Supporting Information

The chiral crown conformation in chiral paddlewheel complexes

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General Considerations

All reactions were carried out in glassware that was flame-dried under vacuum and cooled under nitrogen. Toluene was dried with a column packed with activated neutral alumina. Chromatography was performed on silica gel (silicycle 40-63D, 60Å). For ^{13}C NMR, multiplicities were distinguished using an ATP pulse sequence: typical methylene and quaternary carbons appear 'up' (u); methine and methyl carbons appear 'down' (dn). Reagents were used directly as purchased from commercial sources without further purification. *N*-Phthaloyl (*S*)-*tert*-leuinate,[1] dirhodium tetrakis *N*-phthaloyl (*S*)-*tert*-leucinate (Rh$_2$(*S*-PTTL)$_4$),[1] and dirhodium tetrakis *N*-1,8-naphthoyl (*S*)-*tert*-leucinate (Rh$_2$(*S*-NTTL)$_4$),[2] were prepared according to methods described in the literature.

X-ray structural analysis for compounds **2, 3, 4** and **5** (datasets **joef097f, joef094a, joef099** and **joef086**): Crystals were selected and mounted on plastic mesh using Paratone® oil flash-cooled to the data collection temperature. Data were collected on a Brüker-AXS APEX CCD diffractometer with graphite-monochromated Mo-Kα radiation (λ=0.71073 Å). Unit cell parameters were obtained from 60 data frames, 0.3º ω, from three different sections of the Ewald sphere. The systematic absences in the data and the unit cell parameters were consistent for *P*2$_1$ and *P*2$_1$/*m* for **4** and, uniquely, to the reported space groups for **2, 3** and **5**. The acentric space group is consistent with the chirally resolved **4.** The data-sets were treated with SADABS absorption corrections based on redundant multiscan data (Sheldrick, G.M. 2008. Acta Cryst. A64, 112-122). The structures were solved using direct methods and refined with full-matrix, least-squares procedures on F^2. The absolute structure parameters refined to virtually nil indicating the true hand of the data-sets was established which were confirmed by chiral centers with absolute chirality known from the

synthetic method. Compound **2** has two severely disordered, cocrystallized, acetonitrile solvent molecules per compound molecule which were treated as diffused contributions (Squeeze/Platon: Spek, A. L. 2003, J. Appl. Cryst. 36, 7-13). A severely disordered ethanol coordinated to a copper atom in **2** was treated as a rigid group, modeled on a similar ethanol ligand on an ordered, good quality, dicopper structure (Agterberg, F. P. W. et al. 1998, Inorg. Chim. Acta 267, 183), in two positions with refined 60/40 site occupancy. Compound **3** has a severely disordered thf molecule coordinated to copper in two positions with a refined site occupancy of 51/49 with chemically equivalent bonds and atomic displacement parameters constrained to be similar between disordered contributions. A cocrystallized ethyl acetate solvent molecule was located in **3**. A void of 157 Å^3 in **3** was observed but without any significant electron density that could be assigned as a chemically reasonable solvent molecule. Three disordered acetonitrile molecules per compound molecule were located in **4** constrained to have similar 1,2 and 1,3 atomic distances. Three toluene molecules per monomer are found cocrystallized in **5**. Alerts in checkCIF (http://checkcif.iucr.org) arise from the Squeeze procedure in **2**, a small void in **3**, and unresolvable, minor disorder, mostly in solvent molecules, resulting in Hirshfeld test failures. A peak remaining in the final difference map of **4** is located less than 1 Å from a Rh atom and was ignored as an artifact. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were treated as idealized contributions. Atomic scattering factors and anomalous absorption coefficients are contained in the SHELXTL 6.12 program library (Sheldrick, G. M., *op. cit.*). The structures are filed with the CCDC under depositary numbers 761719 – 761721, and 770533.

Experimental Procedures

Copper(II) tetrakis *N*-phthaloyl-(*S*)-*tert*-leucinate Cu$_2$(*S*-PTTL)$_4$
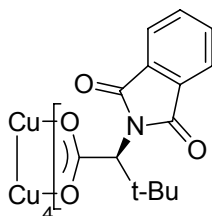
In a dry, 25 mL round-bottomed flask, copper(II) acetate (50 mg, 0.13 mmol) and *N*-phthaloyl-

(*S*)-*tert*-leucine[1] (164 mg, 0.630 mmol) were dissolved in chlorobenzene (6.3 mL). The flask was

fitted with a 10 mL addition funnel that was plugged with glass wool and filled with Na$_2$CO$_3$. The

top of the addition funnel was fitted with a reflux condenser, and the top of the reflux condenser

was fitted with a gas inlet adapter. The solution was heated to reflux in an oil bath at 165°C under

nitrogen atmosphere, with acetic acid being removed from the condensate by the Na$_2$CO$_3$. After

refluxing for 20 hours, the condenser and reflux condenser were removed, and replaced by a short

path distillation apparatus. The chlorobenzene was removed by distillation at atmospheric

pressure. The residue was dissolved in CH$_2$Cl$_2$ and washed twice with water, dried over

anhydrous MgSO$_4$, filtered, concentrated, and quickly chromatographed on silica gel (30-40%

ethyl acetate in hexane) to give 86 mg (0.074 mmol, 57%) of a blue solid. The complex was only

moderately stable in solution at ambient temperature, and broad spectral features were observed in

the ^{1}H NMR spectrum.

Spectral properties of the chromatographed material: $[\alpha]^{20}_{D}$ = 880° (*c*. 0.28, CH$_2$Cl$_2$); ^{1}H-NMR

(400 MHz, CDCl$_3$, δ): 7.64 (broad m, 16H), 4.64 (broad m, 4H), 2.18-0.73 (broad m, 36H). A

peak was observed at 2.46 ppm was attributed to an impurity. IR (neat, cm^{-1}): 2963, 1777, 1718,

1643, 1468, 1385, 1266, 1108, 902, 739, 720; HRMS-ESI m/z: [M+H], calc'd for

$Cu_2C_{56}H_{57}N_4O_{16}$, 1167.2362; found 1167.2380. X-ray quality crystals of $Cu_2(S\text{-PTTL})_4$ were grown as follows: the blue complex was dissolved in acetonitrile (~1 mL), which was then filtered through celite into a small tube (10 cm tall, 5 mm I.D.). This tube was then placed in a larger test tube (15 cm tall, 18 mm I.D.) that was filled with ~15 mL of 1:1 ethanol/water. The larger test tube was capped with a septum and sealed with parafilm. Crystals formed upon slow diffusion.

[Rh₂(S-PTTL)₄(NCC₆H₄CN)]ₙ

12 mg (0.010 mmol) of $Rh_2(S\text{-PTTL})_4$ and 26 mg (0.020 mmol) of 1,4-dicyanobenzene were dissolved in 2 mL 1:1 toluene:hexanes. X-ray quality crystals were grown by slow diffusion of the resulting solution into hexanes.

Rh₂(S-NTTL)₄(EtOAc)(C₄H₈O)

X-ray quality crystals of $Rh_2(S\text{-NTTL})_4$ were grown by slow evaporation of a solution of in 18:1:1 toluene:EtOAc:THF.

Rh₂(S-PTPA)₄(MeCN)₂

X-ray quality crystals of $Rh_2(S\text{-PTPA})_4(MeCN)_2$ were grown as follows: the complex was dissolved in acetonitrile (~1 mL), which was then filtered through celite into a small tube (10 cm tall, 5 mm I.D.). This tube was then placed in a larger test tube (15 cm tall, 18 mm I.D.) that was filled with ~15 mL of 1:1 ethanol/water. The larger test tube was capped with a septum and sealed with parafilm. Crystals formed upon slow diffusion.

^{1}H-NMR spectrum of Cu$_2$(S-PTTL)$_4$ (400 MHz, CD$_3$CN)
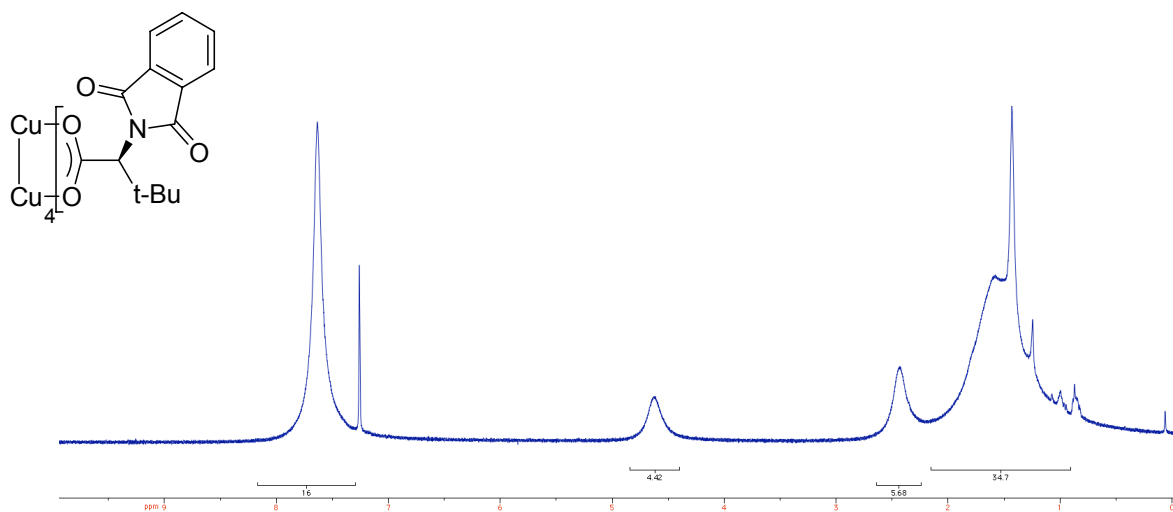
References

[1] Tsutsui, H.; Abe, T.; Nakamura, S.; Anada, M.; Hashimoto, S. *Chem. Pharm. Bull.* **2005**, *10*, 1366-1368.

[2] Müller, P.; Allenbach, Y. F.; Robert, E. *Tetrahedron: Asymmetry* **2003**, *14*, 779.

Summary of crystallographic details

Crystallographic details for **2**: $C_{64}H_{71}Cu_2N_7O_{17}$, 1337.36 dalton, orthorhombic, $P2_12_12$, a=25.068(4)Å, b=26.409(4)Å, c=10.1657(15)Å, V=6730.0(17)Å^3, T=200(2)K, Z=4, $Refl_{coll}$/$Refl_{unique}$/R_{int}=85763/16721/0.0533, $R(I_o>2I\sigma)$=0.0466, CCDC 761721

Crystallographic details for **3**: $C_{84}H_{88}N_4O_{21}Rh_2$, 1695.40 dalton, orthorhombic, $P2_12_12$, a=21.627(10)Å, b=21.826(10)Å, c=17.238(8)Å, V=8137(6)Å^3, T=200(2)K, Z=4, $Refl_{coll}$/$Refl_{unique}$/R_{int}=111612/20130/0.0526, $R(I_o>2I\sigma)$=0.0401, CCDC 761720

Crystallographic details for **4**: $C_{78}H_{63}N_9O_{16}Rh_2$, 1588.19 dalton, monoclinic, $P2_1$, a=12.649(4)Å, b=24.398(7)Å, c=12.670(4)Å, β=107.947(4)°, V = 3719.9(18)Å^3, T=200(2)K, Z=2, $Refl_{coll}$/$Refl_{unique}$/R_{int}=51127/18446/0.0403, $R(I_o>2I\sigma)$=0.0525, CCDC 770533

Crystallographic details for **5**: $C_{85}H_{84}N_6O_{16}Rh_2$, 1651.40 dalton, orthorhombic, $P2_12_12_1$, a=13.412(3)Å, b=21.7183(5)Å, c=27.323(6)Å, V = 7982(3)Å^3, T=170(2)K, Z=4, $Refl_{coll}$/$Refl_{unique}$/R_{int}=94308.19746/0.0469, $R(I_o>2I\sigma)$=0.0297, CCDC 761719.
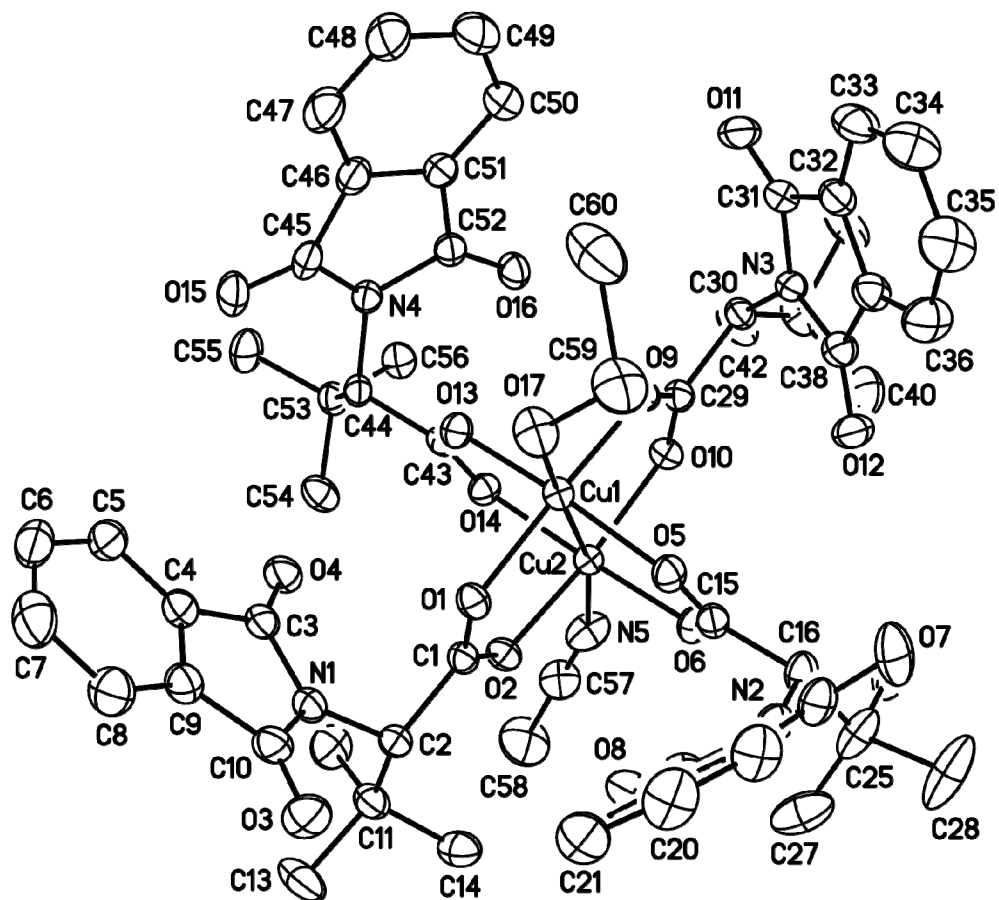
Figure 1. Molecular diagram of **2** with ellipsoids at 30% probability. Minor disordered contributor and H-atoms deleted for clarity.

Table 1. Crystal data and structure refinement for joef097f.

Identification code	joef097f
Empirical formula	C64 H71 Cu2 N7 O17
Formula weight	1337.36
Temperature	200(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2
Unit cell dimensions	a = 25.068(4) A alpha = 90 deg.
	b = 26.409(4) A beta = 90 deg.
	c = 10.1657(15) A gamma = 90 deg.
Volume	6730.0(17) A^3
Z, Calculated density	4, 1.320 Mg/m^3
Absorption coefficient	0.703 mm^-1
F(000)	2792
Crystal size	0.24 x 0.16 x 0.13 mm
Theta range for data collection	1.74 to 28.28 deg.
Limiting indices	-33<=h<=33, -35<=k<=35, -13<=l<=13
Reflections collected / unique	85763 / 16721 [R(int) = 0.0523]
Completeness to theta = 25.00	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9129 and 0.8472
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16721 / 1 / 776
Goodness-of-fit on F^2	1.073
Final R indices [I>2sigma(I)]	R1 = 0.0466, wR2 = 0.1084
R indices (all data)	R1 = 0.0552, wR2 = 0.1137
Absolute structure parameter	-0.009(8)
Largest diff. peak and hole	0.713 and -0.287 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for joef097f.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

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	x	y	z	U(eq)

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Cu(1)	3195(1)	3287(1)	7813(1)	33(1)
Cu(2)	3403(1)	3424(1)	10336(1)	31(1)
N(1)	4036(1)	1745(1)	8010(3)	43(1)
N(2)	1642(1)	2565(1)	9176(3)	47(1)
N(3)	2431(1)	4832(1)	7686(2)	36(1)
N(4)	4795(1)	4040(1)	7040(2)	39(1)
O(1)	3406(1)	2578(1)	8000(2)	40(1)
O(2)	3577(1)	2692(1)	10144(2)	40(1)
O(3)	3538(1)	1060(1)	7335(3)	68(1)
O(4)	4621(1)	2430(1)	8002(3)	54(1)
O(5)	2488(1)	3124(1)	8510(2)	43(1)
O(6)	2654(1)	3259(1)	10655(2)	41(1)
O(7)	956(1)	2900(1)	7940(3)	77(1)
O(8)	2375(1)	2076(1)	9776(3)	57(1)
O(9)	3010(1)	4001(1)	7843(2)	39(1)
O(10)	3182(1)	4129(1)	9987(2)	39(1)
O(11)	2840(1)	5352(1)	6154(2)	56(1)
O(12)	1865(1)	4239(1)	8611(2)	54(1)
O(13)	3947(1)	3472(1)	7623(2)	39(1)
O(14)	4133(1)	3581(1)	9761(2)	38(1)
O(15)	5164(1)	3520(1)	5457(3)	60(1)
O(16)	4233(1)	4636(1)	8008(2)	47(1)
C(1)	3562(1)	2433(1)	9116(3)	36(1)
C(2)	3723(1)	1869(1)	9196(3)	39(1)
C(3)	4451(1)	2046(1)	7507(3)	44(1)
C(4)	4626(1)	1789(1)	6277(3)	50(1)
C(5)	5030(2)	1907(2)	5420(4)	62(1)
C(6)	5111(2)	1597(2)	4354(4)	71(1)
C(7)	4790(2)	1175(2)	4168(4)	81(2)
C(8)	4378(2)	1055(2)	5021(4)	71(1)
C(9)	4305(2)	1368(1)	6089(3)	52(1)
C(10)	3905(2)	1350(1)	7174(4)	51(1)
C(11)	3991(1)	1683(1)	10483(3)	49(1)
C(12)	4498(2)	1967(2)	10823(4)	65(1)
C(13)	4113(2)	1107(1)	10298(5)	80(1)
C(14)	3581(2)	1730(2)	11607(3)	60(1)
C(15)	2358(1)	3142(1)	9708(3)	39(1)
C(16)	1767(1)	3023(1)	9940(3)	48(1)
C(17)	1274(1)	2571(2)	8139(4)	54(1)
C(18)	1377(1)	2098(1)	7374(4)	51(1)
C(19)	1120(2)	1906(2)	6281(4)	65(1)
C(20)	1328(2)	1473(2)	5725(4)	76(1)
C(21)	1773(2)	1234(2)	6251(4)	70(1)
C(22)	2028(2)	1429(1)	7350(4)	58(1)
C(23)	1817(1)	1865(1)	7905(3)	47(1)
C(24)	1999(1)	2156(1)	9063(3)	46(1)
C(25)	1554(2)	3017(2)	11367(4)	67(1)
C(26)	1636(2)	3544(2)	11981(4)	79(1)
C(27)	1811(2)	2616(2)	12204(4)	91(2)
C(28)	943(2)	2927(3)	11275(6)	117(3)

