Chlorido(η^6-*p*-cymene)[2-(5-phenyl-4*H*-1,2,4-triazol-3-yl-κN^2)pyridine-κN]ruthenium(II) chloride. Addendum

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The paper by Sikalov [*IUCrData* (2018), **3**, x180625] is updated.

As requested by the author's institution, the Taras Shevchenko National University of Kyiv, two additional authors and an acknowledgement are added to the data report of Sikalov (2018). The revised author list is Alexander Sikalov, Dmytro M. Khomenko and Roman O. Doroschuk. The affiliation for the two additional authors is the Department of Chemistry, Taras Shevchenko National University of Kyiv, Volodymyrska Street 64/13, Kyiv 01601, Ukraine. In addition, Dr S. Shova, 'Petra Poni' Institute of Macromolecular Chemistry, Iasi, Romania, is thanked for the data collection and structure solution.

References

Sikalov, A. (2018). *IUCrData*, **3**, x180625.
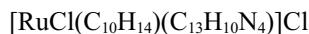
full crystallographic data

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Crystal data

[RuCl(C$_{10}$H$_{14}$)(C$_{13}$H$_{10}$N$_4$)]Cl	$Z = 1$
$M_r = 528.44$	$F(000) = 267.999$
Triclinic, $P1$	$D_x = 1.574$ Mg m^{-3}
Hall symbol: P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 6.4704$ (2) Å	Cell parameters from 8029 reflections
$b = 8.7593$ (3) Å	$\theta = 2$–32°
$c = 10.1975$ (4) Å	$\mu = 0.96$ mm^{-1}
$\alpha = 101.425$ (3)°	$T = 200$ K
$\beta = 97.379$ (3)°	Prism, clear intense red
$\gamma = 95.337$ (3)°	$0.35 \times 0.20 \times 0.20$ mm
$V = 557.62$ (3) Å^3	

Data collection

Agilent Xcalibur, Eos with CCD area detector diffractometer	13071 measured reflections
	7295 independent reflections
Graphite monochromator	7220 reflections with $I > 2.0\sigma(I)$
ω scans	$R_{int} = 0.028$
Absorption correction: multi-scan (DENZO/SCALEPACK; Otwinowski & Minor, 1997)	$\theta_{max} = 32.7°$, $\theta_{min} = 2.1°$
	$h = -9 \rightarrow 9$
	$k = -13 \rightarrow 13$
$T_{min} = 0.81$, $T_{max} = 0.83$	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.032$	Method = Modified Sheldrick $w = 1/[\sigma^2(F^2) + (0.02P)^2 + 0.15P]$,
$wR(F^2) = 0.062$	where $P = (\max(F_o^2, 0) + 2F_c^2)/3$
$S = 0.98$	
7295 reflections	$(\Delta/\sigma)_{max} = 0.001$
276 parameters	$\Delta\rho_{max} = 0.56$ e Å^{-3}
7 restraints	$\Delta\rho_{min} = -0.40$ e Å^{-3}
Primary atom site location: other	Absolute structure: Flack (1983), 3505 Friedel-pairs
Hydrogen site location: difference Fourier map	Absolute structure parameter: -0.03 (2)

