Electronic Supplementary Information

Conformational Isomers of Extraordinary Stability: Carboxamidate-Bridged Dimetalloorganic Compounds

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Synthesis of O: To a dry flask 110.5 mg (150 μ mol) Rh₂(cap)₄(CH₃CN)₂ and 34.0 mg (300 μ mol) ϵ caparolactam was added, followed by 15 mL (0.36 mg/mL, 90 μ mol) of acetic acid in toluene and 10 mL of toluene. The mixture was heated to reflux in an oil bath. The color of the reaction solution changed from purple to blue after refluxing for 10 minutes. Refluxing was continued for 4 hrs after which the solvents were removed under reduced pressure to provide a blue residue. Then 92 mg (0.75 mmol) of phenylboronic acid and 126 mg (1.50 mmol) of sodium bicarbonate were added, followed by 20 mL of dichloromethane (DCM), and the mixture was stirred at room temperature for a few minutes, after which 5.0 mL of a CuSO₄.5H₂O solution (3 μ mol/mL, 15 μ mol) in MeOH was added. After stirring at room temperature for 18 h the solvents were removed under reduced pressure and the residue was chromatographed on silica gel to yield O 34.5 mg (28.5 %) and G 23.6 mg (19.5%). (A small amount of the minor green isomer was also obtained, 2 mg, 1% yield). HPLC analysis of the two conformers that shows O eluting faster than G (Figure S-1) is consistent with their expected behavior based on size exclusion.





Data for G and O

G: ¹H NMR (400 MHz, CD₂Cl₂): δ 7.49–7.46 (comp, 4H), 7.11–7.08 (comp, 6H), 3.07–2.94 (comp, 8H), 2.50-2.34 (comp, 8H), 1.81–1.72 (comp, 4H), 1.66–1.38 (comp, 20H) ppm; ¹³C NMR (100 MHz, CD₂Cl₂) δ 183.71, 147.81 (d, ¹*J*_{C-Rh} = 37.1 Hz), 137.12, 126.16, 123.98, 51.43, 38.61, 30.69, 29.80, 24.36 ppm; UV/Visible (CH₂Cl₂): 430 nm (ε = 6590 M⁻¹cm⁻¹). IR (neat): 1550(s), 1583(s) cm⁻¹; HRMS (ESI) Calcd for for C₃₆H₅₁N₄O₄Rh₂([M+H]⁺) 809.2020; found 809.2018 (M+H).)





O: ¹H NMR (400 MHz, CD₂Cl₂): δ 7.51–7.46 (comp, 4H), 7.19–7.14 (comp, 6H), 3.16–2.98 (comp, 5H), 2.98–2.93 (comp, 3H), 2.68–2.45 (comp, 4H), 2.38–2.31 (comp, 4H), 1.83–1.71 (comp, 4H), 1.68–1.32 (comp, 20H); ¹³C NMR (100 MHz, CD₂Cl₂): δ 185.80, 185.68, 184.16, 183.84, 147.37 (d, ¹J_{C-Rh}= 35.8 Hz), 144.58 (d, ¹J_{C-Rh}= 34.3 Hz), 136.56, 134.28, 126.93, 126.85, 124.77, 124.73, 52.70, 51.06, 50.58, 38.65, 38.39, 38.27, 30.67, 30.53, 30.50, 29.64, 29.66, 29.00, 24.56, 24.40, 24.34, 24.21; UV/Visible (CH₂Cl₂): 430 nm (ε = 2580 M⁻¹cm⁻¹); IR (neat): cm⁻¹; HRMS (ESI): Calcd for C₃₆H₅₀N₄O₄Rh₂ (M⁺): 808.1942; found: 808.1928.

- 7000 7.459 7.451 7.445 7.169 7.162 3.138 3.120 3.079 2.957 2.939 2.939 2.917 2.521 2.515 2.379 2.305 2.287 2.284 1.598 1.580 1.482 1.477 1.497 6000 5000 4000 3000 - 2000 - 1000 Aut." - o ſ T 1 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 ppm (t1) 185.795 185.679 184.159 183.844 147.547 147.189 144.737 144.394 136.555 134.276 134.276 126.930 126.852 124.770 124.726 51.057 <u>50</u>.579 38.646 38.388 38.267 30.672 30.530 30.530 30.496 29.641 29.64 28.990 24.558 24.558 24.341 24.207 52.700 3500(3000(- 2500(- 2000(- 1500(1000(- 5000(II 1 - 0 150 100 50 Ó

ppm (t1)

Synthesis of PhACO: To a dry flask was added 24.0 mg (30 μ mol) Rh₂(aco)₄(CH₃CN)₂, 15 mg (0.15 mmol) of phenylboronic acid and 25.2 mg (0.30 mmol) of sodium bicarbonate, followed by 4.0 mL of dichloromethane (DCM), and the mixture was stirred at room temperature for a few minutes, after which 1.0 mL of a CuSO₄.5H₂O solution (3 μ mol/mL, 3 μ mol) in MeOH was added. After stirring at room temperature for 20 h the solvents were removed under reduced pressure, and the residue was chromatographed on silica gel to yield 8.0 mg of **PhACO** (30.8 %).

PhACO: ¹H NMR (400 MHz, CDCl₃): δ 7.47–7.50 (comp, 4H), 7.08–7.11 (comp, 6H), 3.15–3.26 (comp, 8H), 2.24–2.36 (comp, 8H), 1.22–1.58 (comp, 32H); ¹³C NMR (150 MHz, CDCl₃): δ 182.41, 136.89, 131.09, 128.57 (d, ¹*J*_{C-Rh}= 36.9 Hz), 126.21, 124.04, 120.26, 50.50, 33.83, 32.98, 28.30, 26.42, 25.41; UV/Visible (CH₂Cl₂): 435 nm (ε = 2084 M⁻¹cm⁻¹); HRMS (ESI): Calcd for C₄₀H₅₉N₄O₄Rh₂ (M+H)⁺: 865.2646; found: 865.2652.





X-ray structural determinations of G, O, PhACO, and ACOBF4

Details of the x-ray structural analysis of G (CCDC#615577). The crystal of G suitable X-ray analysis was obtained by evaporation of the solvents from the solution of G in chloroform and dichloromethane. A green prism of $C_{36}H_{50}N_4O_4Rh_2$ ·2CHCl₃, approximate dimensions $0.08 \times 0.095 \times 0.21$ mm³, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 150(2) K on a three-circle diffractometer system equipped with Bruker Smart Apex II CCD area detector using a graphite monochromator and a MoK α fine-focus sealed tube (λ = 0.71073 Å). The detector was placed at a distance of 5.200 cm from the crystal.

A total of 2130 frames was collected with a scan width of 0.5° in ω and an exposure time of 38 sec/frame using Apex2 (Bruker, 2005). The total data collection time was 24 hours. The frames were integrated with Apex2 software package using a narrow-frame integration algorithm. The integration of the data using a triclinic unit cell yielded a total of 13816 reflections to a maximum θ angle of 27.50°, of which 9901 were independent (completeness = 99.3%, R_{int} = 2.00%, R_{sig} = 3.07%) and 8334 were greater than $2\sigma(I)$. The final cell dimensions of a = 11.5388(8) Å, b = 11.6313(8) Å, c = 17.2249(12) Å, $\alpha = 82.9623(12)^{\circ}$, $\beta = 78.2631(12)^{\circ}$, $\gamma = 74.1013(13)^{\circ}$, V = 2171.4(3) Å³, are based upon the refinement of the XYZ-centroids of 14756 reflections with $2.3 < \theta < 30.0^{\circ}$ using Apex2. Analysis of the data showed 0 % decay during data collection. Data were corrected for absorption effects with the Semi-empirical from equivalents method using SADABS (Sheldrick, 1996). The minimum and maximum transmission coefficients were 0.791 and 0.911.

The structure was solved and refined using the SHELXS-97 (Sheldrick, 1990) and SHELXL-97 (Sheldrick, 1997) software in the space group P-1 with Z = 2 for the formula unit

 $C_{36}H_{50}N_4O_4Rh_2$ ·2CHCl₃. The final anisotropic full-matrix least-squares refinement on F² with 487 variables converged at R_1 =3.17 % for the observed data and w R_2 =6.77 % for all data. The goodness-of-fit was 1.000. The largest peak on the final difference map was 0.934 $e/Å^3$ and the largest hole was - 0.884 $e/Å^3$. On the basis of the final model, the calculated density was 1.602 g/cm³ and F(000), 1064 e.

Details of the crystal data and structure refinement (Supplemental Table 1), atomic coordinates and equivalent isotropic atomic displacement parameters (Supplemental Table 2), anisotropic atomic displacement parameters (Supplemental Table 3), Hydrogen atom coordinates and isotropic atomic displacement parameters (Supplemental Table 4), bond lengths and angles (Supplemental Table 5), Torsion angles (Supplemental Table 6) are shown below.

Table 1. Crystal data and structure refinement for G.

Empirical formula Formula weight Temperature Wavelength Crystal size Crystal habit Crystal system Space group	$\begin{array}{c} C_{36}H_{50}N_4O_4Rh_2\cdot 2CHCl_2\\ 1047.36\\ 150(2)\ K\\ 0.71073\ \text{\AA}\\ 0.21\times 0.095\times 0.08\ \text{mm}\\ \text{green prism}\\ \text{Triclinic}\\ P-1 \end{array}$	3
Unit cell dimensions	a = 11.5388(8) Å b = 11.6313(8) Å c = 17.2249(12) Å	$\alpha = 82.9623(12)^{\circ}$ $\beta = 78.2631(12)^{\circ}$ $\gamma = 74.1013(13)^{\circ}$
Volume	2171.4(3) Å ³	• • • •
Z	2	
Density, ρ_{calc}	1.602 g/cm^3	
Absorption coefficient, μ	1.172 mm^{-1}	
F(000) Differentemeter	1064 e Deulier Smort Anar II C	CD area datastar
Difficulture Dediction courses	fina focus scaled tuba	Vol area detector
Detector distance	5 200 cm	VIORU
Detector resolution	8 333 nivels/mm	
Total frames	2130	
Frame size	512 pixels	
Frame width	0.5°	
Exposure per frame	38 sec	
Total measurement time	24 hours	
Data collection method	ω and ϕ scans	
θ range for data collection	1.83 to 27.50°	
Index ranges	$-14 \le h \le 13, -15 \le k \le 1$	$12, -22 \le l \le 22$
Reflections collected	13816	
Independent reflections	9901	
Observed reflection, 1>20(1)	8334	
Variation in check reflections	99.5 %	
Absorption correction	Semi-empirical from eq	uivalents
Ausorption concetion	SADABS (Sheldrick 19	996)
Max, and min, transmission	0.911 and 0.791	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
Structure solution technique	direct	
Structure solution program	SHELXS-97 (Sheldrick	, 1990)
Refinement technique	Full-matrix least-square	es on F ²
Refinement program	SHELXL-97 (Sheldrick	., 1997)
Function minimized	$\Sigma w (F_o^2 - F_c^2)^2$	
Data / restraints / parameters	9901 / 0 / 487	
Goodness-of-fit on F^2	1.000	
$\Delta \sigma_{\rm max}$	0.002	
	7	

Final R indices:	R_1 , $I > 2\sigma(I)$ wR, all data	0.0317
	R _{int}	0.0200
	R _{sig}	0.0307
Weighting scheme	-	$w = 1/[\sigma^2(F_o^2) + (0.01P)^2 + 5.5P], P = [max(F_o^2, 0) + 2F_o^2]/3$
Largest diff. peak and	hole 0.934 and -0.884 $\overline{e}/\text{\AA}$	3

Supplementary Material (ESI) for Chemical Communications This journal is $\ensuremath{\mathbb{O}}$ The Royal Society of Chemistry 2009

 $R_{1} = \Sigma ||F_{o}| - |F_{c}|| / \Sigma |F_{o}|, \quad wR2 = [\Sigma w (F_{o}^{2} - F_{c}^{2})^{2} / \Sigma w (F_{o}^{2})^{2}]^{1/2}$

