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trans-Carbonyl[dihydrobis(1,2,4-triazol-1-yl-κN^2)borato]hydridobis(triphenylphosphine-κP)ruthenium(II) acetonitrile solvate

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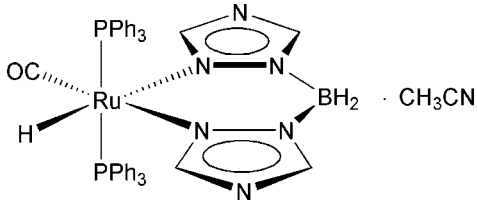
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.080; data-to-parameter ratio = 17.2.

In the crystal structure of the title compound, $[Ru(C_4H_6BN_6)H(C_{18}H_{15}P)_2(CO)]\cdot C_2H_3N$, discrete mononuclear complexes are found in which the Ru atom is coordinated by two triphenylphosphine (PPh_3) ligands, one dihydrobis(1,2,4-triazol-1-yl)borate ligand, one carbonyl ligand and one hydride atom within slightly distorted octahedra. The two P atoms of the PPh_3 ligands are *trans* positioned and the two N atoms of the chelating dihydrobis(1,2,4-triazol-1-yl)borate ligand occupy *cis* positions.

Related literature

For related literature, see: Youm *et al.* (2006); Huh *et al.* (1999, 2000).



Experimental

Crystal data

$[Ru(C_4H_6BN_6)H(C_{18}H_{15}P)_2(CO)]\cdot C_2H_3N$
M_r = 844.64
Triclinic, $P\overline{1}$
a = 9.0733 (1) Å
b = 11.8032 (3) Å
c = 20.2609 (6) Å
α = 74.438 (11)°
β = 89.552 (15)°
γ = 70.731 (14)°
V = 1965.4 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.53 mm^{-1}
T = 100 (2) K
0.35 × 0.30 × 0.28 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*DENZO-SMN*; Otwinowski & Minor, 1997)
T_{min} = 0.838, T_{max} = 0.867
31908 measured reflections
8964 independent reflections
6896 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.079
S = 0.98
8964 reflections
521 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ru1—H1*RU*	1.57 (2)	Ru1—N1	2.1771 (17)
Ru1—C1	1.833 (2)	Ru1—P2	2.3588 (6)
Ru1—N4	2.1396 (19)	Ru1—P1	2.3978 (6)
H1*RU*—Ru1—C1	90.0 (9)	N4—Ru1—P2	95.09 (5)
H1*RU*—Ru1—N4	87.9 (9)	N1—Ru1—P2	98.90 (5)
C1—Ru1—N4	176.92 (8)	H1*RU*—Ru1—P1	91.1 (8)
H1*RU*—Ru1—N1	175.7 (9)	C1—Ru1—P1	91.65 (7)
C1—Ru1—N1	94.31 (8)	N4—Ru1—P1	86.16 (5)
N4—Ru1—N1	87.84 (7)	N1—Ru1—P1	89.15 (5)
H1*RU*—Ru1—P2	81.0 (8)	P2—Ru1—P1	171.884 (18)
C1—Ru1—P2	86.77 (7)		

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Bruker, 1998); software used to prepare material for publication: *SHELXTL/PC*.

The author thanks Dr Alan J. Lough of the University of Toronto for the structure determination.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2075).

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supplementary materials

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trans-Carbonyl[dihydrobis(1,2,4-triazol-1-yl-κN^2)borato]hydridobis(triphenylphosphine-κP)ruthenium(II) acetonitrile solvate

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Comment

In our ongoing investigations on the preparation of one-dimensional coordination polymers containing catalytically active Ru^{II} complex moieties, we recently reported the preparation and spectroscopic data of the title compound (I) (Youm *et al.*, 2006). The proposed structure of (I) which based on the spectroscopic data closely resembles those of the previously structurally characterized analogues, $[RuH(AsPh_3)_2(\eta^2\text{-}H_2Bpz_2)(CO)]$ (II) (pz is pyrazol-1-yl) (Huh *et al.*, 1999) and $[RuH\{P(p\text{-}C_6H_4CH_3)_3\}_2(\eta^2\text{-}H_2Bpz_2)(CO)]$ (III) (Huh *et al*., 2000). Here we report the crystal structure of compound (I).

The crystal structure of compound I shows similar structural features as the analogous structures of (II) and (III) and therefore, confirm the proposed structure of (I) from our spectroscopic investigations.