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

	x	y	z	$U_{iso}*/U_{eq}$
Ru1	0.86321 (8)	0.38802 (6)	0.54014 (6)	0.0176

Cl2	0.67364 (12)	0.60046 (10)	0.49812 (9)	0.0272
Cl3	0.38532 (13)	0.18193 (12)	−0.10651 (9)	0.0382
N4	0.6317 (4)	0.2491 (3)	0.3951 (2)	0.0217
N5	0.9711 (4)	0.4024 (3)	0.3535 (2)	0.0205
N6	0.4495 (3)	0.1562 (3)	0.3969 (2)	0.0224
N7	0.4792 (3)	0.1708 (3)	0.1855 (2)	0.0220
C8	1.0648 (5)	0.5307 (4)	0.7248 (3)	0.0242
C9	0.6471 (4)	0.2555 (3)	0.2682 (2)	0.0197
C10	0.7853 (5)	0.3174 (4)	0.7245 (3)	0.0269
C11	1.1560 (4)	0.4760 (3)	0.3399 (3)	0.0252
C12	0.3595 (4)	0.1103 (3)	0.2695 (3)	0.0212
C13	0.8319 (4)	0.3402 (3)	0.2389 (3)	0.0217
C14	1.1769 (4)	0.4165 (3)	0.6582 (3)	0.0266
C15	0.8723 (4)	0.3530 (3)	0.1111 (3)	0.0294
C16	0.8650 (4)	0.4755 (3)	0.7562 (3)	0.0269
C17	0.1609 (4)	0.0092 (3)	0.2237 (3)	0.0227
C18	−0.1477 (6)	−0.0882 (5)	0.0591 (4)	0.0390
C19	1.0659 (4)	0.4275 (4)	0.0989 (3)	0.0318
C20	1.2075 (4)	0.4896 (4)	0.2144 (3)	0.0299
C21	0.9010 (4)	0.2016 (3)	0.6564 (3)	0.0276
C22	1.1445 (4)	0.7045 (3)	0.7648 (3)	0.0300
C23	0.0847 (5)	−0.0834 (4)	0.3077 (3)	0.0350
C24	1.0990 (4)	0.2552 (4)	0.6249 (3)	0.0279
C25	−0.2238 (5)	−0.1779 (4)	0.1438 (3)	0.0421
C26	0.0434 (4)	0.0051 (4)	0.0982 (3)	0.0310
C27	1.2355 (5)	0.7703 (4)	0.6552 (3)	0.0395
C28	−0.1071 (5)	−0.1770 (4)	0.2670 (3)	0.0433
C29	0.8085 (6)	0.0338 (4)	0.6203 (4)	0.0445
C30	1.3064 (6)	0.7305 (4)	0.8939 (4)	0.0505
H71	0.451 (3)	0.160 (3)	0.1007 (18)	0.0278 (19)*
H111	1.2519	0.5190	0.4165	0.0292*
H141	1.3038	0.4499	0.6226	0.0345*
H151	0.7718	0.3117	0.0351	0.0363*
H161	0.7756	0.5545	0.7899	0.0341*
H181	−0.2263	−0.0894	−0.0232	0.0473*
H191	1.1020	0.4339	0.0136	0.0391*
H201	1.3382	0.5360	0.2072	0.0359*
H221	1.0243	0.7611	0.7874	0.0381*
H231	0.1642	−0.0822	0.3918	0.0421*
H241	1.1754	0.1828	0.5704	0.0352*
H251	−0.3543	−0.2396	0.1181	0.0508*
H261	0.0930	0.0653	0.0394	0.0384*
H271	1.3590	0.7220	0.6351	0.0610*
H272	1.2764	0.8813	0.6860	0.0609*
H273	1.1347	0.7520	0.5733	0.0611*
H281	−0.1561	−0.2397	0.3228	0.0532*
H291	0.8511	−0.0189	0.5382	0.0682*
H293	0.8554	−0.0149	0.6927	0.0682*