Table 2. Atomic coordinates and equivalent [*] isotropic atomic displacement parameters ($Å^2$) for	G.
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Rh1A 0.082005(18) 1.041271(18) 0.455103(11) 0.01524(5) C1A 0.2314(2) 1.0367(2) 0.39700(16) 0.0189(5) C3A 0.4394(3) 1.0435(3) 0.39510(18) 0.0221(6) C3A 0.4921(3) 1.0193(3) 0.3156(17) 0.0305(7) C5A 0.4028(3) 1.013(3) 0.3760(18) 0.0223(6) C1A 0.7355(17) 0.94459(19) 0.54474(11) 0.0223(6) C1A 0.1353(2) 0.8332(3) 0.66239(17) 0.0234(7) C1AA 0.256(3) 0.8324(3) 0.80069(17) 0.0301(7) C1AA 0.0261(3) 0.8324(3) 0.60239(17) 0.0321(7) C1AA 0.0261(3) 0.8324(3) 0.8069(17) 0.0302(7) C1AA 0.0233(17) 0.8869(2) 0.6237(13) 0.0244(6) C1AA 0.023(3) 0.69429(16) 0.0214(6) C2AA 0.01303(17) 0.8869(17) 0.3382(2) 0.0396(8) C2AA 0.0243(3) 0.805(3) 0.2424(4) <th>Atom</th> <th>x/a</th> <th><i>y/b</i></th> <th>z/c</th> <th>U_{eq}</th> <th></th>	Atom	x/a	<i>y/b</i>	z/c	U _{eq}	
$\begin{array}{ccccc} 1.1 \\ C2A & 0.340(c) & 1.0357(2) & 0.39700(16) & 0.0189(5) \\ C3A & 0.4594(3) & 1.0455(3) & 0.33510(18) & 0.0268(6) \\ C4A & 0.4912(3) & 1.0493(3) & 0.31569(19) & 0.0396(7) \\ C5A & 0.4228(3) & 1.0038(3) & 0.27680(18) & 0.0286(6) \\ C6A & 0.2389(2) & 1.0115(3) & 0.31742(16) & 0.0236(6) \\ C6A & 0.2389(2) & 0.0532(3) & 0.060734(16) & 0.0219(6) \\ C11A & 0.1335(17) & 0.94459(19) & 0.54474(11) & 0.0262(4) \\ C11A & 0.1339(2) & 0.8532(3) & 0.60734(16) & 0.0219(6) \\ C12A & 0.0225(7) & 0.8332(3) & 0.060734(16) & 0.0219(6) \\ C13A & 0.086(3) & 0.8894(3) & 0.74218(18) & 0.0294(7) \\ C13A & 0.086(3) & 0.8894(3) & 0.74218(18) & 0.0294(7) \\ C15A & -0.0249(3) & 0.8456(3) & 0.77320(17) & 0.0321(7) \\ C15A & -0.0249(3) & 0.8456(3) & 0.77320(17) & 0.0321(7) \\ C15A & -0.0249(3) & 0.8456(3) & 0.77320(17) & 0.021(6) \\ N1A & 0.0231(2) & 0.86860(17) & 0.3994(61) & 0.0244(6) \\ C21A & 0.0443(3) & 0.7930(3) & 0.69429(16) & 0.0244(6) \\ C21A & 0.0443(3) & 0.8051(3) & 0.42207(16) & 0.0214(5) \\ C22A & -0.029(4) & 0.6258(4) & 0.312(2) & 0.0548(11) \\ C23A & -0.029(3) & 0.6949(3) & 0.3283(2) & 0.0398(8) \\ C23A & -0.029(3) & 0.6949(3) & 0.3283(2) & 0.0398(8) \\ C23A & -0.029(3) & 0.6859(4) & 0.4312(2) & 0.0544(11) \\ C25A & -0.1766(3) & 0.6859(4) & 0.4312(2) & 0.035(7) \\ C1B & 0.2915(2) & 0.373819(18) & 0.0158(19) & 0.0123(7) \\ N2A & -0.0457(2) & 0.3108(2) & 0.48502(13) & 0.0036(5) \\ C1B & 0.2915(2) & 0.373819(18) & 0.0158(17) & 0.0286(6) \\ C23A & -0.096(4) & 0.373819(18) & 0.0158(16) \\ C4B & 0.1164(3) & 0.4990(3) & -0.1821(2) & 0.035(7) \\ C4B & 0.114(4) & 0.4990(3) & -0.1821(2) & 0.035(7) \\ C4B & 0.114(4) & 0.4990(3) & -0.1821(2) & 0.035(7) \\ C4B & 0.128(6) & 0.1786(3) & -0.1583(19) & 0.0238(6) \\ C1B & 0.2915(2) & 0.4758(3) & -0.1683(19) & 0.0238(6) \\ C1B & 0.2915(2) & 0.4758(3) & -0.1632(19) & 0.0328(7) \\ C4B & 0.114(4) & 0.4990(3) & -0.1532(16) & 0.0298(6) \\ C1B & 0.4968(3) & 0.1786(3) & -0.1583(19) & 0.0328(7) \\ C4B & 0.194(3) & 0.1786(3) & -0.1583(19) & 0.0328(7) \\ C1B & 0.3505(2) & 0.45859(1) & 0.3583(1) & 0.0288(6) \\ C1B & 0.4966(10) &$	Rh1A	0.082005(18)	1 041271(18)	0 455103(11)	0.01524(5)	
C2A 0.449(C) 1.0515(3) 0.43615(17) 0.0231(6) C3A 0.4594(3) 1.045(3) 0.33160(18) 0.0268(6) C4A 0.4912(3) 1.0193(3) 0.31569(19) 0.0286(6) C5A 0.4028(3) 1.0115(3) 0.31742(16) 0.0233(6) C1A 0.17365(17) 0.94459(19) 0.54474(11) 0.0224(4) C1AA 0.17365(17) 0.94459(19) 0.54474(11) 0.0224(7) C1AA 0.136(3) 0.8332(3) 0.66239(17) 0.0234(7) C1AA 0.036(3) 0.8332(3) 0.66239(17) 0.0321(7) C1AA 0.036(3) 0.8332(3) 0.69429(16) 0.0214(6) C1AA 0.036(3) 0.7930(3) 0.69429(16) 0.0214(6) C1AA 0.043(3) 0.8051(3) 0.4297(16) 0.0214(6) C2AA 0.0130(17) 0.8869(2) 0.6387(18) 0.0208(6) C2AA 0.0130(3) 0.7920(3) 0.36857(18) 0.0203(6) C2AA 0.0181(3) 0.7834(4)	CIA	0.2514(2)	1.0367(2)	0.39700(16)	0.0189(5)	
$\begin{array}{ccccc} \hline C3A & 0.494(2) & 1.0435(3) & 0.39510(18) & 0.0286(6) \\ C4A & 0.491(23) & 1.093(3) & 0.3156(19) & 0.036(7) \\ C5A & 0.4028(3) & 1.0015(3) & 0.31742(16) & 0.0236(6) \\ C6A & 0.2839(3) & 1.0115(3) & 0.31742(16) & 0.0236(6) \\ C1A & 0.17365(17) & 0.94459(19) & 0.54474(11) & 0.0262(4) \\ C11A & 0.139(2) & 0.8532(3) & 0.66734(16) & 0.0219(6) \\ C12A & 0.2257(3) & 0.8532(3) & 0.66734(16) & 0.0219(6) \\ C13A & 0.1863(3) & 0.8894(3) & 0.74218(18) & 0.0294(7) \\ C13A & 0.086(3) & 0.8894(3) & 0.74218(18) & 0.0294(7) \\ C15A & -0.0249(3) & 0.8852(2) & 0.62374(13) & 0.0190(5) \\ C15A & -0.0249(3) & 0.8456(3) & 0.77320(17) & 0.0321(7) \\ C15A & -0.0249(3) & 0.8866(17) & 0.3994(61) & 0.0241(6) \\ N1A & 0.0231(2) & 0.86869(2) & 0.62374(13) & 0.0190(5) \\ C22A & -0.0130(317) & 0.88660(17) & 0.3994(61) & 0.0236(4) \\ C21A & 0.0443(3) & 0.5051(3) & 0.42207(16) & 0.0214(5) \\ C22A & -0.0294(3) & 0.6949(3) & 0.3283(2) & 0.0398(8) \\ C23A & -0.0294(3) & 0.6489(4) & 0.3312(2) & 0.0548(11) \\ C25A & -0.1766(3) & 0.6889(4) & 0.4576(2) & 0.0489(10) \\ C25A & -0.0964(3) & 0.7094(3) & 0.5159(19) & 0.0323(7) \\ N2A & -0.0457(2) & 0.8108(2) & -0.1482(2) & 0.0544(11) \\ C25A & -0.0964(3) & 0.737819(18) & 0.37819(18) & 0.03787(18) & 0.03787(18) \\ C1B & 0.2915(2) & 0.37819(18) & -0.1582(19) & 0.0326(7) \\ C2B & 0.326(2) & 0.4758(3) & -0.1622(19) & 0.0336(7) \\ C2B & 0.326(2) & 0.4758(3) & -0.1623(19) & 0.0336(7) \\ C4B & 0.1146(3) & 0.4990(3) & -0.1821(2) & 0.0336(7) \\ C4B & 0.1146(3) & 0.4990(3) & -0.1821(2) & 0.0336(7) \\ C4B & 0.1146(3) & 0.4990(3) & -0.1823(19) & 0.0336(7) \\ C4B & 0.1146(3) & 0.4990(3) & -0.1823(19) & 0.0336(7) \\ C4B & 0.196(6) \\ C4B & 0.1692(2) & 0.5734(6) & -0.1152(16) & 0.0291(6) \\ C4B & 0.196(6) \\ C4B & 0.1692(2) & 0.4578(13) & -0.1632(19) & 0.0336(7) \\ C4B & 0.018(6) & -0.1532(19) & 0.0336(7) \\ C4B & 0.018(6) & -0.1532(19) & 0.0336(7) \\ C4B & 0.0283(6) & -0.11537(16) & 0.0293(6) \\ C1B & 0.3526(2) & 0.4559(19) & 0.0532(1) & 0.0396(7) \\ C4B & 0.048(3) & 0.0532(2) & 0.0496(3) \\ C1B & 0.5786(3) & 0.1586(6) & 0.1533(18) & 0.0499(6) $	C2A	0.3406(2)	1.0515(3)	0.43615(17)	0.0231(6)	
$\begin{array}{cccc} C4A & 0.4912(2) & 1.0193(3) & 0.3159(19) & 0.0286(7) \\ C5A & 0.4028(3) & 1.0038(3) & 0.27680(18) & 0.0286(6) \\ C6A & 0.2839(3) & 1.0115(3) & 0.31742(16) & 0.0233(6) \\ C1A & 0.17365(17) & 0.94459(19) & 0.54474(11) & 0.022(4) \\ C11A & 0.1339(2) & 0.8532(3) & 0.66239(17) & 0.0284(7) \\ C13A & 0.0264(3) & 0.8332(3) & 0.66239(17) & 0.0391(7) \\ C14A & 0.096(13) & 0.8332(3) & 0.66239(17) & 0.0391(7) \\ C15A & -0.0136(3) & 0.8332(3) & 0.66239(17) & 0.0391(7) \\ C15A & -0.0136(3) & 0.7930(3) & 0.69429(16) & 0.0214(6) \\ C12A & 0.0136(3) & 0.7930(3) & 0.69429(16) & 0.0214(6) \\ C12A & 0.0136(3) & 0.7930(3) & 0.69429(16) & 0.0214(6) \\ C21A & 0.0136(3) & 0.7930(3) & 0.69429(16) & 0.0214(5) \\ C22A & 0.01303(17) & 0.88690(17) & 0.39946(11) & 0.0236(4) \\ C22A & 0.01303(17) & 0.88690(17) & 0.3832(2) & 0.0598(6) \\ C24A & -0.104(4) & 0.6286(4) & 0.3812(2) & 0.0548(11) \\ C25A & -0.122(3) & 0.6494(3) & 0.51059(19) & 0.0323(7) \\ C26A & -0.0249(3) & 0.6889(4) & 0.3152(2) & 0.0444(11) \\ C25A & -0.0249(3) & 0.63871(18) & 0.0235(7) \\ C2A & -0.0424(2) & 0.35718(9) & 0.0323(7) \\ C2A & -0.0424(2) & 0.35718(9) & 0.04387(11) & 0.01472(5) \\ C1B & 0.2915(2) & 0.4578(3) & -0.1152(16) & 0.0191(5) \\ C2B & 0.3526(3) & 0.4471(3) & -0.1521(19) & 0.0238(7) \\ C3B & 0.315(3) & 0.5378(3) & -0.1153(16) & 0.0191(5) \\ C3B & 0.315(3) & 0.5378(3) & -0.1153(16) & 0.0191(5) \\ C2B & 0.3526(3) & 0.4471(3) & -0.1052(16) & 0.0191(5) \\ C2B & 0.0585(3) & 0.188(17) & -0.09045(12) & 0.0238(6) \\ C3B & 0.116(3) & 0.47990(3) & -0.1839(18) & 0.0238(7) \\ C4B & 0.116(3) & 0.4798(3) & -0.1532(19) & 0.0238(6) \\ C4B & 0.1164(3) & 0.4990(3) & -0.1839(18) & 0.0238(7) \\ C4B & 0.015(3) & 0.5348(17) & -0.09045(12) & 0.0249(4) \\ C1B & 0.6558(18) & 0.3748(3) & -0.1538(19) & 0.0336(7) \\ C3B & 0.0315(3) & 0.1586(19) & 0.0532(19) & 0.0336(7) \\ C4B & 0.8833(3) & 0.1154(3) & -0.10532(1) & 0.0189(4) \\ C1B & 0.45658(19) & 0.5558(16) & 0.7578(17) & 0.0208(6) \\ C1B & 0.786(3) & 0.1586(19) & 0.0532(2) & 0.06578(16) & 0.0207(5) \\ C2B & 0.6585(3) & 0.1586(18) & 0.0138(7) & 0.1889(18) \\ C1B$	C3A	0.4594(3)	1.0435(3)	0.39510(18)	0.0268(6)	
C5A 0.4028(3) 1.0038(3) 0.27680(18) 0.0238(6) C6A 0.2839(3) 1.0115(3) 0.31742(16) 0.0233(6) C1A 0.17356(17) 0.94459(19) 0.54474(11) 0.0226(4) C11A 0.1339(2) 0.8332(3) 0.66734(16) 0.0219(6) C12A 0.2257(3) 0.8332(3) 0.66734(16) 0.0224(7) C13A 0.1863(3) 0.8392(3) 0.66239(17) 0.0301(7) C15A -00249(3) 0.8456(3) 0.77320(17) 0.0321(7) C15A -00231(2) 0.8869(2) 0.62374(13) 0.0190(5) C21A 0.0443(3) 0.895(13) 0.42207(16) 0.0214(6) C1A 0.0231(2) 0.8869(17) 0.39946(11) 0.0236(4) C21A 0.0443(3) 0.805(13) 0.42207(16) 0.0214(6) C21A 0.0443(3) 0.8689(1) 0.3283(2) 0.0356(8) C23A -0.029(3) 0.6494(3) 0.312(2) 0.0489(10) C23A -0.0296(3) 0.7994(3) <td>C4A</td> <td>0.4912(3)</td> <td>1.0193(3)</td> <td>0.31569(19)</td> <td>0.0200(0)</td> <td></td>	C4A	0.4912(3)	1.0193(3)	0.31569(19)	0.0200(0)	
$\begin{array}{cccc} C6A & 0.2839(3) & 1.0115(3) & 0.31742(16) & 0.0233(6) \\ 01A & 0.17565(17) & 0.94459(19) & 0.54474(11) & 0.0202(4) \\ 0.212A & 0.2257(3) & 0.8332(3) & 0.66239(17) & 0.0284(7) \\ 0.12A & 0.2257(3) & 0.8332(3) & 0.66239(17) & 0.0301(7) \\ 0.13A & 0.185(3) & 0.8894(3) & 0.74218(18) & 0.0294(7) \\ 0.14A & 0.0961(3) & 0.8324(3) & 0.80069(17) & 0.0301(7) \\ 0.15A & -0.0249(3) & 0.8456(3) & 0.77320(17) & 0.0321(7) \\ 0.16A & -0.0136(3) & 0.7930(3) & 0.69429(16) & 0.0241(6) \\ 0.22A & 0.10303(17) & 0.88860(17) & 0.39946(11) & 0.0236(4) \\ 0.21A & 0.0434(3) & 0.8051(3) & 0.42207(16) & 0.0124(5) \\ 0.22A & 0.10303(17) & 0.88660(17) & 0.33842(2) & 0.0396(8) \\ 0.23A & -0.0229(3) & 0.6949(3) & 0.3283(2) & 0.0396(8) \\ 0.23A & -0.0229(3) & 0.6949(3) & 0.3283(2) & 0.0396(8) \\ 0.23A & -0.0156(3) & 0.6889(4) & 0.43576(2) & 0.0489(10) \\ 0.25A & -0.1766(3) & 0.6889(4) & 0.4576(2) & 0.0489(10) \\ 0.25A & -0.064(3) & 0.7994(3) & 0.51059(19) & 0.0323(7) \\ 0.26A & -0.096(4) & 0.3718(9) & 0.04877(11) & 0.01472(5) \\ 0.118 & 0.42057(18) & 0.537819(18) & -0.04877(11) & 0.01472(5) \\ 0.218 & 0.2320(3) & 0.4471(13) & -0.17811(17) & 0.0266(6) \\ 0.23B & 0.2362(3) & 0.4471(3) & -0.10521(1) & 0.0191(5) \\ 0.22B & 0.2320(3) & 0.4471(3) & -0.10521(1) & 0.0132(7) \\ 0.25B & 0.0235(3) & 0.4758(3) & -0.1824(2) & 0.0352(7) \\ 0.28 & 0.2320(3) & 0.4758(3) & -0.1821(2) & 0.0336(7) \\ 0.28 & 0.0326(3) & 0.4758(3) & -0.1821(2) & 0.0336(7) \\ 0.28 & 0.0358(7) & 0.0534(3) & -0.1821(2) & 0.0328(6) \\ 0.118 & 0.6970(2) & 0.2552(2) & -0.06675(16) & 0.0291(5) \\ 0.28 & 0.0358(3) & 0.1786(3) & -0.1583(19) & 0.0336(7) \\ 0.128 & 0.6835(3) & 0.1786(3) & -0.1583(19) & 0.0336(7) \\ 0.128 & 0.6835(3) & 0.1786(3) & -0.1583(19) & 0.0336(7) \\ 0.128 & 0.6385(3) & 0.1786(3) & -0.1583(19) & 0.0336(7) \\ 0.128 & 0.6385(3) & 0.1586(19) & 0.0524(11) & 0.0249(4) \\ 0.118 & 0.6833(3) & 0.1586(3) & 0.0257(11) & 0.04387(4) \\ 0.128 & 0.4305(2) & 0.4466(2) & 0.0452(4) & 0.0224(6) \\ 0.128 & 0.3202(3) & 0.3667(3) & 0.1583(6) & 0.0733(6) \\ 0.228 & 0.2315(3) & 0.3667(3) & 0.2580(19) & 0.0323(7) \\ $	C5A	0.4028(3)	1.0038(3)	0.27680(18)	0.0286(6)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6A	0.2839(3)	1.0115(3)	0.31742(16)	0.0233(6)	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	01A	0.17365(17)	0.94459(19)	0.54474(11)	0.0255(0) 0.0262(4)	
$ \begin{array}{cccccc} C12A & 0.2257(3) & 0.8332(3) & 0.66239(17) & 0.0284(7) \\ C13A & 0.1863(3) & 0.8394(3) & 0.74218(18) & 0.0294(7) \\ C15A & 0.0249(3) & 0.8324(3) & 0.80069(17) & 0.0301(7) \\ C15A & 0.0249(3) & 0.8324(3) & 0.80069(17) & 0.0321(7) \\ C15A & 0.0231(2) & 0.8689(2) & 0.63274(13) & 0.0190(5) \\ O2A & 0.033(17) & 0.88660(17) & 0.39946(11) & 0.0236(4) \\ C21A & 0.0443(3) & 0.8051(3) & 0.42207(16) & 0.0214(5) \\ C22A & 0.0811(3) & 0.7024(3) & 0.3687(18) & 0.0280(6) \\ C23A & 0.029(3) & 0.6629(4) & 0.3812(2) & 0.0594(11) \\ C25A & 0.096(4) & 0.7024(3) & 0.3283(2) & 0.0599(8) \\ C24A & 0.1104(4) & 0.6286(4) & 0.3812(2) & 0.0544(11) \\ C25A & 0.096(4) & 0.7094(3) & 0.51059(19) & 0.0323(7) \\ C25A & -0.096(4) & 0.7094(3) & 0.51059(19) & 0.0323(7) \\ C26A & -0.0964(3) & 0.7094(3) & 0.48502(13) & 0.0030(5) \\ Rh1B & 0.420837(18) & 0.537819(18) & -0.043874(11) & 0.01472(5) \\ C1B & 0.2915(2) & 0.5250(2) & -0.10152(16) & 0.0191(5) \\ C2B & 0.3250(3) & 0.4751(3) & -0.17811(17) & 0.0266(6) \\ C3B & 0.146(4) & 0.4990(3) & -0.1821(2) & 0.0336(7) \\ C5B & 0.0815(3) & 0.3334(3) & -0.16323(19) & 0.0281(6) \\ C6B & 0.1992(2) & 0.5472(2) & -0.06441(17) & 0.0218(6) \\ C1B & 0.51586(18) & 0.37488(17) & -0.09045(12) & 0.0249(4) \\ C1B & 0.670(2) & 0.252(2) & -0.06735(16) & 0.0207(5) \\ C1B & 0.670(2) & 0.252(2) & -0.06735(16) & 0.0207(5) \\ C1B & 0.670(2) & 0.252(2) & -0.06735(16) & 0.0238(6) \\ C13B & 0.7916(3) & 0.1786(3) & -0.1839(19) & 0.0238(6) \\ C13B & 0.7916(3) & 0.1786(3) & -0.1839(19) & 0.0238(6) \\ C13B & 0.7946(3) & 0.256(3) & 0.01757(16) & 0.0209(5) \\ C14B & 0.32329(18) & 0.45659(19) & 0.0524(11) & 0.0239(6) \\ C14B & 0.32329(18) & 0.3656(3) & 0.17573(17) & 0.0239(6) \\ C14B & 0.32329(18) & 0.45659(19) & 0.0524(11) & 0.0238(6) \\ C13B & 0.7916(3) & 0.189(4) & 0.7252(2) & 0.00677(13) & 0.189(4) \\ 02B & 0.23239(18) & 0.3656(3) & 0.17573(17) & 0.0238(6) \\ C14B & 0.3202(3) & 0.367(3) & 0.3101(18) & 0.023(6) \\ C14B & 0.3202(3) & 0.367(3) & 0.31051(18) & 0.0238(6) \\ C14B & 0.3202(3) & 0.367(3) & 0.31051(18) & 0.0238(6) \\ C14B & 0.3202(3) & 0.367(3)$	CllA	0.1339(2)	0.8832(3)	0.60734(16)	0.0219(6)	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C12A	0.2257(3)	0.8332(3)	0.66739(17)	0.0219(0) 0.0284(7)	
$\begin{array}{ccccc} C14A & 0.0961(3) & 0.8324(5) & 0.80069(17) & 0.0301(7) \\ C15A & -0.0249(3) & 0.8456(3) & 0.77320(17) & 0.0321(7) \\ C15A & -0.0136(3) & 0.7930(3) & 0.69429(16) & 0.0241(6) \\ N1A & 0.0231(2) & 0.8689(2) & 0.63274(13) & 0.0190(5) \\ O2A & 0.10303(17) & 0.88660(17) & 0.39946(11) & 0.0236(4) \\ C21A & 0.0443(3) & 0.8051(3) & 0.42207(16) & 0.0214(5) \\ C22A & 0.0811(3) & 0.7024(3) & 0.36857(18) & 0.0280(6) \\ C23A & -0.0229(3) & 0.6949(3) & 0.3283(2) & 0.0396(8) \\ C24A & -0.1104(4) & 0.6286(4) & 0.3812(2) & 0.0544(11) \\ C25A & -0.0964(3) & 0.7094(3) & 0.51059(19) & 0.0323(7) \\ C2A & -0.0425(2) & 0.8108(2) & 0.48502(13) & 0.0203(5) \\ Rh1B & 0.420837(18) & 0.537819(18) & -0.043874(11) & 0.01472(5) \\ C1B & 0.2915(2) & 0.550(2) & -0.10152(16) & 0.0191(5) \\ C2B & 0.3250(3) & 0.4871(3) & -0.1881(2) & 0.0332(7) \\ C4B & 0.1146(3) & 0.4990(3) & -0.1821(2) & 0.0332(7) \\ C5B & 0.0815(3) & 0.5334(3) & -0.1884(2) & 0.0332(7) \\ C5B & 0.0815(3) & 0.5334(3) & -0.1881(17) & 0.0266(6) \\ C1B & 0.51586(18) & 0.37488(17) & -0.09045(12) & 0.0231(6) \\ C6B & 0.1692(2) & 0.5472(2) & -0.06441(17) & 0.0218(6) \\ O1B & 0.51586(18) & 0.37488(17) & -0.09045(12) & 0.0238(6) \\ C1B & 0.670(2) & 0.952(2) & -0.0675(16) & 0.0207(5) \\ C1B & 0.673(3) & 0.1180(4) & -0.0232(2) & 0.0336(7) \\ C5B & 0.0815(3) & 0.1384(3) & -0.1833(19) & 0.0238(6) \\ C1B & 0.678(2) & 0.952(2) & -0.0675(16) & 0.0207(5) \\ C1B & 0.678(3) & 0.1786(3) & -0.1835(19) & 0.0334(7) \\ C1B & 0.678(3) & 0.1580(19) & 0.0238(6) \\ C1B & 0.7486(3) & 0.2053(3) & 0.0216(1(18) & 0.0238(6) \\ C1B & 0.7486(3) & 0.2565(19) & 0.0524(11) & 0.0283(6) \\ C1B & 0.7486(3) & 0.2563(3) & 0.017573(17) & 0.0270(6) \\ C23B & 0.23129(18) & 0.3565(3) & 0.17573(17) & 0.0270(6) \\ C23B & 0.23129(18) & 0.3565(3) & 0.17573(17) & 0.0270(6) \\ C23B & 0.23129(18) & 0.3565(3) & 0.17573(17) & 0.0330(7) \\ C44B & 0.3202(3) & 0.3607(3) & 0.31031(18) & 0.0389(8) \\ C26B & 0.5098(3) & 0.3125(3) & 0.1977(16) & 0.0234(6) \\ C11 & 0.3742(3) & 0.717(3) & 0.4466(2) & 0.0424(8) \\ C111 & 0.4966(10) & 0.72562(11) & 0.49853(8) & 0.0653($	C13A	0.1863(3)	0.8894(3)	0.74218(18)	0.0294(7)	
$\begin{array}{cccccc} C15A & -0.0240(3) & 0.8456(3) & 0.77320(17) & 0.0321(7) \\ C16A & -0.0136(3) & 0.7930(3) & 0.69429(16) & 0.0241(6) \\ 0.0241(6) & 0.0236(4) \\ C2A & 0.10303(17) & 0.88660(17) & 0.39946(11) & 0.0236(4) \\ C21A & 0.0443(3) & 0.8051(3) & 0.42207(16) & 0.0214(5) \\ C22A & 0.0811(3) & 0.7024(3) & 0.38857(18) & 0.0280(6) \\ C23A & -0.0229(3) & 0.6949(3) & 0.3283(2) & 0.0396(8) \\ C24A & 0.1104(4) & 0.6286(4) & 0.3812(2) & 0.0544(11) \\ C25A & -0.1766(3) & 0.6889(4) & 0.4576(2) & 0.04489(10) \\ C25A & -0.096(4(3) & 0.7094(3) & 0.51057(19) & 0.0323(7) \\ N2A & -0.0425(2) & 0.8108(2) & 0.48802(13) & 0.0203(5) \\ Rh1B & 0.420837(18) & 0.537819(18) & -0.043874(11) & 0.0472(5) \\ C1B & 0.2915(2) & 0.525(2) & -0.10152(16) & 0.0191(5) \\ C2B & 0.3250(3) & 0.4871(3) & -0.17811(17) & 0.0266(6) \\ C3B & 0.1692(2) & 0.5473(2) & -0.0233(7) \\ C4B & 0.1146(3) & 0.4990(3) & -0.1821(2) & 0.0336(7) \\ C5B & 0.0815(3) & 0.3534(3) & -0.1023(19) & 0.0231(6) \\ C6B & 0.1692(2) & 0.5472(2) & -0.06441(17) & 0.0218(6) \\ C1B & 0.51586(18) & 0.37488(17) & -0.09045(12) & 0.0238(6) \\ C1B & 0.5158(18) & 0.37488(17) & -0.09045(12) & 0.0238(6) \\ C1B & 0.6855(3) & 0.1896(3) & -0.11839(18) & 0.0233(7) \\ C1B & 0.6855(3) & 0.1896(3) & -0.11839(18) & 0.0233(6) \\ C1B & 0.6855(3) & 0.1896(3) & -0.11839(18) & 0.0233(6) \\ C1B & 0.6855(3) & 0.1896(3) & -0.11839(18) & 0.0233(6) \\ C1B & 0.6853(3) & 0.1154(3) & -0.1053(2) & 0.0336(7) \\ C2B & 0.2638(3) & 0.0359(2) & -0.00671(13) & 0.0189(4) \\ O2B & 0.32329(18) & 0.4565(5) & 0.1277(18) & 0.0338(8) \\ C16B & 0.7486(3) & 0.2356(5) & 0.17573(17) & 0.0270(6) \\ C2B & 0.2638(3) & 0.3565(3) & 0.17573(17) & 0.0270(6) \\ C2B & 0.2638(3) & 0.3565(3) & 0.17573(17) & 0.0270(6) \\ C2B & 0.2638(3) & 0.3565(3) & 0.17573(17) & 0.0239(6) \\ C1B & 0.3320(2) & 0.3060(3) & 0.3101(18) & 0.0339(7) \\ C24B & 0.3222(1) & 0.3656(3) & 0.17573(17) & 0.0270(6) \\ C2B & 0.2638(3) & 0.3556(5) & 0.17573(17) & 0.0230(6) \\ C1B & 0.375(4) & 0.3556(5) & 0.17573(17) & 0.0230(6) \\ C2B & 0.2638(3) & 0.3565(5) & 0.17573(17) & 0.0339(7) \\ C2B & 0.2638(3) & 0.356$	C14A	0.0961(3)	0.8324(3)	0.80069(17)	0.0301(7)	
$\begin{array}{ccccc} C16A & -0.0136(3) & 0.7930(5) & 0.69429(16) & 0.0241(6) \\ 0.11A & 0.0231(2) & 0.8869(2) & 0.62374(13) & 0.0190(5) \\ 0.2A & 0.10393(17) & 0.88660(17) & 0.39946(11) & 0.0214(5) \\ 0.21A & 0.0443(3) & 0.8051(3) & 0.42207(16) & 0.0214(5) \\ 0.22A & 0.0811(3) & 0.7024(3) & 0.38857(18) & 0.0280(6) \\ 0.23A & -0.0229(3) & 0.6949(3) & 0.3283(2) & 0.0396(8) \\ 0.24A & 0.1104(4) & 0.6286(4) & 0.3812(2) & 0.0544(11) \\ 0.25A & -0.0964(3) & 0.7094(3) & 0.51059(19) & 0.0323(7) \\ 0.2A & -0.0452(2) & 0.8108(2) & 0.4887(21) & 0.01372(5) \\ 0.25A & -0.0964(3) & 0.7094(3) & 0.51059(19) & 0.0323(7) \\ 0.2A & -0.0425(2) & 0.8108(2) & 0.48874(11) & 0.01472(5) \\ 0.1B & 0.2915(2) & 0.5250(2) & -0.10152(16) & 0.0191(5) \\ 0.2B & 0.3250(3) & 0.4758(3) & -0.2184(2) & 0.0352(7) \\ 0.2B & 0.3250(3) & 0.4758(3) & -0.17811(7) & 0.0266(6) \\ 0.3B & 0.2362(3) & 0.4758(3) & -0.1821(2) & 0.0352(7) \\ 0.2B & 0.0815(3) & 0.5334(3) & -0.1821(2) & 0.0352(7) \\ 0.2B & 0.0815(3) & 0.5348(17) & -0.06755(16) & 0.0207(5) \\ 0.2B & 0.0815(3) & 0.5348(17) & -0.06755(16) & 0.0207(5) \\ 0.2B & 0.0815(3) & 0.5348(17) & -0.06755(16) & 0.0207(5) \\ 0.2B & 0.6585(3) & 0.1896(5) & -0.11839(18) & 0.0283(6) \\ 0.1B & 0.51586(18) & 0.37488(17) & -0.00451(2) & 0.0249(4) \\ 0.11B & 0.6070(2) & 0.2952(2) & -0.06755(16) & 0.0207(5) \\ 0.2B & 0.6585(3) & 0.1896(3) & -0.11839(18) & 0.0283(6) \\ 0.1B & 0.51586(18) & 0.3748(17) & -0.000451(2) & 0.0249(4) \\ 0.11B & 0.6544(2) & 0.3059(2) & -0.0671(13) & 0.0189(4) \\ 0.2B & 0.3229(18) & 0.45659(19) & 0.0524(11) & 0.0249(4) \\ 0.21B & 0.3605(2) & 0.4006(2) & 0.11537(16) & 0.0295(6) \\ 0.23B & 0.2315(3) & 0.158(4) & 0.2781(7) & 0.0229(6) \\ 0.23B & 0.2315(3) & 0.158(4) & 0.2781(7) & 0.0234(6) \\ 0.118 & 0.6544(2) & 0.3552(2) & 0.10671(13) & 0.188(4) \\ 0.21B & 0.3605(2) & 0.4006(2) & 0.11557(16) & 0.0299(5) \\ 0.22B & 0.2638(3) & 0.315(5) & 0.17573(7) & 0.0270(6) \\ 0.23B & 0.2315(3) & 0.4169(3) & 0.228404(19) & 0.0330(7) \\ 0.24B & 0.3202(3) & 0.3607(3) & 0.3101(18) & 0.0380(8) \\ 0.24B & 0.3202(3) & 0.3607(3) & 0.3103(18) & 0.0380(8) \\ 0.24B &$	C15A	-0.0249(3)	0.8456(3)	0.77320(17)	0.0321(7)	
N1A 0.0231(2) 0.8689(2) 0.62374(13) 0.0190(5) 02A 0.10303(17) 0.88660(17) 0.39946(11) 0.0236(4) C21A 0.0443(3) 0.8051(3) 0.42207(16) 0.0214(5) C22A 0.0811(3) 0.7024(3) 0.38687(18) 0.0230(6) C23A -0.0229(3) 0.6949(3) 0.3283(2) 0.0396(8) C24A -0.1104(4) 0.6286(4) 0.3812(2) 0.0489(10) C25A -0.176(3) 0.6889(4) 0.4576(2) 0.0489(10) C26A -0.096(3) 0.7094(3) 0.01323(7) 0.01472(5) C1B 0.42087(18) 0.537819(18) -0.04387(11) 0.01472(5) C1B 0.2915(2) 0.5250(2) -0.10152(16) 0.0191(5) C2B 0.3250(3) 0.4871(3) -0.17811(17) 0.0266(6) C3B 0.3250(3) 0.4878(3) -0.1821(2) 0.0352(7) C4B 0.1146(3) 0.4990(3) -0.1821(2) 0.0352(7) C4B 0.1365(3) 0.37348(17	C16A	-0.0136(3)	0.7930(3)	0.69429(16)	0.0241(6)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	NIA	0.0231(2)	0.8689(2)	0.62374(13)	0.0190(5)	