In the crystal structure of the title compound the Ru atom is coordinated by two phosphorous atoms of two crystallographically independent triphenylphosphine ligands, one carbon atom of the CO ligand, one hydride H atom and two nitrogen atoms of the dihydrobis(1,2,4-triazol-1-yl)borate ligand within a slightly distorted octahedra (Fig. 1). The two phosphorous atoms of the PPh_3 ligands are *trans*-positioned and the two nitrogen atoms of the chelating dihydrobis(1,2,4-triazol-1-yl)borate ligand occupy *cis*-positions. The two Ru—P bond lengths are slightly longer than those in (III) [2.3448 (17) – 2.3699 (17) Å] (Tab. 1). In (I), the Ru1—P1 bond length is slightly longer than the Ru1—P2 bond by about 0.039 Å (Tab. 1). However, the Ru—N bond distances are very similar to those in (III). The H1—Ru—P2 angle of 81.0 (8)° is smaller than the H1—Ru—P1 angle of 91.1 (8)° (Tab. 1).

Experimental

The title compound was prepared according to the literature method (Youm *et al.*, 2006). Single crystals are obtained by slow evaporation of the solvent from a solution of (I) in acetonitrile.

Refinement

H atoms bonded to C atoms were placed in calculated positions [C—H = 0.95 - 0.97 Å] and included in the refinement in a riding-model approximation with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$ for methyl H atoms. The hydride H atom [H1RU], the H atoms connected to B1 and to the nitrogen atom of the acetonitrile molecules were refined with varying coordinates and free isotropic displacement parameters.

Figures

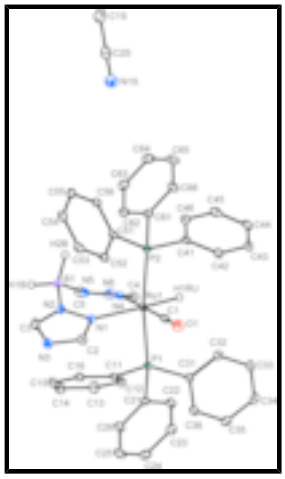


Fig. 1. The molecular structure of the title compound with labeling and displacement ellipsoids drawn at the 50% probability level. All hydrogen atoms except the hydride and hydrogen atoms attached to the B atom are omitted for clarity.

trans-Carbonyl[dihydrobis(1,2,4-triazol-1-yl- κN^2)borato]hydridobis(triphenylphosphine-κ*P*)ruthenium(II) acetonitrile solvate

Crystal data

$[Ru(C_4H_6BN_6)H(C_{18}H_{15}P)_2(CO)]\cdot C_2H_3N$	$Z = 2$
$M_r = 844.64$	$F_{000} = 868$
Triclinic, $P\overline{1}$	$D_x = 1.427$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.0733$ (1) Å	Cell parameters from 31908 reflections
$b = 11.8032$ (3) Å	$\theta = 4.1$–27.5º
$c = 20.2609$ (6) Å	$\mu = 0.53$ mm^{-1}
$\alpha = 74.438$ (11)º	$T = 100$ (2) K
$\beta = 89.552$ (15)º	Block cut from needle, pale yellow
$\gamma = 70.731$ (14)º	0.35 × 0.30 × 0.28 mm
$V = 1965.4$ (2) Å^3	

Data collection

Nonius KappaCCD diffractometer	8964 independent reflections
Radiation source: fine-focus sealed tube	6896 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.060$
Detector resolution: 9 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 100(2)$ K	$\theta_{min} = 4.1$º
φ scan and ω scans with κ offsets	$h = -11\rightarrow11$
Absorption correction: multi-scan (DENZO-SMN; Otwinowski & Minor, 1997)	$k = -13\rightarrow15$
$T_{min} = 0.838$, $T_{max} = 0.867$	$l = -26\rightarrow26$
31908 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.079$	$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} = 0.002$
8964 reflections	$\Delta\rho_{max} = 0.76$ e Å^{-3}
521 parameters	$\Delta\rho_{min} = -0.79$ e Å^{-3}
9 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.991567 (18)	0.597576 (15)	0.723224 (10)	0.01409 (6)
H1RU	0.815 (2)	0.668 (2)	0.6948 (12)	0.022 (6)*
P1	0.97691 (6)	0.40525 (5)	0.71054 (3)	0.01384 (12)
P2	0.97123 (6)	0.80041 (5)	0.72650 (3)	0.01507 (12)
O1	1.09179 (19)	0.66608 (15)	0.58094 (9)	0.0295 (4)
N1	1.23032 (19)	0.49727 (16)	0.77038 (10)	0.0160 (4)
N2	1.2776 (2)	0.46297 (17)	0.83893 (10)	0.0194 (4)
N3	1.4870 (2)	0.38206 (18)	0.78677 (11)	0.0251 (5)
N4	0.91255 (19)	0.54559 (16)	0.82298 (10)	0.0162 (4)
N5	1.0082 (2)	0.49179 (16)	0.88370 (10)	0.0195 (4)
N6	0.7751 (2)	0.47449 (18)	0.90769 (11)	0.0267 (5)
C1	1.0512 (2)	0.63962 (19)	0.63591 (13)	0.0181 (5)
C2	1.3590 (2)	0.44611 (19)	0.74159 (12)	0.0195 (5)
H2A	1.3604	0.4540	0.6937	0.023*
C3	1.4305 (2)	0.3955 (2)	0.84596 (13)	0.0266 (6)
H3A	1.4923	0.3607	0.8889	0.032*

