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Chlorido(η^4-cycloocta-1,5-diene)-[(*S*)-2-(methoxymethyl)pyrrolidine-κN]rhodium(I)

Lutz Dahlenburg,* Harald Treffert and Frank W. Heinemann

Institut für Anorganische Chemie, Universität Erlangen-Nürnberg, Egerlandstrasse 1, D-91058 Erlangen, Germany
Correspondence e-mail: lutz.dahlenburg@chemie.uni-erlangen.de

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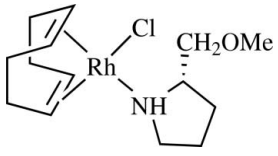
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.016; wR factor = 0.035; data-to-parameter ratio = 22.9.

The title compound, [RhCl(C_8H_{12})($C_6H_{13}NO$)], which is of interest from the point of view of catalysis, crystallizes with two independent molecules in the asymmetric unit, which is the complete unit cell. Neither the Rh—Cl nor the Rh—N bond lengths deviate significantly from the corresponding dimensions observed for closely related chloride–rhodium complexes in the literature. Individual molecules are interlinked through N—H···Cl hydrogen-bonding interactions.

Related literature

For structurally related rhodium complexes with various chiral and achiral β-amino alcohol ligands, see Dahlenburg *et al.* (2007).



Experimental

Crystal data

[RhCl(C_8H_{12})($C_6H_{13}NO$)]
M_r = 361.71
Triclinic, $P1$
a = 6.5499 (2) Å
b = 6.6563 (2) Å
c = 18.8540 (7) Å
α = 92.253 (3)°
β = 95.026 (3)°
γ = 114.841 (2)°
V = 740.44 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 150 (2) K
0.25 × 0.18 × 0.10 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.730, T_{max} = 0.880
19576 measured reflections
7489 independent reflections
7246 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.035
S = 1.06
7489 reflections
327 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Absolute structure: Flack (1983), 3690 Friedel pairs
Flack parameter: −0.013 (13)

Table 1
Selected geometric parameters (Å, °).

Rh1—N1	2.1236 (15)	Rh2—N2	2.1263 (15)
Rh1—Cl1	2.3960 (6)	Rh2—Cl2	2.3870 (5)
Rh1—C11	2.1199 (17)	Rh2—C25	2.0985 (18)
Rh1—C12	2.1021 (17)	Rh2—C26	2.1154 (18)
Rh1—C7	2.1491 (19)	Rh2—C21	2.1242 (18)
Rh1—C8	2.1300 (19)	Rh2—C22	2.150 (2)
N1—Rh1—Cl1	90.47 (4)	N2—Rh2—Cl2	89.43 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl1^{i}	0.93	2.59	3.4888 (16)	163
N2—H2···Cl2^{ii}	0.93	2.51	3.4028 (16)	162

Symmetry codes: (i) $x, y+1, z$; (ii) $x+1, y, z$.

Data collection: *COLLECT* (Bruker, 2002); cell refinement: *EVALCCD* (Duisenberg *et al.*, 2003); data reduction: *EVALCCD*; program(s) used to solve structure: *SHELXTL-NT* (Bruker, 2002); 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG3061).

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supplementary materials

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Chlorido(η^4-cycloocta-1,5-diene)[(*S*)-2-(methoxymethyl)pyrrolidine-κN]rhodium(I)

L. Dahlenburg, H. Treffert and F. W. Heinemann

Comment

Chlorido(η^4-1,5-cyclooctadiene)[κ*N*-(*S*)-2-methoxymethylpyrrolidine]rhodium(I), [Rh(Cl)(η^4-C_8H_{12}){(*S*)-$C_6H_{13}NO$}] (I), represents the *O*-methylated analogue of the previously described prolinol complexes [Rh(Cl)(η^4-C_8H_{12}){(*R*)-$C_5H_{11}NO$}] and [Rh(Cl)(η^4-C_8H_{12}){(*S*)-$C_5H_{11}NO$}] which themselves belong to a family of catalytically attractive rhodium compounds containing β-amino alcohol ligands (Dahlenburg *et al.*, 2007). Complex (I) crystallizes from $CDCl_3$ in the triclinic space group *P*1 with two independent moieties per cell.