C(29)	3029(1)	4267(1)	8864(3)	37(1)
C(30)	2865(1)	4825(1)	8657(3)	37(1)
C(31)	2479(1)	5082(1)	6474(3)	43(1)
C(32)	1990(1)	4940(1)	5704(3)	47(1)
C(33)	1825(2)	5084(2)	4474(3)	60(1)
C(34)	1362(2)	4874(2)	3994(4)	73(1)
C(35)	1076(2)	4533(2)	4719(5)	79(1)
C(36)	1236(2)	4384(2)	5966(4)	68(1)
C(37)	1702(1)	4596(1)	6445(3)	46(1)
C(38)	1984(1)	4515(1)	7721(3)	44(1)
C(39)	2771(2)	5170(1)	9847(3)	50(1)
C(40)	2325(2)	4980(2)	10747(4)	74(1)
C(41)	2633(2)	5700(1)	9322(4)	71(1)
C(42)	3293(2)	5214(1)	10631(4)	65(1)
C(43)	4252(1)	3572(1)	8568(3)	35(1)
C(44)	4832(1)	3674(1)	8136(3)	36(1)
C(45)	4915(1)	3895(1)	5746(3)	47(1)
C(46)	4662(1)	4274(1)	4876(3)	50(1)
C(47)	4654(2)	4308(2)	3517(4)	72(1)
C(48)	4351(2)	4688(2)	2964(4)	86(2)
C(49)	4072(2)	5024(2)	3731(4)	77(1)
C(50)	4078(2)	4994(2)	5096(4)	57(1)
C(51)	4376(1)	4612(1)	5641(3)	44(1)
C(52)	4441(1)	4459(1)	7047(3)	40(1)
C(53)	5261(1)	3797(1)	9176(3)	41(1)
C(54)	5278(1)	3368(1)	10178(4)	54(1)
C(55)	5798(1)	3821(2)	8449(4)	61(1)
C(56)	5165(1)	4296(1)	9877(3)	48(1)
N(5)	3650(1)	3360(1)	12411(3)	61(1)
C(57)	3859(2)	3155(2)	13242(4)	60(1)
C(58)	4124(2)	2879(2)	14313(5)	99(2)
O(17)	2998(5)	3221(4)	5741(9)	58(1)
C(59)	2626(4)	3534(6)	5030(20)	96(3)
C(60)	2875(4)	4014(3)	4533(8)	110(3)
O(17')	2999(7)	3146(6)	5760(13)	58(1)
C(59')	2575(7)	3391(10)	5140(30)	96(3)
C(60')	2019(7)	3258(5)	5573(12)	110(3)

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Table 3.  Bond lengths [A] and angles [deg] for joef097f.
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        Cu(1)-O(9)                   1.9434(19)
        Cu(1)-O(1)                   1.9552(19)
        Cu(1)-O(13)                  1.956(2)
        Cu(1)-O(5)                   1.958(2)
        Cu(1)-O(17')                 2.177(13)
        Cu(1)-O(17)                  2.170(8)
        Cu(1)-Cu(2)                  2.6423(6)
        Cu(2)-O(6)                   1.954(2)
        Cu(2)-O(14)                  1.965(2)
        Cu(2)-O(10)                  1.975(2)
        Cu(2)-O(2)                   1.992(2)
        Cu(2)-N(5)                   2.205(3)
        N(1)-C(10)                   1.386(4)
        N(1)-C(3)                    1.404(4)
        N(1)-C(2)                    1.476(4)
        N(2)-C(17)                   1.400(4)
        N(2)-C(24)                   1.409(4)
        N(2)-C(16)                   1.471(4)
        N(3)-C(38)                   1.399(4)
        N(3)-C(31)                   1.402(4)
        N(3)-C(30)                   1.469(4)
        N(4)-C(45)                   1.403(4)
        N(4)-C(52)                   1.418(4)
        N(4)-C(44)                   1.479(4)
        O(1)-C(1)                    1.259(3)
        O(2)-C(1)                    1.249(3)
        O(3)-C(10)                   1.207(4)
        O(4)-C(3)                    1.209(4)
        O(5)-C(15)                   1.261(4)
        O(6)-C(15)                   1.253(4)
        O(7)-C(17)                   1.198(4)
        O(8)-C(24)                   1.207(4)
        O(9)-C(29)                   1.254(3)
        O(10)-C(29)                  1.258(3)
        O(11)-C(31)                  1.198(4)
        O(12)-C(38)                  1.199(4)
        O(13)-C(43)                  1.257(3)
        O(14)-C(43)                  1.250(3)
        O(15)-C(45)                  1.207(4)
        O(16)-C(52)                  1.202(4)
        C(1)-C(2)                    1.545(4)
        C(2)-C(11)                   1.550(4)
        C(3)-C(4)                    1.490(5)
        C(4)-C(5)                    1.372(5)
        C(4)-C(9)                    1.386(5)
        C(5)-C(6)                    1.372(6)
        C(6)-C(7)                    1.387(7)
        C(7)-C(8)                    1.385(6)
        C(8)-C(9)                    1.376(5)
        C(9)-C(10)                   1.492(5)
        C(11)-C(12)                  1.515(5)
        C(11)-C(14)                  1.540(5)
        C(11)-C(13)                  1.565(5)
        C(15)-C(16)                  1.534(4)
        C(16)-C(25)                  1.545(5)
        C(17)-C(18)                  1.492(5)
        C(18)-C(23)                  1.375(5)
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C(18)-C(19)                          1.381(5)
C(19)-C(20)                          1.377(6)
C(20)-C(21)                          1.388(6)
C(21)-C(22)                          1.387(5)
C(22)-C(23)                          1.386(5)
C(23)-C(24)                          1.478(5)
C(25)-C(27)                          1.506(7)
C(25)-C(26)                          1.539(6)
C(25)-C(28)                          1.553(6)
C(29)-C(30)                          1.544(4)
C(30)-C(39)                          1.534(4)
C(31)-C(32)                          1.501(5)
C(32)-C(33)                          1.370(5)
C(32)-C(37)                          1.385(5)
C(33)-C(34)                          1.375(6)
C(34)-C(35)                          1.366(6)
C(35)-C(36)                          1.387(6)
C(36)-C(37)                          1.382(5)
C(37)-C(38)                          1.494(4)
C(39)-C(40)                          1.530(6)
C(39)-C(41)                          1.537(5)
C(39)-C(42)                          1.538(5)
C(43)-C(44)                          1.543(4)
C(44)-C(53)                          1.543(4)
C(45)-C(46)                          1.479(5)
C(46)-C(51)                          1.382(5)
C(46)-C(47)                          1.385(5)
C(47)-C(48)                          1.378(6)
C(48)-C(49)                          1.373(6)
C(49)-C(50)                          1.390(6)
C(50)-C(51)                          1.373(5)
C(51)-C(52)                          1.495(4)
C(53)-C(56)                          1.516(4)
C(53)-C(54)                          1.525(5)
C(53)-C(55)                          1.536(5)
N(5)-C(57)                           1.131(5)
C(57)-C(58)                          1.469(6)
O(17)-C(59)                          1.4388
C(59)-C(60)                          1.5016
O(17')-C(59')                        1.3921
C(59')-C(60')                        1.5016

O(9)-Cu(1)-O(1)                    173.24(9)
O(9)-Cu(1)-O(13)                    89.39(9)
O(1)-Cu(1)-O(13)                    89.33(9)
O(9)-Cu(1)-O(5)                     89.52(9)
O(1)-Cu(1)-O(5)                     89.94(9)
O(13)-Cu(1)-O(5)                   164.43(9)
O(9)-Cu(1)-O(17')                   97.3(4)
O(1)-Cu(1)-O(17')                   89.4(4)
O(13)-Cu(1)-O(17')                  99.5(5)
O(5)-Cu(1)-O(17')                   96.0(5)
O(9)-Cu(1)-O(17)                    92.2(3)
O(1)-Cu(1)-O(17)                    94.6(3)
O(13)-Cu(1)-O(17)                   98.2(3)
O(5)-Cu(1)-O(17)                    97.3(3)
O(17')-Cu(1)-O(17)                   5.3(6)
O(9)-Cu(1)-Cu(2)                    84.22(6)
O(1)-Cu(1)-Cu(2)                    89.04(6)
O(13)-Cu(1)-Cu(2)                   82.65(6)
O(5)-Cu(1)-Cu(2)                    81.80(7)
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O(17')-Cu(1)-Cu(2)        177.3(5)
O(17)-Cu(1)-Cu(2)         176.3(3)
O(6)-Cu(2)-O(14)          172.21(9)
O(6)-Cu(2)-O(10)           88.22(9)
O(14)-Cu(2)-O(10)          90.49(9)
O(6)-Cu(2)-O(2)            90.61(9)
O(14)-Cu(2)-O(2)           88.45(9)
O(10)-Cu(2)-O(2)          163.54(8)
O(6)-Cu(2)-N(5)            95.42(10)
O(14)-Cu(2)-N(5)           92.26(10)
O(10)-Cu(2)-N(5)          108.87(11)
O(2)-Cu(2)-N(5)            87.58(11)
O(6)-Cu(2)-Cu(1)           86.61(6)
O(14)-Cu(2)-Cu(1)          85.62(6)
O(10)-Cu(2)-Cu(1)          84.21(6)
O(2)-Cu(2)-Cu(1)           79.33(6)
N(5)-Cu(2)-Cu(1)          166.79(10)
C(10)-N(1)-C(3)           112.3(3)
C(10)-N(1)-C(2)           122.8(3)
C(3)-N(1)-C(2)            124.4(3)
C(17)-N(2)-C(24)          111.4(3)
C(17)-N(2)-C(16)          121.9(3)
C(24)-N(2)-C(16)          122.6(3)
C(38)-N(3)-C(31)          111.9(3)
C(38)-N(3)-C(30)          124.5(2)
C(31)-N(3)-C(30)          122.3(2)


C(45)-N(4)-C(52)          110.6(3)
C(45)-N(4)-C(44)          120.9(2)
C(52)-N(4)-C(44)          123.1(2)
C(1)-O(1)-Cu(1)           117.55(18)
C(1)-O(2)-Cu(2)           127.34(19)
C(15)-O(5)-Cu(1)          125.06(19)
C(15)-O(6)-Cu(2)          119.73(19)
C(29)-O(9)-Cu(1)          123.14(18)
C(29)-O(10)-Cu(2)         121.42(18)
C(43)-O(13)-Cu(1)         124.29(19)
C(43)-O(14)-Cu(2)         120.52(19)
O(2)-C(1)-O(1)            126.6(3)
O(2)-C(1)-C(2)            118.4(2)
O(1)-C(1)-C(2)            114.9(2)
N(1)-C(2)-C(1)            108.0(2)
N(1)-C(2)-C(11)           112.9(2)
C(1)-C(2)-C(11)           117.5(2)
O(4)-C(3)-N(1)            125.7(3)
O(4)-C(3)-C(4)            128.9(3)
N(1)-C(3)-C(4)            105.4(3)
C(5)-C(4)-C(9)            121.6(4)
C(5)-C(4)-C(3)            130.4(4)
C(9)-C(4)-C(3)            108.1(3)
C(6)-C(5)-C(4)            118.3(4)
C(5)-C(6)-C(7)            120.1(4)
C(8)-C(7)-C(6)            122.0(4)
C(9)-C(8)-C(7)            117.1(4)
C(8)-C(9)-C(4)            120.9(4)
C(8)-C(9)-C(10)           130.8(4)
C(4)-C(9)-C(10)           108.3(3)
O(3)-C(10)-N(1)           125.1(3)
O(3)-C(10)-C(9)           129.3(3)
N(1)-C(10)-C(9)           105.6(3)
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C(12)-C(11)-C(14)	110.5(3)
C(12)-C(11)-C(2)	113.6(3)
C(14)-C(11)-C(2)	108.2(3)
C(12)-C(11)-C(13)	110.0(3)
C(14)-C(11)-C(13)	107.3(3)
C(2)-C(11)-C(13)	106.9(3)
O(6)-C(15)-O(5)	126.8(3)
O(6)-C(15)-C(16)	120.3(3)
O(5)-C(15)-C(16)	112.9(3)
N(2)-C(16)-C(15)	107.0(2)
N(2)-C(16)-C(25)	114.4(3)
C(15)-C(16)-C(25)	118.7(3)
O(7)-C(17)-N(2)	125.0(3)
O(7)-C(17)-C(18)	129.3(3)
N(2)-C(17)-C(18)	105.7(3)
C(23)-C(18)-C(19)	121.6(4)
C(23)-C(18)-C(17)	108.0(3)
C(19)-C(18)-C(17)	130.3(4)
C(20)-C(19)-C(18)	117.4(4)
C(19)-C(20)-C(21)	121.6(4)
C(22)-C(21)-C(20)	120.8(4)
C(23)-C(22)-C(21)	117.4(4)
C(18)-C(23)-C(22)	121.2(3)

C(18)-C(23)-C(24)	109.1(3)
C(22)-C(23)-C(24)	129.7(3)
O(8)-C(24)-N(2)	125.5(3)
O(8)-C(24)-C(23)	129.0(3)
N(2)-C(24)-C(23)	105.5(3)
C(27)-C(25)-C(26)	110.5(4)
C(27)-C(25)-C(16)	112.9(4)
C(26)-C(25)-C(16)	109.0(3)
C(27)-C(25)-C(28)	110.4(4)
C(26)-C(25)-C(28)	107.1(4)
C(16)-C(25)-C(28)	106.6(4)
O(9)-C(29)-O(10)	127.0(3)
O(9)-C(29)-C(30)	114.2(2)
O(10)-C(29)-C(30)	118.8(3)
N(3)-C(30)-C(39)	114.1(2)
N(3)-C(30)-C(29)	107.6(2)
C(39)-C(30)-C(29)	120.1(2)
O(11)-C(31)-N(3)	125.7(3)
O(11)-C(31)-C(32)	128.6(3)
N(3)-C(31)-C(32)	105.8(3)
C(33)-C(32)-C(37)	121.4(3)
C(33)-C(32)-C(31)	130.8(3)
C(37)-C(32)-C(31)	107.8(3)
C(32)-C(33)-C(34)	117.8(4)
C(35)-C(34)-C(33)	121.1(4)
C(34)-C(35)-C(36)	121.9(4)
C(37)-C(36)-C(35)	116.8(4)
C(36)-C(37)-C(32)	121.0(3)
C(36)-C(37)-C(38)	130.5(3)
C(32)-C(37)-C(38)	108.6(3)
O(12)-C(38)-N(3)	125.7(3)
O(12)-C(38)-C(37)	128.6(3)
N(3)-C(38)-C(37)	105.8(3)
C(40)-C(39)-C(30)	112.9(3)
C(40)-C(39)-C(41)	110.0(3)
C(30)-C(39)-C(41)	107.6(3)

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C(40)-C(39)-C(42)          109.7(3)
C(30)-C(39)-C(42)          108.8(3)
C(41)-C(39)-C(42)          107.6(3)
O(14)-C(43)-O(13)          126.9(3)
O(14)-C(43)-C(44)          119.9(3)
O(13)-C(43)-C(44)          113.1(2)
N(4)-C(44)-C(53)           114.9(2)
N(4)-C(44)-C(43)           105.6(2)
C(53)-C(44)-C(43)          119.9(2)
O(15)-C(45)-N(4)           124.3(3)
O(15)-C(45)-C(46)          129.2(3)
N(4)-C(45)-C(46)           106.5(3)
C(51)-C(46)-C(47)          120.8(4)
C(51)-C(46)-C(45)          108.8(3)
C(47)-C(46)-C(45)          130.3(4)
C(48)-C(47)-C(46)          117.5(4)
C(49)-C(48)-C(47)          121.3(4)
C(48)-C(49)-C(50)          121.6(4)
C(51)-C(50)-C(49)          116.8(4)
C(50)-C(51)-C(46)          122.0(3)
C(50)-C(51)-C(52)          130.0(3)
C(46)-C(51)-C(52)          107.9(3)
O(16)-C(52)-N(4)           125.4(3)
O(16)-C(52)-C(51)          128.7(3)
N(4)-C(52)-C(51)           105.9(3)
C(56)-C(53)-C(54)          109.7(3)
C(56)-C(53)-C(55)          109.3(3)
C(54)-C(53)-C(55)          109.1(3)
C(56)-C(53)-C(44)          113.3(2)
C(54)-C(53)-C(44)          108.6(2)
C(55)-C(53)-C(44)          106.8(3)
C(57)-N(5)-Cu(2)           151.8(3)
N(5)-C(57)-C(58)           178.9(5)
C(59)-O(17)-Cu(1)          126.0(11)
O(17)-C(59)-C(60)          112.6
C(59')-O(17')-Cu(1)        121.6(16)
O(17')-C(59')-C(60')       118.0
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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for joef097f.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	33(1)	34(1)	31(1)	-3(1)	-3(1)	2(1)
Cu(2)	31(1)	32(1)	31(1)	-1(1)	-3(1)	0(1)
N(1)	44(1)	32(1)	52(2)	-4(1)	3(1)	2(1)
N(2)	35(1)	50(2)	56(2)	-8(1)	-3(1)	-11(1)
N(3)	33(1)	35(1)	39(1)	7(1)	-1(1)	1(1)
N(4)	34(1)	38(1)	44(1)	-1(1)	4(1)	1(1)
O(1)	42(1)	35(1)	43(1)	-6(1)	-2(1)	2(1)
O(2)	45(1)	32(1)	44(1)	-3(1)	-4(1)	-1(1)
O(3)	80(2)	51(1)	73(2)	-18(1)	13(2)	-20(1)
O(4)	42(1)	39(1)	81(2)	2(1)	-2(1)	-4(1)
O(5)	35(1)	42(1)	50(1)	-4(1)	-2(1)	-1(1)
O(6)	31(1)	46(1)	47(1)	-7(1)	-3(1)	-5(1)
O(7)	44(1)	88(2)	99(2)	-28(2)	-21(2)	16(1)
O(8)	64(2)	46(1)	61(2)	1(1)	-22(1)	-4(1)
O(9)	47(1)	34(1)	36(1)	1(1)	-1(1)	6(1)
O(10)	42(1)	36(1)	39(1)	2(1)	-3(1)	2(1)
O(11)	53(2)	54(1)	63(2)	20(1)	-1(1)	-8(1)
O(12)	49(1)	60(1)	54(1)	18(1)	0(1)	-8(1)
O(13)	35(1)	43(1)	40(1)	-3(1)	0(1)	-1(1)
O(14)	34(1)	41(1)	39(1)	0(1)	-2(1)	-3(1)
O(15)	57(2)	66(2)	58(1)	-7(1)	15(1)	17(1)
O(16)	50(1)	43(1)	47(1)	-6(1)	4(1)	9(1)
C(1)	31(1)	33(1)	43(1)	1(1)	-1(1)	0(1)
C(2)	41(2)	32(1)	43(2)	-2(1)	3(1)	-1(1)
C(3)	38(2)	38(2)	56(2)	6(1)	-1(1)	5(1)
C(4)	49(2)	49(2)	52(2)	8(2)	3(2)	12(2)
C(5)	52(2)	70(2)	64(2)	21(2)	7(2)	16(2)
C(6)	61(2)	96(3)	56(2)	21(2)	13(2)	27(2)
C(7)	97(4)	97(4)	49(2)	-1(2)	7(2)	35(3)
C(8)	93(3)	66(2)	54(2)	-7(2)	11(2)	8(2)
C(9)	60(2)	46(2)	51(2)	-2(2)	5(2)	7(2)
C(10)	62(2)	36(2)	54(2)	-4(2)	6(2)	-2(2)
C(11)	57(2)	42(2)	49(2)	5(2)	0(2)	10(2)
C(12)	49(2)	85(3)	60(2)	11(2)	-16(2)	6(2)
C(13)	113(4)	47(2)	79(3)	10(2)	-5(3)	29(2)
C(14)	78(3)	52(2)	51(2)	6(2)	2(2)	-2(2)
C(15)	33(1)	34(1)	50(2)	-4(1)	0(1)	-1(1)
C(16)	34(2)	50(2)	61(2)	-15(1)	-1(1)	-3(1)
C(17)	32(2)	67(2)	63(2)	-9(2)	-4(2)	-9(2)
C(18)	39(2)	57(2)	58(2)	-9(2)	-1(2)	-12(2)
C(19)	53(2)	76(3)	66(2)	-16(2)	-14(2)	-10(2)
C(20)	68(3)	86(3)	72(3)	-30(2)	-8(2)	-17(2)
C(21)	79(3)	57(2)	72(3)	-18(2)	-1(2)	-8(2)
C(22)	73(2)	44(2)	58(2)	0(2)	-4(2)	-6(2)
C(23)	47(2)	45(2)	48(2)	3(1)	-2(2)	-13(1)
C(24)	47(2)	40(2)	51(2)	2(1)	-2(2)	-12(1)
C(25)	47(2)	95(3)	60(2)	-25(2)	17(2)	-27(2)
C(26)	50(2)	103(3)	84(3)	-47(3)	9(2)	-10(2)
C(27)	125(4)	94(3)	55(2)	-7(2)	17(3)	-48(3)
C(28)	57(3)	190(7)	105(4)	-67(4)	33(3)	-52(4)
C(29)	32(2)	34(1)	43(2)	2(1)	1(1)	1(1)