C4	0.7767 (2)	0.5315 (2)	0.84039 (13)	0.0212 (5)
H4A	0.6879	0.5592	0.8081	0.025*
C5	0.9212 (3)	0.4511 (2)	0.93188 (13)	0.0258 (5)
H5A	0.9600	0.4098	0.9786	0.031*
C11	1.0065 (2)	0.28484 (19)	0.79288 (12)	0.0161 (4)
C12	0.8863 (2)	0.2443 (2)	0.82195 (12)	0.0200 (5)
H12A	0.7859	0.2746	0.7974	0.024*
C13	0.9140 (3)	0.1595 (2)	0.88699 (13)	0.0254 (5)
H13A	0.8317	0.1326	0.9067	0.031*
C14	1.0599 (3)	0.1136 (2)	0.92364 (13)	0.0260 (5)
H14A	1.0778	0.0549	0.9678	0.031*
C15	1.1800 (2)	0.1544 (2)	0.89514 (13)	0.0216 (5)
H15A	1.2802	0.1241	0.9200	0.026*
C16	1.1531 (2)	0.23893 (19)	0.83086 (12)	0.0182 (5)
H16A	1.2354	0.2667	0.8118	0.022*
C21	1.1176 (2)	0.32556 (19)	0.65704 (12)	0.0165 (5)
C22	1.1077 (2)	0.3869 (2)	0.58734 (12)	0.0216 (5)
H22A	1.0322	0.4681	0.5696	0.026*
C23	1.2054 (3)	0.3322 (2)	0.54338 (13)	0.0245 (5)
H23A	1.1967	0.3757	0.4960	0.029*
C24	1.3165 (3)	0.2133 (2)	0.56868 (13)	0.0245 (5)
H24A	1.3847	0.1758	0.5388	0.029*
C25	1.3268 (3)	0.1503 (2)	0.63731 (14)	0.0298 (6)
H25A	1.4016	0.0687	0.6546	0.036*
C26	1.2285 (3)	0.2052 (2)	0.68153 (13)	0.0240 (5)
H26A	1.2367	0.1607	0.7288	0.029*
C31	0.7951 (2)	0.4155 (2)	0.66621 (11)	0.0161 (4)
C32	0.6824 (2)	0.5310 (2)	0.63387 (12)	0.0189 (5)
H32A	0.6943	0.6055	0.6386	0.023*
C33	0.5524 (2)	0.5382 (2)	0.59473 (12)	0.0221 (5)
H33A	0.4775	0.6174	0.5721	0.026*
C34	0.5322 (2)	0.4303 (2)	0.58883 (12)	0.0226 (5)
H34A	0.4429	0.4353	0.5626	0.027*
C35	0.6424 (3)	0.3145 (2)	0.62120 (13)	0.0235 (5)
H35A	0.6281	0.2403	0.6173	0.028*
C36	0.7736 (2)	0.3071 (2)	0.65924 (12)	0.0208 (5)
H36A	0.8495	0.2277	0.6807	0.025*
C41	0.9074 (2)	0.91694 (19)	0.64166 (12)	0.0177 (5)
C42	0.7850 (3)	0.9175 (2)	0.60011 (13)	0.0239 (5)
H42A	0.7373	0.8555	0.6151	0.029*
C43	0.7320 (3)	1.0073 (2)	0.53737 (13)	0.0259 (5)
H43A	0.6486	1.0064	0.5097	0.031*
C44	0.8006 (3)	1.0989 (2)	0.51474 (13)	0.0262 (5)
H44A	0.7643	1.1604	0.4717	0.031*
C45	0.9218 (3)	1.0994 (2)	0.55539 (13)	0.0244 (5)
H45A	0.9691	1.1616	0.5401	0.029*
C46	0.9751 (2)	1.0099 (2)	0.61834 (12)	0.0210 (5)
H46A	1.0582	1.0116	0.6459	0.025*
C51	1.1555 (2)	0.81957 (19)	0.74822 (12)	0.0170 (5)

