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# Acetonitriletrichloridobis(cyclohexyldiphenylphosphane)rhodium(III) acetonitrile disolvate

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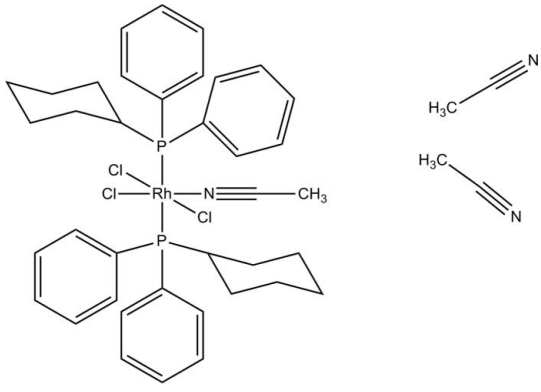
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; disorder in solvent or counterion; $R$ factor = 0.022; $wR$ factor = 0.055; data-to-parameter ratio = 19.1.

In the title compound, $[RhCl_3(CH_3CN)(C_{18}H_{21}P)_2]\cdot 2CH_3CN$, the complex molecule lies on a twofold rotation axis that passes through the $Rh^{III}$ atom, one Cl atom, and the C and N atoms of the coordinated acetonitrile molecule. The $Rh^{III}$ atom is coordinated by two P atoms in *trans* positions, three Cl atoms and an acetonitrile molecule in a distorted octahedral geometry. Intramolecular C—H···Cl interactions are observed. The uncoordinated acetonitrile molecule is disordered over two sites with occupancies of 0.588 (4) and 0.412 (4).

## Related literature

For background to the catalytic activity of rhodium–phosphane adducts, see: Brink *et al.* (2010); Marko & Heil (1974); Nagy-Magos *et al.* (1978); Oro *et al.* (1978); Roodt *et al.* (2003). For related structures, see: Archer *et al.* (1993); Aslanov *et al.* (1970); Clegg *et al.* (2002); Drew *et al.* (1970).




## Experimental

### Crystal data

$[RhCl_3(C_2H_3N)(C_{18}H_{21}P)_2]\cdot 2C_2H_3N$
$M_r$ = 869.06
Monoclinic, $C2/c$
$a$ = 24.995 (1) Å
$b$ = 10.041 (1) Å
$c$ = 16.258 (1) Å
$\beta$ = 96.763 (1)°
$V$ = 4052.0 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.73 mm$^{-1}$
$T$ = 100 K
0.32 × 0.25 × 0.16 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min}$ = 0.797, $T_{max}$ = 0.889
33882 measured reflections
5038 independent reflections
4615 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.055
$S$ = 1.04
5038 reflections
264 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.63 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Rh1—N1 | 1.9978 (17) | Rh1—Cl1 | 2.3486 (3) |
| Rh1—Cl2 | 2.3297 (5) | Rh1—P1 | 2.4013 (3) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C10—H10···Cl2 | 0.95 | 2.59 | 3.4452 (14) | 150 |
| C20—H20$B$···Cl2 | 0.99 | 2.72 | 3.4797 (14) | 134 |

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT-Plus* (Bruker, 2008); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); 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: IS2783).

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# supporting information

*Acta Cryst.* (2011). E**67**, m1785–m1786 [https://doi.org/10.1107/S1600536811047477]

## Acetonitriletrichloridobis(cyclohexyldiphenylphosphane)rhodium(III) acetonitrile disolvate

**Theunis J. Muller, Hendrik G. Visser and Andreas Roodt**

### S1. Comment

Rhodium catalysts formed *in situ* from $RhCl_3xH_2O$ and phosphanes have been used for the hydrogenation (Marko & Heil, 1974; Nagy-Magos *et al.*, 1978) and hydroformylation (Oro *et al.*, 1978) of olefins. The catalytic activity is determined by the electronic and steric effects of the phosphane ligand (Roodt *et al.*, 2003; Brink *et al.*, 2010).