C(30)	34(1)	34(1)	43(2)	3(1)	-3(1)	2(1)
C(31)	45(2)	37(2)	46(2)	7(1)	1(1)	5(1)
C(32)	48(2)	42(2)	49(2)	4(1)	-2(1)	8(1)
C(33)	73(2)	60(2)	47(2)	13(2)	-7(2)	9(2)
C(34)	88(3)	76(3)	55(2)	6(2)	-27(2)	-1(2)
C(35)	71(3)	89(3)	77(3)	0(3)	-33(2)	-12(2)
C(36)	59(2)	72(3)	73(3)	8(2)	-13(2)	-16(2)
C(37)	43(2)	47(2)	49(2)	4(1)	-8(1)	1(1)
C(38)	41(2)	45(2)	47(2)	6(1)	-3(1)	0(1)
C(39)	55(2)	42(2)	52(2)	-9(1)	-12(2)	14(2)
C(40)	73(3)	88(3)	60(2)	-17(2)	9(2)	21(2)
C(41)	94(3)	44(2)	76(3)	-11(2)	-25(2)	25(2)
C(42)	72(3)	45(2)	78(3)	-11(2)	-29(2)	11(2)
C(43)	37(2)	26(1)	44(2)	2(1)	0(1)	4(1)
C(44)	33(1)	35(1)	41(2)	-3(1)	5(1)	3(1)
C(45)	37(2)	56(2)	48(2)	-4(1)	13(1)	2(1)
C(46)	40(2)	62(2)	48(2)	6(2)	8(1)	2(2)
C(47)	73(3)	97(3)	46(2)	7(2)	16(2)	16(2)
C(48)	93(4)	113(4)	52(2)	16(3)	17(2)	33(3)
C(49)	87(3)	83(3)	62(2)	21(2)	-1(2)	24(3)
C(50)	58(2)	57(2)	57(2)	9(2)	0(2)	9(2)
C(51)	38(2)	44(2)	52(2)	5(1)	3(1)	-2(1)
C(52)	36(2)	35(1)	48(2)	-3(1)	2(1)	-3(1)
C(53)	34(2)	38(2)	51(2)	-3(1)	0(1)	1(1)
C(54)	49(2)	47(2)	64(2)	4(2)	-15(2)	4(2)
C(55)	34(2)	72(2)	77(3)	-8(2)	3(2)	0(2)
C(56)	46(2)	44(2)	53(2)	-9(1)	-4(1)	-4(1)
N(5)	62(2)	83(2)	39(1)	2(2)	-6(1)	-18(2)
C(57)	67(2)	68(2)	47(2)	-3(2)	-6(2)	-2(2)
C(58)	100(4)	120(5)	78(3)	21(3)	-28(3)	17(3)
O(17)	70(2)	64(3)	40(1)	-10(2)	-13(1)	17(2)
C(59)	137(5)	86(11)	66(5)	-11(4)	-46(4)	38(5)
C(60)	171(9)	95(5)	64(4)	-8(4)	-9(5)	61(6)
O(17')	70(2)	64(3)	40(1)	-10(2)	-13(1)	17(2)
C(59')	137(5)	86(11)	66(5)	-11(4)	-46(4)	38(5)
C(60')	171(9)	95(5)	64(4)	-8(4)	-9(5)	61(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic
displacement parameters (A^2 x 10^3) for joef097f.

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	x	y	z	U(eq)
H(2A)	3383	1673	9117	47
H(5A)	5249	2195	5560	74
H(6A)	5387	1671	3744	85
H(7A)	4854	962	3433	97
H(8A)	4155	770	4874	85
H(12A)	4418	2328	10924	97
H(12B)	4760	1921	10117	97
H(12C)	4644	1834	11649	97
H(13A)	4248	966	11126	119
H(13B)	4382	1064	9608	119
H(13C)	3786	929	10045	119
H(14A)	3485	2087	11728	90
H(14B)	3737	1598	12422	90
H(14C)	3261	1535	11384	90
H(16A)	1568	3303	9494	58
H(19A)	813	2065	5926	78
H(20A)	1163	1335	4964	91
H(21A)	1904	933	5854	84
H(22A)	2336	1270	7708	70
H(26A)	2017	3598	12147	118
H(26B)	1440	3565	12812	118
H(26C)	1505	3804	11375	118
H(27A)	2200	2649	12155	137
H(27B)	1706	2280	11884	137
H(27C)	1695	2656	13119	137
H(28A)	875	2594	10888	176
H(28B)	782	3190	10720	176
H(28C)	786	2942	12157	176
H(30A)	3175	4980	8188	44
H(33A)	2024	5320	3969	72
H(34A)	1239	4968	3145	88
H(35A)	759	4394	4358	95
H(36A)	1036	4148	6467	81
H(40A)	2404	4634	11031	110
H(40B)	1986	4984	10269	110
H(40C)	2299	5201	11520	110
H(41A)	2909	5810	8701	107
H(41B)	2615	5940	10057	107
H(41C)	2287	5689	8874	107
H(42A)	3587	5296	10030	97
H(42B)	3368	4892	11071	97
H(42C)	3259	5483	11290	97
H(44A)	4954	3351	7720	43
H(47A)	4851	4079	2986	86
H(48A)	4335	4718	2034	103
H(49A)	3871	5284	3319	93
H(50A)	3884	5226	5627	69
H(54A)	5593	3408	10742	80
H(54B)	5298	3043	9717	80
H(54C)	4955	3377	10720	80
H(55A)	6085	3880	9084	92
H(55B)	5790	4097	7807	92

H(55C)	5861	3499	7993	92
H(56A)	5435	4342	10566	71
H(56B)	4809	4294	10275	71
H(56C)	5190	4575	9243	71
H(58A)	3933	2562	14484	149
H(58B)	4124	3088	15110	149
H(58C)	4493	2804	14059	149
H(17A)	3174	2963	5258	70
H(59A)	2323	3620	5618	116
H(59B)	2482	3339	4279	116
H(60A)	2595	4242	4217	165
H(60B)	3119	3935	3810	165
H(60C)	3072	4178	5247	165
H(17B)	3208	2911	5272	70
H(59C)	2602	3323	4189	116
H(59D)	2624	3759	5270	116
H(60D)	1775	3294	4827	165
H(60E)	1909	3486	6283	165
H(60F)	2012	2907	5889	165

Table 6. Torsion angles [deg] for joef097f.

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O(9)-Cu(1)-Cu(2)-O(6)                          88.70(9)
O(1)-Cu(1)-Cu(2)-O(6)                         -91.72(9)
O(13)-Cu(1)-Cu(2)-O(6)                        178.83(9)
O(5)-Cu(1)-Cu(2)-O(6)                          -1.65(9)
O(9)-Cu(1)-Cu(2)-O(14)                        -90.79(9)
O(1)-Cu(1)-Cu(2)-O(14)                         88.78(9)
O(13)-Cu(1)-Cu(2)-O(14)                        -0.67(9)
O(5)-Cu(1)-Cu(2)-O(14)                        178.86(9)
O(9)-Cu(1)-Cu(2)-O(10)                          0.15(9)
O(1)-Cu(1)-Cu(2)-O(10)                        179.72(9)
O(13)-Cu(1)-Cu(2)-O(10)                        90.28(9)
O(5)-Cu(1)-Cu(2)-O(10)                        -90.20(9)
O(9)-Cu(1)-Cu(2)-O(2)                         179.96(9)
O(1)-Cu(1)-Cu(2)-O(2)                          -0.46(9)
O(13)-Cu(1)-Cu(2)-O(2)                        -89.91(9)
O(5)-Cu(1)-Cu(2)-O(2)                          89.61(9)
O(9)-Cu(1)-Cu(2)-N(5)                        -172.0(4)
O(1)-Cu(1)-Cu(2)-N(5)                           7.6(4)
O(13)-Cu(1)-Cu(2)-N(5)                        -81.9(4)
O(5)-Cu(1)-Cu(2)-N(5)                          97.6(4)
O(13)-Cu(1)-O(1)-C(1)                          81.6(2)
O(5)-Cu(1)-O(1)-C(1)                          -82.8(2)
O(17')-Cu(1)-O(1)-C(1)                       -178.8(5)
O(17)-Cu(1)-O(1)-C(1)                         179.8(4)
Cu(2)-Cu(1)-O(1)-C(1)                          -1.0(2)
O(6)-Cu(2)-O(2)-C(1)                           88.8(2)
O(14)-Cu(2)-O(2)-C(1)                         -83.5(2)
O(10)-Cu(2)-O(2)-C(1)                           3.0(5)
N(5)-Cu(2)-O(2)-C(1)                         -175.8(3)
Cu(1)-Cu(2)-O(2)-C(1)                           2.3(2)
O(9)-Cu(1)-O(5)-C(15)                         -82.4(2)
O(1)-Cu(1)-O(5)-C(15)                          90.9(2)
O(13)-Cu(1)-O(5)-C(15)                          3.6(5)
O(17')-Cu(1)-O(5)-C(15)                      -179.7(5)
O(17)-Cu(1)-O(5)-C(15)                       -174.5(3)
Cu(2)-Cu(1)-O(5)-C(15)                          1.8(2)
O(10)-Cu(2)-O(6)-C(15)                         86.4(2)
O(2)-Cu(2)-O(6)-C(15)                         -77.2(2)
N(5)-Cu(2)-O(6)-C(15)                        -164.8(2)
Cu(1)-Cu(2)-O(6)-C(15)                          2.1(2)
O(13)-Cu(1)-O(9)-C(29)                        -84.0(2)
O(5)-Cu(1)-O(9)-C(29)                          80.5(2)
O(17')-Cu(1)-O(9)-C(29)                       176.5(5)
O(17)-Cu(1)-O(9)-C(29)                        177.8(4)
Cu(2)-Cu(1)-O(9)-C(29)                         -1.3(2)
O(6)-Cu(2)-O(10)-C(29)                        -85.9(2)
O(14)-Cu(2)-O(10)-C(29)                        86.5(2)
O(2)-Cu(2)-O(10)-C(29)                          0.3(5)
N(5)-Cu(2)-O(10)-C(29)                        179.0(2)
Cu(1)-Cu(2)-O(10)-C(29)                         0.9(2)
O(9)-Cu(1)-O(13)-C(43)                         85.5(2)
O(1)-Cu(1)-O(13)-C(43)                        -87.9(2)
O(5)-Cu(1)-O(13)-C(43)                         -0.6(5)
O(17')-Cu(1)-O(13)-C(43)                     -177.2(5)
O(17)-Cu(1)-O(13)-C(43)                       177.6(3)
Cu(2)-Cu(1)-O(13)-C(43)                         1.2(2)
O(10)-Cu(2)-O(14)-C(43)                       -83.8(2)
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O(2)-Cu(2)-O(14)-C(43)        79.8(2)
N(5)-Cu(2)-O(14)-C(43)       167.3(2)
Cu(1)-Cu(2)-O(14)-C(43)        0.38(19)
Cu(2)-O(2)-C(1)-O(1)          -4.2(5)
Cu(2)-O(2)-C(1)-C(2)         179.13(19)
Cu(1)-O(1)-C(1)-O(2)           3.2(4)
Cu(1)-O(1)-C(1)-C(2)         179.98(18)
C(10)-N(1)-C(2)-C(1)        -125.5(3)
C(3)-N(1)-C(2)-C(1)           45.7(4)
C(10)-N(1)-C(2)-C(11)        102.8(3)
C(3)-N(1)-C(2)-C(11)         -86.0(3)
O(2)-C(1)-C(2)-N(1)         -140.2(3)
O(1)-C(1)-C(2)-N(1)           42.8(3)
O(2)-C(1)-C(2)-C(11)         -11.1(4)
O(1)-C(1)-C(2)-C(11)         171.9(3)
C(10)-N(1)-C(3)-O(4)         175.6(3)
C(2)-N(1)-C(3)-O(4)            3.6(5)
C(10)-N(1)-C(3)-C(4)          -4.9(3)
C(2)-N(1)-C(3)-C(4)         -176.9(3)
O(4)-C(3)-C(4)-C(5)            2.3(6)
N(1)-C(3)-C(4)-C(5)         -177.2(3)
O(4)-C(3)-C(4)-C(9)         -178.6(3)
N(1)-C(3)-C(4)-C(9)            1.9(4)
C(9)-C(4)-C(5)-C(6)            0.2(5)
C(3)-C(4)-C(5)-C(6)          179.2(3)
C(4)-C(5)-C(6)-C(7)           -0.3(6)
C(5)-C(6)-C(7)-C(8)            1.0(7)
C(6)-C(7)-C(8)-C(9)           -1.5(6)
C(7)-C(8)-C(9)-C(4)            1.4(6)
C(7)-C(8)-C(9)-C(10)         179.6(4)
C(5)-C(4)-C(9)-C(8)           -0.8(6)
C(3)-C(4)-C(9)-C(8)         -180.0(3)
C(5)-C(4)-C(9)-C(10)        -179.4(3)
C(3)-C(4)-C(9)-C(10)           1.4(4)
C(3)-N(1)-C(10)-O(3)        -174.3(4)
C(2)-N(1)-C(10)-O(3)          -2.1(5)
C(3)-N(1)-C(10)-C(9)           5.7(4)
C(2)-N(1)-C(10)-C(9)         177.9(3)
C(8)-C(9)-C(10)-O(3)          -2.6(7)
C(4)-C(9)-C(10)-O(3)         175.8(4)
C(8)-C(9)-C(10)-N(1)         177.3(4)
C(4)-C(9)-C(10)-N(1)          -4.3(4)
N(1)-C(2)-C(11)-C(12)         68.7(4)
C(1)-C(2)-C(11)-C(12)        -58.0(4)
N(1)-C(2)-C(11)-C(14)       -168.2(3)
C(1)-C(2)-C(11)-C(14)         65.1(4)
N(1)-C(2)-C(11)-C(13)        -52.9(4)
C(1)-C(2)-C(11)-C(13)       -179.6(3)
Cu(2)-O(6)-C(15)-O(5)         -1.5(4)
Cu(2)-O(6)-C(15)-C(16)      -178.7(2)
Cu(1)-O(5)-C(15)-O(6)         -0.8(4)
Cu(1)-O(5)-C(15)-C(16)       176.56(19)
C(17)-N(2)-C(16)-C(15)      -116.6(3)
C(24)-N(2)-C(16)-C(15)        38.8(4)
C(17)-N(2)-C(16)-C(25)       109.7(4)
C(24)-N(2)-C(16)-C(25)       -94.9(4)
O(6)-C(15)-C(16)-N(2)       -135.4(3)
O(5)-C(15)-C(16)-N(2)         47.1(4)
O(6)-C(15)-C(16)-C(25)        -4.0(5)
O(5)-C(15)-C(16)-C(25)       178.4(3)
C(24)-N(2)-C(17)-O(7)       -173.6(4)
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C(16)-N(2)-C(17)-O(7)	-15.8(6)
C(24)-N(2)-C(17)-C(18)	5.5(4)
C(16)-N(2)-C(17)-C(18)	163.4(3)
O(7)-C(17)-C(18)-C(23)	173.8(4)
N(2)-C(17)-C(18)-C(23)	-5.2(4)
O(7)-C(17)-C(18)-C(19)	-3.2(7)
N(2)-C(17)-C(18)-C(19)	177.8(4)
C(23)-C(18)-C(19)-C(20)	-1.0(6)
C(17)-C(18)-C(19)-C(20)	175.6(4)
C(18)-C(19)-C(20)-C(21)	1.0(7)
C(19)-C(20)-C(21)-C(22)	-1.0(7)
C(20)-C(21)-C(22)-C(23)	0.9(6)
C(19)-C(18)-C(23)-C(22)	1.0(5)
C(17)-C(18)-C(23)-C(22)	-176.3(3)
C(19)-C(18)-C(23)-C(24)	-179.7(3)
C(17)-C(18)-C(23)-C(24)	3.0(4)
C(21)-C(22)-C(23)-C(18)	-1.0(5)
C(21)-C(22)-C(23)-C(24)	179.9(3)
C(17)-N(2)-C(24)-O(8)	175.4(3)
C(16)-N(2)-C(24)-O(8)	17.7(5)
C(17)-N(2)-C(24)-C(23)	-3.8(4)
C(16)-N(2)-C(24)-C(23)	-161.4(3)
C(18)-C(23)-C(24)-O(8)	-178.8(4)
C(22)-C(23)-C(24)-O(8)	0.4(6)
C(18)-C(23)-C(24)-N(2)	0.3(4)
C(22)-C(23)-C(24)-N(2)	179.5(3)
N(2)-C(16)-C(25)-C(27)	65.3(4)
C(15)-C(16)-C(25)-C(27)	-62.7(4)
N(2)-C(16)-C(25)-C(26)	-171.5(3)
C(15)-C(16)-C(25)-C(26)	60.5(5)
N(2)-C(16)-C(25)-C(28)	-56.2(5)
C(15)-C(16)-C(25)-C(28)	175.9(4)
Cu(1)-O(9)-C(29)-O(10)	2.6(4)
Cu(1)-O(9)-C(29)-C(30)	179.95(18)
Cu(2)-O(10)-C(29)-O(9)	-2.3(4)
Cu(2)-O(10)-C(29)-C(30)	-179.60(19)
C(38)-N(3)-C(30)-C(39)	-88.7(4)
C(31)-N(3)-C(30)-C(39)	105.7(3)
C(38)-N(3)-C(30)-C(29)	47.1(4)
C(31)-N(3)-C(30)-C(29)	-118.4(3)
O(9)-C(29)-C(30)-N(3)	36.3(3)
O(10)-C(29)-C(30)-N(3)	-146.1(3)
O(9)-C(29)-C(30)-C(39)	169.0(3)
O(10)-C(29)-C(30)-C(39)	-13.4(4)
C(38)-N(3)-C(31)-O(11)	-175.5(3)
C(30)-N(3)-C(31)-O(11)	-8.3(5)
C(38)-N(3)-C(31)-C(32)	5.0(3)
C(30)-N(3)-C(31)-C(32)	172.2(2)
O(11)-C(31)-C(32)-C(33)	-1.0(6)
N(3)-C(31)-C(32)-C(33)	178.4(4)
O(11)-C(31)-C(32)-C(37)	176.6(4)
N(3)-C(31)-C(32)-C(37)	-3.9(3)
C(37)-C(32)-C(33)-C(34)	0.0(5)
C(31)-C(32)-C(33)-C(34)	177.4(4)
C(32)-C(33)-C(34)-C(35)	-0.1(7)
C(33)-C(34)-C(35)-C(36)	0.2(8)
C(34)-C(35)-C(36)-C(37)	-0.2(7)
C(35)-C(36)-C(37)-C(32)	0.1(6)
C(35)-C(36)-C(37)-C(38)	-179.3(4)
C(33)-C(32)-C(37)-C(36)	0.0(6)
C(31)-C(32)-C(37)-C(36)	-177.9(3)