C52	1.2868 (2)	0.7637 (2)	0.71679 (12)	0.0201 (5)
H52A	1.2784	0.7169	0.6864	0.024*
C53	1.4298 (2)	0.7767 (2)	0.73004 (13)	0.0230 (5)
H53A	1.5186	0.7390	0.7084	0.028*
C54	1.4430 (2)	0.8441 (2)	0.77453 (13)	0.0238 (5)
H54A	1.5413	0.8516	0.7839	0.029*
C55	1.3140 (2)	0.9007 (2)	0.80537 (13)	0.0221 (5)
H55A	1.3232	0.9478	0.8355	0.027*
C56	1.1690 (2)	0.8885 (2)	0.79220 (12)	0.0194 (5)
H56A	1.0801	0.9275	0.8134	0.023*
C61	0.8356 (2)	0.8771 (2)	0.78193 (12)	0.0182 (5)
C62	0.8375 (2)	0.8146 (2)	0.85103 (12)	0.0213 (5)
H62A	0.9069	0.7311	0.8690	0.026*
C63	0.7396 (3)	0.8727 (2)	0.89403 (14)	0.0259 (5)
H63A	0.7418	0.8290	0.9410	0.031*
C64	0.6377 (3)	0.9956 (2)	0.86808 (14)	0.0280 (6)
H64A	0.5704	1.0357	0.8974	0.034*
C65	0.6349 (3)	1.0586 (2)	0.80013 (15)	0.0283 (6)
H65A	0.5663	1.1425	0.7827	0.034*
C66	0.7322 (2)	1.0002 (2)	0.75667 (13)	0.0223 (5)
H66A	0.7283	1.0441	0.7096	0.027*
B1	1.1701 (3)	0.5070 (3)	0.89352 (15)	0.0241 (6)
H1B	1.227 (3)	0.447 (2)	0.9452 (14)	0.031 (7)*
H2B	1.147 (3)	0.615 (2)	0.8855 (13)	0.029 (7)*
N1S	0.5802 (3)	1.1379 (2)	1.00400 (13)	0.0398 (6)
C1S	0.5862 (3)	1.3314 (3)	1.04008 (15)	0.0385 (7)
C2S	0.5840 (3)	1.2214 (3)	1.02053 (13)	0.0290 (6)
H1S	0.660 (2)	1.3039 (18)	1.0804 (9)	0.044*
H2S	0.620 (2)	1.3844 (17)	1.0025 (10)	0.044*
H3S	0.483 (2)	1.3758 (17)	1.0506 (10)	0.044*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01425 (9)	0.01286 (9)	0.01445 (11)	−0.00458 (6)	0.00124 (6)	−0.00273 (7)
P1	0.0149 (3)	0.0122 (3)	0.0137 (3)	−0.0046 (2)	0.0013 (2)	−0.0025 (2)
P2	0.0144 (3)	0.0128 (3)	0.0181 (3)	−0.0048 (2)	0.0018 (2)	−0.0045 (2)
O1	0.0422 (10)	0.0280 (9)	0.0200 (11)	−0.0163 (8)	0.0089 (8)	−0.0041 (8)
N1	0.0166 (9)	0.0157 (9)	0.0158 (11)	−0.0067 (7)	0.0022 (7)	−0.0034 (8)
N2	0.0185 (9)	0.0210 (10)	0.0162 (11)	−0.0039 (7)	−0.0015 (7)	−0.0044 (8)
N3	0.0171 (9)	0.0275 (11)	0.0251 (13)	−0.0010 (8)	−0.0002 (8)	−0.0066 (9)
N4	0.0177 (9)	0.0141 (9)	0.0158 (11)	−0.0042 (7)	0.0027 (7)	−0.0040 (8)
N5	0.0215 (9)	0.0169 (9)	0.0164 (11)	−0.0024 (7)	0.0018 (7)	−0.0040 (8)
N6	0.0318 (11)	0.0277 (11)	0.0235 (13)	−0.0134 (9)	0.0118 (9)	−0.0078 (9)
C1	0.0190 (11)	0.0122 (11)	0.0225 (14)	−0.0055 (8)	−0.0011 (9)	−0.0034 (9)
C2	0.0178 (11)	0.0192 (11)	0.0192 (13)	−0.0057 (8)	0.0037 (9)	−0.0025 (10)
C3	0.0193 (11)	0.0276 (13)	0.0260 (15)	−0.0007 (9)	−0.0055 (10)	−0.0051 (11)
C4	0.0198 (11)	0.0208 (12)	0.0243 (14)	−0.0078 (9)	0.0054 (9)	−0.0076 (10)