The title compound (Fig. 1) crystallizes in the monoclinic space group *C*2/*c*. The $Rh^{III}$ atom is situated on a twofold rotation axis, which passes atoms Cl2, N1 and C2. Two cyclohexyldiphenylphosphane ligands are positioned *trans* to each other, with the other four coordination sites occupied by three *mer*-chloroligands and one molecule of the acetonitrile solvent. In contrast to the structure reported by Clegg *et al.* (2002) the solvent molecule lies opposite the shortest Rh—Cl2 bond [2.3297 (5) Å] in the complex. Deviations from ideal octahedral geometry are minor (Table 1). The Rh—P1 bond length is 2.4013 (5) Å, while the Rh—Cl1 bond length is 2.3486 (6) Å. The P1—Rh—$P1^i$ angle is 176.462 (17)° which is close to the Cl1—Rh—$Cl1^i$ at 176.185 (18)° [symmetry code: (i) -*x*, *y*, -*z* + 1/2]. This complex is therefore structurally related to *trans*-$ReCl_3(PMe_2Ph)_3$ (Aslanov *et al.*, 1970) and $ReCl_3(PPh_3)_2MeCN$ (Drew *et al.*, 1970), and other metal halide derivatives of this type (Archer *et al.*, 1993). The uncoordinated acetonitrile molecule is disordered over two positions with occupancies of 0.588 (4) and 0.412 (4). The molecular structure of the complex is stabilized by intramolecular C—H···Cl interactions (Table 2).

### S2. Experimental

$RhCl_3.H_2O$ (20 mg, $9.557\times10^{-5}$ mol) was added to acetonitrile (5 ml) and heated to reflux. Cyclohexyldiphenylphosphane (2 eq, $1.911\times10^{-4}$ mol, 51,2 mg) was added to the solution. The solution was refluxed for 15 min before it was cooled to room temperature. Crystals suitable for X-ray analysis was grown overnight by the slow evaporation of acetonitrile at room temperature (yield 0.0750 g, 89%)

### S3. Refinement

H atoms were positioned geometrically (C—H = 0.93–9.97 Å) and allowed to ride on their parent atoms, with $U_{iso}$(H) = 1.2$U_{eq}$(phenyl C) or 1.5$U_{eq}$(methyl and methylene C). The distance restraints [1.45 (1) Å] were applied for C21A—C22A and C21B—C22B.

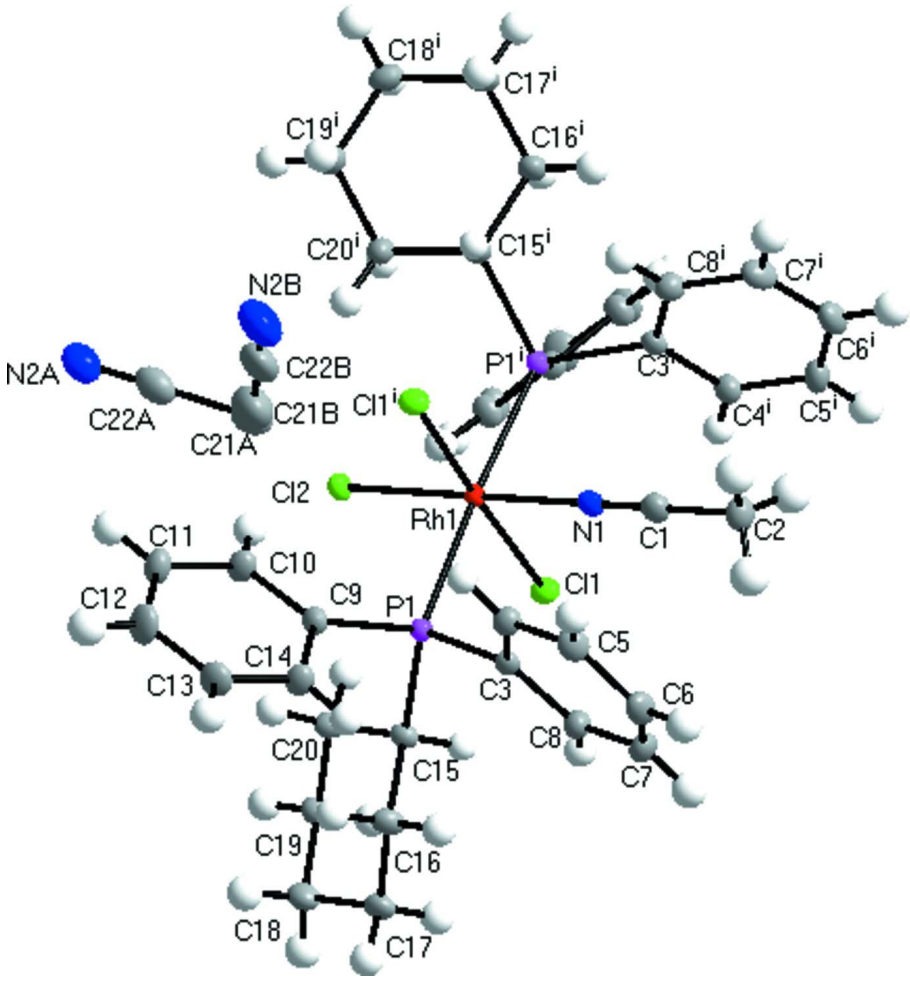


**Figure 1**

Diamond representation of the title compound, showing the numbering scheme and displacement ellipsoids (50% probability).