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C(33)-C(32)-C(37)-C(38)	179.5(3)
C(31)-C(32)-C(37)-C(38)	1.6(4)
C(31)-N(3)-C(38)-O(12)	176.0(3)
C(30)-N(3)-C(38)-O(12)	9.1(5)
C(31)-N(3)-C(38)-C(37)	-4.1(3)
C(30)-N(3)-C(38)-C(37)	-170.9(3)
C(36)-C(37)-C(38)-O(12)	0.8(6)
C(32)-C(37)-C(38)-O(12)	-178.7(4)
C(36)-C(37)-C(38)-N(3)	-179.2(4)
C(32)-C(37)-C(38)-N(3)	1.4(4)
N(3)-C(30)-C(39)-C(40)	69.6(4)
C(29)-C(30)-C(39)-C(40)	-60.3(4)
N(3)-C(30)-C(39)-C(41)	-52.0(4)
C(29)-C(30)-C(39)-C(41)	178.1(3)
N(3)-C(30)-C(39)-C(42)	-168.3(3)
C(29)-C(30)-C(39)-C(42)	61.8(4)
Cu(2)-O(14)-C(43)-O(13)	0.4(4)
Cu(2)-O(14)-C(43)-C(44)	-177.29(18)
Cu(1)-O(13)-C(43)-O(14)	-1.4(4)
Cu(1)-O(13)-C(43)-C(44)	176.46(17)
C(45)-N(4)-C(44)-C(53)	115.5(3)
C(52)-N(4)-C(44)-C(53)	-92.9(3)
C(45)-N(4)-C(44)-C(43)	-110.0(3)
C(52)-N(4)-C(44)-C(43)	41.6(3)
O(14)-C(43)-C(44)-N(4)	-133.0(3)
O(13)-C(43)-C(44)-N(4)	49.0(3)
O(14)-C(43)-C(44)-C(53)	-1.3(4)
O(13)-C(43)-C(44)-C(53)	-179.3(2)
C(52)-N(4)-C(45)-O(15)	-172.5(3)
C(44)-N(4)-C(45)-O(15)	-17.7(5)
C(52)-N(4)-C(45)-C(46)	5.6(3)
C(44)-N(4)-C(45)-C(46)	160.4(3)
O(15)-C(45)-C(46)-C(51)	174.4(4)
N(4)-C(45)-C(46)-C(51)	-3.6(4)
O(15)-C(45)-C(46)-C(47)	-1.9(7)
N(4)-C(45)-C(46)-C(47)	-179.8(4)
C(51)-C(46)-C(47)-C(48)	-0.4(7)
C(45)-C(46)-C(47)-C(48)	175.5(4)
C(46)-C(47)-C(48)-C(49)	0.9(8)
C(47)-C(48)-C(49)-C(50)	-0.8(9)
C(48)-C(49)-C(50)-C(51)	0.2(8)
C(49)-C(50)-C(51)-C(46)	0.4(6)
C(49)-C(50)-C(51)-C(52)	-176.2(4)
C(47)-C(46)-C(51)-C(50)	-0.3(6)
C(45)-C(46)-C(51)-C(50)	-176.9(3)
C(47)-C(46)-C(51)-C(52)	176.9(4)
C(45)-C(46)-C(51)-C(52)	0.3(4)
C(45)-N(4)-C(52)-O(16)	173.0(3)
C(44)-N(4)-C(52)-O(16)	18.9(5)
C(45)-N(4)-C(52)-C(51)	-5.4(3)
C(44)-N(4)-C(52)-C(51)	-159.5(3)
C(50)-C(51)-C(52)-O(16)	1.6(6)
C(46)-C(51)-C(52)-O(16)	-175.3(3)
C(50)-C(51)-C(52)-N(4)	179.9(4)
C(46)-C(51)-C(52)-N(4)	3.1(3)
N(4)-C(44)-C(53)-C(56)	62.0(3)
C(43)-C(44)-C(53)-C(56)	-65.5(3)
N(4)-C(44)-C(53)-C(54)	-175.9(2)
C(43)-C(44)-C(53)-C(54)	56.6(3)
N(4)-C(44)-C(53)-C(55)	-58.4(3)
C(43)-C(44)-C(53)-C(55)	174.1(3)

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O(6)-Cu(2)-N(5)-C(57)                                    106.1(7)
O(14)-Cu(2)-N(5)-C(57)                                   -72.6(7)
O(10)-Cu(2)-N(5)-C(57)                                  -163.9(7)
O(2)-Cu(2)-N(5)-C(57)                                     15.7(7)
Cu(1)-Cu(2)-N(5)-C(57)                                    7.9(10)
O(9)-Cu(1)-O(17)-C(59)                                   -26.1(6)
O(1)-Cu(1)-O(17)-C(59)                                   154.2(6)
O(13)-Cu(1)-O(17)-C(59)                                 -115.8(6)
O(5)-Cu(1)-O(17)-C(59)                                    63.7(6)
O(17')-Cu(1)-O(17)-C(59)                                  140(9)
Cu(1)-O(17)-C(59)-C(60)                                   85.4(15)
O(9)-Cu(1)-O(17')-C(59')                                 -34.9(10)
O(1)-Cu(1)-O(17')-C(59')                                 145.3(10)
O(13)-Cu(1)-O(17')-C(59')                               -125.5(9)
O(5)-Cu(1)-O(17')-C(59')                                  55.4(10)
O(17)-Cu(1)-O(17')-C(59')                                 -49(8)
Cu(1)-O(17')-C(59')-C(60')                                -69(3)
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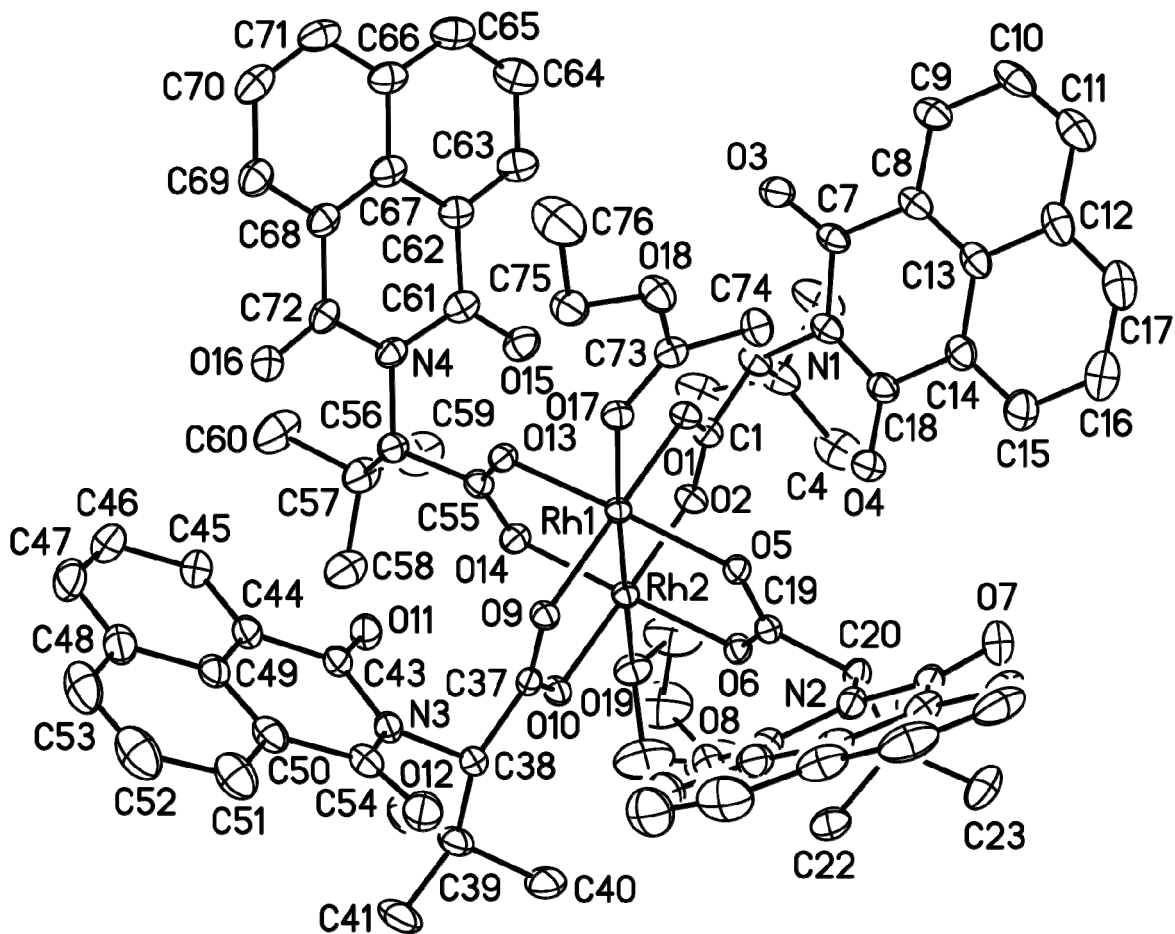Symmetry transformations used to generate equivalent atoms:

Figure 2. Molecular diagram of **3** with ellipsoids at 30% probability. Minor disordered contributor, cocrystallized ethyl acetate solvent and H-atoms deleted for clarity.

Table 1. Crystal data and structure refinement for joef094a.

Identification code	joef094a
Empirical formula	C84 H88 N4 O21 Rh2
Formula weight	1695.40
Temperature	200(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2
Unit cell dimensions	a = 21.627(10) A alpha = 90 deg. b = 21.826(10) A beta = 90 deg. c = 17.238(8) A gamma = 90 deg.
Volume	8137(6) A^3
Z, Calculated density	4, 1.384 Mg/m^3
Absorption coefficient	0.480 mm^-1
F(000)	3512
Crystal size	0.30 x 0.11 x 0.08 mm
Theta range for data collection	1.33 to 28.27 deg.
Limiting indices	-28<=h<=28, -29<=k<=29, -22<=l<=22
Reflections collected / unique	111612 / 20130 [R(int) = 0.0526]
Completeness to theta = 25.00	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9622 and 0.8694
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	20130 / 181 / 1032
Goodness-of-fit on F^2	1.065
Final R indices [I>2sigma(I)]	R1 = 0.0401, wR2 = 0.0975
R indices (all data)	R1 = 0.0479, wR2 = 0.1038
Absolute structure parameter	-0.035(17)
Largest diff. peak and hole	1.048 and -0.400 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for joef094a.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

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	x	y	z	U(eq)
Rh(1)	2566(1)	2340(1)	2035(1)	24(1)
Rh(2)	2578(1)	2004(1)	3351(1)	28(1)
C(1)	2085(2)	1131(2)	2298(2)	33(1)
C(2)	1786(2)	528(2)	2035(2)	36(1)
C(3)	1650(2)	41(2)	2668(2)	54(1)
C(4)	2234(3)	-197(2)	3073(3)	76(2)
C(5)	1317(3)	-507(2)	2282(3)	78(2)
C(6)	1198(3)	313(2)	3261(3)	71(2)
C(7)	1759(2)	120(2)	705(2)	36(1)
C(8)	2090(2)	-203(2)	67(2)	38(1)
C(9)	1744(2)	-484(2)	-511(2)	44(1)
C(10)	2042(2)	-827(2)	-1082(2)	53(1)
C(11)	2661(2)	-855(2)	-1116(2)	54(1)
C(12)	3036(2)	-547(2)	-558(2)	49(1)
C(13)	2729(2)	-239(2)	71(2)	41(1)
C(14)	3088(2)	13(2)	673(2)	41(1)
C(15)	3718(2)	-12(2)	656(3)	53(1)
C(16)	4019(2)	-293(2)	20(3)	65(1)
C(17)	3690(2)	-548(2)	-559(3)	61(1)
C(18)	2767(2)	280(2)	1355(2)	38(1)
C(19)	3689(2)	1745(1)	2502(2)	31(1)
C(20)	4347(2)	1496(2)	2379(2)	34(1)
C(21)	4684(2)	1229(2)	3103(2)	45(1)
C(22)	4748(2)	1680(2)	3764(2)	56(1)
C(23)	5338(2)	1018(2)	2859(3)	64(1)
C(24)	4317(2)	662(2)	3371(3)	58(1)
C(25)	5063(2)	1745(2)	1316(2)	39(1)
C(26)	5406(2)	2215(2)	854(2)	41(1)
C(27)	5768(2)	2028(2)	243(2)	48(1)
C(28)	6050(2)	2465(3)	-248(3)	60(1)
C(29)	5962(2)	3073(3)	-113(3)	64(1)
C(30)	5598(2)	3287(2)	516(3)	53(1)
C(31)	5318(2)	2841(2)	1007(2)	42(1)
C(32)	4939(2)	3035(2)	1624(2)	43(1)
C(33)	4832(2)	3650(2)	1760(3)	54(1)
C(34)	5111(3)	4082(2)	1268(3)	71(1)
C(35)	5479(2)	3913(2)	680(3)	66(1)
C(36)	4648(2)	2577(2)	2144(2)	39(1)
C(37)	3039(1)	3212(1)	3140(2)	30(1)
C(38)	3328(2)	3821(1)	3402(2)	35(1)
C(39)	3452(2)	3898(2)	4296(2)	46(1)
C(40)	3931(2)	3418(2)	4540(3)	61(1)
C(41)	3751(3)	4536(2)	4423(3)	68(1)
C(42)	2877(2)	3851(2)	4797(2)	63(1)
C(43)	2335(2)	4335(2)	3091(2)	35(1)
C(44)	2007(2)	4889(2)	2792(2)	40(1)
C(45)	1368(2)	4904(2)	2810(3)	53(1)
C(46)	1059(2)	5432(2)	2562(3)	66(1)
C(47)	1381(3)	5926(2)	2306(3)	66(1)
C(48)	2025(2)	5922(2)	2259(2)	50(1)

C(49)	2350(2)	5385(2)	2504(2)	40(1)
C(50)	2993(2)	5357(2)	2441(2)	41(1)
C(51)	3323(2)	5849(2)	2150(3)	57(1)
C(52)	3010(3)	6385(2)	1928(3)	70(1)
C(53)	2386(3)	6418(2)	1975(2)	65(1)
C(54)	3332(2)	4800(2)	2691(2)	38(1)
C(55)	1471(2)	2621(2)	2904(2)	33(1)
C(56)	849(2)	2936(2)	3020(2)	37(1)
C(57)	523(2)	2879(2)	3826(2)	54(1)
C(58)	940(2)	3194(3)	4424(2)	69(2)
C(59)	378(3)	2226(3)	4075(3)	79(2)
C(60)	-87(2)	3242(3)	3781(3)	84(2)
C(61)	372(2)	2170(2)	2144(2)	41(1)
C(62)	-72(2)	2030(2)	1515(2)	39(1)
C(63)	-205(2)	1428(2)	1336(3)	51(1)
C(64)	-605(2)	1289(2)	719(3)	59(1)
C(65)	-857(2)	1752(2)	284(3)	54(1)
C(66)	-733(2)	2367(2)	443(2)	46(1)
C(67)	-341(2)	2513(2)	1086(2)	41(1)
C(68)	-200(2)	3124(2)	1256(2)	41(1)
C(69)	-440(2)	3592(2)	801(2)	48(1)
C(70)	-819(2)	3451(2)	173(3)	54(1)
C(71)	-961(2)	2864(2)	-11(2)	52(1)
C(72)	208(2)	3279(2)	1907(2)	39(1)
C(73)	2554(2)	2301(1)	123(2)	32(1)
C(74)	2605(2)	1617(1)	115(2)	40(1)
C(75)	2406(2)	3185(2)	-659(2)	44(1)
C(76)	2249(3)	3323(2)	-1486(3)	81(2)
C(81)	1340(4)	2480(4)	6665(5)	108(2)
C(82)	1857(5)	2875(6)	6363(5)	172(5)
C(83)	685(3)	1646(3)	6413(4)	98(2)
C(84)	678(5)	1094(4)	5937(7)	166(4)
N(1)	2118(2)	289(1)	1352(2)	36(1)
N(2)	4712(1)	1957(1)	1941(2)	36(1)
N(3)	2984(1)	4345(1)	3063(2)	33(1)
N(4)	439(1)	2790(2)	2347(2)	38(1)
O(1)	2169(1)	1520(1)	1763(1)	31(1)
O(2)	2201(1)	1203(1)	3007(1)	35(1)
O(3)	1207(1)	218(1)	693(2)	47(1)
O(4)	3050(1)	487(1)	1910(2)	48(1)
O(5)	3432(1)	1976(1)	1907(1)	30(1)
O(6)	3442(1)	1669(1)	3157(1)	33(1)
O(7)	5078(1)	1203(1)	1151(2)	50(1)
O(8)	4352(1)	2722(1)	2711(2)	43(1)
O(9)	2945(1)	3154(1)	2419(1)	30(1)
O(10)	2953(1)	2812(1)	3656(1)	33(1)
O(11)	2064(1)	3895(1)	3352(2)	43(1)
O(12)	3887(1)	4740(1)	2592(2)	52(1)
O(13)	1705(1)	2691(1)	2235(1)	31(1)
O(14)	1722(1)	2366(1)	3477(1)	36(1)
O(15)	671(1)	1777(1)	2475(2)	51(1)
O(16)	341(1)	3810(1)	2078(2)	48(1)
O(17)	2560(1)	2627(1)	698(1)	31(1)
O(18)	2491(1)	2531(1)	-590(1)	41(1)
O(20)	1095(2)	2549(3)	7289(3)	111(2)
O(21)	1187(2)	2023(3)	6168(3)	117(2)
O(19)	2594(11)	1675(14)	4612(10)	47(1)
C(77)	2373(8)	1095(8)	4791(7)	94(4)
C(78)	2481(8)	1077(9)	5701(8)	114(5)
C(79)	3208(7)	1140(7)	5510(8)	112(4)
C(80)	3103(8)	1826(8)	5125(9)	97(4)

O(19')	2610(12)	1710(15)	4621(11)	47(1)
C(77')	2208(8)	1314(9)	4972(9)	94(4)
C(78')	2650(9)	909(9)	5503(10)	114(5)
C(79')	3040(8)	1490(8)	5823(7)	112(4)
C(80')	3226(8)	1627(10)	4938(9)	97(4)

Table 3. Bond lengths [A] and angles [deg] for joef094a.