H292	0.6578	0.0253	0.6089	0.0680*
H301	1.2398	0.7033	0.9668	0.0790*
H303	1.4155	0.6662	0.8771	0.0789*
H302	1.3657	0.8396	0.9189	0.0788*
H101	0.6409	0.2853	0.7369	0.0348*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01437 (7)	0.02394 (8)	0.01423 (7)	0.00019 (5)	0.00201 (5)	0.00478 (6)
Cl2	0.0199 (3)	0.0299 (3)	0.0327 (4)	0.0052 (3)	0.0026 (3)	0.0090 (3)
Cl3	0.0336 (4)	0.0593 (5)	0.0200 (3)	−0.0087 (3)	0.0005 (3)	0.0134 (3)
N4	0.0213 (11)	0.0260 (11)	0.0172 (12)	−0.0043 (9)	0.0043 (9)	0.0054 (9)
N5	0.0156 (10)	0.0278 (12)	0.0182 (10)	0.0016 (9)	0.0031 (8)	0.0055 (9)
N6	0.0204 (10)	0.0244 (10)	0.0204 (10)	−0.0055 (8)	0.0013 (8)	0.0052 (8)
N7	0.0222 (10)	0.0261 (11)	0.0165 (10)	−0.0041 (8)	0.0020 (8)	0.0052 (8)
C8	0.0198 (13)	0.0308 (15)	0.0185 (15)	−0.0021 (11)	−0.0049 (10)	0.0041 (12)
C9	0.0194 (11)	0.0237 (12)	0.0156 (11)	−0.0009 (9)	0.0022 (8)	0.0053 (9)
C10	0.0234 (14)	0.0414 (18)	0.0177 (12)	−0.0001 (12)	0.0040 (10)	0.0121 (13)
C11	0.0186 (11)	0.0336 (14)	0.0226 (12)	−0.0014 (10)	0.0041 (9)	0.0058 (11)
C12	0.0193 (11)	0.0235 (12)	0.0211 (12)	0.0004 (9)	0.0043 (9)	0.0056 (10)
C13	0.0185 (11)	0.0261 (12)	0.0198 (12)	−0.0011 (9)	0.0022 (9)	0.0055 (10)
C14	0.0184 (11)	0.0393 (15)	0.0224 (12)	0.0025 (10)	−0.0030 (9)	0.0119 (11)
C15	0.0288 (14)	0.0392 (15)	0.0193 (12)	−0.0043 (12)	0.0043 (10)	0.0073 (11)
C16	0.0259 (13)	0.0371 (15)	0.0159 (11)	0.0025 (11)	0.0019 (9)	0.0030 (11)
C17	0.0212 (11)	0.0231 (12)	0.0224 (12)	−0.0026 (9)	0.0029 (9)	0.0038 (10)
C18	0.0271 (14)	0.052 (3)	0.032 (2)	−0.0112 (16)	−0.0040 (14)	0.0070 (18)
C19	0.0312 (14)	0.0440 (17)	0.0217 (13)	−0.0024 (12)	0.0088 (11)	0.0106 (12)
C20	0.0210 (12)	0.0405 (16)	0.0293 (14)	−0.0038 (11)	0.0085 (10)	0.0103 (12)
C21	0.0326 (14)	0.0282 (13)	0.0220 (12)	0.0020 (11)	−0.0011 (10)	0.0094 (10)
C22	0.0247 (13)	0.0341 (15)	0.0262 (13)	0.0011 (11)	−0.0008 (10)	−0.0013 (11)
C23	0.0360 (15)	0.0386 (16)	0.0280 (14)	−0.0129 (13)	−0.0004 (12)	0.0127 (12)
C24	0.0260 (14)	0.0356 (16)	0.0238 (14)	0.0114 (12)	0.0006 (11)	0.0088 (12)
C25	0.0306 (15)	0.0471 (19)	0.0424 (18)	−0.0161 (13)	0.0014 (13)	0.0071 (15)
C26	0.0255 (13)	0.0375 (16)	0.0279 (14)	−0.0049 (11)	0.0017 (11)	0.0073 (12)
C27	0.0418 (17)	0.0321 (15)	0.0435 (18)	−0.0019 (13)	0.0135 (14)	0.0037 (14)
C28	0.0392 (17)	0.0482 (19)	0.0393 (18)	−0.0180 (15)	0.0049 (14)	0.0131 (15)
C29	0.051 (2)	0.0342 (16)	0.050 (2)	0.0026 (15)	0.0041 (16)	0.0180 (15)
C30	0.051 (2)	0.048 (2)	0.0396 (19)	−0.0053 (17)	−0.0179 (16)	−0.0004 (16)

Geometric parameters (Å, °)