**Acetonitriletrichloridobis(cyclohexyldiphenylphosphane)rhodium(III) acetonitrile disolvate**

*Crystal data*

$[RhCl_3(C_2H_3N)(C_{18}H_{21}P)_2]\cdot 2C_2H_3N$
$M_r = 869.06$
Monoclinic, $C2/c$
$a = 24.995$ (1) Å
$b = 10.041$ (1) Å
$c = 16.258$ (1) Å
$\beta = 96.763$ (1)°
$V = 4052.0$ (5) Å$^3$
$Z = 4$
$F(000) = 1800$
$D_x = 1.425$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9837 reflections
$\theta = 2.5$–28.3°
$\mu = 0.73$ mm$^{-1}$
$T = 100$ K
Cuboid, red
0.32 × 0.25 × 0.16 mm

*Data collection*

Bruker APEXII CCD diffractometer
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.797$, $T_{max} = 0.889$
33882 measured reflections

5038 independent reflections
4615 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 28.4°$, $\theta_{min} = 1.6°$
$h = -33 \rightarrow 33$
$k = -13 \rightarrow 13$
$l = -21 \rightarrow 19$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.055$
$S = 1.04$
5038 reflections
264 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0236P)^2 + 4.9122P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å$^{-3}$
$\Delta\rho_{min} = -0.63$ e Å$^{-3}$

*Special details*

**Experimental**. The intensity data was collected on a Bruker X8 ApexII 4 K Kappa CCD diffractometer using an exposure time of 20 s/frame. A total of 1963 frames were collected with a frame width of 0.5° covering up to $\theta = 28.35°$ with 99.6% completeness accomplished

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Rh1 | 0 | 0.145288 (14) | 0.25 | 0.01099 (5) | |
| Cl1 | −0.053994 (13) | 0.13750 (3) | 0.35876 (2) | 0.01819 (7) | |
| Cl2 | 0 | 0.37731 (4) | 0.25 | 0.01635 (9) | |
| P1 | 0.079330 (13) | 0.13791 (3) | 0.34878 (2) | 0.01236 (7) | |
| N1 | 0 | −0.05368 (17) | 0.25 | 0.0166 (3) | |
| C15 | 0.07347 (5) | 0.20332 (14) | 0.45392 (8) | 0.0160 (3) | |
| H15 | 0.0418 | 0.1572 | 0.4734 | 0.019* | |
| C11 | 0.18508 (6) | 0.40163 (15) | 0.26099 (10) | 0.0230 (3) | |
| H11 | 0.1831 | 0.479 | 0.2271 | 0.028* | |
| C2 | 0 | −0.3095 (2) | 0.25 | 0.0238 (4) | |
| H2A | 0.019 | −0.3421 | 0.2046 | 0.036* | 0.5 |
| H2B | −0.0372 | −0.3421 | 0.2426 | 0.036* | 0.5 |
| H2C | 0.0182 | −0.3421 | 0.3029 | 0.036* | 0.5 |
| C5 | 0.14501 (6) | −0.23233 (15) | 0.32610 (10) | 0.0228 (3) | |
| H5 | 0.1671 | −0.2744 | 0.29 | 0.027* | |
| C4 | 0.13087 (6) | −0.09925 (15) | 0.31407 (9) | 0.0186 (3) | |
| H4 | 0.1431 | −0.0512 | 0.2696 | 0.022* | |
| C18 | 0.10192 (7) | 0.36857 (16) | 0.60247 (9) | 0.0242 (3) | |