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Rh(1)-O(13)            2.042(2)
Rh(1)-O(1)             2.041(2)
Rh(1)-O(5)             2.048(2)
Rh(1)-O(9)             2.064(2)
Rh(1)-Rh(2)            2.3843(10)
Rh(1)-O(17)            2.388(2)
Rh(2)-O(10)            2.011(2)
Rh(2)-O(2)             2.018(2)
Rh(2)-O(14)            2.025(2)
Rh(2)-O(6)             2.032(2)
Rh(2)-O(19')           2.282(11)
Rh(2)-O(19)            2.290(10)
C(1)-O(2)              1.258(4)


C(1)-O(1)              1.265(4)
C(1)-C(2)              1.536(5)
C(2)-N(1)              1.474(5)
C(2)-C(3)              1.552(5)
C(3)-C(4)              1.534(7)
C(3)-C(6)              1.535(7)
C(3)-C(5)              1.546(6)
C(7)-O(3)              1.214(5)
C(7)-N(1)              1.408(5)
C(7)-C(8)              1.489(5)
C(8)-C(13)             1.384(6)
C(8)-C(9)              1.389(5)
C(9)-C(10)             1.394(6)
C(10)-C(11)            1.342(7)
C(11)-C(12)            1.425(6)
C(12)-C(17)            1.415(7)
C(12)-C(13)            1.438(5)
C(13)-C(14)            1.408(5)
C(14)-C(15)            1.365(6)
C(14)-C(18)            1.484(5)
C(15)-C(16)            1.414(6)
C(16)-C(17)            1.345(7)
C(18)-O(4)             1.223(4)
C(18)-N(1)             1.403(5)
C(19)-O(6)             1.259(4)
C(19)-O(5)             1.270(4)
C(19)-C(20)            1.539(5)
C(20)-N(2)             1.485(4)
C(20)-C(21)            1.558(5)
C(21)-C(22)            1.513(6)
C(21)-C(24)            1.540(6)
C(21)-C(23)            1.547(6)
C(25)-O(7)             1.217(4)
C(25)-N(2)             1.396(5)
C(25)-C(26)            1.495(5)
C(26)-C(27)            1.374(5)
C(26)-C(31)            1.404(5)
C(27)-C(28)            1.414(6)
C(28)-C(29)            1.361(8)
C(29)-C(30)            1.419(7)
C(30)-C(35)            1.419(7)
C(30)-C(31)            1.425(6)
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C(31)-C(32)	1.409(6)
C(32)-C(33)	1.381(5)
C(32)-C(36)	1.483(5)
C(33)-C(34)	1.405(7)
C(34)-C(35)	1.340(8)
C(36)-O(8)	1.210(4)
C(36)-N(2)	1.405(4)
C(37)-O(10)	1.261(4)
C(37)-O(9)	1.266(4)
C(37)-C(38)	1.537(4)
C(38)-N(3)	1.485(4)
C(38)-C(39)	1.572(5)
C(39)-C(42)	1.517(6)
C(39)-C(40)	1.532(6)
C(39)-C(41)	1.551(6)
C(43)-O(11)	1.212(4)
C(43)-N(3)	1.403(5)
C(43)-C(44)	1.495(5)
C(44)-C(45)	1.383(6)
C(44)-C(49)	1.402(5)
C(45)-C(46)	1.398(6)
C(46)-C(47)	1.357(8)
C(47)-C(48)	1.394(7)
C(48)-C(53)	1.422(7)
C(48)-C(49)	1.432(5)
C(49)-C(50)	1.396(6)
C(50)-C(51)	1.384(6)
C(50)-C(54)	1.483(5)
C(51)-C(52)	1.405(7)
C(52)-C(53)	1.354(8)
C(54)-O(12)	1.219(5)
C(54)-N(3)	1.402(4)
C(55)-O(14)	1.257(4)
C(55)-O(13)	1.269(4)
C(55)-C(56)	1.524(4)
C(56)-N(4)	1.494(5)
C(56)-C(57)	1.564(5)
C(57)-C(59)	1.521(8)
C(57)-C(58)	1.532(7)
C(57)-C(60)	1.541(6)
C(61)-O(15)	1.217(4)
C(61)-N(4)	1.405(5)
C(61)-C(62)	1.481(5)
C(62)-C(63)	1.381(6)
C(62)-C(67)	1.413(5)
C(63)-C(64)	1.404(6)
C(64)-C(65)	1.372(7)
C(65)-C(66)	1.395(6)
C(66)-C(67)	1.429(5)
C(66)-C(71)	1.427(6)
C(67)-C(68)	1.399(6)
C(68)-C(69)	1.388(5)
C(68)-C(72)	1.468(5)
C(69)-C(70)	1.394(6)
C(70)-C(71)	1.354(7)
C(72)-O(16)	1.231(5)
C(72)-N(4)	1.401(5)
C(73)-O(17)	1.219(3)
C(73)-O(18)	1.335(3)

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C(73)-C(74)                        1.498(4)
C(75)-O(18)                        1.445(4)
C(75)-C(76)                        1.497(5)
C(81)-O(20)                        1.207(9)
C(81)-O(21)                        1.357(10)
C(81)-C(82)                        1.505(11)
C(83)-O(21)                        1.425(8)
C(83)-C(84)                        1.458(11)
O(19)-C(77)                        1.388(16)
O(19)-C(80)                        1.450(14)
C(77)-C(78)                        1.586(15)
C(78)-C(79)                        1.611(18)
C(79)-C(80)                        1.654(16)
O(19')-C(77')                      1.368(14)
O(19')-C(80')                      1.451(17)
C(77')-C(78')                      1.592(17)
C(78')-C(79')                      1.619(18)
C(79')-C(80')                      1.606(15)

O(13)-Rh(1)-O(1)                   89.13(9)
O(13)-Rh(1)-O(5)                  176.39(9)
O(1)-Rh(1)-O(5)                    91.03(9)
O(13)-Rh(1)-O(9)                   89.22(9)
O(1)-Rh(1)-O(9)                   174.51(8)
O(5)-Rh(1)-O(9)                    90.29(9)
O(13)-Rh(1)-Rh(2)                  88.03(6)
O(1)-Rh(1)-Rh(2)                   87.28(6)
O(5)-Rh(1)-Rh(2)                   88.38(6)
O(9)-Rh(1)-Rh(2)                   87.43(6)
O(13)-Rh(1)-O(17)                  93.42(8)
O(1)-Rh(1)-O(17)                   90.37(8)
O(5)-Rh(1)-O(17)                   90.18(8)
O(9)-Rh(1)-O(17)                   94.95(8)
Rh(2)-Rh(1)-O(17)                 177.22(5)
O(10)-Rh(2)-O(2)                  178.10(9)
O(10)-Rh(2)-O(14)                  89.88(10)
O(2)-Rh(2)-O(14)                   89.97(10)
O(10)-Rh(2)-O(6)                   89.36(10)
O(2)-Rh(2)-O(6)                    90.67(10)
O(14)-Rh(2)-O(6)                  176.30(9)
O(10)-Rh(2)-O(19')                 89.0(7)
O(2)-Rh(2)-O(19')                  92.9(7)
O(14)-Rh(2)-O(19')                 91.9(9)
O(6)-Rh(2)-O(19')                  91.7(9)
O(10)-Rh(2)-O(19)                  91.2(7)
O(2)-Rh(2)-O(19)                   90.7(7)
O(14)-Rh(2)-O(19)                  91.9(8)
O(6)-Rh(2)-O(19)                   91.7(8)
O(19')-Rh(2)-O(19)                  2.1(13)
O(10)-Rh(2)-Rh(1)                  89.05(6)
O(2)-Rh(2)-Rh(1)                   89.05(7)
O(14)-Rh(2)-Rh(1)                  88.38(6)
O(6)-Rh(2)-Rh(1)                   87.99(6)
O(19')-Rh(2)-Rh(1)                178.1(6)
O(19)-Rh(2)-Rh(1)                 179.6(10)
O(2)-C(1)-O(1)                    126.7(3)
O(2)-C(1)-C(2)                    118.5(3)
O(1)-C(1)-C(2)                    114.8(3)
N(1)-C(2)-C(1)                    109.5(3)
N(1)-C(2)-C(3)                    114.3(3)
C(1)-C(2)-C(3)                    117.4(3)
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C(4)-C(3)-C(6)	110.6(4)
C(4)-C(3)-C(5)	108.5(4)
C(6)-C(3)-C(5)	106.9(4)
C(4)-C(3)-C(2)	113.3(4)
C(6)-C(3)-C(2)	108.9(4)
C(5)-C(3)-C(2)	108.4(3)
O(3)-C(7)-N(1)	120.6(3)
O(3)-C(7)-C(8)	123.0(3)
N(1)-C(7)-C(8)	116.4(3)
C(13)-C(8)-C(9)	121.1(4)
C(13)-C(8)-C(7)	120.2(3)
C(9)-C(8)-C(7)	118.7(4)
C(8)-C(9)-C(10)	119.7(4)
C(11)-C(10)-C(9)	121.0(4)
C(10)-C(11)-C(12)	121.1(4)
C(17)-C(12)-C(11)	124.5(4)
C(17)-C(12)-C(13)	117.6(4)
C(11)-C(12)-C(13)	117.8(4)
C(8)-C(13)-C(14)	122.1(4)
C(8)-C(13)-C(12)	118.9(4)
C(14)-C(13)-C(12)	119.0(4)
C(15)-C(14)-C(13)	121.2(4)
C(15)-C(14)-C(18)	120.1(4)
C(13)-C(14)-C(18)	118.6(3)
C(14)-C(15)-C(16)	119.5(5)
C(17)-C(16)-C(15)	120.8(5)
C(16)-C(17)-C(12)	121.8(4)
O(4)-C(18)-N(1)	119.8(4)
O(4)-C(18)-C(14)	122.1(4)
N(1)-C(18)-C(14)	118.1(3)
O(6)-C(19)-O(5)	126.2(3)
O(6)-C(19)-C(20)	118.1(3)
O(5)-C(19)-C(20)	115.6(3)
N(2)-C(20)-C(19)	108.9(3)
N(2)-C(20)-C(21)	114.4(3)
C(19)-C(20)-C(21)	117.0(3)
C(22)-C(21)-C(24)	110.2(4)
C(22)-C(21)-C(23)	108.3(4)
C(24)-C(21)-C(23)	108.2(3)
C(22)-C(21)-C(20)	113.7(3)
C(24)-C(21)-C(20)	107.5(3)
C(23)-C(21)-C(20)	108.8(3)
O(7)-C(25)-N(2)	121.1(3)
O(7)-C(25)-C(26)	122.0(3)
N(2)-C(25)-C(26)	117.0(3)
C(27)-C(26)-C(31)	120.7(4)
C(27)-C(26)-C(25)	119.1(4)
C(31)-C(26)-C(25)	120.0(3)
C(26)-C(27)-C(28)	120.2(4)
C(29)-C(28)-C(27)	119.7(4)
C(28)-C(29)-C(30)	121.9(4)
C(35)-C(30)-C(31)	117.5(4)
C(35)-C(30)-C(29)	124.8(4)
C(31)-C(30)-C(29)	117.7(4)
C(26)-C(31)-C(32)	120.9(3)
C(26)-C(31)-C(30)	119.8(4)
C(32)-C(31)-C(30)	119.3(4)
C(33)-C(32)-C(31)	121.2(4)
C(33)-C(32)-C(36)	118.7(4)
C(31)-C(32)-C(36)	120.0(3)
C(32)-C(33)-C(34)	118.5(5)

C(35)-C(34)-C(33)	121.8(4)
C(34)-C(35)-C(30)	121.6(4)
O(8)-C(36)-N(2)	120.4(3)
O(8)-C(36)-C(32)	122.4(3)
N(2)-C(36)-C(32)	117.2(3)
O(10)-C(37)-O(9)	126.8(3)
O(10)-C(37)-C(38)	116.9(3)
O(9)-C(37)-C(38)	116.2(3)
N(3)-C(38)-C(37)	110.2(3)
N(3)-C(38)-C(39)	112.9(3)
C(37)-C(38)-C(39)	116.7(3)
C(42)-C(39)-C(40)	110.6(4)
C(42)-C(39)-C(41)	108.8(4)
C(40)-C(39)-C(41)	107.0(4)
C(42)-C(39)-C(38)	114.3(3)
C(40)-C(39)-C(38)	108.2(3)
C(41)-C(39)-C(38)	107.8(3)
O(11)-C(43)-N(3)	120.5(3)
O(11)-C(43)-C(44)	122.7(3)
N(3)-C(43)-C(44)	116.8(3)
C(45)-C(44)-C(49)	121.2(4)
C(45)-C(44)-C(43)	119.1(4)
C(49)-C(44)-C(43)	119.6(3)
C(44)-C(45)-C(46)	119.3(5)
C(47)-C(46)-C(45)	120.6(5)
C(46)-C(47)-C(48)	121.8(4)
C(47)-C(48)-C(53)	124.4(4)
C(47)-C(48)-C(49)	118.5(4)
C(53)-C(48)-C(49)	117.1(4)
C(50)-C(49)-C(44)	121.4(3)
C(50)-C(49)-C(48)	120.1(4)
C(44)-C(49)-C(48)	118.5(4)
C(51)-C(50)-C(49)	120.6(4)
C(51)-C(50)-C(54)	119.1(4)
C(49)-C(50)-C(54)	120.4(3)
C(50)-C(51)-C(52)	119.8(5)
C(53)-C(52)-C(51)	120.4(5)
C(52)-C(53)-C(48)	122.0(4)
O(12)-C(54)-N(3)	121.1(3)
O(12)-C(54)-C(50)	122.3(3)
N(3)-C(54)-C(50)	116.6(3)
O(14)-C(55)-O(13)	126.6(3)
O(14)-C(55)-C(56)	118.6(3)
O(13)-C(55)-C(56)	114.5(3)
N(4)-C(56)-C(55)	109.1(3)
N(4)-C(56)-C(57)	113.9(3)
C(55)-C(56)-C(57)	118.6(3)
C(59)-C(57)-C(58)	110.6(4)
C(59)-C(57)-C(60)	108.7(4)
C(58)-C(57)-C(60)	107.8(4)
C(59)-C(57)-C(56)	114.7(4)
C(58)-C(57)-C(56)	107.2(3)
C(60)-C(57)-C(56)	107.5(4)
O(15)-C(61)-N(4)	120.5(3)
O(15)-C(61)-C(62)	122.9(4)
N(4)-C(61)-C(62)	116.7(3)
C(63)-C(62)-C(67)	120.5(4)
C(63)-C(62)-C(61)	119.7(4)
C(67)-C(62)-C(61)	119.8(3)
C(62)-C(63)-C(64)	120.2(4)
C(65)-C(64)-C(63)	120.0(4)

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C(64)-C(65)-C(66)          121.7(4)
C(65)-C(66)-C(67)          118.7(4)
C(65)-C(66)-C(71)          123.8(4)
C(67)-C(66)-C(71)          117.4(4)
C(68)-C(67)-C(62)          120.8(3)
C(68)-C(67)-C(66)          120.2(4)
C(62)-C(67)-C(66)          118.9(4)
C(69)-C(68)-C(67)          120.2(4)
C(69)-C(68)-C(72)          119.1(4)
C(67)-C(68)-C(72)          120.7(3)
C(68)-C(69)-C(70)          119.6(4)
C(71)-C(70)-C(69)          121.7(4)
C(70)-C(71)-C(66)          120.8(4)
O(16)-C(72)-N(4)           120.3(3)
O(16)-C(72)-C(68)          122.7(3)
N(4)-C(72)-C(68)           117.0(3)
O(17)-C(73)-O(18)          122.0(3)
O(17)-C(73)-C(74)          126.1(3)
O(18)-C(73)-C(74)          111.9(3)
O(18)-C(75)-C(76)          107.8(3)
O(20)-C(81)-O(21)          123.1(8)
O(20)-C(81)-C(82)          124.3(9)
O(21)-C(81)-C(82)          112.6(8)
O(21)-C(83)-C(84)          108.6(7)
C(18)-N(1)-C(7)            123.4(3)
C(18)-N(1)-C(2)            119.3(3)
C(7)-N(1)-C(2)             117.2(3)
C(25)-N(2)-C(36)           124.4(3)
C(25)-N(2)-C(20)           117.3(3)
C(36)-N(2)-C(20)           118.2(3)
C(54)-N(3)-C(43)           124.3(3)
C(54)-N(3)-C(38)           117.1(3)
C(43)-N(3)-C(38)           118.4(3)
C(61)-N(4)-C(72)           124.1(3)
C(61)-N(4)-C(56)           117.4(3)
C(72)-N(4)-C(56)           118.1(3)
C(1)-O(1)-Rh(1)            118.8(2)
C(1)-O(2)-Rh(2)            118.2(2)
C(19)-O(5)-Rh(1)           117.8(2)
C(19)-O(6)-Rh(2)           119.4(2)
C(37)-O(9)-Rh(1)           117.7(2)
C(37)-O(10)-Rh(2)          118.8(2)
C(55)-O(13)-Rh(1)          118.1(2)
C(55)-O(14)-Rh(2)          118.9(2)
C(73)-O(17)-Rh(1)          129.13(19)
C(73)-O(18)-C(75)          117.4(2)
C(81)-O(21)-C(83)          115.0(6)
C(77)-O(19)-C(80)          109.5(11)
C(77)-O(19)-Rh(2)          119.5(15)
C(80)-O(19)-Rh(2)          121.2(10)
O(19)-C(77)-C(78)          101.0(12)
C(77)-C(78)-C(79)           86.5(12)
C(80)-C(79)-C(78)           91.5(11)
O(19)-C(80)-C(79)           98.2(14)
C(77')-O(19')-C(80')       109.7(12)
C(77')-O(19')-Rh(2)        125.6(12)
C(80')-O(19')-Rh(2)        115.1(15)
O(19')-C(77')-C(78')       102.9(15)
C(77')-C(78')-C(79')        94.3(12)
C(80')-C(79')-C(78')        87.3(12)
O(19')-C(80')-C(79')        98.7(12)
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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Aˆ2 x 10ˆ3) for joef094a.
The anisotropic displacement factor exponent takes the form:
-2 piˆ2 [hˆ2 a*ˆ2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Rh(1)	28(1)	26(1)	20(1)	0(1)	-1(1)	1(1)
Rh(2)	34(1)	29(1)	20(1)	1(1)	-1(1)	2(1)
C(1)	36(2)	34(2)	29(2)	1(1)	3(1)	-2(1)
C(2)	50(2)	33(2)	25(2)	1(1)	2(1)	-8(1)
C(3)	85(3)	42(2)	35(2)	6(2)	-2(2)	-20(2)
C(4)	134(5)	50(2)	46(2)	21(2)	-15(3)	-13(3)
C(5)	131(5)	53(3)	49(3)	5(2)	4(3)	-46(3)
C(6)	91(4)	78(3)	45(2)	3(2)	14(2)	-39(3)
C(7)	52(2)	26(2)	30(2)	1(1)	-4(2)	-5(1)
C(8)	65(2)	24(2)	26(2)	5(1)	-3(2)	-3(2)
C(9)	65(3)	37(2)	30(2)	4(2)	-5(2)	-5(2)
C(10)	97(4)	37(2)	26(2)	-1(2)	-2(2)	-5(2)
C(11)	96(4)	37(2)	29(2)	6(1)	7(2)	5(2)
C(12)	78(3)	33(2)	37(2)	5(2)	13(2)	10(2)
C(13)	64(3)	26(2)	32(2)	3(1)	2(2)	5(2)
C(14)	49(2)	29(2)	44(2)	2(2)	1(2)	2(2)
C(15)	54(2)	45(2)	61(3)	1(2)	2(2)	6(2)
C(16)	58(3)	58(3)	78(3)	6(3)	16(2)	15(2)
C(17)	79(3)	48(2)	58(3)	3(2)	17(2)	17(2)
C(18)	47(2)	29(2)	37(2)	-1(1)	-5(2)	-1(1)
C(19)	33(2)	25(1)	35(2)	-3(1)	-4(1)	2(1)
C(20)	34(2)	30(2)	38(2)	2(1)	-1(1)	6(1)
C(21)	46(2)	45(2)	44(2)	10(2)	-7(2)	12(2)
C(22)	55(2)	69(3)	45(2)	2(2)	-21(2)	8(2)
C(23)	47(2)	75(3)	71(3)	15(3)	-7(2)	24(2)
C(24)	63(3)	47(2)	62(3)	18(2)	-4(2)	10(2)
C(25)	33(2)	41(2)	42(2)	0(2)	-2(1)	9(1)
C(26)	27(2)	53(2)	43(2)	6(2)	-4(1)	2(1)
C(27)	29(2)	66(3)	49(2)	2(2)	-2(2)	3(2)
C(28)	27(2)	102(4)	52(2)	6(3)	-5(2)	-6(2)
C(29)	38(2)	95(4)	59(3)	23(3)	-8(2)	-22(2)
C(30)	41(2)	64(3)	55(2)	16(2)	-12(2)	-13(2)
C(31)	31(2)	48(2)	47(2)	6(2)	-10(2)	-3(1)
C(32)	39(2)	38(2)	51(2)	0(2)	-10(2)	-2(2)
C(33)	61(3)	36(2)	66(3)	3(2)	-5(2)	-2(2)
C(34)	85(4)	40(2)	87(4)	9(2)	-12(3)	-6(2)
C(35)	72(3)	53(3)	73(3)	19(2)	-10(3)	-24(2)
C(36)	33(2)	35(2)	48(2)	-2(2)	-7(2)	4(1)
C(37)	28(1)	31(2)	30(2)	-3(1)	-2(1)	7(1)
C(38)	36(2)	29(2)	38(2)	-5(1)	-6(2)	3(1)
C(39)	61(2)	40(2)	38(2)	-7(2)	-18(2)	0(2)
C(40)	71(3)	55(3)	57(3)	-1(2)	-33(2)	3(2)
C(41)	103(4)	46(2)	55(3)	-14(2)	-36(3)	-4(2)
C(42)	88(3)	71(3)	30(2)	-14(2)	0(2)	13(3)
C(43)	40(2)	34(2)	32(2)	-6(1)	-2(1)	4(1)
C(44)	48(2)	36(2)	37(2)	-8(1)	-4(2)	9(2)
C(45)	48(2)	46(2)	65(3)	-10(2)	-7(2)	13(2)
C(46)	54(3)	66(3)	77(3)	-12(3)	-19(2)	23(2)
C(47)	89(4)	56(3)	55(3)	-5(2)	-24(3)	34(3)
C(48)	76(3)	42(2)	33(2)	-4(2)	-11(2)	17(2)
C(49)	55(2)	34(2)	29(2)	-5(1)	-9(2)	9(2)