Ru1—Cl2	2.399 (3)	C15—H151	0.933
Ru1—N4	2.072 (3)	C16—H161	0.981
Ru1—N5	2.132 (2)	C17—C23	1.394 (4)
Ru1—C8	2.223 (3)	C17—C26	1.394 (4)
Ru1—C10	2.195 (3)	C18—C25	1.382 (5)
Ru1—C14	2.189 (3)	C18—C26	1.383 (5)

Ru1—C16	2.183 (3)	C18—H181	0.922
Ru1—C21	2.213 (3)	C19—C20	1.378 (4)
Ru1—C24	2.195 (3)	C19—H191	0.940
N4—N6	1.373 (3)	C20—H201	0.922
N4—C9	1.322 (3)	C21—C24	1.421 (4)
N5—C11	1.342 (3)	C21—C29	1.490 (4)
N5—C13	1.363 (4)	C22—C27	1.513 (4)
N6—C12	1.320 (3)	C22—C30	1.538 (4)
N7—C9	1.345 (3)	C22—H221	0.988
N7—C12	1.374 (3)	C23—C28	1.388 (4)
N7—H71	0.846 (17)	C23—H231	0.939
C8—C14	1.407 (4)	C24—H241	0.972
C8—C16	1.435 (4)	C25—C28	1.379 (5)
C8—C22	1.518 (4)	C25—H251	0.936
C9—C13	1.444 (3)	C26—H261	0.940
C10—C16	1.391 (4)	C27—H271	0.964
C10—C21	1.438 (4)	C27—H272	0.961
C10—H101	0.982	C27—H273	0.967
C11—C20	1.388 (4)	C28—H281	0.930
C11—H111	0.924	C29—H291	0.959
C12—C17	1.458 (3)	C29—H293	0.955
C13—C15	1.386 (3)	C29—H292	0.961
C14—C24	1.414 (4)	C30—H301	0.963
C14—H141	0.983	C30—H303	0.955
C15—C19	1.390 (4)	C30—H302	0.967
Cl2—Ru1—N4	84.77 (8)	Ru1—C14—H141	122.1
Cl2—Ru1—N5	83.97 (7)	C8—C14—H141	119.4
N4—Ru1—N5	76.14 (9)	C24—C14—H141	118.0
Cl2—Ru1—C8	94.13 (9)	C13—C15—C19	118.5 (3)
N4—Ru1—C8	168.20 (9)	C13—C15—H151	120.5
N5—Ru1—C8	115.48 (10)	C19—C15—H151	121.0
Cl2—Ru1—C10	109.97 (9)	Ru1—C16—C8	72.50 (16)
N4—Ru1—C10	101.13 (11)	Ru1—C16—C10	71.95 (16)
N5—Ru1—C10	165.66 (9)	C8—C16—C10	122.3 (3)
C8—Ru1—C10	68.16 (12)	Ru1—C16—H161	121.8
Cl2—Ru1—C14	124.65 (8)	C8—C16—H161	117.5
N4—Ru1—C14	148.83 (11)	C10—C16—H161	119.7
N5—Ru1—C14	95.31 (9)	C12—C17—C23	119.5 (2)
C8—Ru1—C14	37.19 (11)	C12—C17—C26	121.3 (2)
C10—Ru1—C14	79.71 (11)	C23—C17—C26	119.2 (2)
Cl2—Ru1—C16	88.32 (8)	C25—C18—C26	120.5 (4)
N4—Ru1—C16	130.20 (10)	C25—C18—H181	119.6
N5—Ru1—C16	151.76 (10)	C26—C18—H181	119.9
C8—Ru1—C16	38.00 (11)	C15—C19—C20	118.8 (2)
C10—Ru1—C16	37.05 (11)	C15—C19—H191	121.1
Cl2—Ru1—C21	146.94 (8)	C20—C19—H191	120.1
N4—Ru1—C21	93.12 (10)	C11—C20—C19	119.9 (2)