C5	0.0350 (13)	0.0227 (12)	0.0174 (14)	−0.0085 (10)	0.0070 (10)	−0.0035 (10)
C11	0.0204 (10)	0.0103 (10)	0.0165 (13)	−0.0038 (8)	0.0018 (8)	−0.0037 (9)
C12	0.0172 (11)	0.0192 (11)	0.0211 (14)	−0.0059 (8)	0.0013 (9)	−0.0023 (10)
C13	0.0253 (12)	0.0268 (13)	0.0226 (15)	−0.0132 (10)	0.0036 (10)	0.0009 (11)
C14	0.0300 (13)	0.0230 (12)	0.0188 (14)	−0.0080 (10)	0.0009 (10)	0.0031 (10)
C15	0.0199 (11)	0.0177 (11)	0.0226 (14)	−0.0034 (9)	−0.0010 (9)	−0.0020 (10)
C16	0.0178 (10)	0.0155 (11)	0.0203 (13)	−0.0054 (8)	0.0014 (9)	−0.0041 (9)
C21	0.0158 (10)	0.0174 (11)	0.0196 (13)	−0.0081 (8)	0.0019 (8)	−0.0072 (9)
C22	0.0229 (11)	0.0192 (12)	0.0195 (14)	−0.0038 (9)	0.0018 (9)	−0.0044 (10)
C23	0.0263 (12)	0.0294 (13)	0.0172 (14)	−0.0085 (10)	0.0052 (9)	−0.0068 (10)
C24	0.0229 (12)	0.0295 (13)	0.0271 (15)	−0.0103 (10)	0.0093 (10)	−0.0162 (11)
C25	0.0298 (13)	0.0216 (12)	0.0321 (16)	0.0003 (10)	0.0061 (11)	−0.0094 (11)
C26	0.0264 (12)	0.0182 (12)	0.0225 (14)	−0.0032 (9)	0.0033 (10)	−0.0036 (10)
C31	0.0160 (10)	0.0189 (11)	0.0134 (12)	−0.0063 (8)	0.0024 (8)	−0.0043 (9)
C32	0.0209 (11)	0.0204 (11)	0.0167 (13)	−0.0092 (9)	0.0035 (9)	−0.0046 (9)
C33	0.0170 (11)	0.0267 (12)	0.0183 (13)	−0.0045 (9)	−0.0016 (9)	−0.0033 (10)
C34	0.0207 (11)	0.0343 (14)	0.0158 (13)	−0.0133 (10)	0.0015 (9)	−0.0069 (10)
C35	0.0257 (12)	0.0263 (12)	0.0244 (14)	−0.0142 (10)	0.0043 (10)	−0.0102 (11)
C36	0.0211 (11)	0.0175 (11)	0.0221 (14)	−0.0055 (9)	0.0006 (9)	−0.0044 (10)
C41	0.0190 (10)	0.0128 (10)	0.0183 (13)	−0.0025 (8)	0.0014 (8)	−0.0029 (9)
C42	0.0255 (12)	0.0175 (11)	0.0263 (15)	−0.0063 (9)	−0.0031 (10)	−0.0034 (10)
C43	0.0230 (12)	0.0221 (12)	0.0260 (15)	−0.0005 (9)	−0.0063 (10)	−0.0049 (11)
C44	0.0309 (13)	0.0186 (12)	0.0200 (14)	0.0007 (9)	0.0015 (10)	−0.0019 (10)
C45	0.0288 (12)	0.0176 (11)	0.0245 (15)	−0.0078 (9)	0.0080 (10)	−0.0024 (10)
C46	0.0199 (11)	0.0189 (11)	0.0237 (14)	−0.0062 (9)	0.0026 (9)	−0.0056 (10)
C51	0.0168 (10)	0.0124 (10)	0.0189 (13)	−0.0044 (8)	0.0011 (8)	−0.0002 (9)
C52	0.0209 (11)	0.0164 (11)	0.0225 (14)	−0.0065 (8)	0.0013 (9)	−0.0044 (10)
C53	0.0157 (11)	0.0214 (12)	0.0303 (15)	−0.0051 (9)	0.0061 (9)	−0.0065 (11)
C54	0.0179 (11)	0.0221 (12)	0.0297 (15)	−0.0094 (9)	−0.0018 (9)	−0.0013 (10)
C55	0.0237 (11)	0.0199 (12)	0.0236 (14)	−0.0103 (9)	−0.0023 (9)	−0.0039 (10)
C56	0.0208 (11)	0.0156 (11)	0.0210 (13)	−0.0056 (8)	0.0013 (9)	−0.0045 (9)
C61	0.0131 (10)	0.0183 (11)	0.0269 (14)	−0.0068 (8)	0.0027 (9)	−0.0101 (10)
C62	0.0216 (11)	0.0217 (12)	0.0219 (14)	−0.0075 (9)	0.0032 (9)	−0.0081 (10)
C63	0.0236 (12)	0.0335 (14)	0.0270 (15)	−0.0127 (10)	0.0072 (10)	−0.0153 (11)
C64	0.0212 (12)	0.0300 (13)	0.0409 (18)	−0.0093 (10)	0.0109 (10)	−0.0225 (13)
C65	0.0219 (12)	0.0190 (12)	0.0458 (18)	−0.0062 (9)	0.0074 (11)	−0.0129 (12)
C66	0.0180 (11)	0.0164 (11)	0.0324 (15)	−0.0066 (8)	0.0059 (9)	−0.0059 (10)
B1	0.0225 (13)	0.0284 (15)	0.0204 (16)	−0.0031 (11)	−0.0001 (11)	−0.0123 (12)
N1S	0.0555 (15)	0.0322 (13)	0.0298 (15)	−0.0145 (11)	0.0069 (11)	−0.0064 (11)
C1S	0.0487 (17)	0.0355 (16)	0.0321 (18)	−0.0222 (13)	−0.0020 (13)	−0.0006 (13)
C2S	0.0287 (13)	0.0345 (15)	0.0178 (14)	−0.0105 (11)	0.0033 (10)	0.0022 (11)