$\begin{array}{cccccc} C21A & 0.0443(3) & 0.8051(3) & 0.42207(16) & 0.0214(5) \\ C22A & 0.0811(3) & 0.7024(3) & 0.38657(18) & 0.0280(6) \\ C23A & -0.0229(3) & 0.6949(3) & 0.3283(2) & 0.0396(8) \\ C24A & -0.1104(4) & 0.6286(4) & 0.3812(2) & 0.0544(11) \\ C25A & -0.1766(3) & 0.6889(4) & 0.4576(2) & 0.0489(10) \\ C26A & -0.0964(3) & 0.7094(3) & 0.51059(19) & 0.0323(7) \\ N2A & -0.0425(2) & 0.8108(2) & 0.48502(13) & 0.0203(5) \\ Rh1B & 0.420837(18) & 0.537819(18) & -0.043874(11) & 0.01472(5) \\ C1B & 0.2915(2) & 0.5250(2) & -0.10152(16) & 0.0191(5) \\ C2B & 0.3250(3) & 0.4871(3) & -0.17811(17) & 0.0266(6) \\ C3B & 0.3250(3) & 0.4758(3) & -0.2184(2) & 0.0352(7) \\ C4B & 0.1146(3) & 0.4990(3) & -0.1821(2) & 0.0353(7) \\ C5B & 0.0815(3) & 0.5334(3) & -0.16523(19) & 0.0218(6) \\ C6B & 0.1692(2) & 0.5472(2) & -0.06441(17) & 0.0218(6) \\ O1B & 0.51586(18) & 0.37488(17) & -0.09045(12) & 0.0249(4) \\ O1B & 0.51586(18) & 0.37488(17) & -0.036441(17) & 0.0218(6) \\ C1B & 0.6585(3) & 0.1896(3) & -0.11839(18) & 0.0283(6) \\ C13B & 0.7916(3) & 0.1786(3) & -0.15836(19) & 0.0343(7) \\ C14B & 0.8833(3) & 0.1154(3) & -0.10532(2) & 0.0423(9) \\ C16B & 0.7486(3) & 0.2063(3) & 0.0216(118) & 0.0283(6) \\ C13B & 0.7916(3) & 0.1896(3) & -0.15836(19) & 0.0383(6) \\ C13B & 0.7916(3) & 0.1810(4) & -0.0322(2) & 0.0423(9) \\ C16B & 0.7486(3) & 0.2063(3) & 0.216(118) & 0.0283(6) \\ C13B & 0.32329(18) & 0.45559(19) & 0.05244(11) & 0.0249(4) \\ O2B & 0.32329(18) & 0.45559(19) & 0.05244(11) & 0.0249(4) \\ O2B & 0.32329(18) & 0.3565(3) & 0.17573(17) & 0.0270(6) \\ C23B & 0.2315(3) & 0.4169(3) & 0.25400(19) & 0.0320(7) \\ C24B & 0.3202(3) & 0.3667(3) & 0.11573(16) & 0.0396(8) \\ C16B & 0.7486(3) & 0.3565(3) & 0.17573(17) & 0.0270(6) \\ C24B & 0.3202(3) & 0.3665(3) & 0.17573(17) & 0.0270(6) \\ C24B & 0.3202(3) & 0.3665(3) & 0.17573(17) & 0.0270(6) \\ C24B & 0.3202(3) & 0.3665(3) & 0.17573(17) & 0.0270(6) \\ C24B & 0.3098(3) & 0.3125(3) & 0.19974(16) & 0.0249(4) \\ C11 & 0.3742(3) & 0.7173(3) & 0.4486(2) & 0.0653(3) \\ C114 & 0.4966(10) & 7.72552(11) & 0.48953(8) & 0.0653(3) \\ C115 & 0.29758(11)$	O2A	0.10303(17)	0.88660(17)	0.39946(11)	0.0236(4)	
$\begin{array}{cccccc} C22A & 0.0811(3) & 0.7024(3) & 0.36857(18) & 0.0280(6) \\ C23A & -0.0229(3) & 0.6949(3) & 0.3283(2) & 0.0396(8) \\ C23A & -0.0229(3) & 0.6949(3) & 0.3283(2) & 0.0594(11) \\ C25A & -0.1766(3) & 0.6889(4) & 0.4576(2) & 0.0489(10) \\ C26A & -0.0964(3) & 0.7094(3) & 0.51059(19) & 0.0323(7) \\ N2A & -0.0425(2) & 0.8108(2) & 0.488502(13) & 0.0203(5) \\ Rh1B & 0.2915(2) & 0.5250(2) & -0.10152(16) & 0.0191(5) \\ C2B & 0.3250(3) & 0.4871(3) & -0.17811(17) & 0.0266(6) \\ C3B & 0.2362(3) & 0.4758(3) & -0.1281(2) & 0.0352(7) \\ C4B & 0.1146(3) & 0.4990(3) & -0.1821(2) & 0.0353(7) \\ C5B & 0.0815(3) & 0.5334(3) & -0.10523(19) & 0.0281(6) \\ C6B & 0.1692(2) & 0.5472(2) & -0.06755(16) & 0.0207(5) \\ C1B & 0.6170(2) & 0.2952(2) & -0.06755(16) & 0.0207(5) \\ C1B & 0.61853(3) & 0.1786(3) & -0.1839(18) & 0.0283(6) \\ C1B & 0.7916(3) & 0.1786(3) & -0.15836(19) & 0.0343(7) \\ C1B & 0.8833(3) & 0.1154(3) & -0.1053(2) & 0.0395(8) \\ C13B & 0.7916(3) & 0.1786(3) & -0.1533(2) & 0.0395(8) \\ C13B & 0.7916(3) & 0.1810(4) & -0.0322(2) & 0.0423(9) \\ C16B & 0.7486(3) & 0.2063(3) & 0.02161(18) & 0.0283(6) \\ C15B & 0.8729(3) & 0.1810(4) & -0.0322(2) & 0.0423(9) \\ C16B & 0.7486(3) & 0.2063(3) & 0.02161(18) & 0.0283(6) \\ C13B & 0.7486(3) & 0.2063(3) & 0.02161(18) & 0.0283(6) \\ C13B & 0.6730(2) & 0.405659(19) & 0.05244(11) & 0.0249(4) \\ C21B & 0.3605(2) & 0.4060(2) & 0.11557(16) & 0.0209(5) \\ C22B & 0.2638(3) & 0.3556(3) & 0.17873(17) & 0.0270(6) \\ C22B & 0.2638(3) & 0.3556(3) & 0.17873(17) & 0.0270(6) \\ C22B & 0.2638(3) & 0.355(2) & 0.0423(19) & 0.0330(7) \\ C23B & 0.2315(3) & 0.3469(3) & 0.3125(3) & 0.19974(16) & 0.0254(6) \\ D190 & 0.5024(11) & 0.0349(7) \\ C24B & 0.5098(3) & 0.3125(3) & 0.19974(16) & 0.0254(6) \\ D102B & 0.5098(3) & 0.355(2) & 0.109773(17) & 0.0270(6) \\ C22B & 0.2638(3) & 0.355(2) & 0.109773(17) & 0.0270(6) \\ C22B & 0.2638(3) & 0.355(2) & 0.19974(16) & 0.0254(6) \\ D111 & 0.4966(10) & 0.72562(11) & 0.48953(8) & 0.0653(3) \\ C112 & 0.42543(12) & 0.67570(13) & 0.3486(48) & 0.0753(4) \\ C113 & 0.29758(11) & 0.61567(10) & 0.59463(8) & 0.065$	C21A	0.0443(3)	0.8051(3)	0.42207(16)	0.0214(5)	
$\begin{array}{ccccc} C23A & -0.0229(3) & 0.6949(3) & 0.3283(2) & 0.0396(8) \\ C24A & -0.1104(4) & 0.6286(4) & 0.3812(2) & 0.0544(11) \\ C25A & -0.0766(3) & 0.7094(3) & 0.51059(19) & 0.0323(7) \\ N2A & -0.0425(2) & 0.8108(2) & 0.48502(13) & 0.0203(5) \\ Rh1B & 0.420837(18) & 0.537819(18) & -0.04874(11) & 0.01472(5) \\ C1B & 0.2915(2) & 0.5250(2) & -0.101521(6) & 0.0191(5) \\ C2B & 0.3250(3) & 0.4758(3) & -0.1871(17) & 0.0266(6) \\ C3B & 0.2362(3) & 0.4758(3) & -0.1821(2) & 0.0336(7) \\ C4B & 0.1146(3) & 0.4990(3) & -0.1821(2) & 0.0336(7) \\ C6B & 0.1692(2) & 0.5472(2) & -0.06441(17) & 0.0218(6) \\ C1B & 0.51586(18) & 0.37488(17) & -0.0945(12) & 0.0221(6) \\ C1B & 0.6585(3) & 0.1896(3) & -0.11839(18) & 0.0238(6) \\ C1B & 0.6585(3) & 0.1896(3) & -0.11839(18) & 0.0238(6) \\ C13B & 0.7916(3) & 0.1786(3) & -0.1839(18) & 0.0238(6) \\ C13B & 0.7916(3) & 0.1786(3) & -0.1839(19) & 0.0343(7) \\ C14B & 0.8833(3) & 0.1154(3) & -0.0057(2) & 0.0395(8) \\ C15B & 0.8729(3) & 0.1810(4) & -0.0322(2) & 0.0423(9) \\ C16B & 0.7486(3) & 0.2056(2) & -0.0671(13) & 0.189(4) \\ O2B & 0.32329(18) & 0.45659(19) & 0.05244(11) & 0.0249(4) \\ C21B & 0.6552(2) & 0.4066(2) & 0.11557(16) & 0.0207(5) \\ C12B & 0.6583(3) & 0.1810(4) & -0.0322(2) & 0.0433(7) \\ C14B & 0.8833(3) & 0.1154(3) & -0.1053(2) & 0.0395(8) \\ C16B & 0.7486(3) & 0.2063(3) & 0.2161(18) & 0.0283(6) \\ N1B & 0.6544(2) & 0.3059(2) & -0.0671(13) & 0.189(4) \\ O2B & 0.32329(18) & 0.45659(19) & 0.05244(11) & 0.0249(4) \\ C21B & 0.3605(2) & 0.4006(2) & 0.11557(16) & 0.0209(5) \\ C22B & 0.2638(3) & 0.3565(3) & 0.17573(17) & 0.0270(6) \\ C24B & 0.5098(3) & 0.3125(3) & 0.1974(16) & 0.0380(8) \\ C26B & 0.5098(3) & 0.3125(3) & 0.1974(16) & 0.0380(8) \\ C26B & 0.5098(3) & 0.3125(3) & 0.1974(16) & 0.0249(4) \\ C111 & 0.4966(10) & 0.7252(211) & 0.48853(8) & 0.0653(3) \\ C112 & 0.42543(12) & 0.67570(13) & 0.34864(8) & 0.0753(4) \\ C113 & 0.29758(11) & 0.61567(10) & 0.50463(8) & 0.0653(3) \\ C114 & 0.84970(9) & 0.77018(11) & -0.00131(7) & 0.0632(3) \\ \end{array}$	C22A	0.0811(3)	0.7024(3)	0.36857(18)	0.0280(6)	
$\begin{array}{ccccc} C24A & -0.1104(4) & 0.6286(4) & 0.3812(2) & 0.0544(11) \\ C25A & -0.1766(3) & 0.6889(4) & 0.4576(2) & 0.0489(10) \\ C26A & -0.0964(3) & 0.7094(3) & 0.51059(19) & 0.0323(7) \\ N2A & -0.0425(2) & 0.8108(2) & 0.48502(13) & 0.0203(5) \\ Rh B & 0.420837(18) & 0.537819(18) & -0.043874(11) & 0.01472(5) \\ C1B & 0.2915(2) & 0.520(2) & -0.10152(16) & 0.0191(5) \\ C2B & 0.3250(3) & 0.4871(3) & -0.17811(17) & 0.0266(6) \\ C3B & 0.1236(3) & 0.4973(3) & -0.1821(2) & 0.0356(7) \\ C5B & 0.0815(3) & 0.5334(3) & -0.01821(2) & 0.0336(7) \\ C6B & 0.1692(2) & 0.5472(2) & -0.06441(17) & 0.0218(6) \\ C1B & 0.51586(18) & 0.37488(17) & -0.09045(12) & 0.0249(4) \\ C11B & 0.6070(2) & 0.2952(2) & -0.06755(16) & 0.0207(5) \\ C12B & 0.6585(3) & 0.1896(3) & -0.1839(18) & 0.0283(6) \\ C13B & 0.7916(3) & 0.1786(3) & -0.0532(2) & 0.0343(7) \\ C14B & 0.8833(3) & 0.1154(3) & -0.0532(2) & 0.0343(7) \\ C14B & 0.8833(3) & 0.1154(3) & -0.0532(2) & 0.0423(9) \\ C16B & 0.7486(3) & 0.205(3) & 0.0221(61(18) & 0.0283(6) \\ C13B & 0.6584(12) & 0.3059(2) & -0.00671(13) & 0.0189(4) \\ O2B & 0.32329(18) & 0.45659(19) & 0.05244(11) & 0.0249(4) \\ C21B & 0.3605(2) & 0.4006(2) & 0.11557(16) & 0.0209(5) \\ C22B & 0.2638(3) & 0.3565(3) & 0.17573(17) & 0.0230(7) \\ C24B & 0.3202(3) & 0.3607(3) & 0.31031(18) & 0.0380(8) \\ C23B & 0.2315(3) & 0.416(93) & 0.27817(18) & 0.0380(8) \\ C23B & 0.2315(3) & 0.3162(4) & 0.27817(18) & 0.0380(8) \\ C23B & 0.4510(3) & 0.3682(4) & 0.27817(18) & 0.0380(8) \\ C24B & 0.3202(3) & 0.3607(3) & 0.31031(18) & 0.0183(4) \\ C11 & 0.3742(3) & 0.7173(3) & 0.4466(8) & 0.0753(4) \\ C11 & 0.3742(3) & 0.7173(3) & 0.4466(8) & 0.0753(4) \\ C11 & 0.3742(3) & 0.7173(3) & 0.4466(8) & 0.0753(4) \\ C11 & 0.4966(10) & 0.72562(111) & 0.6485(8) & 0.0653(3) \\ C12 & 0.42543(12) & 0.67570(13) & 0.34864(8) & 0.0753(4) \\ C12 & 0.42543(12) & 0.67570(13) & 0.34864(8) & 0.0753(4) \\ C12 & 0.42543(12) & 0.67570(13) & 0.34864(8) & 0.0753(4) \\ C12 & 0.84970(9) & 0.77018(11) & -0.00131(7) & 0.0632(3) \\ \end{array}$	C23A	-0.0229(3)	0.6949(3)	0.3283(2)	0.0396(8)	
$\begin{array}{ccccc} C25A & -0.1766(3) & 0.6889(4) & 0.4576(2) & 0.0489(10) \\ C26A & -0.0964(3) & 0.7094(3) & 0.51059(19) & 0.0323(7) \\ N2A & -0.0425(2) & 0.8108(2) & 0.48502(13) & 0.0203(5) \\ Rh1B & 0.420837(18) & 0.537819(18) & -0.043874(11) & 0.01472(5) \\ C1B & 0.2915(2) & 0.5250(2) & -0.10152(16) & 0.0191(5) \\ C2B & 0.3250(3) & 0.4871(3) & -0.17811(17) & 0.0266(6) \\ C3B & 0.2362(3) & 0.4758(3) & -0.1821(2) & 0.0336(7) \\ C4B & 0.1146(3) & 0.4990(3) & -0.1821(2) & 0.0336(7) \\ C5B & 0.015(3) & 0.53743(17) & -0.09045(12) & 0.0281(6) \\ C6B & 0.1692(2) & 0.5472(2) & -0.06441(17) & 0.0218(6) \\ O1B & 0.51586(18) & 0.37488(17) & -0.09045(12) & 0.0281(6) \\ C11B & 0.6070(2) & 0.2952(2) & -0.06755(16) & 0.0207(5) \\ C12B & 0.6585(3) & 0.1896(3) & -0.1839(18) & 0.0283(6) \\ C13B & 0.7916(3) & 0.1786(3) & -0.15836(19) & 0.0343(7) \\ C14B & 0.8833(3) & 0.1154(3) & -0.1053(2) & 0.0395(8) \\ C15B & 0.8729(3) & 0.1810(4) & -0.0322(2) & 0.0423(9) \\ C16B & 0.7486(3) & 0.2063(3) & 0.02161(18) & 0.0283(6) \\ N1B & 0.6544(2) & 0.3059(2) & -0.00671(13) & 0.0189(4) \\ O2B & 0.3229(18) & 0.45659(19) & 0.05244(11) & 0.0249(4) \\ C21B & 0.3605(2) & 0.4006(2) & 0.11557(16) & 0.0209(5) \\ C22B & 0.2638(3) & 0.356(3) & 0.17573(17) & 0.0290(6) \\ C23B & 0.2315(3) & 0.4169(3) & 0.22810(13) & 0.0189(4) \\ C21B & 0.3605(2) & 0.4006(2) & 0.11557(16) & 0.0209(5) \\ C22B & 0.2638(3) & 0.356(3) & 0.17573(17) & 0.0270(6) \\ C22B & 0.2638(3) & 0.356(3) & 0.17573(17) & 0.0270(6) \\ C23B & 0.2315(3) & 0.3607(3) & 0.31031(18) & 0.0380(8) \\ C26B & 0.5098(3) & 0.3125(3) & 0.19974(16) & 0.0254(6) \\ N2B & 0.4716(2) & 0.3852(2) & 0.12914(13) & 0.0183(4) \\ C11 & 0.3742(3) & 0.7173(3) & 0.4466(2) & 0.0424(8) \\ C111 & 0.4966(10) & 0.7256(111) & 0.48953(8) & 0.0653(3) \\ C12 & 0.42543(12) & 0.67570(13) & 0.34864(8) & 0.0753(4) \\ C12 & 0.42543(12) & 0.67570(13) & 0.34864(8) & 0.0753(4) \\ C12 & 0.6956(3) & 0.77018(11) & -0.00131(7) & 0.0632(3) \\ \end{array}$	C24A	-0.1104(4)	0.6286(4)	0.3812(2)	0.0544(11)	
$\begin{array}{ccccc} C26A & -0.0964(3) & 0.7094(3) & 0.51059(19) & 0.0323(7) \\ N2A & -0.0425(2) & 0.8108(2) & 0.48502(13) & 0.0203(5) \\ Rh1B & 0.420837(18) & 0.537819(18) & -0.043874(11) & 0.01472(5) \\ C1B & 0.2915(2) & 0.5250(2) & -0.0152(16) & 0.0191(5) \\ C2B & 0.3250(3) & 0.4871(3) & -0.17811(17) & 0.0266(6) \\ C3B & 0.1362(3) & 0.4758(3) & -0.2184(2) & 0.0352(7) \\ C4B & 0.1146(3) & 0.4990(3) & -0.1821(2) & 0.0352(7) \\ C5B & 0.0815(3) & 0.37488(17) & -0.06441(17) & 0.0218(6) \\ C6B & 0.1692(2) & 0.5474(2) & -0.06441(17) & 0.0218(6) \\ C1B & 0.51586(18) & 0.37488(17) & -0.09045(12) & 0.029(4) \\ C11B & 0.6070(2) & 0.2952(2) & -0.06755(16) & 0.0207(5) \\ C12B & 0.6585(3) & 0.1896(3) & -0.1839(18) & 0.0283(6) \\ C13B & 0.7916(3) & 0.1786(3) & -0.1839(18) & 0.0283(6) \\ C13B & 0.7916(3) & 0.1786(3) & -0.1633(2) & 0.0395(8) \\ C15B & 0.8729(3) & 0.11810(4) & -0.0322(2) & 0.0395(8) \\ C16B & 0.7486(3) & 0.2063(3) & 0.02161(18) & 0.0283(6) \\ N1B & 0.6544(2) & 0.3059(2) & -0.00671(13) & 0.0189(4) \\ C21B & 0.3605(2) & 0.4006(2) & 0.11557(16) & 0.0209(5) \\ C22B & 0.2638(3) & 0.3565(3) & 0.17573(17) & 0.0270(6) \\ C23B & 0.3215(3) & 0.4169(3) & 0.25404(19) & 0.0320(7) \\ C24B & 0.3202(3) & 0.3607(3) & 0.31031(18) & 0.0380(8) \\ C23B & 0.2315(3) & 0.3167(3) & 0.31031(18) & 0.0380(8) \\ C22B & 0.2638(3) & 0.3565(3) & 0.17573(17) & 0.0270(6) \\ C22B & 0.2638(3) & 0.3567(3) & 0.31031(18) & 0.0380(8) \\ C22B & 0.2638(3) & 0.3567(3) & 0.31031(18) & 0.0380(8) \\ C22B & 0.2638(3) & 0.3567(3) & 0.31031(18) & 0.0380(8) \\ C22B & 0.4510(3) & 0.3682(4) & 0.27817(18) & 0.0380(8) \\ C22B & 0.4510(3) & 0.3682(2) & 0.125740(4) & 0.0753(4) \\ C111 & 0.4966(610) & 0.72552(11) & 0.48953(8) & 0.0653(3) \\ C122 & 0.4556(3) & 0.7173(3) & 0.4486(8) & 0.0753(4) \\ C113 & 0.29758(11) & 0.61567(10) & 0.50463(8) & 0.0652(3) \\ C221 & 0.84970(9) & 0.77018(11) & -0.00131(7) & 0.0632(3) \\ \end{array}$	C25A	-0.1766(3)	0.6889(4)	0.4576(2)	0.0489(10)	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C26A	-0.0964(3)	0.7094(3)	0.51059(19)	0.0323(7)	
Rh1B $0.420837(18)$ $0.537819(18)$ $-0.043874(11)$ $0.01472(5)$ C1B $0.2915(2)$ $0.5250(2)$ $-0.10152(16)$ $0.0191(5)$ C2B $0.3250(3)$ $0.4871(3)$ $-0.17811(17)$ $0.0266(6)$ C3B $0.2362(3)$ $0.4758(3)$ $-0.1821(2)$ $0.0332(7)$ C4B $0.1146(3)$ $0.4990(3)$ $-0.1821(2)$ $0.0336(7)$ C5B $0.0815(3)$ $0.5374(3)$ $-0.00441(17)$ $0.0281(6)$ C6B $0.1692(2)$ $0.5472(2)$ $-0.06441(17)$ $0.0249(4)$ C11B $0.6070(2)$ $0.2952(2)$ $-0.06755(16)$ $0.0207(5)$ C12B $0.6585(3)$ $0.1896(3)$ $-0.11839(18)$ $0.0283(6)$ C13B $0.7916(3)$ $0.1786(3)$ $-0.15836(19)$ $0.0343(7)$ C14B $0.8833(3)$ $0.1154(3)$ $-0.1053(2)$ $0.0939(8)$ C15B $0.8729(3)$ $0.1810(4)$ $-0.0322(2)$ $0.0423(9)$ C16B $0.7486(3)$ $0.2063(3)$ $0.0216(18)$ $0.0283(6)$ N1B $0.6544(2)$ $0.3059(2)$ $-0.0671(13)$ $0.189(4)$ O2B $0.32329(18)$ $0.45659(19)$ $0.02540(11)$ $0.029(5)$ C22B $0.2638(3)$ $0.3565(3)$ $0.17573(17)$ $0.0270(6)$ C23B $0.2315(3)$ $0.3607(3)$ $0.3101(18)$ $0.0380(8)$ C24B $0.3202(3)$ $0.3607(3)$ $0.3101(18)$ $0.0380(8)$ C24B $0.3202(3)$ $0.3682(4)$ $0.27817(18)$ $0.0380(8)$ C24B $0.3202(3)$ $0.3125(3)$ <	N2A	-0.0425(2)	0.8108(2)	0.48502(13)	0.0203(5)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Rh1B	0.420837(18)	0.537819(18)	-0.043874(11)	0.01472(5)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1B	0.2915(2)	0.5250(2)	-0.10152(16)	0.0191(5)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2B	0.3250(3)	0.4871(3)	-0.17811(17)	0.0266(6)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C3B	0.2362(3)	0.4758(3)	-0.2184(2)	0.0352(7)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4B	0.1146(3)	0.4990(3)	-0.1821(2)	0.0336(7)	
C6B $0.1692(2)$ $0.5472(2)$ $-0.06441(17)$ $0.0218(6)$ O1B $0.5188(618)$ $0.37488(17)$ $-0.09045(12)$ $0.0249(4)$ C11B $0.6070(2)$ $0.2952(2)$ $-0.06755(16)$ $0.0207(5)$ C12B $0.6585(3)$ $0.1896(3)$ $-0.11839(18)$ $0.0283(6)$ C13B $0.7916(3)$ $0.1786(3)$ $-0.15836(19)$ $0.0343(7)$ C14B $0.8833(3)$ $0.1154(3)$ $-0.1053(2)$ $0.0395(8)$ C15B $0.8729(3)$ $0.1810(4)$ $-0.0322(2)$ $0.0423(9)$ C16B $0.7486(3)$ $0.2063(3)$ $0.0216(18)$ $0.0283(6)$ N1B $0.6544(2)$ $0.3059(2)$ $-0.00671(13)$ $0.0189(4)$ O2B $0.32329(18)$ $0.45659(19)$ $0.05244(11)$ $0.0229(5)$ C22B $0.2638(3)$ $0.3565(3)$ $0.17573(17)$ $0.0270(6)$ C22B $0.2638(3)$ $0.3565(3)$ $0.17573(17)$ $0.0320(7)$ C24B $0.3202(3)$ $0.3607(3)$ $0.31031(18)$ $0.0349(7)$ C25B $0.4510(3)$ $0.3582(2)$ $0.12914(13)$ $0.0183(4)$ C1 $0.3742(3)$ $0.7173(3)$ $0.4466(2)$ $0.0424(8)$ C111 $0.4966(10)$ $0.72562(11)$ $0.48953(8)$ $0.0653(3)$ C12 $0.29758(11)$ $0.61567(10)$ $0.34864(8)$ $0.0753(4)$ C112 $0.29758(11)$ $0.61567(10)$ $0.0349(2)$ C121 $0.84970(9)$ $0.77018(11)$ $-0.00131(7)$ $0.0632(3)$	C5B	0.0815(3)	0.5334(3)	-0.10523(19)	0.0281(6)	
O1B $0.51586(18)$ $0.37488(17)$ $-0.09045(12)$ $0.0249(4)$ C11B $0.6070(2)$ $0.2952(2)$ $-0.06755(16)$ $0.0207(5)$ C12B $0.6585(3)$ $0.1896(3)$ $-0.11839(18)$ $0.0283(6)$ C13B $0.7916(3)$ $0.1786(3)$ $-0.15836(19)$ $0.0343(7)$ C14B $0.8833(3)$ $0.1154(3)$ $-0.1053(2)$ $0.0395(8)$ C15B $0.8729(3)$ $0.1810(4)$ $-0.0322(2)$ $0.0423(9)$ C16B $0.7486(3)$ $0.2063(3)$ $0.02161(18)$ $0.0283(6)$ N1B $0.6544(2)$ $0.3059(2)$ $-0.00671(13)$ $0.0189(4)$ O2B $0.32329(18)$ $0.45659(19)$ $0.05244(11)$ $0.0249(4)$ C21B $0.3605(2)$ $0.4006(2)$ $0.11557(16)$ $0.0209(5)$ C22B $0.2638(3)$ $0.3565(3)$ $0.17573(17)$ $0.0270(6)$ C23B $0.2315(3)$ $0.4169(3)$ $0.25404(19)$ $0.0320(7)$ C24B $0.3202(3)$ $0.3607(3)$ $0.31031(18)$ $0.0349(7)$ C25B $0.4510(3)$ $0.3682(4)$ $0.27817(18)$ $0.0380(8)$ C26B $0.5098(3)$ $0.3125(3)$ $0.19974(16)$ $0.0254(6)$ N2B $0.4716(2)$ $0.3852(2)$ $0.12914(13)$ $0.0183(4)$ C1 $0.3742(3)$ $0.7173(3)$ $0.4466(2)$ $0.0424(8)$ C111 $0.4966(10)$ $0.72562(11)$ $0.48953(8)$ $0.0653(3)$ C122 $0.6956(3)$ $0.7848(3)$ $0.0391(2)$ $0.0444(9)$ C121 $0.84970(9)$ $0.77018(11)$ <td>C6B</td> <td>0.1692(2)</td> <td>0.5472(2)</td> <td>-0.06441(17)</td> <td>0.0218(6)</td> <td></td>	C6B	0.1692(2)	0.5472(2)	-0.06441(17)	0.0218(6)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O1B	0.51586(18)	0.37488(17)	-0.09045(12)	0.0249(4)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11B	0.6070(2)	0.2952(2)	-0.06755(16)	0.0207(5)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12B	0.6585(3)	0.1896(3)	-0.11839(18)	0.0283(6)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C13B	0.7916(3)	0.1786(3)	-0.15836(19)	0.0343(7)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C14B	0.8833(3)	0.1154(3)	-0.1053(2)	0.0395(8)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C15B	0.8729(3)	0.1810(4)	-0.0322(2)	0.0423(9)	
N1B $0.6544(2)$ $0.3059(2)$ $-0.00671(13)$ $0.0189(4)$ O2B $0.32329(18)$ $0.45659(19)$ $0.05244(11)$ $0.0249(4)$ C21B $0.3605(2)$ $0.4006(2)$ $0.11557(16)$ $0.0209(5)$ C22B $0.2638(3)$ $0.3565(3)$ $0.17573(17)$ $0.0270(6)$ C23B $0.2315(3)$ $0.4169(3)$ $0.25404(19)$ $0.0320(7)$ C24B $0.3202(3)$ $0.3607(3)$ $0.31031(18)$ $0.0349(7)$ C25B $0.4510(3)$ $0.3682(4)$ $0.27817(18)$ $0.0380(8)$ C26B $0.5098(3)$ $0.3125(3)$ $0.19974(16)$ $0.0254(6)$ N2B $0.4716(2)$ $0.3852(2)$ $0.12914(13)$ $0.0183(4)$ C1 $0.3742(3)$ $0.7173(3)$ $0.4466(2)$ $0.0424(8)$ C111 $0.49666(10)$ $0.72562(11)$ $0.48953(8)$ $0.0653(3)$ C112 $0.42543(12)$ $0.67570(13)$ $0.34864(8)$ $0.0753(4)$ C113 $0.29758(11)$ $0.61567(10)$ $0.50463(8)$ $0.0632(3)$ C210 $0.84970(9)$ $0.77018(11)$ $-0.00131(7)$ $0.0632(3)$	C16B	0.7486(3)	0.2063(3)	0.02161(18)	0.0283(6)	
O2B $0.32329(18)$ $0.45659(19)$ $0.05244(11)$ $0.0249(4)$ $C21B$ $0.3605(2)$ $0.4006(2)$ $0.11557(16)$ $0.0209(5)$ $C22B$ $0.2638(3)$ $0.3565(3)$ $0.17573(17)$ $0.0270(6)$ $C23B$ $0.2315(3)$ $0.4169(3)$ $0.25404(19)$ $0.0320(7)$ $C24B$ $0.3202(3)$ $0.3607(3)$ $0.31031(18)$ $0.0349(7)$ $C25B$ $0.4510(3)$ $0.3682(4)$ $0.27817(18)$ $0.0380(8)$ $C26B$ $0.5098(3)$ $0.3125(3)$ $0.19974(16)$ $0.0254(6)$ $N2B$ $0.4716(2)$ $0.3852(2)$ $0.12914(13)$ $0.0183(4)$ $C1$ $0.3742(3)$ $0.7173(3)$ $0.4466(2)$ $0.0424(8)$ $C111$ $0.49666(10)$ $0.72562(11)$ $0.48953(8)$ $0.0653(3)$ $C112$ $0.42543(12)$ $0.67570(13)$ $0.34864(8)$ $0.0753(4)$ $C113$ $0.29758(11)$ $0.61567(10)$ $0.50463(8)$ $0.0632(3)$ $C22$ $0.6956(3)$ $0.7848(3)$ $0.0391(2)$ $0.0444(9)$ $C121$ $0.84970(9)$ $0.77018(11)$ $-0.00131(7)$ $0.0632(3)$	N1B	0.6544(2)	0.3059(2)	-0.00671(13)	0.0189(4)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2B	0.32329(18)	0.45659(19)	0.05244(11)	0.0249(4)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C21B	0.3605(2)	0.4006(2)	0.11557(16)	0.0209(5)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C22B	0.2638(3)	0.3565(3)	0.17573(17)	0.0270(6)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C23B	0.2315(3)	0.4169(3)	0.25404(19)	0.0320(7)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C24B	0.3202(3)	0.3607(3)	0.31031(18)	0.0349(7)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C25B	0.4510(3)	0.3682(4)	0.27817(18)	0.0380(8)	
N2B $0.4716(2)$ $0.3852(2)$ $0.12914(13)$ $0.0183(4)$ C1 $0.3742(3)$ $0.7173(3)$ $0.4466(2)$ $0.0424(8)$ C11 $0.49666(10)$ $0.72562(11)$ $0.48953(8)$ $0.0653(3)$ C112 $0.42543(12)$ $0.67570(13)$ $0.34864(8)$ $0.0753(4)$ C113 $0.29758(11)$ $0.61567(10)$ $0.50463(8)$ $0.0632(3)$ C2 $0.6956(3)$ $0.7848(3)$ $0.0391(2)$ $0.0444(9)$ C121 $0.84970(9)$ $0.77018(11)$ $-0.00131(7)$ $0.0632(3)$	C26B	0.5098(3)	0.3125(3)	0.19974(16)	0.0254(6)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2B	0.4716(2)	0.3852(2)	0.12914(13)	0.0183(4)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1	0.3742(3)	0.7173(3)	0.4466(2)	0.0424(8)	
Cl120.42543(12)0.67570(13)0.34864(8)0.0753(4)Cl130.29758(11)0.61567(10)0.50463(8)0.0632(3)C20.6956(3)0.7848(3)0.0391(2)0.0444(9)Cl210.84970(9)0.77018(11)-0.00131(7)0.0632(3)	Cl11	0.49666(10)	0.72562(11)	0.48953(8)	0.0653(3)	
C1130.29758(11)0.61567(10)0.50463(8)0.0632(3)C20.6956(3)0.7848(3)0.0391(2)0.0444(9)C1210.84970(9)0.77018(11)-0.00131(7)0.0632(3)	Cl12	0.42543(12)	0.67570(13)	0.34864(8)	0.0753(4)	
C20.6956(3)0.7848(3)0.0391(2)0.0444(9)C1210.84970(9)0.77018(11)-0.00131(7)0.0632(3)	Cl13	0.29758(11)	0.61567(10)	0.50463(8)	0.0632(3)	
CI21 $0.84970(9)$ $0.77018(11)$ $-0.00131(7)$ $0.0632(3)$	C2	0.6956(3)	0.7848(3)	0.0391(2)	0.0444(9)	
	CI21	0.84970(9)	0.77018(11)	-0.00131(7)	0.0632(3)	