| | | | | | |
|---|---|---|---|---|---|
| H18A | 0.1342 | 0.4175 | 0.5893 | 0.029* | |
| H18B | 0.0942 | 0.3966 | 0.6582 | 0.029* | |
| C3 | 0.09890 (5) | −0.03580 (13) | 0.36674 (8) | 0.0151 (3) | |
| C8 | 0.07948 (6) | −0.10963 (15) | 0.42960 (9) | 0.0197 (3) | |
| H8 | 0.0562 | −0.069 | 0.4644 | 0.024* | |
| C16 | 0.12161 (6) | 0.17108 (15) | 0.51730 (9) | 0.0217 (3) | |
| H16A | 0.1273 | 0.0735 | 0.5193 | 0.026* | |
| H16B | 0.1544 | 0.2129 | 0.5 | 0.026* | |
| C10 | 0.13773 (6) | 0.33469 (15) | 0.27481 (9) | 0.0205 (3) | |
| H10 | 0.1037 | 0.369 | 0.2525 | 0.025* | |
| C7 | 0.09408 (7) | −0.24283 (15) | 0.44145 (10) | 0.0250 (3) | |
| H7 | 0.0812 | −0.2921 | 0.485 | 0.03* | |
| C19 | 0.05461 (6) | 0.40325 (16) | 0.53948 (9) | 0.0220 (3) | |
| H19A | 0.0505 | 0.5013 | 0.537 | 0.026* | |
| H19B | 0.0214 | 0.3657 | 0.5579 | 0.026* | |
| C14 | 0.19135 (6) | 0.17214 (15) | 0.35757 (10) | 0.0209 (3) | |
| H14 | 0.1936 | 0.0956 | 0.3922 | 0.025* | |
| C9 | 0.14076 (5) | 0.21728 (14) | 0.32148 (9) | 0.0166 (3) | |
| C13 | 0.23812 (6) | 0.23857 (16) | 0.34300 (10) | 0.0243 (3) | |
| H13 | 0.2723 | 0.2043 | 0.3647 | 0.029* | |
| C20 | 0.06056 (6) | 0.35127 (14) | 0.45333 (9) | 0.0201 (3) | |
| H20A | 0.0897 | 0.4009 | 0.4305 | 0.024* | |
| H20B | 0.0267 | 0.3673 | 0.4167 | 0.024* | |
| C17 | 0.11302 (6) | 0.22091 (16) | 0.60265 (9) | 0.0214 (3) | |
| H17A | 0.0823 | 0.1728 | 0.6221 | 0.026* | |
| H17B | 0.1455 | 0.2016 | 0.6418 | 0.026* | |
| C6 | 0.12719 (6) | −0.30370 (15) | 0.39021 (10) | 0.0253 (3) | |
| H6 | 0.1376 | −0.394 | 0.3991 | 0.03* | |
| C12 | 0.23475 (6) | 0.35541 (17) | 0.29659 (11) | 0.0281 (4) | |
| H12 | 0.2666 | 0.4036 | 0.2893 | 0.034* | |
| C1 | 0 | −0.1644 (2) | 0.25 | 0.0199 (4) | |
| N2A | 0.22420 (12) | 0.4183 (3) | 0.0550 (2) | 0.0384 (8) | 0.588 (4) |
| C21A | 0.2017 (4) | 0.1790 (4) | 0.1017 (6) | 0.0345 (17) | 0.588 (4) |
| H21A | 0.1631 | 0.173 | 0.1067 | 0.052* | 0.588 (4) |
| H21B | 0.2223 | 0.1594 | 0.1554 | 0.052* | 0.588 (4) |
| H21C | 0.211 | 0.1144 | 0.0605 | 0.052* | 0.588 (4) |
| C22A | 0.21444 (12) | 0.3123 (3) | 0.07576 (19) | 0.0331 (8) | 0.588 (4) |
| N2B | 0.2558 (2) | 0.0458 (6) | −0.0078 (4) | 0.0611 (16) | 0.412 (4) |
| C21B | 0.2042 (7) | 0.1588 (10) | 0.1007 (9) | 0.060 (4) | 0.412 (4) |
| H21D | 0.2034 | 0.2552 | 0.0914 | 0.09* | 0.412 (4) |
| H21E | 0.2224 | 0.1399 | 0.1563 | 0.09* | 0.412 (4) |
| H21F | 0.1673 | 0.1243 | 0.096 | 0.09* | 0.412 (4) |
| C22B | 0.2333 (2) | 0.0950 (6) | 0.0394 (4) | 0.0523 (17) | 0.412 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Rh1 | 0.01107 (7) | 0.00977 (7) | 0.01209 (7) | 0 | 0.00121 (5) | 0 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Cl1 | 0.01540 (15) | 0.02406 (18) | 0.01562 (16) | −0.00089 (12) | 0.00398 (12) | 0.00129 (12) |
| Cl2 | 0.0172 (2) | 0.0117 (2) | 0.0195 (2) | 0 | −0.00028 (17) | 0 |
| P1 | 0.01149 (15) | 0.01268 (16) | 0.01287 (16) | −0.00007 (12) | 0.00121 (12) | 0.00040 (12) |
| N1 | 0.0136 (7) | 0.0180 (9) | 0.0173 (8) | 0 | −0.0018 (6) | 0 |
| C15 | 0.0154 (6) | 0.0181 (7) | 0.0141 (6) | 0.0006 (5) | 0.0003 (5) | −0.0021 (5) |
| C11 | 0.0214 (7) | 0.0184 (7) | 0.0299 (8) | −0.0017 (6) | 0.0054 (6) | 0.0036 (6) |
| C2 | 0.0263 (11) | 0.0165 (10) | 0.0285 (11) | 0 | 0.0033 (9) | 0 |
| C5 | 0.0222 (7) | 0.0179 (7) | 0.0278 (8) | 0.0047 (6) | 0.0007 (6) | −0.0026 (6) |
| C4 | 0.0168 (6) | 0.0190 (7) | 0.0199 (7) | 0.0011 (5) | 0.0018 (5) | 0.0012 (6) |
| C18 | 0.0279 (8) | 0.0275 (8) | 0.0170 (7) | −0.0023 (6) | 0.0019 (6) | −0.0044 (6) |
| C3 | 0.0144 (6) | 0.0146 (6) | 0.0154 (6) | −0.0001 (5) | −0.0016 (5) | 0.0009 (5) |
| C8 | 0.0219 (7) | 0.0187 (7) | 0.0185 (7) | −0.0024 (5) | 0.0022 (5) | 0.0010 (5) |
| C16 | 0.0238 (7) | 0.0224 (7) | 0.0178 (7) | 0.0031 (6) | −0.0026 (6) | −0.0019 (6) |
| C10 | 0.0154 (6) | 0.0212 (7) | 0.0250 (7) | 0.0004 (5) | 0.0022 (5) | 0.0044 (6) |
| C7 | 0.0322 (8) | 0.0196 (7) | 0.0222 (8) | −0.0048 (6) | −0.0006 (6) | 0.0060 (6) |
| C19 | 0.0246 (7) | 0.0207 (7) | 0.0201 (7) | 0.0025 (6) | 0.0004 (6) | −0.0046 (6) |
| C14 | 0.0161 (6) | 0.0217 (7) | 0.0247 (7) | 0.0002 (5) | 0.0014 (5) | 0.0038 (6) |
| C9 | 0.0138 (6) | 0.0177 (7) | 0.0185 (7) | −0.0020 (5) | 0.0025 (5) | −0.0004 (5) |
| C13 | 0.0147 (6) | 0.0283 (8) | 0.0295 (8) | −0.0003 (6) | 0.0007 (6) | 0.0013 (6) |
| C20 | 0.0251 (7) | 0.0184 (7) | 0.0165 (7) | 0.0033 (6) | 0.0014 (5) | −0.0010 (5) |
| C17 | 0.0191 (7) | 0.0275 (8) | 0.0168 (7) | −0.0026 (6) | −0.0020 (5) | −0.0011 (6) |
| C6 | 0.0302 (8) | 0.0152 (7) | 0.0285 (8) | 0.0014 (6) | −0.0051 (6) | 0.0020 (6) |
| C12 | 0.0166 (7) | 0.0297 (9) | 0.0390 (9) | −0.0052 (6) | 0.0073 (6) | 0.0039 (7) |
| C1 | 0.0174 (9) | 0.0200 (11) | 0.0217 (10) | 0 | −0.0004 (7) | 0 |
| N2A | 0.0365 (16) | 0.0417 (17) | 0.0367 (17) | −0.0067 (12) | 0.0033 (12) | −0.0085 (13) |
| C21A | 0.027 (3) | 0.040 (3) | 0.037 (4) | −0.005 (2) | 0.007 (2) | −0.007 (2) |
| C22A | 0.0247 (14) | 0.0420 (19) | 0.0323 (16) | −0.0032 (13) | 0.0020 (11) | −0.0101 (14) |
| N2B | 0.063 (3) | 0.066 (4) | 0.052 (3) | −0.027 (3) | −0.002 (3) | −0.014 (3) |
| C21B | 0.073 (8) | 0.047 (4) | 0.055 (8) | −0.014 (5) | −0.021 (5) | 0.009 (5) |
| C22B | 0.056 (4) | 0.049 (3) | 0.046 (3) | −0.023 (3) | −0.017 (3) | 0.000 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Rh1—N1 | 1.9978 (17) | C16—C17 | 1.514 (2) |
| Rh1—Cl2 | 2.3297 (5) | C16—H16A | 0.99 |
| Rh1—Cl1 | 2.3486 (3) | C16—H16B | 0.99 |
| Rh1—Cl1$^{i}$ | 2.3486 (3) | C10—C9 | 1.399 (2) |
| Rh1—P1 | 2.4013 (3) | C10—H10 | 0.95 |
| Rh1—P1$^{i}$ | 2.4013 (3) | C7—C6 | 1.384 (2) |
| P1—C3 | 1.8257 (14) | C7—H7 | 0.95 |
| P1—C9 | 1.8304 (14) | C19—C20 | 1.518 (2) |
| P1—C15 | 1.8529 (14) | C19—H19A | 0.99 |
| N1—C1 | 1.112 (3) | C19—H19B | 0.99 |
| C15—C20 | 1.520 (2) | C14—C13 | 1.390 (2) |
| C15—C16 | 1.5240 (18) | C14—C9 | 1.4049 (19) |
| C15—H15 | 1 | C14—H14 | 0.95 |
| C11—C12 | 1.387 (2) | C13—C12 | 1.392 (2) |
| C11—C10 | 1.402 (2) | C13—H13 | 0.95 |