Not unexpectedly, neither the Rh—Cl distances nor the Rh—N bond lengths deviate significantly from the corresponding dimensions observed fo closely related chlorido rhodium complexes in the literature possessing *N*-bonded ethanolamine, valinol, prolinol, and norephedrine ligands [Rh—Cl = 2.381 → 2.398 Å and Rh—N = 2.127→ 2.137 Å] (Dahlenburg *et al.*, 2007).

In the solid state the individual complexes of (I) are assembled through N—H···Cl hydrogen bonds (Table 2). The (*R*)-enantiomer of the parent prolinol compound [Rh(Cl)(η^4-C_8H_{12})($C_5H_{11}NO$)] shows similar N—H···Cl (and O—H···Cl) hydrogen-bonding between two crystallographically independent molecules (Dahlenburg *et al.*, 2007).

Experimental

Compound (I) was prepared by the bridge-opening reaction of [{Rh(η^4-C_8H_{12})}$_2$(μ-Cl)$_2$] with (*S*)-2-methoxymethylpyrrolidine, similar to the procedure previously communicated for the syntheses of a number of chlorido(η^4-1,5-cyclooctadiene)rhodium(I) derivatives bearing diverse *N*-bonded β-amino alcohol ligands (Dahlenburg *et al.*, 2007). The specimen used for the X-ray diffraction study was collected from a partially evaporated NMR sample in $CDCl_3$ solution.

Refinement

Carbon-and nitrogen-bound H atoms were positioned geometrically (C—H = 0.95–0.99 Å; N—H = 0.93 Å) and refined using appropriate riding models. All hydrogen U_{iso} values were fixed at 1.2 times U_{eq} of the preceding carrier atom.

Figures

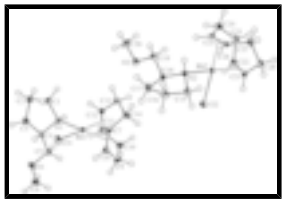


Fig. 1. Structures of the two crystallographically independent molecules of (I). Displacement ellipsoids are drawn at the 50% probability level.

Chlorido(η^4-cycloocta-1,5-diene)[(*S*)-2-(methoxymethyl)pyrrolidine- κ*N*]rhodium(I)

Crystal data

[RhCl(C_8H_{12})($C_6H_{13}NO$)]	Z = 2
M_r = 361.71	F_{000} = 372
Triclinic, $P\overline{1}$	D_x = 1.622 Mg m^{-3}
Hall symbol: P -1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 6.5499 (2) Å	Cell parameters from 98 reflections
b = 6.6563 (2) Å	θ = 6.0–20.0º
c = 18.8540 (7) Å	μ = 1.32 mm^{-1}
α = 92.253 (3)º	T = 150 (2) K
β = 95.026 (3)º	Plate, yellow
γ = 114.841 (2)º	0.25 × 0.18 × 0.10 mm
V = 740.44 (4) Å^3	

Data collection

Bruker–Nonius KappaCCD diffractometer	7489 independent reflections
Radiation source: fine-focus sealed tube	7246 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019
Detector resolution: 9 pixels mm^{-1}	θ_{max} = 28.7º
T = 150(2) K	θ_{min} = 3.3º
ω–rotations with 1.70 ° and 76 sec per frame scans	h = −8→8
Absorption correction: multi-scan (SADABS; Bruker, 2002)	k = −8→8
T_{min} = 0.730, T_{max} = 0.880	l = −25→25
19576 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.016	$w = 1/[\sigma^2(F_o^2) + (0.0125P)^2 + 0.1842P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.035	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.06	$\Delta\rho_{max}$ = 0.37 e Å^{-3}
7489 reflections	$\Delta\rho_{min}$ = −0.35 e Å^{-3}
327 parameters	Extinction correction: none
3 restraints	Absolute structure: Flack (1983)
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.013 (13)
Secondary atom site location: difference Fourier map	