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Cl22	0.60417(10)	0.86489(9)	-0.03093(8)	0.0607(3)	
Cl23	0.65541(13)	0.85715(15)	0.12702(9)	0.0895(5)	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic atomic displacement parameters (A^2) f	for G
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Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Rh1A	0.01323(10)	0.01872(11)	0.01437(10)	-0.00012(8)	-0.00175(7)	-0.00603(8)
CIA	0.01320(10)	0.0195(13)	0.0219(13)	0.0019(10)	-0.0013(10)	-0.0058(10)
C2A	0.0211(12)	0.0170(15) 0.0270(15)	0.0219(13) 0.0218(14)	0.0013(11)	-0.0012(10)	-0.0075(12)
C3A	0.0177(13)	0.0316(16)	0.0339(16)	0.0029(13)	-0.0081(12)	-0.0104(12)
C4A	0.0170(13)	0.0341(17)	0.0375(17)	0.0029(13)	0.0001(12) 0.0043(12)	-0.0098(13)
C5A	0.0254(15)	0.0312(16)	0.0373(17) 0.0257(15)	-0.0005(12)	0.0019(12)	-0.0079(13)
C6A	0.0202(13)	0.0269(15)	0.0235(14)	-0.0032(11)	-0.0021(11)	-0.0079(12)
O1A	0.0181(9)	0.0374(12)	0.0211(10)	0.0095(9)	-0.0054(8)	-0.0076(9)
C11A	0.0200(13)	0.0246(14)	0.0198(13)	0.0014(11)	-0.0040(10)	-0.0049(11)
C12A	0.0195(14)	0.0388(18)	0.0257(15)	0.0118(13)	-0.0080(11)	-0.0086(13)
C13A	0.0305(16)	0.0304(16)	0.0331(16)	0.0082(13)	-0.0196(13)	-0.0119(13)
C14A	0.0324(16)	0.0393(18)	0.0179(14)	0.0015(12)	-0.0094(12)	-0.0057(14)
C15A	0.0259(15)	0.047(2)	0.0219(15)	0.0019(13)	-0.0045(12)	-0.0086(14)
C16A	0.0233(14)	0.0263(15)	0.0240(14)	0.0059(11)	-0.0057(11)	-0.0108(12)
N1A	0.0191(11)	0.0217(12)	0.0171(11)	0.0015(9)	-0.0051(9)	-0.0068(9)
O2A	0.0217(10)	0.0230(10)	0.0264(10)	-0.0066(8)	0.0040(8)	-0.0100(8)
C21A	0.0221(13)	0.0226(14)	0.0211(13)	-0.0039(11)	-0.0038(10)	-0.0071(11)
C22A	0.0285(15)	0.0270(16)	0.0293(16)	-0.0110(12)	0.0022(12)	-0.0099(13)
C23A	0.0409(19)	0.047(2)	0.0343(18)	-0.0216(16)	-0.0047(15)	-0.0105(16)
C24A	0.047(2)	0.072(3)	0.060(3)	-0.037(2)	-0.0010(19)	-0.033(2)
C25A	0.0365(19)	0.065(3)	0.057(2)	-0.032(2)	0.0082(17)	-0.0334(19)
C26A	0.0365(17)	0.0297(17)	0.0329(17)	-0.0083(13)	0.0067(13)	-0.0188(14)
N2A	0.0215(11)	0.0222(12)	0.0192(11)	-0.0036(9)	-0.0022(9)	-0.0092(10)
Rh1B	0.01424(10)	0.01630(10)	0.01497(10)	0.00061(7)	-0.00448(7)	-0.00554(8)
C1B	0.0198(13)	0.0192(13)	0.0213(13)	0.0038(10)	-0.0099(10)	-0.0075(11)
C2B	0.0237(14)	0.0297(16)	0.0281(15)	-0.0050(12)	-0.0075(12)	-0.0063(12)
C3B	0.0367(18)	0.043(2)	0.0318(17)	-0.0104(14)	-0.0144(14)	-0.0107(15)
C4B	0.0327(17)	0.0372(18)	0.0404(18)	-0.0031(14)	-0.0226(14)	-0.0130(14)
C5B	0.0204(14)	0.0293(16)	0.0392(17)	0.0044(13)	-0.0125(12)	-0.0117(12)
C6B	0.0223(13)	0.0235(14)	0.0217(13)	0.0019(11)	-0.0069(11)	-0.0086(11)
O1B	0.0250(10)	0.0202(10)	0.0322(11)	-0.0070(8)	-0.0134(8)	-0.0021(8)
C11B	0.0210(13)	0.0190(13)	0.0234(14)	-0.0031(11)	-0.0044(11)	-0.0062(11)
C12B	0.0312(16)	0.0226(15)	0.0343(16)	-0.0096(12)	-0.0142(13)	-0.0025(12)
C13B	0.0422(19)	0.0324(17)	0.0256(16)	-0.0116(13)	-0.0001(13)	-0.0054(15)
C14B	0.0283(17)	0.045(2)	0.043(2)	-0.0209(16)	-0.0003(14)	-0.0017(15)
C15B	0.0244(16)	0.051(2)	0.050(2)	-0.0241(18)	-0.0120(15)	0.0060(15)
C16B	0.0306(16)	0.0262(15)	0.0254(15)	-0.0041(12)	-0.0114(12)	0.0027(13)
N1B	0.0160(11)	0.0208(12)	0.0198(11)	-0.0017(9)	-0.0039(8)	-0.0041(9)
O2B	0.0219(10)	0.0349(12)	0.0217(10)	0.0107(9)	-0.0090(8)	-0.0153(9)
C21B	0.0211(13)	0.0223(14)	0.0206(13)	0.0010(11)	-0.0038(10)	-0.0089(11)
C22B	0.0220(14)	0.0340(17)	0.0265(15)	0.0100(12)	-0.0053(11)	-0.0144(13)
C23B	0.0238(15)	0.0283(16)	0.0355(17)	0.0059(13)	0.0066(12)	-0.0049(13)
C24B	0.0364(18)	0.044(2)	0.0224(15)	-0.0022(14)	0.0044(13)	-0.0149(15)
C25B	0.0361(18)	0.061(2)	0.0207(15)	0.0026(15)	-0.0055(13)	-0.0218(17)
C26B	0.0226(14)	0.0282(15)	0.0229(14)	0.0071(12)	-0.0059(11)	-0.0050(12)
N2B	0.0193(11)	0.0200(11)	0.0151(10)	0.0029(9)	-0.0026(8)	-0.0066(9)
C1	0.0377(19)	0.0328(19)	0.058(2)	-0.0128(17)	-0.0137(17)	-0.0040(15)
C111	0.0466(6)	0.0634(7)	0.0958(9)	-0.0096(6)	-0.0308(6)	-0.0155(5)
C112	0.0703(8)	0.0799(9)	0.0726(8)	-0.0396(7)	0.0011(6)	-0.0095(7)
C113	0.0645(7)	0.0477(6)	0.0863(8)	0.0059(5)	-0.0271(6)	-0.0236(5)
C2	0.0340(19)	0.0351(19)	0.060(2)	-0.0102(17)	0.0102(16)	-0.0133(16)
Cl21	0.0356(5)	0.0625(7)	0.0794(8)	0.0037(6)	0.0100(5)	-0.0109(5)
Cl22	0.0532(6)	0.0373(5)	0.0865(8)	0.0029(5)	-0.0091(5)	-0.0088(5)
Cl23	0.0683(8)	0.1161(12)	0.0842(9)	-0.0592(9)	0.0088(7)	-0.0176(8)

