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Table 1: Fractional coordinates and equivalent isotropic[a] thermal parameters ($Å^2$) for the non-H atoms of compound **3**.

Atom	x	y	z	U
Ru	0.24616(2)	0.13779(2)	0.20040(2)	0.0343(1)
Cl	0.10361(8)	0.17821(6)	0.35800(6)	0.0462(3)
P1	0.18145(8)	0.29353(6)	0.15779(6)	0.0357(3)
P2	0.05496(8)	0.50717(6)	0.21734(6)	0.0416(4)
P3	0.41311(7)	0.14970(6)	0.24657(6)	0.0352(3)
P4	0.49051(9)	-0.05997(6)	0.31043(7)	0.0462(4)
C1	0.3143(4)	0.0659(3)	0.0678(3)	0.056(2)
C2	0.1771(4)	0.0886(3)	0.0996(3)	0.053(2)
C3	0.1401(4)	0.0410(3)	0.1827(3)	0.055(2)
C4	0.2529(4)	-0.0131(2)	0.2022(3)	0.053(2)
C5	0.3593(4)	0.0028(3)	0.1309(3)	0.054(2)
C6	0.0291(3)	0.3214(2)	0.1321(2)	0.040(1)
C7	0.0026(3)	0.3813(3)	0.0622(3)	0.057(2)
C8	-0.1164(4)	0.4009(3)	0.0492(3)	0.071(2)
C9	-0.2100(4)	0.3633(3)	0.1069(3)	0.067(2)
C10	-0.1855(3)	0.3045(3)	0.1768(3)	0.057(2)
C11	-0.0664(3)	0.2831(2)	0.1890(2)	0.046(1)
C12	0.2898(3)	0.3268(2)	0.0503(2)	0.043(1)
C13	0.3637(4)	0.3872(3)	0.0462(3)	0.063(2)
C14	0.4502(5)	0.4022(4)	-0.0373(3)	0.093(3)
C15	0.4651(5)	0.3585(4)	-0.1160(3)	0.096(3)
C16	0.3957(5)	0.2976(3)	-0.1128(3)	0.082(2)
C17	0.3080(4)	0.2825(3)	-0.0307(2)	0.060(2)
C18	0.1478(3)	0.3872(2)	0.2406(2)	0.042(1)
C19	-0.1128(3)	0.5130(2)	0.2857(2)	0.044(1)
C20	-0.2039(4)	0.5932(3)	0.2745(3)	0.070(2)
C21	-0.3335(4)	0.6072(4)	0.3247(3)	0.084(2)
C22	-0.3721(4)	0.5396(4)	0.3836(3)	0.077(2)
C23	-0.2845(4)	0.4590(3)	0.3936(3)	0.070(2)
C24	-0.1544(4)	0.4452(3)	0.3454(3)	0.057(2)
C25	0.0935(3)	0.5767(2)	0.2915(3)	0.049(2)
C26	0.1838(4)	0.6263(3)	0.2503(3)	0.073(2)
C27	0.2139(5)	0.6810(3)	0.3037(5)	0.100(3)
C28	0.1541(6)	0.6891(4)	0.3963(5)	0.106(3)
C29	0.0659(6)	0.6416(4)	0.4364(4)	0.093(3)
C30	0.0357(4)	0.5849(3)	0.3858(3)	0.064(2)
C31	0.4015(3)	0.2597(2)	0.2988(2)	0.037(1)
C32	0.3200(3)	0.2839(3)	0.3880(2)	0.048(2)
C33	0.3054(3)	0.3701(3)	0.4260(3)	0.059(2)
C34	0.3719(4)	0.4314(3)	0.3756(3)	0.061(2)
C35	0.4544(3)	0.4071(3)	0.2877(3)	0.057(2)
C36	0.4698(3)	0.3217(2)	0.2496(3)	0.045(1)
C37	0.5738(3)	0.1279(2)	0.1598(2)	0.042(1)
C38	0.6859(3)	0.0967(3)	0.1835(3)	0.057(2)
C39	0.8045(4)	0.0865(3)	0.1161(4)	0.076(2)
C40	0.8135(4)	0.1086(3)	0.0270(4)	0.079(2)
C41	0.7037(4)	0.1408(3)	0.0026(3)	0.072(2)

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Table 1 continued.