| | | | |
|---|---|---|---|
| C11—H11 | 0.95 | C20—H20A | 0.99 |
| C2—C1 | 1.457 (3) | C20—H20B | 0.99 |
| C2—H2A | 0.98 | C17—H17A | 0.99 |
| C2—H2B | 0.98 | C17—H17B | 0.99 |
| C2—H2C | 0.98 | C6—H6 | 0.95 |
| C5—C6 | 1.381 (2) | C12—H12 | 0.95 |
| C5—C4 | 1.390 (2) | N2A—C22A | 1.151 (5) |
| C5—H5 | 0.95 | C21A—C22A | 1.4501 (10) |
| C4—C3 | 1.392 (2) | C21A—H21A | 0.98 |
| C4—H4 | 0.95 | C21A—H21B | 0.98 |
| C18—C17 | 1.508 (2) | C21A—H21C | 0.98 |
| C18—C19 | 1.511 (2) | N2B—C22B | 1.119 (9) |
| C18—H18A | 0.99 | C21B—C22B | 1.4498 (10) |
| C18—H18B | 0.99 | C21B—H21D | 0.98 |
| C3—C8 | 1.395 (2) | C21B—H21E | 0.98 |
| C8—C7 | 1.394 (2) | C21B—H21F | 0.98 |
| C8—H8 | 0.95 | | |