* The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2$ [$h^2a^{*2}U_{11} + ... + 2hka^{*b}U_{12}$]

Atom	x/a	у/b	z/c	U _{iso}	
H2A	0.3202	1.0671	0.4908	0.028	
H3A	0.5193	1.0547	0.4219	0.032	
H4A	0.5725	1.0134	0.2881	0.037	
H5A	0.4236	0.9878	0.2222	0.034	
H6A	0.2244	0.9994	0.2906	0.028	
H12A	0.3058	0.8475	0.6363	0.034	
H12B	0.2365	0.7455	0.6717	0.034	
H13A	0.2597	0.8811	0.7658	0.035	
H13B	0.1480	0.9760	0.7332	0.035	
H14A	0.0787	0.8693	0.8520	0.036	
H14B	0.1352	0.7461	0.8100	0.036	
H15A	-0.0773	0.8065	0.8147	0.039	
H15B	-0.0671	0.9320	0.7685	0.039	
H16A	0.0474	0.7143	0.6933	0.029	
H16B	-0.0934	0.7791	0.6912	0.029	
H22A	0.1077	0.6263	0.4004	0.034	
H22B	0.1518	0.7124	0.3272	0.034	
H23A	-0.0694	0.7771	0.3136	0.048	
H23B	0.0125	0.6534	0.2787	0.048	
H24A	-0.0637	0.5462	0.3953	0.065	
H24B	-0.1721	0.6221	0.3507	0.065	
H25A	-0.2307	0.7674	0.4430	0.059	
H25B	-0.2297	0.6392	0.4886	0.059	
H26A	-0.1456	0.7217	0.5646	0.039	
H26B	-0.0293	0.6359	0.5144	0.039	
H2B	0.4087	0.4688	-0.2030	0.032	
H3B	0.2593	0.4520	-0.2713	0.042	
H4B	0.0543	0.4914	-0.2099	0.040	
H5B	-0.0018	0.5479	-0.0798	0.034	
H6B	0.1455	0.5715	-0.0116	0.026	
H12C	0.6081	0.1979	-0.1598	0.034	
H12D	0.6531	0.1152	-0.0848	0.034	
H13C	0.8088	0.1343	-0.2067	0.041	
H13D	0.8028	0.2599	-0.1753	0.041	
H14C	0.9670	0.1056	-0.1367	0.047	
H14D	0.8716	0.0343	-0.0880	0.047	
H15C	0.9346	0.1329	-0.0006	0.051	
H15D	0.8939	0.2582	-0.0498	0.051	
H16C	0.7188	0.1329	0.0290	0.034	
H16D	0.7589	0.2235	0.0743	0.034	
H22C	0.2935	0.2689	0.1867	0.032	
H22D	0.1888	0.3714	0.1525	0.032	
H23C	0.2304	0.5027	0.2424	0.038	
H23D	0.1481	0.4125	0.2806	0.038	
H24C	0.3200	0.2753	0.3225	0.042	
H24D	0.2908	0.4008	0.3607	0.042	
H25C	0.4519	0.4538	0.2715	0.046	
H25D	0.5021	0.3286	0.3184	0.046	
H26C	0.5998	0.2968	0.1940	0.030	
H26D	0.4904	0.2343	0.2017	0.030	
H1	0.3154	0.7984	0.4457	0.051	
H2	0.6813	0.7030	0.0510	0.053	

Table 4. Hydrogen atom coordinates and isotropic atomic displacement parameters (Å²) for G.

Table 5. Bond lengths (Å) and angles (°) for G.

Rh1A-C1A	1.996(3)	Rh1A-N1A#1	2.009(2)
Rh1A-N2A#1	2.011(2)	Rh1A-O2A	2.0743(19)
Rh1A-O1A	2.0865(19)	Rh1A-Rh1A#1	2.5172(4)
C1A-C6A	1.391(4)	C1A-C2A	1.397(4)
C2A-C3A	1.393(4)	C3A-C4A	1.385(4)
C4A-C5A	1.390(4)	C5A-C6A	1.392(4)
01A-C11A	1.293(3)	C11A-N1A	1.303(3)
C11A-C12A	1.516(4)	C12A-C13A	1.525(4)
C13A-C14A	1.525(4)	C14A-C15A	1.526(4)
C15A-C16A	1.526(4)	C16A-N1A	1.472(3)
N1A-Rh1A#1	2.009(2)	O2A-C21A	1.290(3)
C21A-N2A	1.313(3)	C21A-C22A	1.513(4)
C22A-C23A	1.530(4)	C23A-C24A	1.526(5)
C24A-C25A	1.527(5)	C25A-C26A	1.504(5)
C26A-N2A	1.462(3)	N2A-Rh1A#1	2.011(2)
Rh1B-C1B	1.999(2)	Rh1B-N1B#2	2.008(2)
Rh1B-N2B#2	2.011(2)	Rh1B-O1B	2.077(2)
Rh1B-O2B	2.0858(18)	Rh1B-Rh1B#2	2.5126(4)
C1B-C2B	1 388(4)	C1B-C6B	1 393(4)
C2B-C3B	1 390(4)	C3B-C4B	1.390(1)
C4B-C5B	1.378(5)	C5B-C6B	1 396(4)
01B-C11B	1.290(3)	C11B-N1B	1 310(3)
C11B-C12B	1.290(3) 1.510(4)	C12B-C13B	1.510(5) 1.527(4)
C13B-C14B	1.516(5)0	C14B-C15B	1.527(1) 1.520(4)
C15B-C16B	1.516(3)0 1.516(4)	C16B-N1B	1.526(1) 1 466(4)0
N1B_Rh1B#2	2.008(2)	$O^2B_{-}C^21B$	1.400(4)0
C21B-N2B	1.310(3)	C21B-C22B	1.200(3) 1.515(4)
$C_{21}D_{11}C_{23}D_{12}C_{2$	1.510(5) 1.529(4)	C23B-C24B	1.515(4) 1.515(5)
C24B C25B	1.529(4) 1.521(4)	C25B-C24B	1.515(5) 1.510(4)
C24D-C25D C26B-N2B	1.321(4) 1.466(3)	N2B_Rh1B#2	1.319(4) 2.011(2)
C1-C112	1.400(3) 1.752(4)	C1-C111	1.752(4)
C1 C112	1.752(4) 1.762(4)	$C_2 C_{122}$	1.732(4) 1.740(4)
C2-Cl21	1.742(4)	C2-Cl23	1.772(4)
C1A-Rh1A-N1A#1	103.00(10)	C1A-Rh1A-N2A#1	101.49(10)
N1A#1-Rh1A-N2A#1	90.50(9)	C1A-Rh1A-O2A	85.05(9)
N1A#1-Rh1A-O2A	88.07(9)	N2A#1-Rh1A-O2A	173.46(8)
C1A-Rh1A-O1A	83.25(9)	N1A#1-Rh1A-O1A	173.71(8)
N2A#1-Rh1A-O1A	88.94(9)	O2A-Rh1A-O1A	91.78(8)
C1A-Rh1A-Rh1A#1	155.57(8)	N1A#1-Rh1A-Rh1A#1	96.04(6)
N2A#1-Rh1A-Rh1A#1	93.42(6)	O2A-Rh1A-Rh1A#1	80.39(5)
O1A-Rh1A-Rh1A#1	77.74(5)	C6A-C1A-C2A	119.0(2)
C6A-C1A-Rh1A	119.82(19)	C2A-C1A-Rh1A	121.0(2)
C3A-C2A-C1A	120.0(3)	C4A-C3A-C2A	120.8(3)
C3A-C4A-C5A	119.3(3)	C4A-C5A-C6A	120.3(3)
C1A-C6A-C5A	120.6(3)	C11A-O1A-Rh1A	129.62(17)
01A-C11A-N1A	123.4(2)	01A-C11A-C12A	114.1(2)
N1A-C11A-C12A	122.4(2)	C11A-C12A-C13A	112.6(3)
C14A-C13A-C12A	113.0(2)	C13A-C14A-C15A	114.2(2)
C16A-C15A-C14A	115.2(3)	N1A-C16A-C15A	114.3(2)
C11A-N1A-C16A	120.2(2)	C11A-N1A-Rh1A#1	113.13(18)
C16A-N1A-Rh1A#1	126.71(17)	C21A-O2A-Rh1A	127.14(17)
02A-C21A-N2A	123 5(2)	02A-C21A-C22A	114 4(2)
N2A-C21A-C22A	122.1(2)	C21A-C22A-C23A	112.7(3)
C24A-C23A-C22A	112.7(3)	C23A-C24A-C25A	113.8(3)
C26A-C25A-C24A	116 1(3)	N2A-C26A-C25A	115 5(3)
C21A-N2A-C26A	119.8(2)	C21A-N2A-Rh1A#1	115.5(3) 115.47(18)
C26A-N2A-Rh1A#1	12452(18)	C1B-Rh1B-N1B#2	102 58(10)
C1B-Rh1B-N2B#2	101 94(10)	N1B#2-Rh1B-N2B#2	91 08(9)
C1B-Rh1B-O1B	83 92(9)	N1B#2-Rh1B-01B	173 50(8)
N2B#2-Rh1B-O1B	87 40(9)	C1B-Rh1B-O2B	84 30(9)
N1B#2-Rh1B-O2B	88 01(9)	N2B#2-Rh1B-O2B	173 73(8)
01B-Rh1B-02B	92.81(8)	C1B-Rh1B-Rh1B#2	155 20(8)
N1B#2-Rh1B-Rh1B#?	95.11(6)	N2B#2-Rh1B-Rh1B#?	94.89(6)
$O1B_{Rh}1B_{Rh}1B_{H}2$			/
$O I D^{-} K I I D^{-} K I I D^{\pi} L$	78.74(5)	O2B-Rh1B-Rh1B#2	79.03(5)

C6B-C1B-Rh1B	121.0(2)	C1B-C2B-C3B	120.0(3)
C4B-C3B-C2B	120.6(3)	C5B-C4B-C3B	119.5(3)
C4B-C5B-C6B	120.6(3)	C1B-C6B-C5B	119.7(3)
C11B-O1B-Rh1B	128.94(17)	O1B-C11B-N1B	123.2(2)
O1B-C11B-C12B	114.7(2)	N1B-C11B-C12B	122.1(2)
C11B-C12B-C13B	112.9(2)	C14B-C13B-C12B	113.6(3)
C13B-C14B-C15B	113.8(3)	C16B-C15B-C14B	115.6(3)
N1B-C16B-C15B	115.5(3)	C11B-N1B-C16B	120.4(2)
C11B-N1B-Rh1B#2	113.89(18)	C16B-N1B-Rh1B#2	125.66(18)
C21B-O2B-Rh1B	128.34(17)	O2B-C21B-N2B	123.6(2)
O2B-C21B-C22B	114.7(2)	N2B-C21B-C22B	121.7(2)
C21B-C22B-C23B	113.2(2)	C24B-C23B-C22B	113.2(3)
C23B-C24B-C25B	114.1(3)	C26B-C25B-C24B	115.7(3)
N2B-C26B-C25B	115.0(3)	C21B-N2B-C26B	120.3(2)
C21B-N2B-Rh1B#2	114.10(17)	C26B-N2B-Rh1B#2	125.51(17)
Cl12-C1-Cl11	110.8(2)	Cl12-C1-Cl13	110.92(19)
Cl11-C1-Cl13	109.8(2)	Cl23-C2-Cl21	110.9(2)
Cl23-C2-Cl22	110.5(2)	Cl21-C2-Cl22	109.6(2)
Symmetry transformation	codes:#1 -x,-y+2,-z+1	#2 -x+1,-y+1,-z	
	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		

Table 6. Torsion angles (°) for G.

	42 1 (2)	
NIA#I-RhIA-CIA-C6A	-43.1(2)	N2A#I-RhIA-CIA-C6A - 136.3(2)
O2A-RhIA-CIA-C6A	43.8(2)	OIA-RhIA-CIA-C6A = 136.2(2)
KNIA#I-KNIA-CIA-C6A	97.2(3)	NIA#I-KNIA-CIA-C2A = 140.8(2)
N2A#I-RhIA-CIA-C2A	4/.5(2)	O2A-RhIA-CIA-C2A -132.4(2)
OIA-RhIA-CIA-C2A	-40.0(2)	Rh1A#1-Rh1A-C1A-C2A -/9.0(3)
C6A-C1A-C2A-C3A	1.3(4)	Rh1A-C1A-C2A-C3A 177.5(2)
C1A-C2A-C3A-C4A	-0.8(5)	C2A-C3A-C4A-C5A 0.4(5)
C3A-C4A-C5A-C6A	-0.5(5)	C2A-C1A-C6A-C5A -1.5(4)
Rh1A-C1A-C6A-C5A	-177.7(2)	C4A-C5A-C6A-C1A 1.0(5)
C1A-Rh1A-O1A-C11A	-164.8(3)	N2A#1-Rh1A-O1A-C11A 93.5(3)
O2A-Rh1A-O1A-C11A	-80.0(2)	Rh1A#1-Rh1A-O1A-C11A -0.2(2)
Rh1A-O1A-C11A-N1A	2.1(4)	Rh1A-O1A-C11A-C12A -175.37(19)
O1A-C11A-C12A-C13A	113.4(3)	N1A-C11A-C12A-C13A -64.2(4)
C11A-C12A-C13A-C14A	82.2(3)	C12A-C13A-C14A-C15A -62.1(4)
C13A-C14A-C15A-C16A	58.4(4)	C14A-C15A-C16A-N1A -78.7(3)
O1A-C11A-N1A-C16A	177.1(3)	C12A-C11A-N1A-C16A -5.5(4)
O1A-C11A-N1A-Rh1A#1	-3.0(4)	C12A-C11A-N1A-Rh1A#1 174.4(2)
C15A-C16A-N1A-C11A	70.0(3)	C15A-C16A-N1A-Rh1A#1 -109.9(2)
C1A-Rh1A-O2A-C21A	157.6(2)	N1A#1-Rh1A-O2A-C21A -99.2(2)
O1A-Rh1A-O2A-C21A	74.5(2)	Rh1A#1-Rh1A-O2A-C21A -2.7(2)
Rh1A-O2A-C21A-N2A	1.8(4)	Rh1A-O2A-C21A-C22A -179.78(18)
O2A-C21A-C22A-C23A	-115.6(3)	N2A-C21A-C22A-C23A 62.9(4)
C21A-C22A-C23A-C24A	-83.3(4)	C22A-C23A-C24A-C25A 62.2(5)
C23A-C24A-C25A-C26A	-56.9(5)	C24A-C25A-C26A-N2A 77.6(4)
O2A-C21A-N2A-C26A	-174.3(3)	C22A-C21A-N2A-C26A 7.4(4)
O2A-C21A-N2A-Rh1A#1	1.0(4)	C22A-C21A-N2A-Rh1A#1 -177.3(2)
C25A-C26A-N2A-C21A	-70.8(4)	C25A-C26A-N2A-Rh1A#1 114.4(3)
N1B#2-Rh1B-C1B-C2B	136.9(2)	N2B#2-Rh1B-C1B-C2B 43.1(2)
O1B-Rh1B-C1B-C2B	-42.9(2)	O2B-Rh1B-C1B-C2B -136.4(2)
Rh1B#2-Rh1B-C1B-C2B	-88.6(3)	N1B#2-Rh1B-C1B-C6B -46.7(2)
N2B#2-Rh1B-C1B-C6B	-140.5(2)	O1B-Rh1B-C1B-C6B 133.5(2)
O2B-Rh1B-C1B-C6B	40.0(2)	Rh1B#2-Rh1B-C1B-C6B 87.8(3)
C6B-C1B-C2B-C3B	2.5(4)	Rh1B-C1B-C2B-C3B 178.9(2)
C1B-C2B-C3B-C4B	-1.7(5)	C2B-C3B-C4B-C5B -0.1(5)
C3B-C4B-C5B-C6B	1.2(5)	C2B-C1B-C6B-C5B -1.3(4)
Rh1B-C1B-C6B-C5B	-177.7(2)	C4B-C5B-C6B-C1B = -0.5(4)
C1B-Rh1B-O1B-C11B	-160.9(2)	N2B#2-Rh1B-O1B-C11B 96.8(2)
O2B-Rh1B-O1B-C11B	-76.9(2)	Rh1B#2-Rh1B-O1B-C11B = 1.3(2)
Rh1B-O1B-C11B-N1B	1.2(4)	Rh1B-O1B-C11B-C12B -176 70(18)
01B-C11B-C12B-C13B	117.5(3)	N1B-C11B-C12B-C13B -60 4(4)
C11B-C12B-C13B-C14B	83.0(3)	C12B-C13B-C14B-C15B -63 3(4)
end end end end	05.0(5)	CI CI CI CI CI 05.5(1)

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C13B-C14B-C15B-C16B	57.0(4)	C14B-C15B-C16B-N1B -76.8(4)
O1B-C11B-N1B-C16B	173.1(3)	C12B-C11B-N1B-C16B -9.2(4)
O1B-C11B-N1B-Rh1B#2	-3.5(3)	C12B-C11B-N1B-Rh1B#2 174.2(2)
C15B-C16B-N1B-C11B	71.2(3)	C15B-C16B-N1B-Rh1B#2 -112.6(3)
C1B-Rh1B-O2B-C21B	160.3(3)	N1B#2-Rh1B-O2B-C21B -96.8(2)
O1B-Rh1B-O2B-C21B	76.7(2)	Rh1B#2-Rh1B-O2B-C21B -1.2(2)
Rh1B-O2B-C21B-N2B	-0.3(4)	Rh1B-O2B-C21B-C22B 177.62(19)
O2B-C21B-C22B-C23B	-115.1(3)	N2B-C21B-C22B-C23B 62.8(4)
C21B-C22B-C23B-C24B	-82.6(3)	C22B-C23B-C24B-C25B 62.0(4)
C23B-C24B-C25B-C26B	-57.5(4)	C24B-C25B-C26B-N2B 77.9(4)
O2B-C21B-N2B-C26B	-175.4(3)	C22B-C21B-N2B-C26B 6.9(4)
O2B-C21B-N2B-Rh1B#2	2.0(4)	C22B-C21B-N2B-Rh1B#2 -175.7(2)
C25B-C26B-N2B-C21B	-70.3(3)	C25B-C26B-N2B-Rh1B#2 112.6(2)

Symmetry transformation codes:#1 -x,-y+2,-z+1 #2 -x+1,-y+1,-z

Details of the x-ray structural analysis of O. The crystal of **O** suitable X-ray analysis was obtained by evaporation of the solvents from the solution of **O** in Et₂O and acetone. An orange/green prism of $C_{36}H_{50}N_4O_4Rh_2$, approximate dimensions $0.041 \times 0.092 \times 0.147 \text{ mm}^3$, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 150(2) K on a three-circle diffractometer system equipped with Bruker Smart Apex II CCD area detector using a graphite monochromator and a MoK α fine-focus sealed tube (λ = 0.71073 Å). The detector was placed at a distance of 5.2 cm from the crystal.