Atom	x	y	z	U
C42	0.5839(3)	0.1494(3)	0.0684(3)	0.054(2)
C43	0.4375(3)	0.0675(2)	0.3407(2)	0.043(1)
C44	0.6575(3)	-0.0970(3)	0.3107(3)	0.052(2)
C45	0.6977(4)	-0.0805(3)	0.3809(3)	0.069(2)
C46	0.8263(5)	-0.1089(4)	0.3739(5)	0.100(3)
C47	0.9155(5)	-0.1514(4)	0.2952(6)	0.116(4)
C48	0.8790(5)	-0.1687(4)	0.2248(5)	0.102(3)
C49	0.7491(4)	-0.1409(3)	0.2314(3)	0.071(2)
C50	0.4015(3)	-0.1063(2)	0.4187(2)	0.045(1)
C51	0.4578(4)	-0.1791(3)	0.4687(3)	0.056(2)
C52	0.3824(4)	-0.2164(3)	0.5445(3)	0.071(2)
C53	0.2518(4)	-0.1819(3)	0.5719(3)	0.074(2)
C54	0.1935(4)	-0.1108(3)	0.5240(3)	0.067(2)
C55	0.2668(3)	-0.0724(3)	0.4478(3)	0.056(2)

[a]For anisotropic atoms, the U value is U_{eq}, calculated as $U_{eq} = 1/3\ \Sigma_i\Sigma_j\ U_{ij}\ a_i^*\ a_j^*\ A_{ij}$ where A_{ij} is the dot product of the i^{th} and j^{th} direct space unit cell vectors.

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Table 2: Bond Lengths (Å) and Angles (°) for the non-H atoms of compound **3**.

1	2	3	1-2	1-2-3
Cl	Ru	P1	2.452(1)	89.91(3)
Cl	Ru	P3		87.97(3)
Cl	Ru	C1		154.9(1)
Cl	Ru	C2		120.4(1)
Cl	Ru	C3		92.5(1)
Cl	Ru	C4		98.2(1)
P1	Ru	P3	2.319(1)	97.20(4)
P1	Ru	C1		101.2(1)
P1	Ru	C2		92.1(1)
P1	Ru	C3		117.6(1)
P1	Ru	C4		153.5(1)
P1	Ru	C5		136.9(1)
P3	Ru	C1	2.314(1)	112.5(1)
P3	Ru	C2		150.2(1)
P3	Ru	C3		145.1(1)
P3	Ru	C4		108.2(1)
P3	Ru	C5		92.5(1)
C1	Ru	C2	2.191(4)	37.7(1)
C1	Ru	C3		62.4(1)
C1	Ru	C4		62.6(1)
C1	Ru	C5		37.4(1)
C2	Ru	C3	2.229(5)	36.7(1)
C2	Ru	C4		62.0(2)
C2	Ru	C5		62.3(2)
C3	Ru	C4	2.226(5)	37.3(1)
C3	Ru	C5		62.2(1)
C4	Ru	C5	2.221(4)	37.3(1)
C5	Ru	Cl	2.194(3)	132.5(1)
C6	P1	C12	1.843(4)	101.9(2)
C6	P1	C18		102.1(2)
C6	P1	Ru		112.2(1)
C12	P1	C18	1.839(3)	104.9(2)
C12	P1	Ru		115.0(1)
C18	P1	Ru	1.848(4)	118.8(1)
C18	P2	C19	1.861(3)	103.9(1)
C19	P2	C25	1.844(3)	100.1(2)
C25	P2	C18	1.845(5)	99.5(2)
C31	P3	C37	1.842(4)	100.8(2)
C31	P3	C43		99.1(2)
C31	P3	Ru		112.0(1)
C37	P3	C43	1.842(3)	104.4(1)
C37	P3	Ru		117.7(1)
C43	P3	Ru	1.851(3)	112.3(1)
C43	P4	C44	1.866(3)	103.0(2)
C44	P4	C50	1.835(4)	104.1(2)
C50	P4	C43	1.837(3)	99.7(1)
C2	C1	C5	1.429(6)	107.5(3)

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Table 2 continued.