Geometric parameters (Å, °)

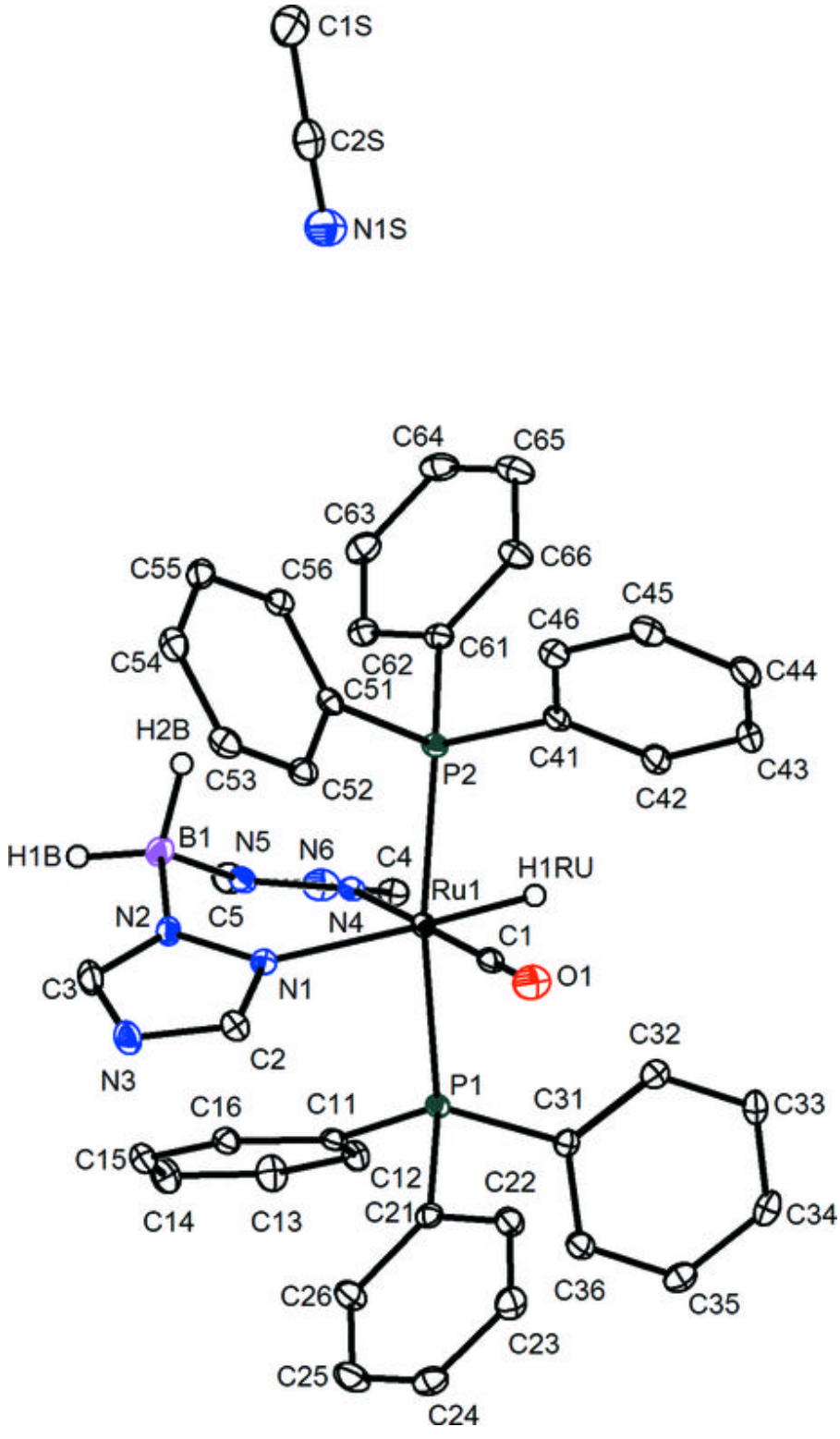
Ru1—H1RU	1.57 (2)	C31—C32	1.394 (3)
Ru1—C1	1.833 (2)	C31—C36	1.398 (3)
Ru1—N4	2.1396 (19)	C32—C33	1.392 (3)
Ru1—N1	2.1771 (17)	C32—H32A	0.9500
Ru1—P2	2.3588 (6)	C33—C34	1.380 (3)