Special details

Refinement. 3690 Friedel pairs were used in the refinement of the Flack parameter.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Rh1	0.084451 (15)	0.914650 (14)	0.609209 (7)	0.01109 (4)
Cl1	0.20120 (12)	0.67363 (10)	0.67548 (3)	0.02427 (14)
N1	0.2502 (3)	1.1749 (3)	0.69167 (8)	0.0131 (3)
H1	0.2092	1.2887	0.6803	0.016*
O1	−0.0795 (3)	1.0168 (3)	0.84488 (8)	0.0287 (4)
C1	0.5026 (3)	1.2725 (3)	0.69824 (10)	0.0180 (4)
H1A	0.5599	1.3537	0.6561	0.022*
H1B	0.5570	1.1549	0.7026	0.022*
C2	0.5807 (3)	1.4316 (3)	0.76628 (11)	0.0217 (4)
H2A	0.6092	1.5844	0.7549	0.026*
H2B	0.7209	1.4340	0.7916	0.026*
C3	0.3818 (3)	1.3363 (3)	0.81205 (10)	0.0210 (4)
H3A	0.4312	1.2943	0.8580	0.025*
H3B	0.3209	1.4465	0.8220	0.025*
C4	0.2023 (3)	1.1302 (4)	0.76651 (10)	0.0142 (4)
H4A	0.2276	0.9970	0.7788	0.017*
C5	−0.0394 (3)	1.0849 (4)	0.77490 (10)	0.0178 (4)
H5A	−0.0633	1.2207	0.7686	0.021*
H5B	−0.1442	0.9663	0.7387	0.021*
C6	−0.2952 (4)	0.9857 (4)	0.86247 (12)	0.0254 (4)
H6A	−0.3208	0.9189	0.9081	0.038*
H6B	−0.4116	0.8871	0.8250	0.038*
H6C	−0.3029	1.1295	0.8665	0.038*
C7	0.0141 (3)	0.7171 (3)	0.50952 (10)	0.0179 (4)
H7A	0.1378	0.6841	0.5249	0.021*
C8	−0.1764 (3)	0.6376 (3)	0.54673 (10)	0.0177 (4)
H8A	−0.1753	0.5469	0.5843	0.021*
C9	−0.3832 (3)	0.6819 (3)	0.53303 (12)	0.0229 (4)
H9A	−0.4747	0.6343	0.5735	0.028*
H9B	−0.4764	0.5903	0.4894	0.028*
C10	−0.3300 (3)	0.9254 (3)	0.52363 (12)	0.0219 (4)
H10A	−0.3216	0.9514	0.4724	0.026*
H10B	−0.4537	0.9584	0.5394	0.026*
C11	−0.1070 (3)	1.0805 (3)	0.56654 (11)	0.0165 (4)
H11A	−0.1115	1.1258	0.6146	0.020*
C12	0.1055 (3)	1.1619 (3)	0.54041 (10)	0.0155 (4)
H12A	0.2311	1.2644	0.5717	0.019*
C13	0.1534 (4)	1.1028 (3)	0.46791 (10)	0.0213 (4)
H13A	0.3187	1.1521	0.4682	0.026*
H13B	0.1049	1.1838	0.4322	0.026*
C14	0.0326 (4)	0.8540 (3)	0.44560 (11)	0.0238 (4)