1	2	3	1-2	1-2-3
C5	C1		1.406(6)	
C3	C2	C1	1.404(5)	107.8(3)
C4	C3	C2	1.422(6)	108.4(3)
C5	C4	C3	1.410(5)	107.4(3)
C1	C5	C4		108.8(3)
C7	C6	C11	1.390(5)	118.5(3)
C7	C6	P1		123.9(3)
C11	C6	P1	1.389(5)	117.5(3)
C8	C7	C6	1.391(7)	120.3(4)
C9	C8	C7	1.373(6)	120.3(4)
C10	C9	C8	1.375(6)	120.0(4)
C11	C10	C9	1.385(6)	120.0(4)
C6	C11	C10		120.8(3)
C13	C12	C17	1.389(6)	117.8(3)
C13	C12	P1		123.8(3)
C17	C12	P1	1.394(6)	118.2(3)
C14	C13	C12	1.387(6)	119.5(5)
C15	C14	C13	1.369(8)	121.5(6)
C16	C15	C14	1.359(9)	119.8(4)
C17	C16	C15	1.380(5)	119.7(5)
C12	C17	C16		121.7(5)
P1	C18	P2		116.9(2)
C20	C19	C24	1.376(5)	118.0(3)
C20	C19	P2		115.6(3)
C24	C19	P2	1.383(5)	126.4(3)
C21	C20	C19	1.393(6)	121.0(4)
C22	C21	C20	1.363(8)	119.9(4)
C23	C22	C21	1.354(6)	120.0(4)
C24	C23	C22	1.392(6)	120.5(4)
C19	C24	C23		120.5(3)
C26	C25	C30	1.396(6)	117.5(4)
C26	C25	P2		118.4(3)
C30	C25	P2	1.387(5)	124.0(3)
C27	C26	C25	1.393(9)	120.2(4)
C28	C27	C26	1.364(10)	121.1(5)
C29	C28	C27	1.353(9)	118.9(7)
C30	C29	C28	1.384(9)	121.5(5)

Table 2 continued.

1	2	3	1-2	1-2-3
C25	C30	C29		120.7(4)
C32	C31	C36	1.393(4)	118.7(3)
C32	C31	P3		120.1(3)
C36	C31	P3	1.393(5)	121.2(2)
C33	C32	C31	1.401(6)	120.2(3)
C34	C33	C32	1.379(6)	120.3(3)
C35	C34	C33	1.380(5)	119.7(4)
C36	C35	C34	1.388(6)	120.4(4)
C31	C36	C35		120.7(3)
C38	C37	C42	1.393(6)	118.7(3)
C38	C37	P3		122.0(3)
C42	C37	P3	1.391(5)	119.1(3)
C39	C38	C37	1.388(5)	119.8(4)
C40	C39	C38	1.361(8)	121.2(4)
C41	C40	C39	1.375(7)	119.7(4)
C42	C41	C40	1.391(5)	120.2(4)
P3	C43	P4		115.3(2)
C37	C42	C41		120.4(4)
C45	C44	C49	1.379(7)	118.7(4)
C49	C44		1.386(5)	
C46	C45	C44	1.382(7)	121.1(4)
C47	C46	C45	1.364(9)	119.5(7)
C48	C47	C46	1.358(12)	120.8(6)
C49	C48	C47	1.398(7)	120.1(5)
C44	C49	C48		119.7(5)
C51	C50	C55	1.397(5)	118.0(3)
C55	C50		1.404(5)	
C52	C51	C50	1.384(6)	120.7(4)
C53	C52	C51	1.364(6)	120.3(4)
C54	C53	C52	1.372(6)	120.5(4)
C55	C54	C53	1.385(6)	120.3(4)
C50	C55	C54		120.3(4)

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Table 3: Anisotropic thermal parameters[a] for the non-H atoms of compound **3.**

