1	0.9500	C9—H9	0.9500
C2—C3	1.377 (4)	C10—H10	0.9500
C2—H2	0.9500		
N2—Ru—N2^{i}	180.00 (9)	C3—C2—H2	120.3
N2—Ru—N1	77.38 (7)	C2—C3—C4	118.5 (2)
N2^{i}—Ru—N1	102.62 (7)	C2—C3—H3	120.8
N2—Ru—N1^{i}	102.62 (7)	C4—C3—H3	120.8
N2^{i}—Ru—N1^{i}	77.38 (7)	C5—C4—C3	119.6 (2)
N1—Ru—N1^{i}	180.00 (12)	C5—C4—H4	120.2
N2—Ru—Cl1^{i}	89.32 (5)	C3—C4—H4	120.2
N2^{i}—Ru—Cl1^{i}	90.68 (5)	N1—C5—C4	121.4 (2)
N1—Ru—Cl1^{i}	87.32 (5)	N1—C5—C6	114.42 (19)
N1^{i}—Ru—Cl1^{i}	92.68 (5)	C4—C5—C6	123.7 (2)
N2—Ru—Cl1	90.68 (5)	N2—C6—C7	121.9 (2)
N2^{i}—Ru—Cl1	89.32 (5)	N2—C6—C5	113.6 (2)
N1—Ru—Cl1	92.68 (5)	C7—C6—C5	123.8 (2)
N1^{i}—Ru—Cl1	87.31 (5)	C8—C7—C6	119.6 (2)
Cl1^{i}—Ru—Cl1	180.00 (3)	C8—C7—H7	120.2
C1—N1—C5	117.97 (19)	C6—C7—H7	120.2
C1—N1—Ru	127.93 (16)	C7—C8—C9	118.4 (2)
C5—N1—Ru	113.93 (15)	C7—C8—H8	120.8
C10—N2—C6	117.5 (2)	C9—C8—H8	120.8
C10—N2—Ru	127.67 (16)	C10—C9—C8	119.3 (2)
C6—N2—Ru	114.84 (16)	C10—C9—H9	120.4
N1—C1—C2	122.8 (2)	C8—C9—H9	120.4
N1—C1—H1	118.6	N2—C10—C9	123.0 (2)
C2—C1—H1	118.6	N2—C10—H10	118.5
C1—C2—C3	119.3 (2)	C9—C10—H10	118.5
C1—C2—H2	120.3		

N2—Ru—N1—C1	−163.6 (2)	C1—N1—C5—C4	−7.4 (3)
N2^{i}—Ru—N1—C1	16.4 (2)	Ru—N1—C5—C4	168.23 (18)
Cl1^{i}—Ru—N1—C1	106.46 (19)	C1—N1—C5—C6	164.8 (2)
Cl1—Ru—N1—C1	−73.54 (19)	Ru—N1—C5—C6	−19.6 (2)
N2—Ru—N1—C5	21.26 (15)	C3—C4—C5—N1	3.9 (4)
N2^{i}—Ru—N1—C5	−158.74 (15)	C3—C4—C5—C6	−167.5 (2)
Cl1^{i}—Ru—N1—C5	−68.65 (15)	C10—N2—C6—C7	6.1 (3)
Cl1—Ru—N1—C5	111.35 (15)	Ru—N2—C6—C7	−173.60 (18)
N1—Ru—N2—C10	160.5 (2)	C10—N2—C6—C5	−164.9 (2)
N1^{i}—Ru—N2—C10	−19.5 (2)	Ru—N2—C6—C5	15.4 (2)
Cl1^{i}—Ru—N2—C10	−112.12 (19)	N1—C5—C6—N2	2.9 (3)
Cl1—Ru—N2—C10	67.88 (19)	C4—C5—C6—N2	174.9 (2)
N1—Ru—N2—C6	−19.82 (15)	N1—C5—C6—C7	−168.0 (2)
N1^{i}—Ru—N2—C6	160.18 (15)	C4—C5—C6—C7	4.0 (4)
Cl1^{i}—Ru—N2—C6	67.58 (15)	N2—C6—C7—C8	−4.3 (4)
Cl1—Ru—N2—C6	−112.42 (15)	C5—C6—C7—C8	165.8 (2)
C5—N1—C1—C2	5.6 (3)	C6—C7—C8—C9	0.1 (4)
Ru—N1—C1—C2	−169.29 (17)	C7—C8—C9—C10	2.0 (4)
N1—C1—C2—C3	−0.4 (4)	C6—N2—C10—C9	−4.0 (3)
C1—C2—C3—C4	−3.2 (4)	Ru—N2—C10—C9	175.73 (18)
C2—C3—C4—C5	1.5 (4)	C8—C9—C10—N2	0.0 (4)

Symmetry codes: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···Cl1^{ii}	0.95	2.72	3.573 (3)	150

Symmetry codes: (ii) −*x*−1, *y*−1/2, −*z*−1/2.

Fig. 1

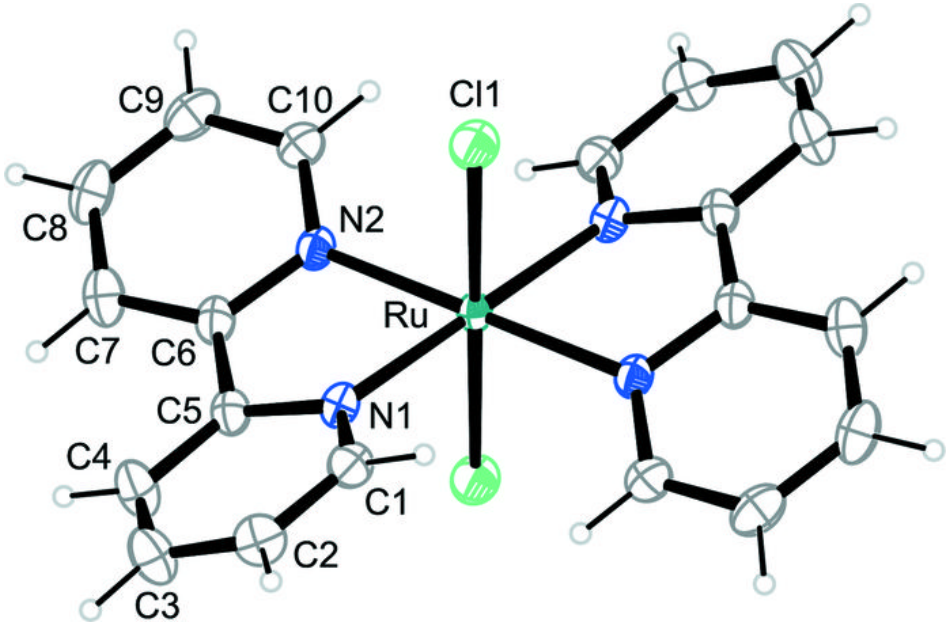

Fig. 2