H14A	−0.1211	0.8179	0.4219	0.029*
H14B	0.1170	0.8144	0.4107	0.029*
Rh2	0.094539 (15)	0.761289 (15)	0.114302 (7)	0.01106 (4)
Cl2	−0.21538 (8)	0.68239 (9)	0.18309 (3)	0.02146 (10)
N2	0.2549 (3)	0.6455 (3)	0.19530 (9)	0.0143 (3)
H2	0.3952	0.6673	0.1815	0.017*
O2	0.5079 (2)	1.0692 (2)	0.34836 (7)	0.0215 (3)
C15	0.1275 (3)	0.4022 (3)	0.20168 (11)	0.0198 (4)
H15A	0.1370	0.3147	0.1594	0.024*
H15B	−0.0339	0.3633	0.2063	0.024*
C16	0.2431 (4)	0.3587 (4)	0.26888 (11)	0.0248 (4)
H16A	0.3738	0.3297	0.2580	0.030*
H16B	0.1360	0.2297	0.2912	0.030*
C17	0.3211 (4)	0.5724 (3)	0.31814 (11)	0.0235 (4)
H17A	0.4806	0.6220	0.3388	0.028*
H17B	0.2254	0.5483	0.3576	0.028*
C18	0.2969 (3)	0.7465 (3)	0.27071 (9)	0.0149 (3)
H18A	0.1607	0.7682	0.2819	0.018*
C19	0.4995 (3)	0.9695 (3)	0.27987 (10)	0.0183 (4)
H19A	0.6400	0.9502	0.2758	0.022*
H19B	0.4847	1.0644	0.2425	0.022*
C20	0.7024 (4)	1.2750 (4)	0.36377 (12)	0.0264 (4)
H20A	0.6966	1.3446	0.4099	0.040*
H20B	0.7055	1.3735	0.3262	0.040*
H20C	0.8392	1.2488	0.3659	0.040*
C21	−0.1169 (3)	0.7272 (3)	0.01827 (10)	0.0168 (4)
H21A	−0.2417	0.6306	0.0408	0.020*
C22	−0.0168 (4)	0.9508 (4)	0.04382 (14)	0.0185 (5)
H22A	−0.0744	0.9937	0.0834	0.022*
C23	0.1775 (4)	1.1297 (3)	0.01277 (11)	0.0234 (4)
H23A	0.1619	1.2711	0.0173	0.028*
H23B	0.1697	1.0881	−0.0387	0.028*
C24	0.4096 (4)	1.1644 (3)	0.05044 (12)	0.0244 (4)
H24A	0.5235	1.2168	0.0161	0.029*
H24B	0.4556	1.2818	0.0902	0.029*
C25	0.4086 (3)	0.9560 (3)	0.07954 (10)	0.0181 (4)
H25A	0.4751	0.9678	0.1273	0.022*
C26	0.3173 (3)	0.7468 (3)	0.04160 (10)	0.0169 (4)
H26A	0.3207	0.6251	0.0656	0.020*
C27	0.2129 (3)	0.7032 (4)	−0.03583 (11)	0.0210 (4)
H27A	0.2477	0.5885	−0.0601	0.025*
H27B	0.2814	0.8411	−0.0603	0.025*
C28	−0.0445 (4)	0.6248 (4)	−0.04210 (11)	0.0195 (4)
H28A	−0.0959	0.6644	−0.0882	0.023*
H28B	−0.1185	0.4610	−0.0420	0.023*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rh1	0.01358 (9)	0.00928 (8)	0.01085 (8)	0.00528 (7)	0.00132 (6)	0.00121 (6)
Cl1	0.0390 (3)	0.0184 (3)	0.0208 (3)	0.0188 (3)	−0.0037 (2)	0.0012 (2)
N1	0.0149 (7)	0.0133 (7)	0.0125 (7)	0.0072 (6)	0.0014 (6)	0.0026 (6)
O1	0.0225 (8)	0.0499 (10)	0.0204 (7)	0.0196 (7)	0.0088 (6)	0.0144 (7)
C1	0.0147 (8)	0.0203 (9)	0.0174 (9)	0.0060 (7)	0.0018 (7)	0.0006 (7)