Atom	U11	U22	U33	U12	U13	U23
Ru	0.0314(1)	0.0361(2)	0.0358(2)	-0.0112(1)	-0.0084(1)	-0.0049(1)
Cl	0.0391(5)	0.0566(5)	0.0393(5)	-0.0156(4)	-0.0052(4)	-0.0026(4)
P1	0.0341(4)	0.0401(5)	0.0341(5)	-0.0126(4)	-0.0098(4)	-0.0024(4)
P2	0.0416(5)	0.0399(5)	0.0406(5)	-0.0096(4)	-0.0113(4)	0.0006(4)
P3	0.0301(4)	0.0360(5)	0.0391(5)	-0.0094(3)	-0.0091(4)	-0.0043(4)
P4	0.0466(5)	0.0415(5)	0.0495(6)	-0.0104(4)	-0.0156(4)	0.0001(4)
C1	0.064(3)	0.057(2)	0.047(2)	-0.019(2)	-0.012(2)	-0.018(2)
C2	0.063(2)	0.050(2)	0.060(2)	-0.016(2)	-0.034(2)	-0.010(2)
C3	0.051(2)	0.052(2)	0.070(3)	-0.024(2)	-0.018(2)	-0.013(2)
C4	0.070(3)	0.039(2)	0.058(2)	-0.021(2)	-0.026(2)	-0.003(2)
C5	0.053(2)	0.046(2)	0.061(2)	-0.003(2)	-0.022(2)	-0.021(2)
C6	0.040(2)	0.041(2)	0.041(2)	-0.013(2)	-0.014(2)	-0.001(2)
C7	0.055(2)	0.065(3)	0.063(2)	-0.030(2)	-0.029(2)	0.020(2)
C8	0.072(3)	0.080(3)	0.079(3)	-0.032(2)	-0.048(3)	0.035(2)
C9	0.053(2)	0.078(3)	0.089(3)	-0.028(2)	-0.043(2)	0.019(3)
C10	0.048(2)	0.066(3)	0.064(3)	-0.027(2)	-0.023(2)	0.012(2)
C11	0.041(2)	0.051(2)	0.044(2)	-0.011(2)	-0.014(2)	0.002(2)
C12	0.039(2)	0.047(2)	0.041(2)	-0.015(2)	-0.008(2)	0.001(2)
C13	0.060(2)	0.072(3)	0.062(3)	-0.036(2)	-0.008(2)	-0.009(2)
C14	0.090(4)	0.107(4)	0.085(4)	-0.071(3)	0.009(3)	-0.009(3)
C15	0.091(4)	0.118(4)	0.063(3)	-0.059(3)	0.019(3)	0.002(3)
C16	0.101(4)	0.098(4)	0.043(2)	-0.046(3)	0.001(2)	-0.006(2)
C17	0.072(3)	0.067(3)	0.041(2)	-0.034(2)	-0.007(2)	-0.002(2)
C18	0.038(2)	0.042(2)	0.043(2)	-0.004(1)	-0.014(2)	-0.006(2)
C19	0.046(2)	0.043(2)	0.045(2)	-0.012(2)	-0.017(2)	-0.002(2)
C20	0.053(2)	0.073(3)	0.071(3)	-0.006(2)	-0.018(2)	0.015(2)
C21	0.052(3)	0.104(4)	0.079(3)	0.007(3)	-0.024(2)	0.000(3)
C22	0.040(2)	0.120(4)	0.068(3)	-0.023(3)	-0.006(2)	-0.030(3)
C23	0.063(3)	0.073(3)	0.067(3)	-0.035(2)	0.006(2)	-0.017(2)
C24	0.055(2)	0.048(2)	0.059(2)	-0.014(2)	-0.007(2)	-0.006(2)
C25	0.038(2)	0.038(2)	0.066(3)	-0.005(2)	-0.015(2)	-0.007(2)
C26	0.060(3)	0.060(3)	0.096(3)	-0.017(2)	-0.012(2)	-0.023(2)
C27	0.061(3)	0.065(3)	0.180(6)	-0.018(2)	-0.036(4)	-0.038(4)
C28	0.092(4)	0.076(4)	0.167(6)	0.006(3)	-0.076(4)	-0.059(4)
C29	0.110(4)	0.090(4)	0.090(4)	-0.010(3)	-0.054(3)	-0.034(3)
C30	0.071(3)	0.066(3)	0.060(3)	-0.017(2)	-0.027(2)	-0.009(2)
C31	0.031(2)	0.039(2)	0.045(2)	-0.008(1)	-0.017(1)	-0.006(1)
C32	0.040(2)	0.054(2)	0.053(2)	-0.011(2)	-0.017(2)	-0.013(2)
C33	0.049(2)	0.070(3)	0.057(2)	-0.005(2)	-0.019(2)	-0.027(2)
C34	0.054(2)	0.049(2)	0.088(3)	-0.009(2)	-0.031(2)	-0.021(2)
C35	0.053(2)	0.044(2)	0.079(3)	-0.017(2)	-0.024(2)	-0.003(2)
C36	0.037(2)	0.044(2)	0.057(2)	-0.013(2)	-0.017(2)	-0.004(2)
C37	0.032(2)	0.037(2)	0.054(2)	-0.012(1)	-0.005(2)	-0.009(2)
C38	0.038(2)	0.057(2)	0.075(3)	-0.018(2)	-0.013(2)	0.001(2)
C39	0.035(2)	0.071(3)	0.114(4)	-0.016(2)	-0.012(2)	-0.005(3)
C40	0.047(3)	0.081(3)	0.094(4)	-0.032(2)	0.018(3)	-0.032(3)
C41	0.067(3)	0.092(3)	0.053(3)	-0.041(3)	0.007(2)	-0.022(2)
C42	0.045(2)	0.066(3)	0.051(2)	-0.020(2)	-0.005(2)	-0.019(2)

Table 3 continued.