Ru1—P1	2.3978 (6)	C33—H33A	0.9500
P1—C11	1.833 (2)	C34—C35	1.387 (3)
P1—C31	1.837 (2)	C34—H34A	0.9500
P1—C21	1.850 (2)	C35—C36	1.389 (3)
P2—C51	1.831 (2)	C35—H35A	0.9500
P2—C61	1.839 (2)	C36—H36A	0.9500
P2—C41	1.845 (2)	C41—C42	1.396 (3)
O1—C1	1.165 (3)	C41—C46	1.403 (3)
N1—C2	1.334 (3)	C42—C43	1.386 (3)
N1—N2	1.367 (3)	C42—H42A	0.9500
N2—C3	1.339 (3)	C43—C44	1.392 (3)
N2—B1	1.550 (3)	C43—H43A	0.9500
N3—C3	1.328 (3)	C44—C45	1.382 (3)
N3—C2	1.351 (3)	C44—H44A	0.9500
N4—C4	1.330 (3)	C45—C46	1.388 (3)
N4—N5	1.380 (2)	C45—H45A	0.9500
N5—C5	1.339 (3)	C46—H46A	0.9500
N5—B1	1.558 (3)	C51—C56	1.389 (3)
N6—C5	1.330 (3)	C51—C52	1.398 (3)
N6—C4	1.351 (3)	C52—C53	1.392 (3)
C2—H2A	0.9500	C52—H52A	0.9500
C3—H3A	0.9500	C53—C54	1.382 (3)
C4—H4A	0.9500	C53—H53A	0.9500
C5—H5A	0.9500	C54—C55	1.380 (3)
C11—C12	1.396 (3)	C54—H54A	0.9500
C11—C16	1.404 (3)	C55—C56	1.405 (3)
C12—C13	1.390 (3)	C55—H55A	0.9500
C12—H12A	0.9500	C56—H56A	0.9500
C13—C14	1.387 (3)	C61—C62	1.393 (3)
C13—H13A	0.9500	C61—C66	1.401 (3)
C14—C15	1.393 (3)	C62—C63	1.387 (3)
C14—H14A	0.9500	C62—H62A	0.9500
C15—C16	1.378 (3)	C63—C64	1.396 (3)
C15—H15A	0.9500	C63—H63A	0.9500
C16—H16A	0.9500	C64—C65	1.374 (4)
C21—C22	1.392 (3)	C64—H64A	0.9500
C21—C26	1.401 (3)	C65—C66	1.393 (3)
C22—C23	1.384 (3)	C65—H65A	0.9500
C22—H22A	0.9500	C66—H66A	0.9500
C23—C24	1.391 (3)	B1—H1B	1.11 (3)
C23—H23A	0.9500	B1—H2B	1.19 (2)
C24—C25	1.377 (3)	N1S—C2S	1.133 (3)
C24—H24A	0.9500	C1S—C2S	1.463 (4)
C25—C26	1.391 (3)	C1S—H1S	0.969 (16)
C25—H25A	0.9500	C1S—H2S	0.966 (16)
C26—H26A	0.9500	C1S—H3S	0.960 (16)
H1RU—Ru1—C1	90.0 (9)	C25—C26—H26A	119.7
H1RU—Ru1—N4	87.9 (9)	C21—C26—H26A	119.7
C1—Ru1—N4	176.92 (8)	C32—C31—C36	118.57 (19)