C2	0.0181 (9)	0.0188 (10)	0.0235 (10)	0.0044 (8)	−0.0007 (8)	−0.0036 (8)
C3	0.0201 (9)	0.0253 (10)	0.0161 (9)	0.0092 (8)	−0.0008 (7)	−0.0040 (8)
C4	0.0168 (9)	0.0160 (10)	0.0114 (9)	0.0085 (8)	0.0006 (7)	0.0031 (7)
C5	0.0171 (9)	0.0231 (10)	0.0140 (9)	0.0091 (8)	0.0021 (7)	0.0032 (8)
C6	0.0226 (10)	0.0322 (12)	0.0246 (10)	0.0129 (9)	0.0106 (8)	0.0070 (9)
C7	0.0212 (9)	0.0145 (9)	0.0152 (9)	0.0053 (8)	0.0021 (7)	−0.0023 (7)
C8	0.0193 (9)	0.0110 (8)	0.0175 (9)	0.0021 (7)	−0.0009 (7)	−0.0004 (7)
C9	0.0152 (9)	0.0183 (10)	0.0287 (11)	0.0009 (8)	0.0009 (8)	0.0019 (8)
C10	0.0167 (9)	0.0228 (10)	0.0259 (10)	0.0089 (8)	−0.0022 (8)	0.0030 (8)
C11	0.0172 (9)	0.0145 (9)	0.0202 (10)	0.0092 (8)	0.0008 (8)	0.0052 (8)
C12	0.0192 (9)	0.0125 (8)	0.0137 (8)	0.0059 (7)	0.0001 (7)	0.0041 (7)
C13	0.0228 (10)	0.0235 (10)	0.0165 (9)	0.0077 (8)	0.0055 (8)	0.0073 (8)
C14	0.0297 (11)	0.0233 (10)	0.0146 (9)	0.0070 (9)	0.0061 (8)	0.0008 (8)
Rh2	0.00948 (8)	0.01340 (8)	0.01073 (8)	0.00511 (7)	0.00209 (6)	0.00113 (6)
Cl2	0.0144 (2)	0.0360 (3)	0.0181 (2)	0.0139 (2)	0.00577 (17)	0.00443 (19)
N2	0.0146 (8)	0.0178 (8)	0.0128 (8)	0.0088 (7)	0.0032 (6)	0.0012 (6)
O2	0.0210 (7)	0.0207 (7)	0.0169 (7)	0.0040 (6)	0.0009 (5)	−0.0041 (5)
C15	0.0245 (10)	0.0155 (9)	0.0197 (9)	0.0097 (8)	−0.0005 (8)	−0.0005 (7)
C16	0.0330 (12)	0.0209 (10)	0.0244 (10)	0.0152 (9)	0.0014 (9)	0.0052 (8)
C17	0.0299 (11)	0.0212 (10)	0.0183 (9)	0.0105 (9)	−0.0015 (8)	0.0035 (8)
C18	0.0146 (8)	0.0192 (9)	0.0123 (8)	0.0084 (7)	0.0018 (7)	0.0001 (7)
C19	0.0208 (9)	0.0179 (9)	0.0173 (9)	0.0094 (8)	0.0028 (7)	−0.0002 (7)
C20	0.0235 (10)	0.0200 (10)	0.0290 (11)	0.0050 (8)	−0.0063 (9)	−0.0043 (8)
C21	0.0163 (9)	0.0189 (9)	0.0136 (8)	0.0063 (7)	−0.0011 (7)	0.0025 (7)
C22	0.0223 (11)	0.0187 (12)	0.0160 (10)	0.0106 (10)	−0.0004 (8)	0.0016 (9)
C23	0.0339 (11)	0.0130 (9)	0.0204 (10)	0.0075 (8)	0.0003 (8)	0.0038 (7)
C24	0.0234 (10)	0.0158 (9)	0.0250 (10)	−0.0009 (8)	0.0049 (8)	0.0022 (8)
C25	0.0128 (8)	0.0214 (10)	0.0159 (9)	0.0027 (7)	0.0045 (7)	0.0021 (7)
C26	0.0158 (9)	0.0207 (9)	0.0170 (9)	0.0088 (8)	0.0087 (7)	0.0054 (7)
C27	0.0261 (11)	0.0213 (10)	0.0163 (9)	0.0098 (9)	0.0082 (8)	0.0003 (8)
C28	0.0250 (11)	0.0172 (11)	0.0124 (9)	0.0059 (9)	−0.0014 (8)	0.0003 (8)