C43	0.041(2)	0.040(2)	0.045(2)	-0.007(2)	-0.015(2)	0.001(2)
C44	0.045(2)	0.042(2)	0.063(2)	-0.010(2)	-0.012(2)	0.003(2)
C45	0.055(3)	0.065(3)	0.085(3)	-0.007(2)	-0.026(2)	-0.002(2)
C46	0.066(3)	0.084(4)	0.165(6)	-0.009(3)	-0.064(4)	-0.005(4)
C47	0.050(3)	0.083(4)	0.206(8)	-0.004(3)	-0.038(4)	-0.014(5)
C48	0.056(3)	0.073(4)	0.140(5)	-0.004(3)	0.008(3)	-0.019(3)
C49	0.061(3)	0.056(3)	0.084(3)	-0.015(2)	-0.006(2)	-0.007(2)
C50	0.045(2)	0.044(2)	0.051(2)	-0.017(2)	-0.017(2)	0.001(2)
C51	0.051(2)	0.051(2)	0.070(3)	-0.014(2)	-0.025(2)	0.007(2)
C52	0.071(3)	0.071(3)	0.079(3)	-0.030(2)	-0.032(2)	0.027(2)
C53	0.075(3)	0.081(3)	0.071(3)	-0.044(3)	-0.016(2)	0.021(2)
C54	0.051(2)	0.076(3)	0.077(3)	-0.029(2)	-0.015(2)	0.003(2)
C55	0.051(2)	0.053(2)	0.064(2)	-0.016(2)	-0.019(2)	0.005(2)

a Uij are the mean-square amplitudes of vibration in $Å^2$ from the general temperature factor expression

$\exp[-2\pi^2(h^2a^{*2}U11 + k^2b^{*2}U22 + l^2c^{*2}U33 + 2hka^*b^*U12 + 2hla^*c^*U13 + 2klb^*c^*U23)]$

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Table 4: Fractional coordinates and isotropic thermal parameters ($Å^2$) for the H atoms of compound 3.

Atom	x	y	z	U
H1	0.36627	0.08951	0.01327	0.08
H2	0.12044	0.12903	0.06950	0.08
H3	0.05328	0.04454	0.22000	0.08
H4	0.25603	-0.05319	0.25437	0.08
H5	0.44786	-0.02491	0.12620	0.08
H7	0.06678	0.40927	0.02275	0.08
H8	-0.13317	0.44086	-0.00035	0.08
H9	-0.29268	0.37812	0.09839	0.08
H10	-0.25104	0.27824	0.21706	0.08
H11	-0.04951	0.24138	0.23745	0.08
H13	0.35481	0.41826	0.10071	0.08
H14	0.50078	0.44417	-0.03985	0.08
H15	0.52421	0.37095	-0.17325	0.08
H16	0.40792	0.26509	-0.16734	0.08
H17	0.25796	0.24048	-0.02930	0.08
H18a	0.10019	0.36845	0.29981	0.08
H18b	0.22882	0.39144	0.24216	0.08
H20	-0.17770	0.64019	0.23161	0.08
H21	-0.39553	0.66443	0.31770	0.08
H22	-0.46140	0.54906	0.41795	0.08
H23	-0.31229	0.41105	0.43421	0.08
H24	-0.09308	0.38812	0.35376	0.08
H26	0.22535	0.62274	0.18503	0.08
H27	0.27776	0.71350	0.27483	0.08
H28	0.17426	0.72790	0.43233	0.08
H29	0.02332	0.64726	0.50154	0.08
H30	-0.02598	0.55102	0.41645	0.08
H32	0.27374	0.24144	0.42352	0.08
H33	0.24880	0.38651	0.48739	0.08
H34	0.36091	0.49071	0.40149	0.08
H35	0.50144	0.44939	0.25282	0.08
H36	0.52800	0.30534	0.18861	0.08
H38	0.68118	0.08229	0.24623	0.08
H39	0.88152	0.06336	0.13257	0.08
H40	0.89625	0.10190	-0.01868	0.08
H41	0.70975	0.15725	-0.06000	0.08
H42	0.50769	0.17035	0.05070	0.08
H43a	0.50161	0.08052	0.36076	0.08
H43b	0.35765	0.07936	0.39029	0.08
H45	0.63538	-0.04884	0.43556	0.08
H46	0.85276	-0.09858	0.42407	0.08
H47	1.00506	-0.16945	0.28963	0.08
H48	0.94259	-0.19983	0.17029	0.08
H49	0.72337	-0.15236	0.18127	0.08
H51	0.54964	-0.20349	0.45018	0.08
H52	0.42226	-0.26667	0.57805	0.08