A total of 1731 frames was collected with a scan width of 0.3° in ω and an exposure time of 30 sec/frame using Apex2 (Bruker, 2005). The total data collection time was 21.9 hours. The frames were integrated with Apex2 software package using a narrow-frame integration algorithm. The integration of the data using a monoclinic unit cell yielded a total of 12334 reflections to a maximum θ angle of 25.00°, of which 2923 were independent (completeness = 99.7%, R_{int} = 2.51%, R_{sig} = 2.02%) and 2684 were greater than $2\sigma(I)$. The final cell dimensions of a = 8.5366(8) Å, b = 20.8840(19) Å, c = 10.0597(9) Å, $\alpha = 90^{\circ}$, $\beta = 111.8290(10)^{\circ}$, $\gamma = 90^{\circ}$, V = 1664.8(3) Å³, are based upon the refinement of the XYZ-centroids of 6253 reflections with $2.4 < \theta < 28.9^{\circ}$ using Apex2. Analysis of the data showed 0% decay during data collection. Data were corrected for absorption effects with the Semi-empirical from equivalents method using SADABS (Sheldrick, 1996). The minimum and maximum transmission coefficients were 0.813 and 0.958.

The structure was solved and refined using the SHELXS-97 (Sheldrick, 1990) and SHELXL-97 (Sheldrick, 1997) software in the space group $P2_1/c$ with Z = 2 for the formula unit $C_{36}H_{50}N_4O_4Rh_2$. The final anisotropic full-matrix least-squares refinement on F² with 208 variables converged at R₁=5.17 % for the observed data and wR₂=11.76 % for all data. The goodness-of-fit was 1.000. The largest peak on the final difference map was 0.600 $e/Å^3$ and the largest hole was -0.983 $e/Å^3$. On the basis of the final model, the calculated density was 1.613 g/cm³ and F(000), 832 e.

Details of the crystal data and structure refinement (Supplemental Table 7), atomic coordinates and equivalent isotropic atomic displacement parameters (Supplemental Table 8), anisotropic atomic displacement parameters (Supplemental Table 9), Hydrogen atom coordinates and isotropic atomic displacement parameters (Supplemental Table 10), bond lengths and angles (Supplemental Table 11) are shown below.

Table 7. Crystal data and structure refinement for **O**.

Empirical formula Formula weight $\begin{array}{c} C_{36}H_{50}N_4O_4Rh_2\\ 808.62 \end{array}$

_					
Temperature		150(2) K			
Wavelength		0.71073 Å			
Crystal size		$0.147 \times 0.092 \times 0.041 \text{ mm}^3$			
Crystal habit		orange/green prism			
Crystal system		Monoclinic			
Space group		$P2_1/c$			
Unit cell dimensions	5	a = 8.5366(8) Å	$\alpha = 90^{\circ}$		
		b = 20.8840(19) Å	$\beta = 111.8290(10)^{\circ}$		
		c = 10.0597(9)Å	$\gamma = 90^{\circ}$		
Volume		$1664.8(3) Å^3$			
Z		2			
Density $\rho_{\rm sole}$		$\frac{1}{1}$ 613 g/cm ³			
Absorption coefficie	ent II	1.037 mm^{-1}			
F(000)	μin, μ	832 6			
Diffractometer		Bruker Smart Apex II C	CD area detector		
Radiation source		fine-focus sealed tube	MoK a		
Detector distance		5.2 cm	violea		
Detector distance		$\frac{3.2}{2}$ nivels/mm			
Total frames		1721			
From aire		1/31 1024 minula			
Frame size		1024 pixels			
Frame width		0.3			
Exposure per frame		30 sec			
Total measurement t	lime	21.9 hours			
Data collection meth	nod	(i) scans			
θ range for data colle	ection	2.57 to 25.00°			
Index ranges		$-10 \le h \le 10, -24 \le k \le 24, -11 \le l \le 11$			
Reflections collected	1	12334			
Independent reflection	ons	2923			
Observed reflection,	$I > 2\sigma(I)$	2684			
Coverage of indepen	ident reflections	99.7 %			
Variation in check re	eflections	0 %			
Absorption correction	on	Semi-empirical from eq	uivalents		
*		SADABS (Sheldrick, 19	996)		
Max. and min. transi	mission	0.958 and 0.813	,		
Structure solution te	chnique	direct			
Structure solution pr	ogram	SHELXS-97 (Sheldrick, 1990)			
Refinement techniqu	ie	Full-matrix least-squares on F^2			
Refinement program	1	SHELXL-97 (Sheldrick	. 1997)		
Function minimized		$\Sigma w (F_{2}^{2} - F_{2}^{2})^{2}$	7 7		
Data / restraints / par	rameters	2923 / 0 / 208			
Goodness-of-fit on F	72	1 000			
Λ/σ		0.000			
Einal P indices:	$\mathbf{P} = \mathbf{I} \ge 2\boldsymbol{\sigma}(\mathbf{I})$	0.0517			
i mai ix multes.	$\mathbf{R}_{\mathrm{I}}, \mathbf{P}_{\mathrm{20}(\mathrm{I})}$	0.0017			
	WK_2 , all data	0.1176			
	K _{int}	0.0251			
	R _{sig}	0.0202			
Weighting scheme		$w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 0$	$P], P = [max(F_o^2, 0) + 2F_o^2]/3$		
Correct the scheme a	as in $w=1/[^2(Fo^2)+$	$(0.008P)^{2}+17.6P], P=($	$(\max(Fo^{2^{,0})+2Fc^{2^{,0}}})/3$		
Largest diff. peak an	id hole 0.600 and -0.983 \overline{e}/A	13			

 $R_{1} = \Sigma ||F_{o}| - |F_{c}|| / \Sigma |F_{o}|, \quad wR2 = [\Sigma w (F_{o}^{2} - F_{c}^{2})^{2} / \Sigma w (F_{o}^{2})^{2}]^{1/2}$

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I able 8. Atomic coordinates and	equivalent isotro	pic atomic displac	ement parameters (A-)) for U .

Atom	x/a	<i>y/b</i>	z/c	U _{eq}	
Rh1	1.02301(6)	0.05348(2)	0.45453(5)	0.03395(17)	
C1	1.1472(8)	0.1238(3)	0.4038(7)	0.0372(14)	
C2	1.2782(9)	0.1560(3)	0.5086(8)	0.0430(16)	
C3	1.3566(10)	0.2070(3)	0.4725(9)	0.0512(18)	
C4	1.3120(10)	0.2249(4)	0.3324(9)	0.056(2)	

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05	1 10 45(10)	0.1024(4)	0.0054(0)	0.0524(10)	
05	1.1845(10)	0.1924(4)	0.2254(9)	0.0534(19)	
C6	1.1034(9)	0.1413(3)	0.2623(7)	0.0412(15)	
N1	0.7809(6)	0.0788(2)	0.3592(6)	0.0357(12)	
01	0.7328(5)	-0.0179(2)	0.4410(5)	0.0419(11)	
C11	0.6798(8)	0.0350(3)	0.3730(7)	0.0371(14)	
C12	0.4903(8)	0.0431(4)	0.3085(8)	0.0485(17)	
C13	0.4203(11)	0.0388(4)	0.1472(9)	0.065(2)	
C14	0.4438(11)	0.0987(4)	0.0713(10)	0.068(2)	
C15	0.6248(11)	0.1214(4)	0.1133(10)	0.070(2)	
C16	0.7117(10)	0.1367(4)	0.2727(10)	0.062(2)	
N2	1.0208(7)	0.0928(2)	0.6376(6)	0.0386(13)	
O2	0.9917(6)	-0.0050(2)	0.7265(5)	0.0409(11)	
C21	1.0008(9)	0.0570(3)	0.7334(7)	0.0421(15)	
C22	0.9844(11)	0.0849(4)	0.8652(8)	0.056(2)	
C23	0.8116(15)	0.1150(5)	0.8402(12)	0.090(3)	
C24	0.7940(13)	0.1837(5)	0.7813(10)	0.076(3)	
C25	0.8183(12)	0.1886(5)	0.6385(10)	0.071(2)	
C26	0.9930(13)	0.1646(4)	0.6464(11)	0.075(3)	
* U _{eq} is defined	as one third of the trace of the	he orthogonalized U _{ij} tensor.			

T.I.I. 0	A :		1:	.1	*	· · * 2) 6 4	
Table 9.	Anisotro	pic atomic	dist	placement	parameters	(A-) for (J.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂	
Rh1	0.0377(3)	0.0281(3)	0.0404(3)	-0.0026(2)	0.0195(2)	-0.0022(2)	
C1	0.043(4)	0.026(3)	0.051(4)	0.001(3)	0.027(3)	0.001(3)	
C2	0.044(4)	0.038(4)	0.047(4)	0.000(3)	0.019(3)	-0.004(3)	
C3	0.050(4)	0.042(4)	0.061(5)	0.001(4)	0.021(4)	-0.007(3)	
C4	0.060(5)	0.041(4)	0.073(6)	0.009(4)	0.030(4)	-0.006(4)	
C5	0.064(5)	0.049(4)	0.054(5)	0.012(4)	0.029(4)	0.002(4)	
C6	0.042(4)	0.040(4)	0.043(4)	0.000(3)	0.018(3)	-0.002(3)	
N1	0.030(3)	0.027(3)	0.050(3)	-0.002(2)	0.015(2)	0.005(2)	
O1	0.030(2)	0.045(3)	0.051(3)	0.008(2)	0.016(2)	0.000(2)	
C11	0.034(3)	0.034(3)	0.045(4)	-0.004(3)	0.017(3)	-0.001(3)	
C12	0.039(4)	0.046(4)	0.063(5)	0.004(3)	0.022(3)	0.005(3)	
C13	0.059(5)	0.062(5)	0.075(6)	0.000(4)	0.026(4)	0.001(4)	
C14	0.067(6)	0.069(6)	0.072(6)	0.013(5)	0.030(5)	0.017(5)	
C15	0.073(6)	0.062(5)	0.085(7)	0.018(5)	0.040(5)	0.016(5)	
C16	0.049(5)	0.041(4)	0.103(7)	0.004(4)	0.035(5)	0.007(4)	
N2	0.054(3)	0.028(3)	0.042(3)	-0.009(2)	0.027(3)	-0.011(2)	
O2	0.054(3)	0.031(2)	0.041(3)	-0.0019(19)	0.022(2)	0.000(2)	
C21	0.047(4)	0.038(4)	0.039(4)	-0.007(3)	0.013(3)	0.002(3)	
C22	0.077(6)	0.044(4)	0.049(4)	-0.008(3)	0.026(4)	0.001(4)	
C23	0.124(9)	0.077(7)	0.095(8)	-0.005(6)	0.072(7)	-0.003(6)	
C24	0.083(7)	0.070(6)	0.078(6)	-0.005(5)	0.034(5)	0.012(5)	
C25	0.077(6)	0.068(6)	0.072(6)	-0.002(5)	0.031(5)	0.007(5)	
C26	0.087(7)	0.058(5)	0.092(7)	-0.010(5)	0.047(6)	-0.010(5)	

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2$ [$h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}$]

							7.	
Table 10.	Hydrogen	atom coordinates	and isotropic	atomic	displacement	parameters	(A²)	for O .

Atom	x/a	<i>y/b</i>	z/c	U _{iso}	
H2	1.3138	0.1426	0.6056	0.052	
H3	1.4422	0.2299	0.5454	0.061	
H4	1.3683	0.2596	0.3081	0.068	
H5	1.1529	0.2048	0.1281	0.064	
H6	1.0175	0.1184	0.1895	0.049	
H12A	0.4371	0.0096	0.3473	0.058	
H12B	0.4602	0.0852	0.3374	0.058	
H13A	0.2981	0.0293	0.1143	0.078	
H13B	0.4752	0.0025	0.1184	0.078	
H14A	0.3971	0.0906	-0.0332	0.082	

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H14B	0.3770	0.1338	0.0905	0.082	
H15A	0.6260	0.1603	0.0573	0.084	
H15B	0.6903	0.0879	0.0873	0.084	
H16A	0.8045	0.1675	0.2859	0.075	
H16B	0.6295	0.1572	0.3073	0.075	
H22A	1.0725	0.1180	0.9048	0.067	
H22B	1.0060	0.0507	0.9380	0.067	
H23A	0.7935	0.1154	0.9319	0.108	
H23B	0.7224	0.0880	0.7720	0.108	
H24A	0.6805	0.2001	0.7686	0.091	
H24B	0.8783	0.2113	0.8525	0.091	
H25A	0.8042	0.2338	0.6068	0.086	
H25B	0.7293	0.1632	0.5657	0.086	
H26A	1.0175	0.1855	0.5679	0.090	
H26B	1.0782	0.1803	0.7375	0.090	

Table 11. Bond lengths (Å) and angles (°) for O_{\cdot}

Rh1-C1	1.986(6)	Rh1-N1	1.999(5)
Rh1-N2	2.023(5)	Rh1-O2#1	2.047(4)
Rh1-O1#1	2.091(4)	Rh1-Rh1#1	2.4994(10)
C1-C6	1.380(9)	C1-C2	1.391(9)
C2-C3	1.376(9)	C3-C4	1.369(11)
C4-C5	1.390(11)	C5-C6	1.396(10)
N1-C11	1.300(8)	N1-C16	1.478(9)
01-C11	1.289(8)	O1-Rh1#1	2.091(4)
C11-C12	1.512(9)	C12-C13	1.509(11)
C13-C14	1.518(11)	C14-C15	1.518(12)
C15-C16	1.530(12)	N2-C21	1.281(8)
N2-C26	1.526(10)	O2-C21	1.296(8)
O2-Rh1#1	2.047(4)	C21-C22	1.502(9)
C22-C23	1.536(13)	C23-C24	1.538(13)
C24-C25	1.529(12)	C25-C26	1.547(12)
	()		
C1-Rh1-N1	103.7(2)	C1-Rh1-N2	96.9(2)
N1-Rh1-N2	88.4(2)	C1-Rh1-O2#1	90.0(2)
N1-Rh1-O2#1	89.6(2)	N2-Rh1-O2#1	173.13(19)
C1-Rh1-O1#1	82.2(2)	N1-Rh1-O1#1	174.05(19)
N2-Rh1-O1#1	91.8(2)	O2#1-Rh1-O1#1	89.50(19)
C1-Rh1-Rh1#1	157.90(19)	N1-Rh1-Rh1#1	97.86(15)
N2-Rh1-Rh1#1	88.51(15)	O2#1-Rh1-Rh1#1	85.26(12)
O1#1-Rh1-Rh1#1	76.21(12)	C6-C1-C2	119.2(6)
C6-C1-Rh1	119.6(5)	C2-C1-Rh1	121.2(5)
C3-C2-C1	120.5(7)	C4-C3-C2	120.4(7)
C3-C4-C5	120.1(7)	C4-C5-C6	119.4(7)
C1-C6-C5	120.4(7)	C11-N1-C16	120.2(6)
C11-N1-Rh1	111.8(4)	C16-N1-Rh1	127.9(4)
C11-O1-Rh1#1	131.2(4)	O1-C11-N1	122.9(6)
01-C11-C12	115.6(6)	N1-C11-C12	121.5(6)
C13-C12-C11	112.8(6)	C12-C13-C14	114.8(7)
C15-C14-C13	115.4(7)	C14-C15-C16	113.8(7)
N1-C16-C15	112.3(7)	C21-N2-C26	117.6(6)
C21-N2-Rh1	119.7(4)	C26-N2-Rh1	120.4(5)
C21-O2-Rh1#1	121.6(4)	N2-C21-O2	124.4(6)
N2-C21-C22	121.3(6)	O2-C21-C22	114.3(6)
C21-C22-C23	114.4(7)	C22-C23-C24	113.3(8)
C25-C24-C23	113.4(8)	C24-C25-C26	113.3(8)
N2-C26-C25	118.9(7)		

Symmetry transformation codes:#1 -x+2,-y,-z+1

Details of the x-ray structural analysis of PhACO. A purple prism of $C_{40}H_{58}N_4O_4Rh_2 \cdot 2CH_2Cl_2$, approximate dimensions 0.275′ 0.33′ 0.42 mm³, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 200(2) K on a three-circle diffractometer system equipped with Bruker Smart Apex II CCD area detector using a graphite monochromator and a MoK α fine-focus sealed tube (λ = 0.71073 Å). The detector was placed at a distance of 5.0000 cm from the crystal.

A total of 2184 frames were collected with a scan width of -0.5° in ω and an exposure time of 13 sec/frame using Apex2 (Bruker, 2005). The total data collection time was 11.5 hours. The frames were integrated with Apex2 software package using a narrow-frame integration algorithm. The integration of the data using a Triclinic unit cell yielded a total of 22338 reflections to a maximum θ angle of 30.00°, of which 6347 were independent (completeness = 99.3%, R_{int} = 5.80%, R_{sig} = 3.28%) and 6166 were greater than $2\sigma(I)$. The final cell dimensions of a = 10.0542(3) Å, b = 11.0233(3) Å, c = 11.6576(3) Å, $\alpha = 88.0671(4)^{\circ}$, $\beta = 65.9778(3)^{\circ}$, $\gamma = 69.4042(4)^{\circ}$, V = 1095.59(5) Å³, are based upon the refinement of the XYZ-centroids of 21281 reflections with $2.3 < \theta < 32.1^{\circ}$ using Apex2. Analysis of the data showed 0 % decay during data collection. Data were corrected for absorption effects with the Semi-empirical from equivalents method using SADABS (Sheldrick, 1996). The minimum and maximum transmission coefficients were 0.686 and 0.751.

The structure was solved and refined using the SHELXS-97 (Sheldrick, 1990) and SHELXL-97 (Sheldrick, 1997) software in the space group *P*-1 with Z = 1 for the formula unit $C_{40}H_{58}N_4O_4Rh_2$ (2CH₂Cl₂. The final anisotropic full-matrix least-squares refinement on F² with 290 variables converged at R₁=1.99 % for the observed data and wR₂=4.66 % for all data. The goodness-of-fit was 1.000. The largest peak on the final difference map was 0.721 e/Å³ and the largest hole was - 0.704 e/Å³. On the basis of the final model, the calculated density was 1.568 g/cm³ and F(000), 532 e. Fifteen restraints were employed to restrain geometry and atomic displacement parameters of disordered ligand (C13 to C16) described as superposition of two alternative conformations.

Details of the crystal data and structure refinement (Supplemental Table 12), atomic coordinates and equivalent isotropic atomic displacement parameters (Supplemental Table 13), anisotropic atomic displacement parameters (Supplemental Table 14), Hydrogen atom coordinates and isotropic atomic displacement parameters (Supplemental Table 15), and bond lengths and angles (Supplemental Table 16) are shown below.

Table 12.	Crystal	data	and	structure	refinement	for 1	PhAC	0.
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Formula weight	1034.58
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal size	$0.42 \text{'} 0.33 \text{'} 0.275 \text{mm}^3$
Crystal habit	purple prism
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	$a = 10.0542(3) \text{ Å}$ $a = 88.0671(4)^{\circ}$
	$b = 11.0233(3) \text{ Å}$ $b = 65.9778(3)^{\circ}$
	$c = 11.6576(3)$ Å $g = 69.4042(4)^{\circ}$
Volume	1095.59(5) Å ³
Z	1
Density, r _{calc}	1.568 g/cm^3
Absorption coefficient, m	1.043 mm^{-1}
F(000)	532`e
Diffractometer	Bruker Smart Apex II CCD area detector
Radiation source	fine-focus sealed tube, MoKa

Detector distance		5.0000 cm		
Detector resolution		11.198 pixels/mm		
Total frames		2184		
Frame size		512 pixels		
Frame width		-0.5°		
Exposure per frame		13 sec		
Total measurement tin	me	11.5 hours		
Data collection metho	od	w and ϕ scans		
q range for data colled	ction	1.99 to 30.00°		
Index ranges		-14 £ <i>h</i> £ 14, -15 £ <i>k</i> £ 15, -16 £ <i>l</i> £ 16		
Reflections collected		22338		
Independent reflection	15	6347		
Observed reflection, I	>2s(I)	6166		
Coverage of independ	lent reflections	99.3 %		
Variation in check ref	lections	0 %		
Absorption correction	L	Semi-empirical from equivalents		
1		SADABS (Sheldrick, 1996)		
Max. and min. transm	ission	0.751 and 0.686		
Structure solution tech	nnique	direct		
Structure solution pro	gram	SHELXS-97 (Sheldrick, 1990)		
Refinement technique		Full-matrix least-squares on F ²		
Refinement program		SHELXL-97 (Sheldrick, 1997)		
Function minimized		$Sw(F_0^2 - F_c^2)^2$		
Data / restraints / para	imeters	6347 / 15 / 290		
Goodness-of-fit on F^2		1.003		
D/s _{max}		0.001		
Final R indices:	R_1 , $I > 2s(I)$	0.0199		
	wR ₂ , all data	0.0466		
	R _{int}	0.0580		
	R _{sig}	0.0328		
Weighting scheme	$w = 1/[s^2(F_0^2)+(0.01P)^2+1]$	091P], P = $[max(F_0^2, 0)+2F_0^2]/3$		
Largest diff. peak and	hole 0.721 and -0.704 e/Å	3		

 $\overline{R_1 = S||F_o| - |F_c||/S|F_o|}, \ wR2 = [Sw(F_o^2 - F_c^2)^2/S \ w(F_o^2)^2]^{1/2}$

Table 13. Atomic coordinates and equivalent^{*} isotropic atomic displacement parameters ($Å^2$) for **PhACO**.