Geometric parameters (Å, °)

Rh1—N1	2.1236 (15)	Rh2—N2	2.1263 (15)
Rh1—Cl1	2.3960 (6)	Rh2—Cl2	2.3870 (5)
Rh1—C11	2.1199 (17)	Rh2—C25	2.0985 (18)
Rh1—C12	2.1021 (17)	Rh2—C26	2.1154 (18)
Rh1—C7	2.1491 (19)	Rh2—C21	2.1242 (18)
Rh1—C8	2.1300 (19)	Rh2—C22	2.150 (2)

N1—C4	1.487 (2)	N2—C15	1.494 (2)
N1—C1	1.492 (2)	N2—C18	1.500 (2)
N1—H1	0.9300	N2—H2	0.9300
O1—C6	1.411 (2)	O2—C19	1.415 (2)
O1—C5	1.422 (2)	O2—C20	1.422 (3)
C1—C2	1.534 (3)	C15—C16	1.519 (3)
C1—H1A	0.9900	C15—H15A	0.9900
C1—H1B	0.9900	C15—H15B	0.9900
C2—C3	1.546 (3)	C16—C17	1.533 (3)
C2—H2A	0.9900	C16—H16A	0.9900
C2—H2B	0.9900	C16—H16B	0.9900
C3—C4	1.542 (3)	C17—C18	1.542 (3)
C3—H3A	0.9900	C17—H17A	0.9900
C3—H3B	0.9900	C17—H17B	0.9900
C4—C5	1.506 (3)	C18—C19	1.510 (3)
C4—H4A	1.0000	C18—H18A	1.0000
C5—H5A	0.9900	C19—H19A	0.9900
C5—H5B	0.9900	C19—H19B	0.9900
C6—H6A	0.9800	C20—H20A	0.9800
C6—H6B	0.9800	C20—H20B	0.9800
C6—H6C	0.9800	C20—H20C	0.9800
C7—C8	1.399 (3)	C21—C22	1.395 (3)
C7—C14	1.522 (3)	C21—C28	1.514 (3)
C7—H7A	0.9500	C21—H21A	0.9500
C8—C9	1.506 (3)	C22—C23	1.514 (3)
C8—H8A	0.9500	C22—H22A	0.9500
C9—C10	1.529 (3)	C23—C24	1.540 (3)
C9—H9A	0.9900	C23—H23A	0.9900
C9—H9B	0.9900	C23—H23B	0.9900
C10—C11	1.521 (3)	C24—C25	1.510 (3)
C10—H10A	0.9900	C24—H24A	0.9900
C10—H10B	0.9900	C24—H24B	0.9900
C11—C12	1.407 (3)	C25—C26	1.398 (3)
C11—H11A	0.9500	C25—H25A	0.9500
C12—C13	1.503 (3)	C26—C27	1.519 (3)
C12—H12A	0.9500	C26—H26A	0.9500
C13—C14	1.527 (3)	C27—C28	1.533 (3)
C13—H13A	0.9900	C27—H27A	0.9900
C13—H13B	0.9900	C27—H27B	0.9900
C14—H14A	0.9900	C28—H28A	0.9900
C14—H14B	0.9900	C28—H28B	0.9900
C12—Rh1—C11	38.94 (7)	C25—Rh2—C26	38.76 (8)
C12—Rh1—N1	87.10 (7)	C25—Rh2—C21	98.69 (7)
C11—Rh1—N1	90.70 (7)	C26—Rh2—C21	82.18 (7)
C12—Rh1—C8	98.37 (7)	C25—Rh2—N2	90.73 (7)
C11—Rh1—C8	82.13 (8)	C26—Rh2—N2	90.97 (7)
N1—Rh1—C8	160.31 (7)	C21—Rh2—N2	154.68 (7)
C12—Rh1—C7	81.99 (7)	C25—Rh2—C22	82.24 (9)
C11—Rh1—C7	90.51 (8)	C26—Rh2—C22	90.28 (9)