Table 4 continued.

H53	0.20024	-0.20767	0.62500	0.08
H54	0.10140	-0.08749	0.54344	0.08
H55	0.22539	-0.02250	0.41474	0.08

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Table 5: Bond Lengths (Å) and Angles (°) of the H atoms of compound 3.

1	2	3	1-2	1-2-3
H1	C1	C2	0.96(1)	126.3(4)
H1	C1	C5		126.2(4)
H2	C2	C3	0.96(1)	126.1(4)
H2	C2	C1		126.1(4)
H3	C3	C4	0.96(1)	125.8(4)
H3	C3	C2		125.8(4)
H4	C4	C5	0.96(1)	126.3(4)
H4	C4	C3		126.3(4)
H5	C5	C1	0.96(1)	125.6(4)
H5	C5	C4		125.6(4)
H7	C7	C8	0.96(1)	119.8(4)
H7	C7	C6		119.8(4)
H8	C8	C9	0.96(1)	119.9(5)
H8	C8	C7		119.9(4)
H9	C9	C10	0.96(1)	120.0(4)
H9	C9	C8		120.0(4)
H10	C10	C11	0.96(1)	120.0(4)
H10	C10	C9		120.0(4)
H11	C11	C6	0.96(1)	119.6(4)
H11	C11	C10		119.6(3)
H13	C13	C14	0.96(1)	120.2(5)
H13	C13	C12		120.2(4)
H14	C14	C15	0.96(1)	119.3(5)
H14	C14	C13		119.3(5)
H15	C15	C16	0.96(1)	120.1(6)
H15	C15	C14		120.1(6)
H16	C16	C17	0.96(1)	120.2(6)
H16	C16	C15		120.2(4)
H17	C17	C12	0.96(1)	119.1(3)
H17	C17	C16		119.1(4)
H18a	C18	H18b	0.96(1)	109.5(4)
H18a	C18	P1		107.6(3)
H18a	C18	P2		107.6(2)
H18b	C18	P1	0.96(1)	107.6(2)
H18b	C18	P2		107.6(3)
H20	C20	C21	0.96(1)	119.5(4)
H20	C20	C19		119.5(4)
H21	C21	C22	0.96(1)	120.0(4)
H21	C21	C20		120.0(5)
H22	C22	C23	0.96(1)	120.0(5)
H22	C22	C21		120.0(5)
H23	C23	C24	0.96(1)	119.7(4)
H23	C23	C22		119.7(4)
H24	C24	C19	0.96(1)	119.8(3)
H24	C24	C23		119.7(4)
H26	C26	C27	0.96(1)	119.9(5)
H26	C26	C25		119.9(5)

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Table 5 continued.