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|---|---|---|---|
| N1—Rh1—Cl2 | 180 | C17—C16—C15 | 111.33 (12) |
| N1—Rh1—Cl1 | 88.093 (9) | C17—C16—H16A | 109.4 |
| Cl2—Rh1—Cl1 | 91.907 (9) | C15—C16—H16A | 109.4 |
| N1—Rh1—Cl1$^{i}$ | 88.093 (9) | C17—C16—H16B | 109.4 |
| Cl2—Rh1—Cl1$^{i}$ | 91.907 (9) | C15—C16—H16B | 109.4 |
| Cl1—Rh1—Cl1$^{i}$ | 176.185 (18) | H16A—C16—H16B | 108 |
| N1—Rh1—P1 | 88.231 (9) | C9—C10—C11 | 119.86 (13) |
| Cl2—Rh1—P1 | 91.769 (9) | C9—C10—H10 | 120.1 |
| Cl1—Rh1—P1 | 89.879 (12) | C11—C10—H10 | 120.1 |
| Cl1$^{i}$—Rh1—P1 | 90.003 (12) | C6—C7—C8 | 120.40 (15) |
| N1—Rh1—P1$^{i}$ | 88.231 (9) | C6—C7—H7 | 119.8 |
| Cl2—Rh1—P1$^{i}$ | 91.769 (9) | C8—C7—H7 | 119.8 |
| Cl1—Rh1—P1$^{i}$ | 90.003 (12) | C18—C19—C20 | 113.09 (13) |
| Cl1$^{i}$—Rh1—P1$^{i}$ | 89.879 (12) | C18—C19—H19A | 109 |
| P1—Rh1—P1$^{i}$ | 176.463 (17) | C20—C19—H19A | 109 |
| C3—P1—C9 | 103.78 (6) | C18—C19—H19B | 109 |
| C3—P1—C15 | 103.88 (6) | C20—C19—H19B | 109 |
| C9—P1—C15 | 103.24 (6) | H19A—C19—H19B | 107.8 |
| C3—P1—Rh1 | 108.72 (4) | C13—C14—C9 | 120.50 (14) |
| C9—P1—Rh1 | 118.33 (5) | C13—C14—H14 | 119.8 |
| C15—P1—Rh1 | 117.21 (4) | C9—C14—H14 | 119.8 |
| C1—N1—Rh1 | 180 | C10—C9—C14 | 119.15 (13) |
| C20—C15—C16 | 111.22 (12) | C10—C9—P1 | 120.32 (10) |
| C20—C15—P1 | 112.36 (10) | C14—C9—P1 | 119.84 (11) |
| C16—C15—P1 | 113.99 (10) | C14—C13—C12 | 119.89 (14) |
| C20—C15—H15 | 106.2 | C14—C13—H13 | 120.1 |
| C16—C15—H15 | 106.2 | C12—C13—H13 | 120.1 |
| P1—C15—H15 | 106.2 | C19—C20—C15 | 111.96 (12) |
| C12—C11—C10 | 120.26 (14) | C19—C20—H20A | 109.2 |
| C12—C11—H11 | 119.9 | C15—C20—H20A | 109.2 |