Atom	x/a	<i>y/b</i>	z/c	U_{eq}	
Rh1	0.430393(11)	0.421754(9)	0.043074(9)	0.01432(3)	
N1	0.23041(13)	0.58538(10)	0.13268(10)	0.01771(19)	
O1	0.35742(11)	0.72644(9)	0.04471(9)	0.02028(18)	
C11	0.23351(15)	0.70314(12)	0.11439(12)	0.0180(2)	
C12	0.08951(16)	0.82788(13)	0.17310(15)	0.0248(3)	
C13	0.0728(2)	0.89071(16)	0.29485(17)	0.0349(3)	
C14	0.0101(3)	0.8237(3)	0.4111(2)	0.0392(6)	
C15	0.1205(3)	0.6848(3)	0.4067(2)	0.0421(7)	
C16	0.0780(2)	0.57775(17)	0.36418(16)	0.0380(4)	
C13A	0.0728(2)	0.89071(16)	0.29485(17)	0.0349(3)	
C14A	0.1077(9)	0.7972(6)	0.3919(5)	0.0365(15)	
C15A	-0.0007(7)	0.7209(5)	0.4394(5)	0.0344(14)	
C16A	0.0780(2)	0.57775(17)	0.36418(16)	0.0380(4)	
C17	0.08684(17)	0.57422(14)	0.23106(14)	0.0253(3)	
N2	0.45856(13)	0.39575(11)	0.20473(10)	0.0183(2)	
O2	0.56468(12)	0.55123(9)	0.13796(9)	0.02083(18)	
C21	0.52397(15)	0.47414(12)	0.21950(12)	0.0182(2)	
C22	0.55523(18)	0.48609(14)	0.33449(13)	0.0236(3)	

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C23	0.72368(19)	0.40451(16)	0.31396(15)	0.0296(3)
C24	0.7597(2)	0.25848(17)	0.31725(18)	0.0359(4)
C25	0.7477(2)	0.18945(16)	0.21132(17)	0.0332(3)
C26	0.5933(2)	0.16984(15)	0.24409(18)	0.0326(3)
C27	0.44272(18)	0.29270(14)	0.28619(14)	0.0245(3)
C31	0.31543(15)	0.30861(12)	0.03735(12)	0.0177(2)
C32	0.36004(17)	0.18097(13)	0.06540(14)	0.0228(3)
C33	0.27779(18)	0.10292(14)	0.06224(16)	0.0277(3)
C34	0.15270(18)	0.15130(15)	0.02954(16)	0.0283(3)
C35	0.10948(17)	0.27837(14)	-0.00078(15)	0.0256(3)
C36	0.19097(16)	0.35657(13)	0.00177(13)	0.0211(2)
C1	0.4672(2)	0.15378(18)	0.72168(18)	0.0388(4)
Cl1	0.64585(6)	0.03320(6)	0.62097(6)	0.05963(15)
Cl2	0.34564(7)	0.21663(6)	0.64222(6)	0.05770(14)

^{*} U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor. ^{**} Occupation factors C13 – C16 = 0.718(5), C13A – C16A = 0.282(5) and the same for corresponding H atoms

Table 14.	Anisotropic atomic	displacement parame	eters [*] (Å ²) for	PhACO
	1 misou opie atomie	and placement parameter		I mico.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂	
Rh1	0.01686(5)	0.01331(4)	0.01436(5)	0.00328(3)	-0.00728(3)	-0.00667(3)	
N1	0.0175(5)	0.0171(5)	0.0175(5)	0.0020(4)	-0.0064(4)	-0.0065(4)	
01	0.0197(4)	0.0159(4)	0.0230(5)	0.0036(3)	-0.0073(4)	-0.0062(3)	
C11	0.0193(5)	0.0170(5)	0.0180(5)	0.0014(4)	-0.0098(5)	-0.0047(4)	
C12	0.0200(6)	0.0179(6)	0.0323(7)	0.0009(5)	-0.0110(5)	-0.0022(5)	
C13	0.0344(8)	0.0245(7)	0.0398(9)	-0.0094(6)	-0.0135(7)	-0.0055(6)	
C14	0.0325(14)	0.0424(13)	0.0300(12)	-0.0144(9)	-0.0130(10)	0.0020(10)	
C15	0.0385(14)	0.0512(14)	0.0230(11)	-0.0048(10)	-0.0169(10)	0.0042(11)	
C16	0.0411(9)	0.0349(8)	0.0225(7)	0.0093(6)	-0.0043(7)	-0.0079(7)	
C13A	0.0344(8)	0.0245(7)	0.0398(9)	-0.0094(6)	-0.0135(7)	-0.0055(6)	
C14A	0.046(4)	0.042(3)	0.025(3)	-0.003(2)	-0.016(3)	-0.017(3)	
C15A	0.034(3)	0.040(3)	0.020(2)	-0.0021(19)	-0.007(2)	-0.008(2)	
C16A	0.0411(9)	0.0349(8)	0.0225(7)	0.0093(6)	-0.0043(7)	-0.0079(7)	
C17	0.0213(6)	0.0247(6)	0.0231(6)	0.0008(5)	-0.0018(5)	-0.0096(5)	
N2	0.0216(5)	0.0184(5)	0.0165(5)	0.0057(4)	-0.0094(4)	-0.0079(4)	
O2	0.0289(5)	0.0222(4)	0.0172(4)	0.0066(3)	-0.0121(4)	-0.0135(4)	
C21	0.0201(5)	0.0187(5)	0.0150(5)	0.0028(4)	-0.0082(4)	-0.0056(4)	
C22	0.0314(7)	0.0262(6)	0.0173(6)	0.0039(5)	-0.0137(5)	-0.0113(5)	
C23	0.0324(7)	0.0353(8)	0.0292(7)	0.0059(6)	-0.0199(6)	-0.0135(6)	
C24	0.0386(9)	0.0346(8)	0.0416(9)	0.0089(7)	-0.0278(8)	-0.0091(7)	
C25	0.0319(8)	0.0283(7)	0.0396(9)	0.0029(6)	-0.0208(7)	-0.0044(6)	
C26	0.0411(9)	0.0224(7)	0.0447(9)	0.0128(6)	-0.0284(8)	-0.0120(6)	
C27	0.0317(7)	0.0246(6)	0.0234(6)	0.0117(5)	-0.0146(6)	-0.0149(6)	
C31	0.0191(5)	0.0169(5)	0.0183(5)	0.0023(4)	-0.0071(5)	-0.0087(4)	
C32	0.0243(6)	0.0186(6)	0.0290(7)	0.0063(5)	-0.0136(5)	-0.0093(5)	
C33	0.0313(7)	0.0199(6)	0.0357(8)	0.0074(5)	-0.0147(6)	-0.0137(5)	
C34	0.0287(7)	0.0260(7)	0.0355(8)	0.0035(6)	-0.0128(6)	-0.0169(6)	
C35	0.0240(6)	0.0270(7)	0.0307(7)	0.0029(5)	-0.0142(6)	-0.0118(5)	
C36	0.0224(6)	0.0187(5)	0.0239(6)	0.0032(5)	-0.0113(5)	-0.0077(5)	
C1	0.0437(10)	0.0371(9)	0.0325(8)	-0.0003(7)	-0.0124(7)	-0.0153(8)	
Cl1	0.0351(2)	0.0642(3)	0.0683(4)	-0.0157(3)	-0.0149(2)	-0.0117(2)	
Cl2	0.0453(3)	0.0679(4)	0.0621(3)	0.0021(3)	-0.0276(3)	-0.0171(3)	

* The anisotropic atomic displacement factor exponent takes the form: $-2p^2$ [$h^2a^{*2}U_{11} + ... + 2hka^{*b}U_{12}$]

Atom	x/a	<i>y/b</i>	z/c	U _{iso}	
H12A	-0.0041	0.8081	0.1908	0.039(4)	
H12B	0.0946	0.8908	0.1115	0.039(4)	
H13A	0.0020	0.9823	0.3109	0.033(5)	
H13B	0.1755	0.8894	0.2833	0.033(5)	
H14A	-0.0110	0.8770	0.4866	0.046(6)	
H14B	-0.0898	0.8207	0.4198	0.046(6)	
H15A	0.1181	0.6725	0.4910	0.049(6)	
H15B	0.2277	0.6745	0.3483	0.049(6)	
H16A	0.1480	0.4926	0.3713	0.039(5)	
H16B	-0.0290	0.5886	0.4237	0.039(5)	
H13C	-0.0346	0.9545	0.3378	0.033(5)	
H13D	0.1432	0.9392	0.2721	0.033(5)	
H14C	0.2166	0.7355	0.3516	0.046(6)	
H14D	0.0964	0.8490	0.4644	0.046(6)	
H15C	-0.0977	0.7684	0.4300	0.049(6)	
H15D	-0.0282	0.7145	0.5296	0.049(6)	
H16C	0.1843	0.5372	0.3591	0.039(5)	
H16D	0.0180	0.5253	0.4122	0.039(5)	
H17A	0.0803	0.4920	0.2093	0.037(4)	
H17B	-0.0043	0.6458	0.2303	0.037(4)	
H22A	0.4829	0.4585	0.4060	0.030(3)	
H22B	0.5334	0.5781	0.3571	0.030(3)	
H23A	0.7955	0.4175	0.2318	0.031(3)	
H23B	0.7447	0.4373	0.3794	0.031(3)	
H24A	0.6872	0.2455	0.3991	0.045(4)	
H24B	0.8660	0.2165	0.3118	0.045(4)	
H25A	0.7656	0.2399	0.1394	0.037(4)	
H25B	0.8328	0.1035	0.1832	0.037(4)	
H26A	0.5796	0.1139	0.3118	0.042(4)	
H26B	0.6040	0.1218	0.1696	0.042(4)	
H27A	0.3578	0.2682	0.2866	0.028(3)	
H27B	0.4132	0.3273	0.3730	0.028(3)	
H32	0.4458	0.1471	0.0866	0.028(5)	
H33	0.3076	0.0171	0.0824	0.038(5)	
H34	0.0973	0.0987	0.0278	0.034(5)	
H35	0.0247	0.3115	-0.0231	0.031(5)	
H36	0.1625	0.4417	-0.0204	0.031(5)	
H1A	0.4873	0.2248	0.7513	0.051(5)	
H1B	0.4137	0.1163	0.7958	0.051(5)	

Table 15. Hydrogen atom coordinates and isotropic atomic displacement parameters $(Å^2)$ for **PhACO**.

Table 16. Bond lengths (Å), valence and torsion angles (°) for PhACO.

1.9947(12)	Rh1-N2	2.0137(11)	Rh1-O1#1	2.0373(9)
2.0623(11)	Rh1-O2#1	2.1043(9)	Rh1-Rh1#1	2.52606(19)
1.3175(16)	N1-C17	1.4770(17)	O1-C11	1.2903(16)
2.0373(9)	C11-C12	1.5204(18)	C12-C13	1.521(2)
1.531(3)	C14-C15	1.531(3)	C15-C16	1.545(3)
1.519(2)	C14A-C15A	1.525(7)	N2-C21	1.3079(17)
1.4659(16)	O2-C21	1.2911(15)	O2-Rh1#1	2.1043(9)
1.5157(18)	C22-C23	1.532(2)	C23-C24	1.523(2)
1.539(2)	C25-C26	1.533(2)	C26-C27	1.538(2)
1.3900(17)	C31-C36	1.3998(18)	C32-C33	1.3975(19)
	1.9947(12) 2.0623(11) 1.3175(16) 2.0373(9) 1.531(3) 1.519(2) 1.4659(16) 1.5157(18) 1.539(2) 1.3900(17)	1.9947(12)Rh1-N22.0623(11)Rh1-O2#11.3175(16)N1-C172.0373(9)C11-C121.531(3)C14-C151.519(2)C14A-C15A1.4659(16)O2-C211.5157(18)C22-C231.539(2)C25-C261.3900(17)C31-C36	1.9947(12)Rh1-N22.0137(11)2.0623(11)Rh1-O2#12.1043(9)1.3175(16)N1-C171.4770(17)2.0373(9)C11-C121.5204(18)1.531(3)C14-C151.531(3)1.519(2)C14A-C15A1.525(7)1.4659(16)O2-C211.2911(15)1.5157(18)C22-C231.532(2)1.539(2)C25-C261.533(2)1.3900(17)C31-C361.3998(18)	1.9947(12)Rh1-N22.0137(11)Rh1-O1#12.0623(11)Rh1-O2#12.1043(9)Rh1-Rh1#11.3175(16)N1-C171.4770(17)O1-C112.0373(9)C11-C121.5204(18)C12-C131.531(3)C14-C151.531(3)C15-C161.519(2)C14A-C15A1.525(7)N2-C211.4659(16)O2-C211.2911(15)O2-Rh1#11.5157(18)C22-C231.532(2)C23-C241.539(2)C25-C261.533(2)C26-C271.3900(17)C31-C361.3998(18)C32-C33

C33-C34	1.384(2)	C34-C35	1.393(2)	C35-C36	1.3906(19)
C1-Cl1	1.7550(19)	C1-Cl2	1.765(2)		
C21 D1 1 120	105 55(5)	C21 D11 01//1	00 00(4)	NO DI 1 01//1	07.24(4)
C31-Rh1-N2	105.55(5)	C31-Kh1-O1#1	92.28(4)	N2-Kh1-O1#1	8/.34(4)
C31-Kh1-N1	94.62(5)	N2-Kh1-N1	90.73(4)	O1#1-Kh1-N1	1/3.10(4)
C31-Kn1-O2#1	81.10(4)	N2-Kn1-O2#1	1/1.41(4)	01#1-Kn1-02#1	86.97(4)
NI-KhI-O2#I	94.17(4)	C31-Kh1-Kh1#1	154.42(4)	N2-Kh1-Kh1#1	99.99(3)
Ol#I-KhI-KhI#I	87.47(3)	NI-KhI-KhI#I	86.33(3)	O2#1-Kh1-Kh1#1	73.34(3)
CII-NI-CI7	118.17(11)	CII-NI-RhI	120.48(9)	CI7-NI-Rhl	120.86(8)
C11-O1-Rh1#1	121.10(8)	Ol-Cll-Nl	124.43(12)	01-C11-C12	112.18(11)
N1-C11-C12	123.39(12)	C11-C12-C13	113.75(12)	C12-C13-C14	113.99(15)
C15-C14-C13	114.4(2)	C14-C15-C16	113.4(2)	C17-C16-C15	116.86(15)
N1-C17-C16	114.47(13)	C21-N2-C27	120.39(11)	C21-N2-Rh1	109.07(8)
C27-N2-Rh1	129.53(9)	C21-O2-Rh1#1	134.27(8)	O2-C21-N2	122.70(12)
O2-C21-C22	113.64(11)	N2-C21-C22	123.64(12)	C21-C22-C23	113.44(12)
C24-C23-C22	114.85(13)	C24C23-C24-C25	114.91(13)	C26-C25-C24	116.85(15)
C25-C26-C27	117.52(13)	N2-C27-C26	113.38(12)	C32-C31-C36	119.39(12)
C32-C31-Rh1	120.64(10)	C36-C31-Rh1	119.95(9)	C31-C32-C33	120.18(13)
C34-C33-C32	120.38(13)	C33-C34-C35	119.56(13)	C36-C35-C34	120.43(13)
C35-C36-C31	120.02(12)	Cl1-Cl-Cl2	110.77(10)		
C21 Ph1 N1 C11	150 74(10)	N2 Ph1 N1 C11	103 60(10)	02#1 Pb1 N1 C11	60.24(10)
Dh1#1 Dh1 N1 C11	-130.74(10)	C21 Ph1 N1 C17	37.42(11)	N2 Ph1 N1 C17	-09.34(10)
$\Omega^{2\#1}$ Ph1 N1 C17	3.04(10)	Dh1#1 Dh1 N1 C17	$\frac{57.42(11)}{168.21(10)}$	Dh1#1 O1 C11 N1	-08.24(10)
02#1-M11-M1-C17	110.01(10) 179.52(9)	$\mathbf{KIII} \# \mathbf{I} \cdot \mathbf{KIII} \cdot \mathbf{NII} \cdot \mathbf{CII} $	-108.21(10) 170.02(12)	RIII#1-01-011-N1	-1.60(10) -2.02(10)
C17 N1 C11 C12	1/8.33(8) 10.40(10)	CI/-NI-CII-OI	170.03(12)	C1 C11 C12 C12	-2.03(18)
VI /-NI-CII-CI2	-10.40(19)	C11 C12 C12 C14	177.34(10)	01-011-012-015	-84.10(10)
NI-CII-CI2-CI3	96.29(16)	C11-C12-C13-C14	-77.72(19)	C12-C13-C14-C15	00.2(3)
CI3-CI4-CI3-CI0	-98.8(3)	C14-C15-C16-C17	62.9(3)	C11-N1-C1/-C10	-84.17(10)
Rn1-N1-C1/-C16	87.85(13)	CI5-CI6-CI/-NI	46.0(2)	C31-Kn1-N2-C21	-1/5.6/(9)
01#1-Kh1-N2-C21	92.70(9)	NI-KhI-N2-C21	-80.67(9)	Kh1#1-Kh1-N2-C2	1 5.73(9)
C31-Rh1-N2-C27	16.04(13)	O1#1-Rh1-N2-C27	-75.59(12)	NI-RhI-N2-C2/	111.04(12)
Rh1#1-Rh1-N2-C27	-162.55(11)	Rh1#1-O2-C21-N2	-6.2(2)	Rh1#1-O2-C21-C2	2 175.32(9)
	C27-N2-C21-O2	167.98(12)	Rh1-N2-C21-O	2 -1.56(16)	C27-N2-C21-C22
-13.7(2)		Rh1-N2-C21-C22	176.75(10)	02-C21-C22-C23	-83.94(15)
N2-C21-C22-C23	97.62(16)		C21-C22-C23-C	224	-76.02(17)
C22-C23-C24-C25	63.9(2)	C23-C24-C25-C26	-96.66(18)		C24-C25-C26-C27
60.2(2)	C21-N2-C27-C26	5 -81.17(16)	Rh1-N2-C27-C2	26 85.98(15)	C25-
C26-C27-N2	46.73(19)	N2-Rh1-C31-C32	-45.27(12)	O1#1-Rh1-C31-C32	2 42.60(11)
N1-Rh1-C31-C32	-137.32(11)	O2#1-Rh1-C31-C32	129.17(12)	Rh1#1-Rh1-C31-C3	32 131.52(10)
N2-Rh1-C31-C36	136.32(11)	O1#1-Rh1-C31-C36	-135.82(11)	N1-Rh1-C31-C36	44.27(11)
O2#1-Rh1-C31-C36	-49.24(11)	Rh1#1-Rh1-C31-C36	5 -46.90(16)	C36-C31-C32-C33	-2.2(2)
Rh1-C31-C32-C33	179.41(11)	C31-C32-C33-C34	0.9(2)	C32-C33-C34-C35	0.3(2)
C33-C34-C35-C36	-0.1(2)	C34-C35-C36-C31	-1.2(2)	C32-C31-C36-C35	2.3(2)
Rh1-C31-C36-C35	-179.22(11)				

Symmetry transformation codes:#1: -x+1,-y+1,-z

Details of the x-ray structural analysis of ACOBF4. A purple needle of

 $C_{32}H_{54}N_6O_4Rh_2$ ·BF₄·2CH₃CN, approximate dimensions 0.025x0.07x0.255 mm³, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 200(2) K on a three-circle diffractometer system equipped with Bruker Smart Apex II CCD area detector using a graphite monochromator and a MoK α fine-focus sealed tube (λ = 0.71073 Å). The detector was placed at a distance of 5.0000 cm from the crystal.

A total of 1818 frames were collected with a scan width of -0.5° in and an exposure time of 40 sec/frame using Apex2 (Bruker, 2005). The total data collection time was 23.2 hours. The frames were integrated with Apex2 software package using a narrow-frame integration algorithm. The integration of

the data using a Monoclinic unit cell yielded a total of 19810 reflections to a maximum angle of 25.00°, of which 3653 were independent (completeness = 99.8%, $R_{int} = 3.72\%$, $R_{sig} = 2.54\%$) and 3296 were greater than 2 (I). The final cell dimensions of a = 24.381(2) Å, b = 7.1609(6) Å, c = 24.440(2) Å, $a = 90^\circ$, $\beta = 103.4465(13)^\circ$, $\gamma = 90^\circ$, V = 4150.0(6) Å³, are based upon the refinement of the XYZ-centroids of 8249 reflections with $2.7 < \theta < 30.7^\circ$ using Apex2. Analysis of the data showed 0 % decay during data collection. Data were corrected for absorption effects with the Semi-empirical from equivalents method using SADABS (Sheldrick, 1996). The minimum and maximum transmission coefficients were 0.856 and 0.979. Fifty restraints were employed to geometry and atomic displacement parameters of BF₄ ions disordered around inversion center in two alternative orientations.

The structure was solved and refined using the SHELXS-97 (Sheldrick, 1990) and SHELXL-97 (Sheldrick, 1997) software in the space group C2/c with Z = 4 for the formula unit $C_{32}H_{54}N_6O_4Rh_2$ ·BF₄·2CH₃CN. The final anisotropic full-matrix least-squares refinement on F² with 274 variables converged at R₁=3.14 % for the observed data and wR₂=6.67 % for all data. The goodness-of-fit was 1.000. The largest peak on the final difference map was $0.633\bar{e}/Å^3$ and the largest hole was - $0.753\bar{e}/Å^3$. On the basis of the final model, the calculated density was 1.539 g/cm³ and F(000), 1980 \bar{e} .