C(50)	61(2)	33(2)	30(2)	-4(1)	-1(2)	-1(2)
C(51)	80(3)	43(2)	49(2)	0(2)	8(2)	-6(2)
C(52)	113(5)	42(2)	53(3)	4(2)	7(3)	-7(3)
C(53)	116(4)	37(2)	42(2)	9(2)	-4(3)	15(2)
C(54)	46(2)	31(2)	36(2)	-5(1)	-1(2)	-5(2)
C(55)	35(2)	35(2)	29(2)	-2(1)	1(1)	-1(1)
C(56)	33(2)	46(2)	31(2)	-3(2)	3(1)	2(1)
C(57)	39(2)	86(3)	36(2)	-3(2)	11(2)	8(2)
C(58)	56(3)	118(5)	34(2)	-10(3)	6(2)	18(3)
C(59)	65(3)	120(5)	53(3)	18(3)	20(2)	-5(3)
C(60)	46(3)	153(6)	51(3)	-5(3)	16(2)	31(3)
C(61)	33(2)	49(2)	41(2)	9(2)	2(1)	-6(1)
C(62)	33(2)	44(2)	41(2)	4(2)	4(1)	-9(2)
C(63)	46(2)	54(2)	53(2)	9(2)	-3(2)	-18(2)
C(64)	61(3)	59(3)	57(3)	1(2)	3(2)	-26(2)
C(65)	40(2)	76(3)	46(2)	1(2)	2(2)	-19(2)
C(66)	29(2)	67(3)	41(2)	1(2)	3(1)	-7(2)
C(67)	25(2)	59(2)	40(2)	3(2)	5(1)	-4(1)
C(68)	30(2)	51(2)	41(2)	2(2)	5(1)	4(1)
C(69)	38(2)	55(2)	50(2)	2(2)	4(2)	7(2)
C(70)	38(2)	74(3)	49(2)	14(2)	1(2)	13(2)
C(71)	32(2)	83(3)	39(2)	3(2)	-3(2)	-1(2)
C(72)	29(2)	45(2)	43(2)	4(2)	5(1)	6(1)
C(73)	31(2)	39(2)	28(1)	3(1)	1(1)	-2(1)
C(74)	46(2)	34(2)	41(2)	1(1)	8(2)	0(2)
C(75)	58(2)	36(2)	38(2)	3(1)	-8(2)	0(2)
C(76)	149(6)	50(2)	45(2)	12(2)	-18(3)	-2(3)
C(81)	101(5)	139(7)	84(5)	18(5)	-22(4)	19(5)
C(82)	147(8)	264(13)	105(6)	59(8)	6(6)	-70(9)
C(83)	99(5)	98(5)	98(5)	17(4)	16(4)	21(4)
C(84)	158(9)	107(6)	233(12)	-14(8)	7(9)	55(6)
N(1)	49(2)	28(1)	30(2)	1(1)	0(1)	-6(1)
N(2)	31(1)	35(1)	41(2)	0(1)	-1(1)	4(1)
N(3)	37(1)	28(1)	33(1)	-3(1)	-1(1)	3(1)
N(4)	29(1)	47(2)	37(2)	2(1)	1(1)	3(1)
O(1)	34(1)	31(1)	27(1)	0(1)	-1(1)	-5(1)
O(2)	49(1)	33(1)	24(1)	3(1)	-1(1)	-5(1)
O(3)	48(2)	49(2)	43(2)	-5(1)	-6(1)	-3(1)
O(4)	52(2)	47(2)	44(2)	-7(1)	-10(1)	3(1)
O(5)	33(1)	30(1)	28(1)	-1(1)	-2(1)	5(1)
O(6)	38(1)	32(1)	28(1)	2(1)	-2(1)	7(1)
O(7)	55(2)	41(1)	56(2)	-2(1)	9(1)	12(1)
O(8)	43(1)	38(1)	48(2)	-9(1)	0(1)	3(1)
O(9)	36(1)	29(1)	26(1)	1(1)	-2(1)	1(1)
O(10)	44(1)	29(1)	25(1)	0(1)	-3(1)	3(1)
O(11)	39(1)	37(1)	51(2)	-2(1)	5(1)	1(1)
O(12)	45(2)	44(2)	68(2)	0(1)	3(1)	-7(1)
O(13)	29(1)	37(1)	27(1)	0(1)	0(1)	3(1)
O(14)	34(1)	45(1)	28(1)	1(1)	3(1)	3(1)
O(15)	51(2)	45(2)	59(2)	13(1)	-9(1)	-3(1)
O(16)	48(2)	40(1)	57(2)	-3(1)	-6(1)	5(1)
O(17)	31(1)	35(1)	26(1)	2(1)	0(1)	-2(1)
O(18)	58(2)	35(1)	31(1)	0(1)	3(1)	-2(1)
O(20)	105(3)	138(4)	88(3)	-3(3)	9(3)	13(3)
O(21)	99(4)	165(5)	88(3)	15(4)	7(3)	32(4)
O(19)	53(2)	59(3)	30(1)	10(1)	-5(1)	-2(2)
C(77)	126(7)	110(9)	47(5)	26(5)	-9(5)	-38(6)
C(78)	150(8)	122(9)	69(6)	51(6)	-19(6)	-33(7)
C(79)	132(7)	147(9)	58(6)	41(6)	-28(5)	-12(7)
C(80)	95(6)	152(9)	43(6)	28(6)	-12(5)	-25(6)
O(19')	53(2)	59(3)	30(1)	10(1)	-5(1)	-2(2)

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C(77')	126(7)	110(9)	47(5)	26(5)	-9(5)	-38(6)
C(78')	150(8)	122(9)	69(6)	51(6)	-19(6)	-33(7)
C(79')	132(7)	147(9)	58(6)	41(6)	-28(5)	-12(7)
C(80')	95(6)	152(9)	43(6)	28(6)	-12(5)	-25(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic
displacement parameters (A^2 x 10^3) for joef094a.

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	x	y	z	U(eq)
H(2A)	1370	649	1834	43
H(4A)	2117	-470	3500	115
H(4B)	2471	150	3279	115
H(4C)	2489	-423	2700	115
H(5A)	1214	-813	2677	117
H(5B)	1590	-692	1892	117
H(5C)	937	-364	2031	117
H(6A)	1068	-6	3626	107
H(6B)	835	476	2991	107
H(6C)	1403	645	3547	107
H(9A)	1307	-443	-517	53
H(10A)	1802	-1045	-1453	64
H(11A)	2853	-1084	-1518	65
H(15A)	3954	158	1068	64
H(16A)	4458	-302	1	78
H(17A)	3903	-734	-979	74
H(20A)	4298	1142	2016	41
H(22A)	5019	2017	3605	84
H(22B)	4927	1472	4216	84
H(22C)	4340	1843	3901	84
H(23A)	5583	1374	2701	97
H(23B)	5306	731	2424	97
H(23C)	5541	814	3298	97
H(24A)	3912	790	3567	86
H(24B)	4546	452	3784	86
H(24C)	4261	382	2932	86
H(27A)	5829	1603	150	58
H(28A)	6300	2335	-670	72
H(29A)	6150	3363	-449	77
H(33A)	4575	3777	2177	65
H(34A)	5036	4506	1353	85
H(35A)	5665	4220	366	79
H(38A)	3746	3833	3153	41
H(40A)	4056	3493	5078	92
H(40B)	4294	3447	4201	92
H(40C)	3750	3008	4497	92
H(41A)	3874	4578	4967	102
H(41B)	3452	4857	4292	102
H(41C)	4116	4576	4090	102
H(42A)	2996	3865	5345	94
H(42B)	2665	3464	4688	94
H(42C)	2600	4194	4681	94
H(45A)	1141	4559	2988	64
H(46A)	620	5445	2573	79
H(47A)	1162	6283	2155	80
H(51A)	3760	5824	2100	69
H(52A)	3238	6728	1744	83
H(53A)	2184	6782	1813	78
H(56A)	941	3383	2965	44
H(58A)	727	3209	4926	104
H(58B)	1032	3611	4251	104
H(58C)	1325	2962	4477	104

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H(59A)	241	2225	4617	119
H(59B)	750	1972	4023	119
H(59C)	49	2059	3745	119
H(60A)	-266	3278	4301	125
H(60B)	-378	3028	3440	125
H(60C)	-5	3652	3573	125
H(63A)	-26	1106	1632	61
H(64A)	-702	874	603	71
H(65A)	-1122	1652	-136	65
H(69A)	-345	4007	918	57
H(70A)	-983	3774	-134	65
H(71A)	-1215	2783	-449	62
H(74A)	2844	1481	566	60
H(74B)	2813	1486	-362	60
H(74C)	2190	1436	135	60
H(75A)	2790	3402	-508	53
H(75B)	2068	3323	-313	53
H(76A)	2188	3765	-1549	122
H(76B)	1868	3107	-1628	122
H(76C)	2587	3187	-1823	122
H(82A)	1805	3295	6555	258
H(82B)	1848	2876	5795	258
H(82C)	2254	2712	6543	258
H(83A)	290	1870	6354	118
H(83B)	736	1535	6966	118
H(84A)	422	781	6188	249
H(84B)	1101	939	5877	249
H(84C)	506	1190	5425	249
H(77A)	2612	771	4523	113
H(77B)	1930	1053	4659	113
H(78A)	2364	685	5949	137
H(78B)	2304	1431	5983	137
H(79A)	3472	1145	5979	135
H(79B)	3358	832	5133	135
H(80A)	2985	2135	5519	116
H(80B)	3472	1969	4836	116
H(77C)	1990	1058	4584	113
H(77D)	1899	1536	5288	113
H(78C)	2906	619	5201	137
H(78D)	2424	690	5919	137
H(79C)	2783	1812	6065	135
H(79D)	3393	1378	6159	135
H(80C)	3481	2002	4889	116
H(80D)	3444	1277	4696	116

Table 6. Torsion angles [deg] for joef094a.

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O(13)-Rh(1)-Rh(2)-O(10)                    -89.63(9)
O(1)-Rh(1)-Rh(2)-O(10)                    -178.85(10)
O(5)-Rh(1)-Rh(2)-O(10)                      90.04(9)
O(9)-Rh(1)-Rh(2)-O(10)                      -0.32(9)
O(17)-Rh(1)-Rh(2)-O(10)                    148.8(11)
O(13)-Rh(1)-Rh(2)-O(2)                      90.28(10)
O(1)-Rh(1)-Rh(2)-O(2)                        1.06(9)
O(5)-Rh(1)-Rh(2)-O(2)                      -90.05(10)
O(9)-Rh(1)-Rh(2)-O(2)                      179.59(10)
O(17)-Rh(1)-Rh(2)-O(2)                     -31.3(11)
O(13)-Rh(1)-Rh(2)-O(14)                      0.28(9)
O(1)-Rh(1)-Rh(2)-O(14)                     -88.94(10)
O(5)-Rh(1)-Rh(2)-O(14)                     179.95(10)
O(9)-Rh(1)-Rh(2)-O(14)                      89.59(10)
O(17)-Rh(1)-Rh(2)-O(14)                    -121.3(11)
O(13)-Rh(1)-Rh(2)-O(6)                    -179.02(9)
O(1)-Rh(1)-Rh(2)-O(6)                       91.76(9)
O(5)-Rh(1)-Rh(2)-O(6)                        0.65(9)
O(9)-Rh(1)-Rh(2)-O(6)                      -89.71(9)
O(17)-Rh(1)-Rh(2)-O(6)                      59.4(11)
O(13)-Rh(1)-Rh(2)-O(19')                   -98(29)
O(1)-Rh(1)-Rh(2)-O(19')                    172(29)
O(5)-Rh(1)-Rh(2)-O(19')                     81(29)
O(9)-Rh(1)-Rh(2)-O(19')                     -9(29)
O(17)-Rh(1)-Rh(2)-O(19')                   140(29)
O(13)-Rh(1)-Rh(2)-O(19)                    142(85)
O(1)-Rh(1)-Rh(2)-O(19)                      53(84)
O(5)-Rh(1)-Rh(2)-O(19)                     -38(84)
O(9)-Rh(1)-Rh(2)-O(19)                    -129(84)
O(17)-Rh(1)-Rh(2)-O(19)                     21(84)
O(2)-C(1)-C(2)-N(1)                       -132.9(3)
O(1)-C(1)-C(2)-N(1)                         49.6(4)
O(2)-C(1)-C(2)-C(3)                         -0.4(5)
O(1)-C(1)-C(2)-C(3)                       -178.0(3)
N(1)-C(2)-C(3)-C(4)                         67.5(4)
C(1)-C(2)-C(3)-C(4)                        -62.8(5)
N(1)-C(2)-C(3)-C(6)                       -168.9(3)
C(1)-C(2)-C(3)-C(6)                         60.8(5)
N(1)-C(2)-C(3)-C(5)                        -53.0(5)
C(1)-C(2)-C(3)-C(5)                        176.7(4)
O(3)-C(7)-C(8)-C(13)                       172.6(4)
N(1)-C(7)-C(8)-C(13)                       -10.0(5)
O(3)-C(7)-C(8)-C(9)                         -9.9(5)
N(1)-C(7)-C(8)-C(9)                        167.5(3)
C(13)-C(8)-C(9)-C(10)                        2.2(6)
C(7)-C(8)-C(9)-C(10)                      -175.2(3)
C(8)-C(9)-C(10)-C(11)                       -4.8(6)
C(9)-C(10)-C(11)-C(12)                       1.5(7)
C(10)-C(11)-C(12)-C(17)                    -179.2(4)
C(10)-C(11)-C(12)-C(13)                      4.0(6)
C(9)-C(8)-C(13)-C(14)                      -176.4(3)
C(7)-C(8)-C(13)-C(14)                        1.0(6)
C(9)-C(8)-C(13)-C(12)                        3.3(6)
C(7)-C(8)-C(13)-C(12)                      -179.2(3)
C(17)-C(12)-C(13)-C(8)                      176.7(4)
C(11)-C(12)-C(13)-C(8)                       -6.3(5)
C(17)-C(12)-C(13)-C(14)                      -3.6(5)
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C(11)-C(12)-C(13)-C(14)	173.4(3)
C(8)-C(13)-C(14)-C(15)	-178.1(4)
C(12)-C(13)-C(14)-C(15)	2.2(6)
C(8)-C(13)-C(14)-C(18)	5.2(6)
C(12)-C(13)-C(14)-C(18)	-174.5(3)
C(13)-C(14)-C(15)-C(16)	0.4(6)
C(18)-C(14)-C(15)-C(16)	177.1(4)
C(14)-C(15)-C(16)-C(17)	-1.6(7)
C(15)-C(16)-C(17)-C(12)	0.0(7)
C(11)-C(12)-C(17)-C(16)	-174.2(4)
C(13)-C(12)-C(17)-C(16)	2.5(6)
C(15)-C(14)-C(18)-O(4)	0.7(6)
C(13)-C(14)-C(18)-O(4)	177.4(3)
C(15)-C(14)-C(18)-N(1)	-179.1(4)
C(13)-C(14)-C(18)-N(1)	-2.4(5)
O(6)-C(19)-C(20)-N(2)	-137.7(3)
O(5)-C(19)-C(20)-N(2)	46.4(4)
O(6)-C(19)-C(20)-C(21)	-6.1(4)
O(5)-C(19)-C(20)-C(21)	178.1(3)
N(2)-C(20)-C(21)-C(22)	71.0(4)
C(19)-C(20)-C(21)-C(22)	-58.2(4)
N(2)-C(20)-C(21)-C(24)	-166.8(3)
C(19)-C(20)-C(21)-C(24)	64.1(4)
N(2)-C(20)-C(21)-C(23)	-49.8(4)
C(19)-C(20)-C(21)-C(23)	-178.9(3)
O(7)-C(25)-C(26)-C(27)	-2.5(5)
N(2)-C(25)-C(26)-C(27)	178.6(3)
O(7)-C(25)-C(26)-C(31)	172.5(4)
N(2)-C(25)-C(26)-C(31)	-6.3(5)
C(31)-C(26)-C(27)-C(28)	-1.0(5)
C(25)-C(26)-C(27)-C(28)	174.0(3)
C(26)-C(27)-C(28)-C(29)	0.1(6)
C(27)-C(28)-C(29)-C(30)	0.7(6)
C(28)-C(29)-C(30)-C(35)	-178.8(4)
C(28)-C(29)-C(30)-C(31)	-0.5(6)
C(27)-C(26)-C(31)-C(32)	178.9(3)
C(25)-C(26)-C(31)-C(32)	4.0(5)
C(27)-C(26)-C(31)-C(30)	1.2(5)
C(25)-C(26)-C(31)-C(30)	-173.8(3)
C(35)-C(30)-C(31)-C(26)	178.0(4)
C(29)-C(30)-C(31)-C(26)	-0.4(5)
C(35)-C(30)-C(31)-C(32)	0.1(5)
C(29)-C(30)-C(31)-C(32)	-178.2(4)
C(26)-C(31)-C(32)-C(33)	-177.5(4)
C(30)-C(31)-C(32)-C(33)	0.3(6)
C(26)-C(31)-C(32)-C(36)	2.6(5)
C(30)-C(31)-C(32)-C(36)	-179.6(3)
C(31)-C(32)-C(33)-C(34)	-0.1(6)
C(36)-C(32)-C(33)-C(34)	179.8(4)
C(32)-C(33)-C(34)-C(35)	-0.6(8)
C(33)-C(34)-C(35)-C(30)	1.1(8)
C(31)-C(30)-C(35)-C(34)	-0.9(7)
C(29)-C(30)-C(35)-C(34)	177.4(5)
C(33)-C(32)-C(36)-O(8)	-4.9(6)
C(31)-C(32)-C(36)-O(8)	175.0(3)
C(33)-C(32)-C(36)-N(2)	173.4(3)
C(31)-C(32)-C(36)-N(2)	-6.7(5)
O(10)-C(37)-C(38)-N(3)	-134.0(3)
O(9)-C(37)-C(38)-N(3)	50.0(4)
O(10)-C(37)-C(38)-C(39)	-3.5(4)
O(9)-C(37)-C(38)-C(39)	-179.5(3)