H1RU—Ru1—N1	175.7 (9)	C32—C31—P1	121.10 (16)
C1—Ru1—N1	94.31 (8)	C36—C31—P1	120.10 (16)
N4—Ru1—N1	87.84 (7)	C33—C32—C31	120.6 (2)
H1RU—Ru1—P2	81.0 (8)	C33—C32—H32A	119.7
C1—Ru1—P2	86.77 (7)	C31—C32—H32A	119.7
N4—Ru1—P2	95.09 (5)	C34—C33—C32	120.1 (2)
N1—Ru1—P2	98.90 (5)	C34—C33—H33A	120.0
H1RU—Ru1—P1	91.1 (8)	C32—C33—H33A	120.0
C1—Ru1—P1	91.65 (7)	C33—C34—C35	120.0 (2)
N4—Ru1—P1	86.16 (5)	C33—C34—H34A	120.0
N1—Ru1—P1	89.15 (5)	C35—C34—H34A	120.0
P2—Ru1—P1	171.884 (18)	C34—C35—C36	120.0 (2)
C11—P1—C31	106.50 (10)	C34—C35—H35A	120.0
C11—P1—C21	103.72 (10)	C36—C35—H35A	120.0
C31—P1—C21	98.22 (10)	C35—C36—C31	120.6 (2)
C11—P1—Ru1	112.79 (7)	C35—C36—H36A	119.7
C31—P1—Ru1	116.25 (7)	C31—C36—H36A	119.7
C21—P1—Ru1	117.57 (7)	C42—C41—C46	118.2 (2)
C51—P2—C61	103.14 (10)	C42—C41—P2	120.30 (17)
C51—P2—C41	101.34 (10)	C46—C41—P2	121.40 (17)
C61—P2—C41	101.84 (10)	C43—C42—C41	120.9 (2)
C51—P2—Ru1	115.45 (7)	C43—C42—H42A	119.5
C61—P2—Ru1	120.09 (7)	C41—C42—H42A	119.5
C41—P2—Ru1	112.53 (7)	C42—C43—C44	120.2 (2)
C2—N1—N2	104.51 (16)	C42—C43—H43A	119.9
C2—N1—Ru1	128.99 (15)	C44—C43—H43A	119.9
N2—N1—Ru1	126.25 (13)	C45—C44—C43	119.4 (2)
C3—N2—N1	106.52 (19)	C45—C44—H44A	120.3
C3—N2—B1	129.5 (2)	C43—C44—H44A	120.3
N1—N2—B1	123.77 (17)	C44—C45—C46	120.6 (2)
C3—N3—C2	102.03 (18)	C44—C45—H45A	119.7
C4—N4—N5	104.00 (18)	C46—C45—H45A	119.7
C4—N4—Ru1	129.70 (16)	C45—C46—C41	120.6 (2)
N5—N4—Ru1	124.89 (13)	C45—C46—H46A	119.7
C5—N5—N4	106.46 (18)	C41—C46—H46A	119.7
C5—N5—B1	128.5 (2)	C56—C51—C52	119.42 (19)
N4—N5—B1	123.62 (19)	C56—C51—P2	123.44 (16)
C5—N6—C4	101.79 (19)	C52—C51—P2	117.11 (17)
O1—C1—Ru1	178.72 (18)	C53—C52—C51	120.0 (2)
N1—C2—N3	113.9 (2)	C53—C52—H52A	120.0
N1—C2—H2A	123.1	C51—C52—H52A	120.0
N3—C2—H2A	123.1	C54—C53—C52	120.3 (2)
N3—C3—N2	113.1 (2)	C54—C53—H53A	119.8
N3—C3—H3A	123.5	C52—C53—H53A	119.8
N2—C3—H3A	123.5	C55—C54—C53	120.2 (2)
N4—C4—N6	114.5 (2)	C55—C54—H54A	119.9
N4—C4—H4A	122.7	C53—C54—H54A	119.9
N6—C4—H4A	122.7	C54—C55—C56	120.0 (2)
N6—C5—N5	113.2 (2)	C54—C55—H55A	120.0

N6—C5—H5A	123.4	C56—C55—H55A	120.0
N5—C5—H5A	123.4	C51—C56—C55	120.1 (2)
C12—C11—C16	118.6 (2)	C51—C56—H56A	120.0
C12—C11—P1	122.82 (16)	C55—C56—H56A	120.0
C16—C11—P1	118.38 (16)	C62—C61—C66	118.5 (2)
C13—C12—C11	119.8 (2)	C62—C61—P2	120.30 (16)
C13—C12—H12A	120.1	C66—C61—P2	121.20 (19)
C11—C12—H12A	120.1	C63—C62—C61	121.0 (2)
C14—C13—C12	121.1 (2)	C63—C62—H62A	119.5
C14—C13—H13A	119.4	C61—C62—H62A	119.5
C12—C13—H13A	119.4	C62—C63—C64	119.8 (2)
C13—C14—C15	119.4 (2)	C62—C63—H63A	120.1
C13—C14—H14A	120.3	C64—C63—H63A	120.1
C15—C14—H14A	120.3	C65—C64—C63	119.9 (2)
C16—C15—C14	119.8 (2)	C65—C64—H64A	120.0
C16—C15—H15A	120.1	C63—C64—H64A	120.0
C14—C15—H15A	120.1	C64—C65—C66	120.4 (2)
C15—C16—C11	121.4 (2)	C64—C65—H65A	119.8
C15—C16—H16A	119.3	C66—C65—H65A	119.8
C11—C16—H16A	119.3	C65—C66—C61	120.4 (2)
C22—C21—C26	118.0 (2)	C65—C66—H66A	119.8
C22—C21—P1	117.78 (16)	C61—C66—H66A	119.8
C26—C21—P1	124.19 (18)	H1B—B1—H2B	113.8 (17)
C23—C22—C21	121.4 (2)	H1B—B1—N2	108.0 (13)
C23—C22—H22A	119.3	H2B—B1—N2	108.9 (12)
C21—C22—H22A	119.3	H1B—B1—N5	108.5 (12)
C22—C23—C24	119.9 (2)	H2B—B1—N5	107.4 (11)
C22—C23—H23A	120.0	N2—B1—N5	110.19 (19)
C24—C23—H23A	120.0	C2S—C1S—H1S	108.5 (12)
C25—C24—C23	119.6 (2)	C2S—C1S—H2S	108.8 (12)
C25—C24—H24A	120.2	H1S—C1S—H2S	109.6 (13)
C23—C24—H24A	120.2	C2S—C1S—H3S	109.8 (12)
C24—C25—C26	120.5 (2)	H1S—C1S—H3S	109.6 (14)
C24—C25—H25A	119.7	H2S—C1S—H3S	110.6 (13)
C26—C25—H25A	119.7	N1S—C2S—C1S	178.4 (3)
C25—C26—C21	120.6 (2)		

Fig. 1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