Table 17.	Crystal	data a	and	structure	refinemen	t for	ACOBF4
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Empirical formula Formula weight Temperature Wavelength Crystal size Crystal habit Crystal system Space group Unit cell dimensions	$\begin{array}{l} C_{32}H_{54}N_{6}O_{4}Rh_{2}\cdot BF_{4}\cdot 2CH_{3}CN \\ 961.55 \\ 200(2) K \\ 0.71073 \text{ Å} \\ 0.255 0.07 0.025 \text{ mm}^{3} \\ \text{purple needle} \\ \text{Monoclinic} \\ C2/c \\ a = 24.381(2) \text{ Å} \\ b = 7.1609(6) \text{ Å} \\ c = 24.440(2) \text{ Å} \\ c = 24.440(2) \text{ Å} \\ c = 90^{\circ} \end{array}$
Volume Z	4150.0(6) Å ³ 4
Density, _{calc} Absorption coefficient, F(000)	1.539 g/cm ³ 0.861 mm ⁻¹ 1980 e
Diffractometer Radiation source	Bruker Smart Apex II CCD area detector
Detector distance	5.000 cm
Total frames	11.198 pixels/mm 1818
Frame size Frame width	512 pixels -0 5°
Exposure per frame	40 sec
Data collection method	ω and φ scans
θ range for data collection Index ranges	1.71 to 25.00° -28 $\leq h \leq$ 28, -8 $\leq k \leq$ 8, -29 $\leq l \leq$ 29
Reflections collected	19810
Observed reflection, $I>2$ (I)	3033
Coverage of independent reflections	99.8 %
Variation in check reflections Absorption correction	0 % Semi-empirical from equivalents SADABS (Sheldrick, 1996)
Max. and min. transmission Structure solution technique	0.979 and 0.856 direct

Structure solution p	rogram	SHELXS-97 (Sheldrick, 1990)
Refinement techniq	ue	Full-matrix least-squares on F^2
Refinement program	n	SHELXL-97 (Sheldrick, 1997)
Function minimized	1	$\Sigma w (F_o^2 - F_c^2)^2$
Data / restraints / pa	arameters	3653 / 50 / 274
Goodness-of-fit on	F^2	0.996
Δ/σ_{max}		0.001
Final R indices:	R_1 , $I \ge 2\sigma(I)$	0.0314
	wR ₂ , all data	0.0667
	R _{int}	0.0372
	R _{sig}	0.0254
Weighting scheme	- 0	$w = 1/[\sigma^{2}(F_{o}^{2})+(0.015P)^{2}+25.96P], P = [max(F_{o}^{2},0)+2F_{o}^{2}]/3$
Largest diff. peak a	nd hole 0.633 and -0.7.	53 ē/Å ³

 $R_{1} = \Sigma ||F_{o}| - |F_{c}|| / \Sigma |F_{o}|, \ wR2 = [\Sigma w (F_{o}^{2} - F_{c}^{2})^{2} / \Sigma w (F_{o}^{2})^{2}]^{1/2}$



Figure S-2. Bisacetonitrile complex of dirhodium(II,III) tetrakis(1-aza-2-cyclooctanoate) = **ACOBF4**; view along the Rh-Rh bond axis with BF₄⁻ disordered and not shown. Bond lengths: Rh-Rh, 2.404 Å; Rh-N, 2.007 Å; Rh-O, 2.015 Å. Bond angles: AN-Rh-Rh, 174.1°; N-Rh-Rh, 88.5° and 88.5°; O-Rh-Rh, 87.8° and 87.9°.

Table 18. Atomic coordinates and equivalent^{*} isotropic atomic displacement parameters $(Å^2)$ for **ACOBF4**.

Atom	x/a	<i>y/b</i>	z/c	U _{eq}	
514					
Rhl	0.263/38(10)	0.15140(3)	0.040695(10)	0.01643(8)	
N1	0.28744(11)	-0.0587(4)	0.11101(11)	0.0238(6)	
C1	0.29874(14)	-0.1656(5)	0.14581(15)	0.0289(8)	
C2	0.31362(19)	-0.3003(6)	0.19135(18)	0.0534(12)	
O11	0.19168(8)	0.5020(3)	0.00286(9)	0.0205(5)	
N11	0.21831(10)	0.3154(3)	0.08007(10)	0.0184(5)	
C11	0.19254(12)	0.4644(4)	0.05472(13)	0.0189(6)	
C12	0.16195(14)	0.6062(4)	0.08260(14)	0.0252(7)	
C13	0.10082(14)	0.5561(5)	0.08287(15)	0.0328(8)	
C14	0.09149(15)	0.3973(5)	0.12148(17)	0.0385(9)	
C15	0.10896(16)	0.2033(5)	0.10671(17)	0.0383(9)	
C16	0.16694(15)	0.1375(5)	0.13908(14)	0.0311(8)	
C17	0.21490(13)	0.2728(5)	0.13795(13)	0.0230(7)	
O21	0.30393(8)	0.5088(3)	-0.00810(9)	0.0210(5)	
N21	0.32969(10)	0.3215(4)	0.06888(10)	0.0187(5)	
C21	0.33672(12)	0.4714(4)	0.04007(13)	0.0201(7)	
C22	0.38305(13)	0.6141(4)	0.05949(14)	0.0250(7)	
C23	0.43858(14)	0.5669(5)	0.04345(15)	0.0314(8)	
C24	0.47266(14)	0.4048(5)	0.07499(17)	0.0352(9)	
C25	0.44588(14)	0.2108(5)	0.06513(16)	0.0331(8)	

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C26	0.41625(14)	0.1420(5)	0.10960(15)	0.0323(8)
C27	0.37166(13)	0.2758(5)	0.12080(13)	0.0243(7)
N1A	0.18200(19)	0.7046(7)	0.23776(16)	0.0726(14)
C1A	0.1358(2)	0.7350(7)	0.23172(16)	0.0487(11)
C2A	0.0759(2)	0.7708(8)	0.2238(2)	0.0644(14)
$B1^{**}$	0.4983(5)	0.7356(9)	0.2504(6)	0.052(2)
F1	0.5184(5)	0.9048(10)	0.2438(6)	0.135(4)
F2	0.4878(7)	0.642(2)	0.2024(6)	0.143(7)
F3	0.4503(3)	0.7518(15)	0.2667(5)	0.132(3)
F4	0.5358(6)	0.640(2)	0.2881(7)	0.126(6)

^{*} U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor. ^{**} BF_4 is disordered around special site and occupation factor for all atoms (B1 – F4) was set to 0.5

Table 19. Anisotropic atomic displacement parameters [*] ($Å^2$) for ACOB

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂	
Rh1	0.01461(12)	0.01697(12)	0.01735(13)	0.00297(11)	0.00295(9)	0.00165(10)	
N1	0.0195(14)	0.0241(15)	0.0272(15)	0.0028(13)	0.0045(11)	0.0015(12)	
C1	0.0252(17)	0.0291(19)	0.0325(19)	0.0036(17)	0.0072(15)	0.0025(15)	
C2	0.054(3)	0.056(3)	0.050(3)	0.032(2)	0.010(2)	0.011(2)	
O11	0.0200(11)	0.0198(11)	0.0219(11)	0.0028(9)	0.0056(9)	0.0056(9)	
N11	0.0181(13)	0.0177(14)	0.0195(13)	0.0015(11)	0.0048(10)	0.0010(10)	
C11	0.0143(15)	0.0182(16)	0.0237(16)	-0.0007(13)	0.0035(12)	-0.0005(12)	
C12	0.0289(18)	0.0207(17)	0.0262(18)	-0.0006(14)	0.0069(14)	0.0048(14)	
C13	0.0243(18)	0.038(2)	0.037(2)	-0.0032(17)	0.0091(15)	0.0094(16)	
C14	0.0254(19)	0.046(2)	0.047(2)	-0.0052(19)	0.0149(17)	-0.0014(17)	
C15	0.033(2)	0.038(2)	0.045(2)	-0.0079(18)	0.0129(17)	-0.0150(17)	
C16	0.042(2)	0.0289(19)	0.0268(18)	0.0003(16)	0.0163(16)	-0.0020(17)	
C17	0.0269(17)	0.0234(17)	0.0183(16)	-0.0001(13)	0.0042(13)	0.0029(14)	
O21	0.0184(11)	0.0211(11)	0.0217(11)	0.0030(9)	0.0014(9)	-0.0011(9)	
N21	0.0146(12)	0.0208(14)	0.0194(13)	0.0018(11)	0.0015(10)	0.0008(11)	
C21	0.0184(15)	0.0202(16)	0.0226(16)	-0.0010(13)	0.0064(13)	0.0009(13)	
C22	0.0261(17)	0.0181(17)	0.0281(18)	0.0008(13)	0.0008(14)	-0.0027(13)	
C23	0.0240(18)	0.034(2)	0.035(2)	0.0020(16)	0.0049(15)	-0.0106(16)	
C24	0.0175(17)	0.041(2)	0.047(2)	-0.0004(18)	0.0069(16)	-0.0013(15)	
C25	0.0210(17)	0.032(2)	0.045(2)	-0.0055(17)	0.0041(16)	0.0048(15)	
C26	0.0231(17)	0.0282(19)	0.039(2)	0.0043(17)	-0.0064(15)	0.0001(15)	
C27	0.0224(16)	0.0255(17)	0.0216(16)	0.0022(14)	-0.0019(13)	-0.0044(14)	
N1A	0.058(3)	0.113(4)	0.042(2)	-0.016(2)	0.001(2)	-0.004(3)	
C1A	0.064(3)	0.052(3)	0.027(2)	-0.0037(19)	0.003(2)	-0.002(2)	
C2A	0.062(3)	0.079(4)	0.047(3)	-0.007(3)	0.002(2)	0.018(3)	
B1	0.057(5)	0.047(5)	0.053(5)	-0.016(14)	0.016(4)	0.006(14)	
F1	0.170(14)	0.072(5)	0.180(10)	0.009(7)	0.073(9)	-0.043(6)	
F2	0.216(18)	0.135(11)	0.062(6)	-0.051(7)	0.002(8)	0.056(10)	
F3	0.081(5)	0.154(9)	0.180(9)	-0.041(8)	0.067(6)	-0.002(6)	
F4	0.119(9)	0.121(10)	0.109(10)	-0.011(7)	-0.034(7)	0.067(9)	

* The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2$ [$h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}$]

Table 20. Hydrogen atom coordinates and isotropic atomic displacement parameters ($Å^2$) for ACOBF4.

Atom	x/a	<i>y/b</i>	z/c	U _{iso}	
H2A	0.3530	-0.2820	0.2113	0.080	
H2B	0.3087	-0.4271	0.1759	0.080	
H2C	0.2892	-0.2826	0.2176	0.080	
H12A	0.1620	0.7274	0.0632	0.030	

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H12B	0.1833	0.6230	0.1220	0.030
H13A	0.0825	0.6695	0.0934	0.039
H13B	0.0810	0.5234	0.0439	0.039
H14A	0.1125	0.4271	0.1603	0.046
H14B	0.0509	0.3939	0.1216	0.046
H15A	0.1082	0.2007	0.0660	0.046
H15B	0.0805	0.1128	0.1132	0.046
H16A	0.1656	0.1155	0.1787	0.037
H16B	0.1754	0.0165	0.1232	0.037
H17A	0.2089	0.3899	0.1573	0.028
H17B	0.2510	0.2174	0.1586	0.028
H22A	0.3904	0.6257	0.1009	0.030
H22B	0.3696	0.7369	0.0431	0.030
H23A	0.4300	0.5381	0.0027	0.038
H23B	0.4627	0.6798	0.0494	0.038
H24A	0.4803	0.4321	0.1158	0.042
H24B	0.5095	0.4007	0.0645	0.042
H25A	0.4182	0.2116	0.0284	0.040
H25B	0.4757	0.1200	0.0624	0.040
H26A	0.4448	0.1212	0.1452	0.039
H26B	0.3982	0.0203	0.0974	0.039
H27A	0.3524	0.2184	0.1481	0.029
H27B	0.3901	0.3920	0.1377	0.029
H2D	0.0609	0.8217	0.1860	0.097
H2E	0.0698	0.8609	0.2520	0.097
H2F	0.0564	0.6539	0.2280	0.097

Table 21. Bond lengths (Å), valence and torsion angles (°) for ACOBF4.

DL1 NO1	2.007(2)	DL1 N11	2.007(2)	Dh1 011#1	2.015(2)
KIII-N21 Db1 ()21#1	2.007(2)	KIII-INII Dh1 N1	2.007(2)	KIII - OI I # I Dh1 Dh1#1	2.013(2) 2.4041(5)
KIII-021#1	2.013(2) 1.120(4)	C1 C2	2.230(3)	KIII-KIII#I	2.4041(3)
NI-CI 011 DI:1#1	1.130(4)	VI-02 N11 C11	1.434(3) 1.217(4)	NILL CIT	1.291(4)
OII-KnI#I	2.015(2)	NII-CII CI2 CI2	1.31/(4) 1.524(5)	NTI-CT/ C12 C14	1.408(4)
C11-C12	1.515(4)	015-016	1.534(5)	016 017	1.528(5)
014-015	1.521(5)	CI5-CI6	1.525(5)	C16-C17	1.524(5)
021-021	1.288(4)	O21-Rh1#1	2.015(2)	N21-C21	1.31/(4)
N21-C27	1.470(4)	C21-C22	1.515(4)	C22-C23	1.532(5)
C23-C24	1.528(5)	C24-C25	1.530(5)	C25-C26	1.520(5)
C26-C27	1.521(5)	NIA-CIA	1.122(6)	CIA-C2A	1.452(7)
B1-F2	1.326(9)	B1-F4	1.326(9)	B1-F3	1.326(9)
B1-F1	1.331(8)				
N21-Rh1-N11	88.15(10)	N21-Rh1-O11#1	91.41(9)	N11-Rh1-O11#1	176.44(9)
N21-Rh1-O21#1	176.38(9)	N11-Rh1-O21#1	91.74(9)	O11#1-Rh1-O21#1	88.47(8)
N21-Rh1-N1	95.76(10)	N11-Rh1-N1	95.58(10)	O11#1-Rh1-N1	87.98(9)
O21#1-Rh1-N1	87.85(9)	N21-Rh1-Rh1#1	88.53(7)	N11-Rh1-Rh1#1	88.53(7)
O11#1-Rh1-Rh1#1	87.93(6)	O21#1-Rh1-Rh1#1	87.84(6)	N1-Rh1-Rh1#1	174.14(7)
C1-N1-Rh1	179.0(3)	N1-C1-C2	178.9(4)	C11-O11-Rh1#1	121.13(19)
C11-N11-C17	119.6(3)	C11-N11-Rh1	120.3(2)	C17-N11-Rh1	120.09(19)
O11-C11-N11	121.9(3)	O11-C11-C12	113.9(3)	N11-C11-C12	124.3(3)
C11-C12-C13	115.2(3)	C14-C13-C12	117.4(3)	C15-C14-C13	116.3(3)
C14-C15-C16	115.9(3)	C17-C16-C15	114.6(3)	N11-C17-C16	111.4(3)
C21-O21-Rh1#1	121.33(19)	C21-N21-C27	119.5(3)	C21-N21-Rh1	120.3(2)
C27-N21-Rh1	120.2(2)	O21-C21-N21	121.9(3)	O21-C21-C22	113.9(3)
N21-C21-C22	124.2(3)	C21-C22-C23	114.2(3)	C24-C23-C22	116.6(3)
C23-C24-C25	116.6(3)	C26-C25-C24	116.0(3)	C25-C26-C27	113.8(3)
N21-C27-C26	111.6(3)	N1A-C1A-C2A	179.0(6)	F2-B1-F4	108.3(7)
F2-B1-F3	108.0(10)	F4-B1-F3	110.5(10)	F2-B1-F1	110.8(11)
			25		

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F4-B1-F1	109.8(11)	F3-B1-F1	109.5(9)		
N21-Rh1-N11-C11	86.2(2)	O21#1-Rh1-N11-C1	1 -90.2(2)	N1-Rh1-N11-C11	-178.2(2)
Rh1#1-Rh1-N11-C11	-2.4(2)	N21-Rh1-N11-C17	-92.1(2)	O21#1-Rh1-N11-C17	91.5(2)
N1-Rh1-N11-C17	3.5(2)	Rh1#1-Rh1-N11-C1	7 179.3(2)	Rh1#1-O11-C11-N11	-6.1(4)
Rh1#1-O11-C11-C12	173.60(19)	C17-N11-C11-O11	-176.1(3)	Rh1-N11-C11-O11	5.6(4)
C17-N11-C11-C12	4.3(4)	Rh1-N11-C11-C12	-174.0(2)	O11-C11-C12-C13	96.0(3)
N11-C11-C12-C13	-84.4(4)	C11-C12-C13-C14	71.2(4)	C12-C13-C14-C15	-66.5(4)
C13-C14-C15-C16	97.4(4)	C14-C15-C16-C17	-52.3(4)	C11-N11-C17-C16	94.2(3)
Rh1-N11-C17-C16	-87.5(3)	C15-C16-C17-N11	-56.8(4)	N11-Rh1-N21-C21	-86.7(2)
O11#1-Rh1-N21-C21	89.8(2)	N1-Rh1-N21-C21	177.9(2)	Rh1#1-Rh1-N21-C21	1.9(2)
N11-Rh1-N21-C27	95.6(2)	O11#1-Rh1-N21-C2	-88.0(2)	N1-Rh1-N21-C27	0.1(2)
Rh1#1-Rh1-N21-C27	-175.9(2)	Rh1#1-O21-C21-N2	4.0(4)	Rh1#1-O21-C21-C22	-176.15(19)
C27-N21-C21-O21	173.8(3)	Rh1-N21-C21-O21	-3.9(4)	C27-N21-C21-C22	-6.0(4)
Rh1-N21-C21-C22	176.2(2)	O21-C21-C22-C23	-93.0(3)	N21-C21-C22-C23	86.9(4)
C21-C22-C23-C24	-71.5(4)	C22-C23-C24-C25	65.6(4)	C23-C24-C25-C26	-98.4(4)
C24-C25-C26-C27	54.3(4)	C21-N21-C27-C26	-93.5(3)	Rh1-N21-C27-C26	84.3(3)
C25-C26-C27-N21	55.1(4)				

Symmetry transformation codes:#1 -x+1/2,-y+1/2,-z

DFT Calculations. Optimization of the structures of **G** and **O** of bisphenyldirhodium(III) caprolactamate. The crystal structures were taken as the starting points for the optimizations. The optimized structures were verified using the normal mode analysis which indicated that all frequencies were in positive values. A comparison of the crystal and computational data in bond lengths and angles associated with the metal dirhodium(III) framework is given in Table S-1.

Table S-1. Experimental (Expt.) and calculated (Opt) data for selected bond lengths (in angstroms) and angles (in degrees) associated with the dirhodium(III) framework.

Dropartias	G (C _{2h})			O (Ci)		
Properties	Expt.	Opt-g	Opt-s	Expt.	Opt-g	Opt-s
Rh-Rh	2.514	2.586	2.584	2.499	2.588	2.586
Rh-C	1.998	2.008	2.007	1.986	2.007	2.007
Rh-N	2.004	2.054	2.054	1.995	2.045	2.045
Rh-N	2.012	2.054	2.054	2.023	2.062	2.062
Rh-O	2.072	2.141	2.142	2.047	2.128	2.129
Rh-O	2.092	2.141	2.142	2.091	2.158	2.160
C-N _{amide}	1.304	1.322	1.321	1.280	1.321	1.320
C-N _{amide}	1.307	1.322	1.321	1.300	1.322	1.322
C-Rh-Rh	156.2	156.1	156.2	157.9	155.4	155.5
N-Rh-Rh	94.5	94.8	94.9	88.5	92.8	92.9
N-Rh-Rh	95.3	94.8	94.9	98.0	97.4	97.3
O-Rh-Rh	78.4	77.6	77.7	76.2	79.6	79.6
O-Rh-Rh	79.3	77.6	77.7	75.1	75.1	75.2
$\triangle E_{rel} (kJ/mol)$	-	0.0	0.0	-	0.1	1.1

To investigate the origin of the conformational energies, conformation changes were calculated of the ligands only. The homologous compounds of 6- 7- and 8- member-rings (valarolactamate,

caprolactamate and 1-aza-2-cyclononanoate) were examined. The structural and energetic data are illustrated in the Figure S-3.



Figure S-3. The calculated energy pathways for 6-, 7-, 8-member-ring ligand molecules.

Table S-2. Experimental (Expt.) and calculated (Opt) data for selected bond lengths and angles associated with **PhACN**. The experimental data is based on the observed conformational orientation having a percentage of 78% of the propeller structure.

	Propeller			Biplanar
	Expt.	Opt 1	Opt 2	
Rh-Rh	2.526	2.526	2.526	2.526
Rh-C	1.995	2.017	2.015	2.039
Rh-N	2.014(2.062)	2.045(2.095)	2.041(2.096)	2.062(2.068)
Rh-O	2.037(2.104)	2.103(2.168)	2.099(2.177)	2.133(2.141)
C-Rh-Rh	154.4	153.1	152.7	151.9
N-Rh-Rh	86.3(100.0)	90.8(100.6)	89.9(101.7)	95.6(96.6)
O-Rh-Rh	73.3(87.5)	73.4(82.8)	72.3(83.7)	77.3(78.2)
$\triangle E_{rel}$		0.00	-0.74	9.42

Table S-3. Experimental (Expt.) and calculated (Opt) data for selected bond lengths and angles associated with **ACNBF4**. The experimental data is based on biplanar structure of **ACNBF4**.

	Bipl	Propeller	
	Expt	Opt	Opt
Rh-Rh	2.404	2.404	2.404
Rh-N	2.007	2.045(2.048)	2.052(2.054)
Rh-O	2.015	2.055(2.059)	2.049(2.051)
AN-Ru		2.365	2.364
AN-Rh-Rh	174.1	171.0	171.7
N-Rh-Rh	88.5	89.1(89.3)	88.3(88.4)
O-Rh-Rh	87.8	87.4(87.6)	88.2(88.3)
$\triangle E_{rel}$		0.00	-1.29