N1—Rh1—C7	161.01 (7)	C21—Rh2—C22	38.08 (8)
C8—Rh1—C7	38.17 (7)	N2—Rh2—C22	167.08 (8)
C12—Rh1—Cl1	158.38 (6)	C25—Rh2—Cl2	156.03 (6)
C11—Rh1—Cl1	162.67 (6)	C26—Rh2—Cl2	165.20 (6)
N1—Rh1—Cl1	90.47 (4)	C21—Rh2—Cl2	91.21 (5)
C8—Rh1—Cl1	91.09 (5)	N2—Rh2—Cl2	89.43 (5)
C7—Rh1—Cl1	93.97 (6)	C22—Rh2—Cl2	92.63 (7)
C4—N1—C1	102.50 (14)	C15—N2—C18	103.84 (14)
C4—N1—Rh1	119.03 (12)	C15—N2—Rh2	112.21 (12)
C1—N1—Rh1	114.78 (11)	C18—N2—Rh2	119.48 (12)
C4—N1—H1	106.6	C15—N2—H2	106.9
C1—N1—H1	106.6	C18—N2—H2	106.9
Rh1—N1—H1	106.6	Rh2—N2—H2	106.9
C6—O1—C5	113.45 (15)	C19—O2—C20	111.74 (16)
N1—C1—C2	104.90 (15)	N2—C15—C16	104.54 (16)
N1—C1—H1A	110.8	N2—C15—H15A	110.8
C2—C1—H1A	110.8	C16—C15—H15A	110.8
N1—C1—H1B	110.8	N2—C15—H15B	110.8
C2—C1—H1B	110.8	C16—C15—H15B	110.8
H1A—C1—H1B	108.8	H15A—C15—H15B	108.9
C1—C2—C3	104.37 (16)	C15—C16—C17	104.50 (16)
C1—C2—H2A	110.9	C15—C16—H16A	110.9
C3—C2—H2A	110.9	C17—C16—H16A	110.9
C1—C2—H2B	110.9	C15—C16—H16B	110.9
C3—C2—H2B	110.9	C17—C16—H16B	110.9
H2A—C2—H2B	108.9	H16A—C16—H16B	108.9
C4—C3—C2	104.89 (16)	C16—C17—C18	105.80 (16)
C4—C3—H3A	110.8	C16—C17—H17A	110.6
C2—C3—H3A	110.8	C18—C17—H17A	110.6
C4—C3—H3B	110.8	C16—C17—H17B	110.6
C2—C3—H3B	110.8	C18—C17—H17B	110.6
H3A—C3—H3B	108.8	H17A—C17—H17B	108.7
N1—C4—C5	110.67 (15)	N2—C18—C19	110.83 (15)
N1—C4—C3	104.52 (15)	N2—C18—C17	105.67 (15)
C5—C4—C3	114.78 (18)	C19—C18—C17	114.30 (16)
N1—C4—H4A	108.9	N2—C18—H18A	108.6
C5—C4—H4A	108.9	C19—C18—H18A	108.6
C3—C4—H4A	108.9	C17—C18—H18A	108.6
O1—C5—C4	107.16 (15)	O2—C19—C18	107.61 (15)
O1—C5—H5A	110.3	O2—C19—H19A	110.2
C4—C5—H5A	110.3	C18—C19—H19A	110.2
O1—C5—H5B	110.3	O2—C19—H19B	110.2
C4—C5—H5B	110.3	C18—C19—H19B	110.2
H5A—C5—H5B	108.5	H19A—C19—H19B	108.5
O1—C6—H6A	109.5	O2—C20—H20A	109.5
O1—C6—H6B	109.5	O2—C20—H20B	109.5
H6A—C6—H6B	109.5	H20A—C20—H20B	109.5
O1—C6—H6C	109.5	O2—C20—H20C	109.5
H6A—C6—H6C	109.5	H20A—C20—H20C	109.5