N5—Ru1—C21	127.60 (10)	C11—C20—H201	120.5
C8—Ru1—C21	81.38 (11)	C19—C20—H201	119.6
C10—Ru1—C21	38.07 (11)	Ru1—C21—C10	70.29 (16)
Cl2—Ru1—C24	161.72 (8)	Ru1—C21—C24	70.50 (15)
N4—Ru1—C24	113.51 (12)	C10—C21—C24	117.4 (3)
N5—Ru1—C24	100.26 (10)	Ru1—C21—C29	129.3 (2)
C8—Ru1—C24	67.92 (12)	C10—C21—C29	119.4 (3)
C10—Ru1—C24	67.60 (11)	C24—C21—C29	123.3 (3)
C14—Ru1—C16	67.15 (10)	C8—C22—C27	114.4 (2)
C14—Ru1—C21	68.15 (10)	C8—C22—C30	107.7 (3)
C16—Ru1—C21	68.00 (11)	C27—C22—C30	111.2 (3)
C14—Ru1—C24	37.62 (11)	C8—C22—H221	107.5
C16—Ru1—C24	79.57 (11)	C27—C22—H221	108.0
C21—Ru1—C24	37.60 (11)	C30—C22—H221	107.9
Ru1—N4—N6	135.48 (17)	C17—C23—C28	120.1 (3)
Ru1—N4—C9	115.74 (18)	C17—C23—H231	119.5
N6—N4—C9	108.6 (2)	C28—C23—H231	120.3
Ru1—N5—C11	125.85 (19)	Ru1—C24—C21	71.89 (15)
Ru1—N5—C13	116.14 (17)	Ru1—C24—C14	70.97 (15)
C11—N5—C13	117.8 (2)	C21—C24—C14	121.0 (3)
N4—N6—C12	106.0 (2)	Ru1—C24—H241	123.9
C9—N7—C12	105.0 (2)	C21—C24—H241	120.0
C9—N7—H71	127.5 (12)	C14—C24—H241	118.6
C12—N7—H71	127.5 (12)	C18—C25—C28	120.0 (3)
Ru1—C8—C14	70.11 (16)	C18—C25—H251	120.5
Ru1—C8—C16	69.50 (16)	C28—C25—H251	119.5
C14—C8—C16	116.6 (3)	C17—C26—C18	120.0 (3)
Ru1—C8—C22	131.5 (2)	C17—C26—H261	120.6
C14—C8—C22	123.8 (3)	C18—C26—H261	119.4
C16—C8—C22	119.6 (3)	C22—C27—H271	109.8
N7—C9—N4	109.8 (2)	C22—C27—H272	109.7
N7—C9—C13	130.9 (2)	H271—C27—H272	108.0
N4—C9—C13	119.2 (2)	C22—C27—H273	111.2
Ru1—C10—C16	71.00 (16)	H271—C27—H273	109.1
Ru1—C10—C21	71.64 (15)	H272—C27—H273	109.0
C16—C10—C21	120.7 (3)	C23—C28—C25	120.2 (3)
Ru1—C10—H101	122.9	C23—C28—H281	119.8
C16—C10—H101	120.0	C25—C28—H281	120.0
C21—C10—H101	118.8	C21—C29—H291	110.7
N5—C11—C20	122.1 (3)	C21—C29—H293	108.3
N5—C11—H111	118.9	H291—C29—H293	109.8
C20—C11—H111	119.0	C21—C29—H292	110.6
N7—C12—N6	110.7 (2)	H291—C29—H292	109.1
N7—C12—C17	124.4 (2)	H293—C29—H292	108.3
N6—C12—C17	124.9 (2)	C22—C30—H301	110.0
C9—C13—N5	111.6 (2)	C22—C30—H303	109.2
C9—C13—C15	125.5 (2)	H301—C30—H303	109.5
N5—C13—C15	122.8 (2)	C22—C30—H302	109.4

Ru1—C14—C8	72.71 (16)	H301—C30—H302	109.3
Ru1—C14—C24	71.41 (15)	H303—C30—H302	109.5
C8—C14—C24	122.1 (3)		

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N7—H71⋯Cl3	0.85	2.15	2.984	169