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|---|---|---|---|
| C10—C11—H11 | 119.9 | C19—C20—H20B | 109.2 |
| C1—C2—H2A | 109.5 | C15—C20—H20B | 109.2 |
| C1—C2—H2B | 109.5 | H20A—C20—H20B | 107.9 |
| H2A—C2—H2B | 109.5 | C18—C17—C16 | 111.65 (13) |
| C1—C2—H2C | 109.5 | C18—C17—H17A | 109.3 |
| H2A—C2—H2C | 109.5 | C16—C17—H17A | 109.3 |
| H2B—C2—H2C | 109.5 | C18—C17—H17B | 109.3 |
| C6—C5—C4 | 120.38 (15) | C16—C17—H17B | 109.3 |
| C6—C5—H5 | 119.8 | H17A—C17—H17B | 108 |
| C4—C5—H5 | 119.8 | C5—C6—C7 | 119.61 (14) |
| C5—C4—C3 | 120.53 (14) | C5—C6—H6 | 120.2 |
| C5—C4—H4 | 119.7 | C7—C6—H6 | 120.2 |
| C3—C4—H4 | 119.7 | C11—C12—C13 | 120.15 (14) |
| C17—C18—C19 | 110.91 (12) | C11—C12—H12 | 119.9 |
| C17—C18—H18A | 109.5 | C13—C12—H12 | 119.9 |
| C19—C18—H18A | 109.5 | N1—C1—C2 | 180 |
| C17—C18—H18B | 109.5 | N2A—C22A—C21A | 179.5 (5) |
| C19—C18—H18B | 109.5 | C22B—C21B—H21D | 109.5 |
| H18A—C18—H18B | 108 | C22B—C21B—H21E | 109.5 |
| C4—C3—C8 | 118.80 (13) | H21D—C21B—H21E | 109.5 |
| C4—C3—P1 | 120.07 (11) | C22B—C21B—H21F | 109.5 |
| C8—C3—P1 | 121.00 (11) | H21D—C21B—H21F | 109.5 |
| C7—C8—C3 | 120.21 (14) | H21E—C21B—H21F | 109.5 |
| C7—C8—H8 | 119.9 | N2B—C22B—C21B | 179.9 (11) |
| C3—C8—H8 | 119.9 | | |

Symmetry code: (i) $-x, y, -z+1/2$.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C10—H10···Cl2 | 0.95 | 2.59 | 3.4452 (14) | 150 |
| C20—H20*B*···Cl2 | 0.99 | 2.72 | 3.4797 (14) | 134 |