N(3)-C(38)-C(39)-C(42)	69.4(4)
C(37)-C(38)-C(39)-C(42)	-59.8(4)
N(3)-C(38)-C(39)-C(40)	-166.9(3)
C(37)-C(38)-C(39)-C(40)	63.9(4)
N(3)-C(38)-C(39)-C(41)	-51.6(4)
C(37)-C(38)-C(39)-C(41)	179.2(3)
O(11)-C(43)-C(44)-C(45)	-0.2(5)
N(3)-C(43)-C(44)-C(45)	-179.7(3)
O(11)-C(43)-C(44)-C(49)	179.5(3)
N(3)-C(43)-C(44)-C(49)	-0.1(5)
C(49)-C(44)-C(45)-C(46)	-2.4(6)
C(43)-C(44)-C(45)-C(46)	177.2(4)
C(44)-C(45)-C(46)-C(47)	0.1(7)
C(45)-C(46)-C(47)-C(48)	1.8(8)
C(46)-C(47)-C(48)-C(53)	178.0(4)
C(46)-C(47)-C(48)-C(49)	-1.3(7)
C(45)-C(44)-C(49)-C(50)	-176.0(4)
C(43)-C(44)-C(49)-C(50)	4.4(5)
C(45)-C(44)-C(49)-C(48)	2.8(5)
C(43)-C(44)-C(49)-C(48)	-176.8(3)
C(47)-C(48)-C(49)-C(50)	177.8(4)
C(53)-C(48)-C(49)-C(50)	-1.5(5)
C(47)-C(48)-C(49)-C(44)	-1.0(5)
C(53)-C(48)-C(49)-C(44)	179.6(3)
C(44)-C(49)-C(50)-C(51)	179.5(3)
C(48)-C(49)-C(50)-C(51)	0.7(6)
C(44)-C(49)-C(50)-C(54)	-1.0(5)
C(48)-C(49)-C(50)-C(54)	-179.8(3)
C(49)-C(50)-C(51)-C(52)	1.1(6)
C(54)-C(50)-C(51)-C(52)	-178.4(4)
C(50)-C(51)-C(52)-C(53)	-2.0(7)
C(51)-C(52)-C(53)-C(48)	1.1(8)
C(47)-C(48)-C(53)-C(52)	-178.7(5)
C(49)-C(48)-C(53)-C(52)	0.6(6)
C(51)-C(50)-C(54)-O(12)	-6.1(6)
C(49)-C(50)-C(54)-O(12)	174.4(4)
C(51)-C(50)-C(54)-N(3)	172.9(3)
C(49)-C(50)-C(54)-N(3)	-6.6(5)
O(14)-C(55)-C(56)-N(4)	-137.9(3)
O(13)-C(55)-C(56)-N(4)	47.6(4)
O(14)-C(55)-C(56)-C(57)	-5.4(5)
O(13)-C(55)-C(56)-C(57)	-179.8(3)
N(4)-C(56)-C(57)-C(59)	70.9(5)
C(55)-C(56)-C(57)-C(59)	-59.5(5)
N(4)-C(56)-C(57)-C(58)	-165.8(4)
C(55)-C(56)-C(57)-C(58)	63.8(5)
N(4)-C(56)-C(57)-C(60)	-50.2(5)
C(55)-C(56)-C(57)-C(60)	179.5(4)
O(15)-C(61)-C(62)-C(63)	6.4(6)
N(4)-C(61)-C(62)-C(63)	-173.7(3)
O(15)-C(61)-C(62)-C(67)	-171.5(4)
N(4)-C(61)-C(62)-C(67)	8.3(5)
C(67)-C(62)-C(63)-C(64)	0.7(6)
C(61)-C(62)-C(63)-C(64)	-177.2(4)
C(62)-C(63)-C(64)-C(65)	1.1(7)
C(63)-C(64)-C(65)-C(66)	-0.9(7)
C(64)-C(65)-C(66)-C(67)	-1.1(6)
C(64)-C(65)-C(66)-C(71)	177.2(4)
C(63)-C(62)-C(67)-C(68)	-178.9(4)
C(61)-C(62)-C(67)-C(68)	-1.0(5)
C(63)-C(62)-C(67)-C(66)	-2.6(5)

C(61)-C(62)-C(67)-C(66)	175.3(3)
C(65)-C(66)-C(67)-C(68)	179.1(3)
C(71)-C(66)-C(67)-C(68)	0.8(5)
C(65)-C(66)-C(67)-C(62)	2.8(5)
C(71)-C(66)-C(67)-C(62)	-175.6(3)
C(62)-C(67)-C(68)-C(69)	176.3(3)
C(66)-C(67)-C(68)-C(69)	0.0(5)
C(62)-C(67)-C(68)-C(72)	-2.8(5)
C(66)-C(67)-C(68)-C(72)	-179.1(3)
C(67)-C(68)-C(69)-C(70)	-0.3(5)
C(72)-C(68)-C(69)-C(70)	178.8(3)
C(68)-C(69)-C(70)-C(71)	-0.3(6)
C(69)-C(70)-C(71)-C(66)	1.1(6)
C(65)-C(66)-C(71)-C(70)	-179.6(4)
C(67)-C(66)-C(71)-C(70)	-1.3(6)
C(69)-C(68)-C(72)-O(16)	1.3(5)
C(67)-C(68)-C(72)-O(16)	-179.6(3)
C(69)-C(68)-C(72)-N(4)	-179.9(3)
C(67)-C(68)-C(72)-N(4)	-0.8(5)
O(4)-C(18)-N(1)-C(7)	173.0(3)
C(14)-C(18)-N(1)-C(7)	-7.2(5)
O(4)-C(18)-N(1)-C(2)	-2.2(5)
C(14)-C(18)-N(1)-C(2)	177.5(3)
O(3)-C(7)-N(1)-C(18)	-169.4(3)
C(8)-C(7)-N(1)-C(18)	13.1(5)
O(3)-C(7)-N(1)-C(2)	6.0(5)
C(8)-C(7)-N(1)-C(2)	-171.5(3)
C(1)-C(2)-N(1)-C(18)	45.7(4)
C(3)-C(2)-N(1)-C(18)	-88.3(4)
C(1)-C(2)-N(1)-C(7)	-129.9(3)
C(3)-C(2)-N(1)-C(7)	96.1(4)
O(7)-C(25)-N(2)-C(36)	-176.8(3)
C(26)-C(25)-N(2)-C(36)	2.0(5)
O(7)-C(25)-N(2)-C(20)	-1.7(5)
C(26)-C(25)-N(2)-C(20)	177.2(3)
O(8)-C(36)-N(2)-C(25)	-177.4(3)
C(32)-C(36)-N(2)-C(25)	4.3(5)
O(8)-C(36)-N(2)-C(20)	7.5(5)
C(32)-C(36)-N(2)-C(20)	-170.8(3)
C(19)-C(20)-N(2)-C(25)	-133.4(3)
C(21)-C(20)-N(2)-C(25)	93.6(4)
C(19)-C(20)-N(2)-C(36)	42.1(4)
C(21)-C(20)-N(2)-C(36)	-90.9(4)
O(12)-C(54)-N(3)-C(43)	-169.6(3)
C(50)-C(54)-N(3)-C(43)	11.4(5)
O(12)-C(54)-N(3)-C(38)	6.4(5)
C(50)-C(54)-N(3)-C(38)	-172.7(3)
O(11)-C(43)-N(3)-C(54)	172.3(3)
C(44)-C(43)-N(3)-C(54)	-8.1(5)
O(11)-C(43)-N(3)-C(38)	-3.6(5)
C(44)-C(43)-N(3)-C(38)	176.0(3)
C(37)-C(38)-N(3)-C(54)	-130.3(3)
C(39)-C(38)-N(3)-C(54)	97.2(4)
C(37)-C(38)-N(3)-C(43)	45.9(4)
C(39)-C(38)-N(3)-C(43)	-86.6(4)
O(15)-C(61)-N(4)-C(72)	167.2(3)
C(62)-C(61)-N(4)-C(72)	-12.6(5)
O(15)-C(61)-N(4)-C(56)	-4.7(5)
C(62)-C(61)-N(4)-C(56)	175.5(3)
O(16)-C(72)-N(4)-C(61)	-172.2(3)
C(68)-C(72)-N(4)-C(61)	8.9(5)

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O(16)-C(72)-N(4)-C(56)              -0.3(5)
C(68)-C(72)-N(4)-C(56)            -179.2(3)
C(55)-C(56)-N(4)-C(61)              51.1(4)
C(57)-C(56)-N(4)-C(61)             -83.9(4)
C(55)-C(56)-N(4)-C(72)            -121.3(3)
C(57)-C(56)-N(4)-C(72)             103.7(4)
O(2)-C(1)-O(1)-Rh(1)                 2.8(5)
C(2)-C(1)-O(1)-Rh(1)              -179.9(2)
O(13)-Rh(1)-O(1)-C(1)              -90.3(2)
O(5)-Rh(1)-O(1)-C(1)                86.1(2)
O(9)-Rh(1)-O(1)-C(1)               -17.7(11)
Rh(2)-Rh(1)-O(1)-C(1)               -2.2(2)
O(17)-Rh(1)-O(1)-C(1)              176.3(2)
O(1)-C(1)-O(2)-Rh(2)                -1.5(5)
C(2)-C(1)-O(2)-Rh(2)              -178.8(2)
O(10)-Rh(2)-O(2)-C(1)                3(3)
O(14)-Rh(2)-O(2)-C(1)               88.1(3)
O(6)-Rh(2)-O(2)-C(1)               -88.2(3)
O(19')-Rh(2)-O(2)-C(1)            -180.0(9)
O(19)-Rh(2)-O(2)-C(1)             -180.0(9)
Rh(1)-Rh(2)-O(2)-C(1)               -0.3(2)
O(6)-C(19)-O(5)-Rh(1)                6.5(4)
C(20)-C(19)-O(5)-Rh(1)            -178.1(2)
O(13)-Rh(1)-O(5)-C(19)               1.7(15)
O(1)-Rh(1)-O(5)-C(19)              -90.8(2)
O(9)-Rh(1)-O(5)-C(19)               83.9(2)
Rh(2)-Rh(1)-O(5)-C(19)              -3.5(2)
O(17)-Rh(1)-O(5)-C(19)             178.9(2)
O(5)-C(19)-O(6)-Rh(2)               -5.8(4)
C(20)-C(19)-O(6)-Rh(2)             178.9(2)
O(10)-Rh(2)-O(6)-C(19)             -87.0(2)
O(2)-Rh(2)-O(6)-C(19)               91.1(2)
O(14)-Rh(2)-O(6)-C(19)              -8.9(16)
O(19')-Rh(2)-O(6)-C(19)           -176.0(7)
O(19)-Rh(2)-O(6)-C(19)            -178.2(7)
Rh(1)-Rh(2)-O(6)-C(19)               2.1(2)
O(10)-C(37)-O(9)-Rh(1)               3.8(4)
C(38)-C(37)-O(9)-Rh(1)             179.4(2)
O(13)-Rh(1)-O(9)-C(37)              86.7(2)
O(1)-Rh(1)-O(9)-C(37)               14.1(11)
O(5)-Rh(1)-O(9)-C(37)              -89.8(2)
Rh(2)-Rh(1)-O(9)-C(37)              -1.4(2)
O(17)-Rh(1)-O(9)-C(37)            -180.0(2)
O(9)-C(37)-O(10)-Rh(2)              -4.2(4)
C(38)-C(37)-O(10)-Rh(2)           -179.7(2)
O(2)-Rh(2)-O(10)-C(37)              -1(3)
O(14)-Rh(2)-O(10)-C(37)            -86.2(2)
O(6)-Rh(2)-O(10)-C(37)              90.2(2)
O(19')-Rh(2)-O(10)-C(37)          -178.1(9)
O(19)-Rh(2)-O(10)-C(37)           -178.1(8)
Rh(1)-Rh(2)-O(10)-C(37)              2.2(2)
O(14)-C(55)-O(13)-Rh(1)              1.8(5)
C(56)-C(55)-O(13)-Rh(1)            175.8(2)
O(1)-Rh(1)-O(13)-C(55)              86.2(2)
O(5)-Rh(1)-O(13)-C(55)              -6.3(16)
O(9)-Rh(1)-O(13)-C(55)             -88.5(2)
Rh(2)-Rh(1)-O(13)-C(55)             -1.1(2)
O(17)-Rh(1)-O(13)-C(55)            176.6(2)
O(13)-C(55)-O(14)-Rh(2)             -1.5(5)
C(56)-C(55)-O(14)-Rh(2)           -175.2(2)
O(10)-Rh(2)-O(14)-C(55)             89.5(2)
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O(2)-Rh(2)-O(14)-C(55)          -88.6(3)
O(6)-Rh(2)-O(14)-C(55)           11.4(16)
O(19')-Rh(2)-O(14)-C(55)        178.5(7)
O(19)-Rh(2)-O(14)-C(55)        -179.4(7)
Rh(1)-Rh(2)-O(14)-C(55)           0.4(2)
O(18)-C(73)-O(17)-Rh(1)         173.3(2)
C(74)-C(73)-O(17)-Rh(1)          -5.7(5)
O(13)-Rh(1)-O(17)-C(73)        -113.5(3)
O(1)-Rh(1)-O(17)-C(73)          -24.3(3)
O(5)-Rh(1)-O(17)-C(73)           66.7(3)
O(9)-Rh(1)-O(17)-C(73)          157.0(3)
Rh(2)-Rh(1)-O(17)-C(73)           8.0(13)
O(17)-C(73)-O(18)-C(75)          -2.2(5)
C(74)-C(73)-O(18)-C(75)         177.0(3)
C(76)-C(75)-O(18)-C(73)        -171.3(4)
O(20)-C(81)-O(21)-C(83)           3.7(10)
C(82)-C(81)-O(21)-C(83)        -178.0(7)
C(84)-C(83)-O(21)-C(81)        -165.5(7)
O(10)-Rh(2)-O(19)-C(77)         180(2)
O(2)-Rh(2)-O(19)-C(77)            0(2)
O(14)-Rh(2)-O(19)-C(77)          90(2)
O(6)-Rh(2)-O(19)-C(77)          -91(2)
O(19')-Rh(2)-O(19)-C(77)       -180(100)
Rh(1)-Rh(2)-O(19)-C(77)         -52(84)
O(10)-Rh(2)-O(19)-C(80)         -38(2)
O(2)-Rh(2)-O(19)-C(80)          142(2)
O(14)-Rh(2)-O(19)-C(80)        -128(2)
O(6)-Rh(2)-O(19)-C(80)           52(2)
O(19')-Rh(2)-O(19)-C(80)        -37(45)
Rh(1)-Rh(2)-O(19)-C(80)          90(84)
C(80)-O(19)-C(77)-C(78)          33(3)
Rh(2)-O(19)-C(77)-C(78)         179.6(17)
O(19)-C(77)-C(78)-C(79)         -63(2)
C(77)-C(78)-C(79)-C(80)          64.0(14)
C(77)-O(19)-C(80)-C(79)          11(3)
Rh(2)-O(19)-C(80)-C(79)        -134.5(19)
C(78)-C(79)-C(80)-O(19)         -49.8(19)
O(10)-Rh(2)-O(19')-C(77')       150(3)
O(2)-Rh(2)-O(19')-C(77')        -30(3)
O(14)-Rh(2)-O(19')-C(77')        60(3)
O(6)-Rh(2)-O(19')-C(77')       -120(3)
O(19)-Rh(2)-O(19')-C(77')       -29(45)
Rh(1)-Rh(2)-O(19')-C(77')       159(26)
O(10)-Rh(2)-O(19')-C(80')       -67(2)
O(2)-Rh(2)-O(19')-C(80')        113(2)
O(14)-Rh(2)-O(19')-C(80')      -157(2)
O(6)-Rh(2)-O(19')-C(80')         22(2)
O(19)-Rh(2)-O(19')-C(80')       113(49)
Rh(1)-Rh(2)-O(19')-C(80')       -58(31)
C(80')-O(19')-C(77')-C(78')      -5(3)
Rh(2)-O(19')-C(77')-C(78')      139(2)
O(19')-C(77')-C(78')-C(79')      45(2)
C(77')-C(78')-C(79')-C(80')     -60.1(17)
C(77')-O(19')-C(80')-C(79')     -36(3)
Rh(2)-O(19')-C(80')-C(79')      175.2(18)
C(78')-C(79')-C(80')-O(19')      60(2)
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_____

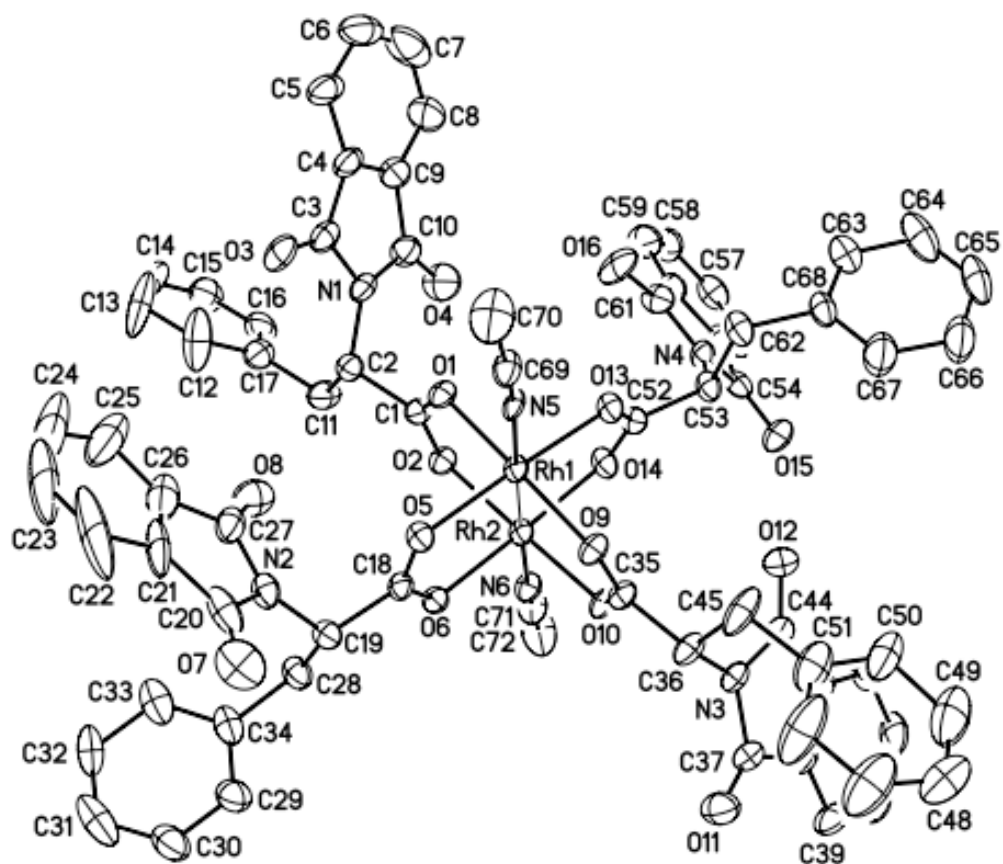Symmetry transformations used to generate equivalent atoms:

Figure 3. Molecular diagram of **4** compound with ellipsoids at 30% probability. Three cocrystallized acetonitrile solvent molecules and H-atoms deleted for clarity.