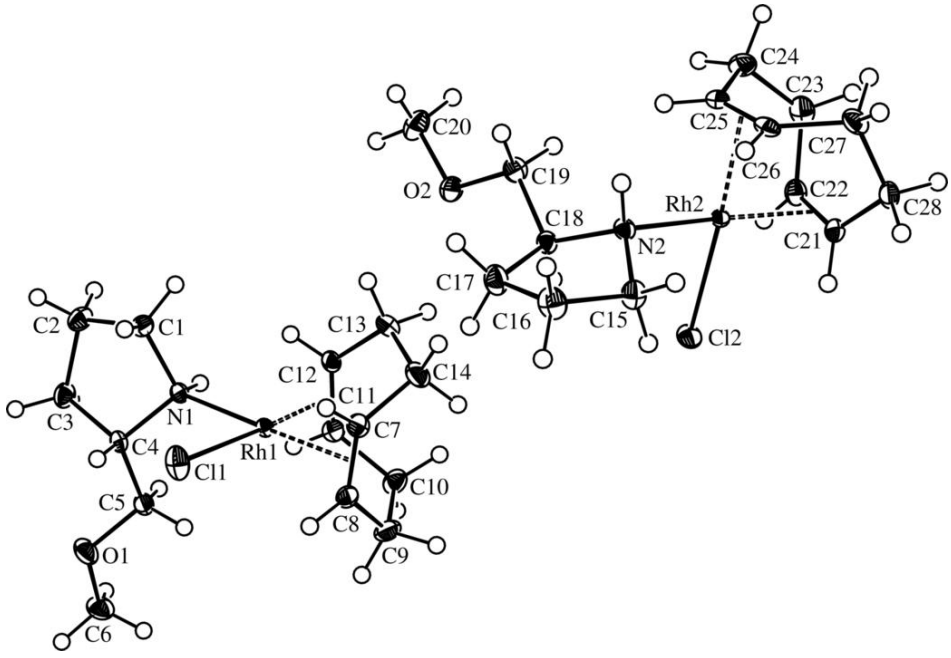
H6B—C6—H6C	109.5	H20B—C20—H20C	109.5
C8—C7—C14	123.11 (18)	C22—C21—C28	125.83 (19)
C8—C7—Rh1	70.17 (11)	C22—C21—Rh2	71.97 (13)
C14—C7—Rh1	112.11 (13)	C28—C21—Rh2	109.72 (13)
C8—C7—H7A	118.4	C22—C21—H21A	117.1
C14—C7—H7A	118.4	C28—C21—H21A	117.1
Rh1—C7—H7A	87.8	Rh2—C21—H21A	88.2
C7—C8—C9	126.34 (17)	C21—C22—C23	124.4 (2)
C7—C8—Rh1	71.66 (11)	C21—C22—Rh2	69.95 (12)
C9—C8—Rh1	109.19 (13)	C23—C22—Rh2	112.47 (16)
C7—C8—H8A	116.8	C21—C22—H22A	117.8
C9—C8—H8A	116.8	C23—C22—H22A	117.8
Rh1—C8—H8A	89.1	Rh2—C22—H22A	87.6
C8—C9—C10	113.95 (16)	C22—C23—C24	112.19 (17)
C8—C9—H9A	108.8	C22—C23—H23A	109.2
C10—C9—H9A	108.8	C24—C23—H23A	109.2
C8—C9—H9B	108.8	C22—C23—H23B	109.2
C10—C9—H9B	108.8	C24—C23—H23B	109.2
H9A—C9—H9B	107.7	H23A—C23—H23B	107.9
C11—C10—C9	111.37 (16)	C25—C24—C23	112.97 (16)
C11—C10—H10A	109.4	C25—C24—H24A	109.0
C9—C10—H10A	109.4	C23—C24—H24A	109.0
C11—C10—H10B	109.4	C25—C24—H24B	109.0
C9—C10—H10B	109.4	C23—C24—H24B	109.0
H10A—C10—H10B	108.0	H24A—C24—H24B	107.8
C12—C11—C10	124.88 (19)	C26—C25—C24	124.98 (18)
C12—C11—Rh1	69.85 (10)	C26—C25—Rh2	71.28 (10)
C10—C11—Rh1	113.50 (13)	C24—C25—Rh2	110.91 (13)
C12—C11—H11A	117.6	C26—C25—H25A	117.5
C10—C11—H11A	117.6	C24—C25—H25A	117.5
Rh1—C11—H11A	86.6	Rh2—C25—H25A	87.8
C11—C12—C13	126.47 (18)	C25—C26—C27	123.65 (18)
C11—C12—Rh1	71.21 (10)	C25—C26—Rh2	69.96 (10)
C13—C12—Rh1	110.29 (13)	C27—C26—Rh2	113.19 (13)
C11—C12—H12A	116.8	C25—C26—H26A	118.2
C13—C12—H12A	116.8	C27—C26—H26A	118.2
Rh1—C12—H12A	88.4	Rh2—C26—H26A	86.9
C12—C13—C14	112.74 (16)	C26—C27—C28	111.86 (16)
C12—C13—H13A	109.0	C26—C27—H27A	109.2
C14—C13—H13A	109.0	C28—C27—H27A	109.2
C12—C13—H13B	109.0	C26—C27—H27B	109.2
C14—C13—H13B	109.0	C28—C27—H27B	109.2
H13A—C13—H13B	107.8	H27A—C27—H27B	107.9
C7—C14—C13	111.54 (16)	C21—C28—C27	112.25 (17)
C7—C14—H14A	109.3	C21—C28—H28A	109.2
C13—C14—H14A	109.3	C27—C28—H28A	109.2
C7—C14—H14B	109.3	C21—C28—H28B	109.2
C13—C14—H14B	109.3	C27—C28—H28B	109.2
H14A—C14—H14B	108.0	H28A—C28—H28B	107.9

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Cl1^{i}	0.93	2.59	3.4888 (16)	163
N2—H2···Cl2^{ii}	0.93	2.51	3.4028 (16)	162

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*+1, *y*, *z*.

Fig. 1


C24
C23
C25
C20
C27
C26
O2
C19
C22
C28
Rh2
C18
N2
C21
C17
C16
C15
Cl2
C2
C1
C13
C12
C14
C11
C3
N1
C7
C4
Rh1
Cl1
C10
C5
C8
O1
C9
C6