H27	C27	C28	0.96(1)	119.5(7)
H27	C27	C26		119.4(6)
H28	C28	C29	0.96(1)	120.5(7)
H28	C28	C27		120.5(6)
H29	C29	C30	0.96(1)	119.3(6)
H29	C29	C28		119.2(7)
H30	C30	C25	0.96(1)	119.7(5)
H30	C30	C29		119.6(4)
H32	C32	C33	0.96(1)	119.9(3)
H32	C32	C31		119.9(4)
H33	C33	C34	0.96(1)	119.9(4)
H33	C33	C32		119.9(4)
H34	C34	C35	0.96(1)	120.1(4)
H34	C34	C33		120.1(4)
H35	C35	C36	0.96(1)	119.8(4)
H35	C35	C34		119.8(4)
H36	C36	C31	0.96(1)	119.7(4)
H36	C36	C35		119.6(3)
H38	C38	C39	0.96(1)	120.1(4)
H38	C38	C37		120.1(3)
H39	C39	C40	0.96(1)	119.4(4)
H39	C39	C38		119.4(5)
H40	C40	C41	0.96(1)	120.1(5)
H40	C40	C39		120.1(5)
H41	C41	C42	0.96(1)	119.9(5)
H41	C41	C40		119.9(4)
H42	C42	C37	0.96(1)	119.8(3)
H42	C42	C41		119.8(4)
H43a	C43	H43b	0.96(1)	109.5(3)
H43a	C43	P3		108.0(3)
H43a	C43	P4		108.0(2)
H43b	C43	P3	0.96(1)	108.0(2)
H43b	C43	P4		108.0(3)
H43a	C43	H43b	0.96(1)	109.5(3)
H43a	C43	P3		108.0(3)
H43b	C43	P3	0.96(1)	108.0(2)
H45	C45	C46	0.96(1)	119.4(6)
H45	C45	C44		119.5(4)
H46	C46	C47	0.96(1)	120.2(6)
H46	C46	C45		120.2(5)
H47	C47	C48	0.96(1)	119.6(6)
H47	C47	C46		119.6(9)
H48	C48	C49	0.96(1)	119.9(7)
H48	C48	C47		119.9(6)
H49	C49	C44	0.96(1)	120.1(4)
H49	C49	C48		120.1(4)
H51	C51	C52	0.96(1)	119.7(4)
H51	C51	C50		119.6(4)
H52	C52	C53	0.96(1)	119.9(4)
H52	C52	C51		119.9(4)

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Table 5 continued.

H53	C53	C54	0.96(1)	119.7(4)
H53	C53	C52		119.8(5)
H54	C54	C55	0.96(1)	119.9(4)
H54	C54	C53		119.9(4)
H55	C55	C50	0.96(1)	119.9(4)
H55	C55	C54		119.9(4)

Table 6: Crystallographic data.

A. Crystal data (298 K)	**I**
a, Å	11.490 (1)
b, Å	14.869 (2)
c, Å	15.447 (2)
α, deg.	84.63 (1)
β, deg.	70.55 (1)
γ, deg.	72.92 (1)
V, Å^3	2378.7 (5)
d_{calc}, g cm^{-3}(298 K)	1.355
Empirical formula	C_{55} H_{49} P_4 Cl Ru
Formula wt, g	970.34
Crystal system	Triclinic
Space group	P 1bar
Z	2
F(000), electrons	1000
Crystal size (mm^3)	0.30 x 0.23 x 0.15
B. Data collection (298 K)	
Radiation, λ (Å)	Mo-K_α, 0.71073
Mode	ω-scan
Scan range	Symmetrically over 1.2° about $K_{\alpha 1,2}$ maximum
Background	offset 1.0 and -1.0 in ω from $K_{\alpha 1,2}$ maximum
Scan rate, deg. min.$^{-1}$	4 – 8
2θ range, deg.	3 – 50
Range of *h k l*	$0 \leq h \leq 13$ $-17 \leq k \leq 17$ $-18 \leq l \leq 18$
Total reflections measured	8848
Unique reflections	8390
Absorption coeff. μ (Mo-K_α), cm^{-1}	0.56
Min. & Max. Transmission	0.883, 0.946
C. Structure refinement	
S, Goodness-of-fit	1.24
Reflections used, I > 2σ(I)	6646
No. of variables	550
R, wR* (%)	3.68, 4.15
$R_{int.}$ (%)	2.16
Max. shift/esd	0.001

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Table 6 continued.

min. peak in diff. four. map (e $Å^{-3}$)	-0.27
max. peak in diff. four. map (e $Å^{-3}$)	0.31

* Relevant expressions are as follows, where in the footnote F_o and F_c represent, respectively, the observed and calculated structure-factor amplitudes.

Function minimized was $w(|F_o| - |F_c|)^2$, where $w = (\sigma(F))^{-2}$

$R = \Sigma(||F_o| - |F_c||) / \Sigma|F_o|$

$wR = [\Sigma w(|F_o| - |F_c|)^2 / \Sigma |F_o|^2]^{1/2}$

$S = [\Sigma w(|F_o| - |F_c|)^2 / (m-n)]^{1/2}$

Figure 1. Full thermal ellipsoids diagram of 3.

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