Table 1. Crystal data and structure refinement for joef099a.

Identification code	joef099a
Empirical formula	C78 H63 N9 O16 Rh2
Formula weight	1588.19
Temperature	200(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 12.649(4) A alpha = 90 deg. b = 24.398(7) A beta = 107.947(4) deg. c = 12.670(4) A gamma = 90 deg.
Volume	3719.9(18) A^3
Z, Calculated density	2, 1.418 Mg/m^3
Absorption coefficient	0.517 mm^-1
F(000)	1624
Crystal size	0.25 x 0.22 x 0.17 mm
Theta range for data collection	1.67 to 28.34 deg.
Limiting indices	-16<=h<=16, -32<=k<=32, -16<=l<=16
Reflections collected / unique	51127 / 18446 [R(int) = 0.0403]
Completeness to theta = 25.00	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9159 and 0.8812
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	18446 / 16 / 903
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0525, wR2 = 0.1383
R indices (all data)	R1 = 0.0597, wR2 = 0.1444
Absolute structure parameter	0.03(2)
Largest diff. peak and hole	1.198 and -0.557 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for joef099a.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

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	x	y	z	U(eq)

_____

Rh(1)	4635(1)	320(1)	3032(1)	32(1)
Rh(2)	5505(1)	-312(1)	2110(1)	33(1)
N(1)	1252(3)	-718(2)	1272(4)	44(1)
N(2)	5036(4)	-1053(2)	5807(4)	47(1)
N(3)	8531(3)	924(2)	2750(4)	43(1)
N(4)	3931(3)	760(2)	-1198(3)	42(1)
N(5)	3844(3)	927(2)	3883(3)	34(1)
N(6)	6333(4)	-889(2)	1231(4)	43(1)
O(1)	3231(3)	-127(2)	2461(3)	39(1)
O(2)	4085(3)	-760(2)	1707(3)	40(1)
O(3)	514(4)	-621(2)	2710(4)	65(1)
O(4)	1436(4)	-745(3)	-499(4)	80(1)
O(5)	5084(3)	-196(2)	4376(3)	39(1)
O(6)	6005(3)	-750(2)	3546(3)	37(1)
O(7)	5883(6)	-775(3)	7555(4)	98(2)
O(8)	3683(4)	-1409(2)	4242(5)	79(1)
O(9)	6087(3)	738(2)	3541(3)	40(1)
O(10)	6895(3)	185(2)	2590(3)	39(1)
O(11)	10179(4)	713(2)	4069(4)	70(1)
O(12)	7237(3)	1209(2)	1114(4)	63(1)
O(13)	4271(3)	795(1)	1647(3)	38(1)
O(14)	4963(3)	159(2)	725(3)	42(1)
O(15)	5475(3)	777(2)	-1805(3)	57(1)
O(16)	2224(4)	569(2)	-1010(4)	75(1)
C(1)	3288(4)	-586(2)	2025(4)	38(1)
C(2)	2304(4)	-971(2)	1899(4)	42(1)
C(3)	428(4)	-589(2)	1743(5)	50(1)
C(4)	-535(5)	-406(2)	815(6)	59(2)
C(5)	-1570(5)	-231(3)	828(8)	82(2)
C(6)	-2309(7)	-74(4)	-230(12)	107(4)
C(7)	-2022(9)	-139(5)	-1211(11)	122(5)
C(8)	-1036(7)	-305(4)	-1200(8)	98(3)
C(9)	-272(5)	-453(3)	-152(6)	64(2)
C(10)	875(5)	-644(3)	124(5)	55(1)
C(11)	2471(5)	-1538(3)	1434(6)	56(2)
C(12)	1039(11)	-2010(4)	2125(9)	120(4)
C(13)	158(13)	-2392(6)	1947(11)	145(6)
C(14)	-248(8)	-2641(4)	963(10)	96(3)
C(15)	192(7)	-2576(3)	154(7)	78(2)
C(16)	1043(6)	-2205(3)	313(7)	74(2)
C(17)	1510(5)	-1922(3)	1303(6)	54(1)
C(18)	5643(4)	-623(2)	4319(4)	36(1)
C(19)	5932(4)	-1004(2)	5328(4)	41(1)
C(20)	5103(8)	-948(3)	6902(5)	72(2)
C(21)	4009(10)	-1125(3)	6983(9)	99(4)
C(22)	3615(18)	-1069(5)	7941(12)	210(10)
C(23)	2630(20)	-1230(7)	7852(19)	232(16)
C(24)	1980(20)	-1417(8)	6900(30)	266(19)
C(25)	2277(10)	-1485(5)	5951(15)	146(6)
C(26)	3344(8)	-1326(3)	5987(10)	88(3)

C(27)	3975(6)	-1282(2)	5214(7)	63(2)
C(28)	6315(5)	-1575(3)	5079(5)	51(1)
C(29)	7604(6)	-1808(3)	7003(6)	66(2)
C(30)	7895(7)	-2114(3)	7936(6)	78(2)
C(31)	7294(10)	-2549(4)	8047(7)	96(3)
C(32)	6329(8)	-2678(3)	7229(7)	80(2)
C(33)	6010(8)	-2358(3)	6241(6)	77(2)
C(34)	6668(6)	-1926(2)	6127(5)	56(2)
C(35)	6853(4)	600(2)	3171(4)	38(1)
C(36)	7877(4)	982(3)	3485(5)	49(1)
C(37)	9679(4)	811(3)	3133(5)	48(1)
C(38)	10057(4)	860(2)	2151(5)	47(1)
C(39)	11104(5)	747(3)	2047(6)	64(2)
C(40)	11237(6)	798(3)	1023(7)	69(2)
C(41)	10365(7)	968(3)	136(7)	78(2)
C(42)	9287(6)	1063(3)	206(6)	67(2)
C(43)	9182(5)	1013(2)	1258(5)	51(1)
C(44)	8191(4)	1073(2)	1640(5)	50(1)
C(45)	7589(6)	1578(3)	3617(8)	76(2)
C(46)	9309(10)	1986(5)	4917(10)	128(5)
C(47)	10265(10)	2294(5)	5123(12)	132(5)
C(48)	10584(8)	2553(5)	4285(10)	109(4)
C(49)	9899(10)	2497(5)	3248(12)	115(4)
C(50)	8866(7)	2199(4)	2991(9)	87(3)
C(51)	8626(7)	1942(4)	3840(8)	84(3)
C(52)	4540(4)	620(2)	823(4)	34(1)
C(53)	4440(4)	1023(2)	-127(4)	40(1)
C(54)	4513(4)	655(2)	-1956(4)	42(1)
C(55)	3701(4)	391(2)	-2917(4)	43(1)
C(56)	3797(5)	221(2)	-3910(4)	53(1)
C(57)	2876(6)	-5(3)	-4672(5)	61(2)
C(58)	1902(6)	-74(3)	-4444(5)	64(2)
C(59)	1801(6)	83(3)	-3423(5)	71(2)
C(60)	2710(4)	329(3)	-2687(4)	51(1)
C(61)	2866(5)	549(3)	-1546(4)	52(1)
C(62)	3841(5)	1551(2)	-3(5)	49(1)
C(63)	3310(7)	2102(3)	-1779(6)	71(2)
C(64)	3476(10)	2532(4)	-2431(7)	93(3)
C(65)	4350(9)	2868(3)	-2043(8)	86(3)
C(66)	5077(8)	2805(4)	-976(9)	95(3)
C(67)	4883(7)	2361(4)	-352(7)	85(2)
C(68)	3991(5)	2012(2)	-756(5)	51(1)
C(69)	3383(5)	1199(2)	4302(5)	48(1)
C(70)	2748(9)	1526(4)	4839(9)	94(3)
C(71)	6636(6)	-1169(3)	705(5)	56(2)
C(72)	7102(9)	-1526(3)	20(8)	93(3)
N(7)	8545(12)	-484(6)	5803(11)	166(5)
C(73)	8723(10)	-629(5)	4966(10)	113(3)
C(74)	8726(11)	-871(6)	3986(10)	140(5)
N(8)	-1170(20)	975(11)	-3140(20)	298(11)
C(75)	-2180(30)	960(20)	-3150(40)	540(30)
C(76)	-3017(17)	630(9)	-3831(17)	220(9)
N(9)	5550(20)	1924(11)	-3827(19)	282(10)
C(77)	6500(20)	1924(12)	-3180(20)	253(11)
C(78)	6940(19)	1870(10)	-2049(19)	241(10)

```
Table 3.  Bond lengths [A] and angles [deg] for joef099a.
_____

Rh(1)-O(1)                2.018(4)
Rh(1)-O(9)                2.025(3)
Rh(1)-O(13)               2.033(3)
Rh(1)-O(5)                2.054(3)
Rh(1)-N(5)                2.241(4)
Rh(1)-Rh(2)               2.3985(5)
Rh(2)-O(14)               2.033(3)
Rh(2)-O(2)                2.028(4)
Rh(2)-O(6)                2.035(3)
Rh(2)-O(10)               2.066(3)
Rh(2)-N(6)                2.244(4)
N(1)-C(3)                 1.388(7)
N(1)-C(10)                1.396(7)
N(1)-C(2)                 1.459(7)
N(2)-C(20)                1.387(7)
N(2)-C(19)                1.447(6)
N(2)-C(27)                1.434(9)
N(3)-C(44)                1.387(7)
N(3)-C(37)                1.409(7)
N(3)-C(36)                1.431(6)
N(4)-C(61)                1.381(7)
N(4)-C(54)                1.402(6)
N(4)-C(53)                1.459(6)
N(5)-C(69)                1.119(7)
N(6)-C(71)                1.102(7)
O(1)-C(1)                 1.261(6)
O(2)-C(1)                 1.268(6)
O(3)-C(3)                 1.198(8)
O(4)-C(10)                1.237(7)
O(5)-C(18)                1.272(6)
O(6)-C(18)                1.241(6)
O(7)-C(20)                1.154(10)
O(8)-C(27)                1.213(9)
O(9)-C(35)                1.246(6)
O(10)-C(35)               1.262(6)
O(11)-C(37)               1.185(7)
O(12)-C(44)               1.231(7)
O(13)-C(52)               1.268(6)
O(14)-C(52)               1.268(6)
O(15)-C(54)               1.209(6)
O(16)-C(61)               1.210(6)
C(1)-C(2)                 1.528(7)
C(2)-C(11)                1.545(8)
C(3)-C(4)                 1.478(9)
C(4)-C(9)                 1.370(10)
C(4)-C(5)                 1.382(9)
C(5)-C(6)                 1.430(14)
C(6)-C(7)                 1.408(16)
C(7)-C(8)                 1.307(16)
C(8)-C(9)                 1.426(10)
C(9)-C(10)                1.461(9)
C(11)-C(17)               1.503(9)
C(12)-C(17)               1.366(11)
C(12)-C(13)               1.415(14)
C(13)-C(14)               1.340(15)
C(14)-C(15)               1.318(13)
C(15)-C(16)               1.374(10)
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C(16)-C(17)	1.394(10)
C(18)-C(19)	1.532(7)
C(19)-C(28)	1.537(8)
C(20)-C(21)	1.483(13)
C(21)-C(26)	1.372(14)
C(21)-C(22)	1.454(10)
C(22)-C(23)	1.28(3)
C(23)-C(24)	1.32(4)
C(24)-C(25)	1.37(2)
C(25)-C(26)	1.392(13)
C(26)-C(27)	1.445(10)
C(28)-C(34)	1.527(8)
C(29)-C(30)	1.350(9)
C(29)-C(34)	1.380(10)
C(30)-C(31)	1.338(13)
C(31)-C(32)	1.372(13)
C(32)-C(33)	1.423(10)
C(33)-C(34)	1.378(10)
C(35)-C(36)	1.545(7)
C(36)-C(45)	1.522(9)
C(37)-C(38)	1.468(8)
C(38)-C(43)	1.369(8)
C(38)-C(39)	1.399(7)
C(39)-C(40)	1.363(10)
C(40)-C(41)	1.374(11)
C(41)-C(42)	1.412(10)
C(42)-C(43)	1.384(8)
C(43)-C(44)	1.484(7)
C(45)-C(51)	1.537(10)
C(46)-C(51)	1.376(14)
C(46)-C(47)	1.379(14)
C(47)-C(48)	1.399(16)
C(48)-C(49)	1.340(15)
C(49)-C(50)	1.443(13)
C(50)-C(51)	1.357(12)
C(52)-C(53)	1.528(7)
C(53)-C(62)	1.527(7)
C(54)-C(55)	1.478(8)
C(55)-C(56)	1.365(7)
C(55)-C(60)	1.381(7)
C(56)-C(57)	1.379(9)
C(57)-C(58)	1.361(10)
C(58)-C(59)	1.392(9)
C(59)-C(60)	1.375(9)
C(60)-C(61)	1.497(7)
C(62)-C(68)	1.523(7)
C(63)-C(68)	1.335(9)
C(63)-C(64)	1.390(11)
C(64)-C(65)	1.341(14)
C(65)-C(66)	1.389(14)
C(66)-C(67)	1.405(11)
C(67)-C(68)	1.381(10)
C(69)-C(70)	1.443(10)
C(71)-C(72)	1.474(8)
N(7)-C(73)	1.204(14)
C(73)-C(74)	1.375(14)
N(8)-C(75)	1.28(2)
C(75)-C(76)	1.40(2)
N(9)-C(77)	1.222(19)
C(77)-C(78)	1.380(19)

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O(1)-Rh(1)-O(9)         176.19(14)
O(1)-Rh(1)-O(13)         93.35(15)
O(9)-Rh(1)-O(13)         86.00(15)
O(1)-Rh(1)-O(5)          87.34(15)
O(9)-Rh(1)-O(5)          93.01(15)
O(13)-Rh(1)-O(5)        175.33(13)
O(1)-Rh(1)-N(5)          93.18(14)
O(9)-Rh(1)-N(5)          90.59(14)
O(13)-Rh(1)-N(5)         91.32(14)
O(5)-Rh(1)-N(5)          93.25(14)
O(1)-Rh(1)-Rh(2)         87.87(10)
O(9)-Rh(1)-Rh(2)         88.35(10)
O(13)-Rh(1)-Rh(2)        87.85(9)
O(5)-Rh(1)-Rh(2)         87.56(9)
N(5)-Rh(1)-Rh(2)        178.70(10)
O(14)-Rh(2)-O(2)         92.89(15)
O(14)-Rh(2)-O(6)        176.40(14)
O(2)-Rh(2)-O(6)          87.15(14)
O(14)-Rh(2)-O(10)        87.25(16)
O(2)-Rh(2)-O(10)        175.42(14)
O(6)-Rh(2)-O(10)         92.43(14)
O(14)-Rh(2)-N(6)         90.66(16)
O(2)-Rh(2)-N(6)          92.88(15)
O(6)-Rh(2)-N(6)          92.94(16)
O(10)-Rh(2)-N(6)         91.70(15)
O(14)-Rh(2)-Rh(1)        88.42(10)
O(2)-Rh(2)-Rh(1)         87.98(10)
O(6)-Rh(2)-Rh(1)         87.98(10)
O(10)-Rh(2)-Rh(1)        87.44(9)
N(6)-Rh(2)-Rh(1)        178.77(12)
C(3)-N(1)-C(10)         111.0(5)
C(3)-N(1)-C(2)          122.8(5)
C(10)-N(1)-C(2)         125.7(4)
C(20)-N(2)-C(19)        126.2(6)
C(20)-N(2)-C(27)        110.8(6)
C(19)-N(2)-C(27)        122.6(5)
C(44)-N(3)-C(37)        111.4(4)
C(44)-N(3)-C(36)        125.0(5)
C(37)-N(3)-C(36)        122.4(5)
C(61)-N(4)-C(54)        112.3(4)
C(61)-N(4)-C(53)        124.6(4)
C(54)-N(4)-C(53)        122.9(4)
C(69)-N(5)-Rh(1)        174.4(4)
C(71)-N(6)-Rh(2)        172.3(5)
C(1)-O(1)-Rh(1)         118.3(3)
C(1)-O(2)-Rh(2)         118.0(3)
C(18)-O(5)-Rh(1)        118.1(3)
C(18)-O(6)-Rh(2)        119.1(3)
C(35)-O(9)-Rh(1)        118.6(3)
C(35)-O(10)-Rh(2)       117.3(3)
C(52)-O(13)-Rh(1)       118.1(3)
C(52)-O(14)-Rh(2)       117.3(3)
O(2)-C(1)-O(1)          126.5(5)
O(2)-C(1)-C(2)          117.6(5)
O(1)-C(1)-C(2)          115.9(4)
N(1)-C(2)-C(1)          112.0(4)
N(1)-C(2)-C(11)         112.3(4)
C(1)-C(2)-C(11)         112.8(5)
O(3)-C(3)-N(1)          125.5(6)
O(3)-C(3)-C(4)          128.8(6)
N(1)-C(3)-C(4)          105.7(5)
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C(9)-C(4)-C(5)            121.9(7)
C(9)-C(4)-C(3)            108.6(5)
C(5)-C(4)-C(3)            129.4(7)
C(4)-C(5)-C(6)            114.8(9)
C(7)-C(6)-C(5)            121.7(8)
C(8)-C(7)-C(6)            122.0(9)
C(7)-C(8)-C(9)            117.3(10)
C(4)-C(9)-C(8)            122.0(7)
C(4)-C(9)-C(10)           108.0(5)
C(8)-C(9)-C(10)           129.9(7)
O(4)-C(10)-N(1)           124.1(6)
O(4)-C(10)-C(9)           129.2(6)
N(1)-C(10)-C(9)           106.6(5)
C(17)-C(11)-C(2)          113.6(5)
C(17)-C(12)-C(13)         119.3(9)
C(14)-C(13)-C(12)         120.2(9)
C(15)-C(14)-C(13)         122.5(8)
C(14)-C(15)-C(16)         117.7(9)
C(15)-C(16)-C(17)         123.6(8)
C(12)-C(17)-C(16)         116.4(7)
C(12)-C(17)-C(11)         122.8(7)
C(16)-C(17)-C(11)         120.7(7)
O(6)-C(18)-O(5)           126.5(5)
O(6)-C(18)-C(19)          117.1(4)
O(5)-C(18)-C(19)          116.3(4)
N(2)-C(19)-C(18)          112.5(4)
N(2)-C(19)-C(28)          110.4(5)
C(18)-C(19)-C(28)         112.9(4)
O(7)-C(20)-N(2)           124.0(8)
O(7)-C(20)-C(21)          131.8(7)
N(2)-C(20)-C(21)          104.2(8)
C(26)-C(21)-C(22)         122.0(12)
C(26)-C(21)-C(20)         111.1(6)
C(22)-C(21)-C(20)         126.7(13)
C(23)-C(22)-C(21)         118.2(19)
C(22)-C(23)-C(24)         120.3(13)
C(23)-C(24)-C(25)         126(2)
C(26)-C(25)-C(24)         117.5(19)
C(25)-C(26)-C(21)         116.3(11)
C(25)-C(26)-C(27)         136.9(13)
C(21)-C(26)-C(27)         106.7(7)
O(8)-C(27)-N(2)           125.1(6)
O(8)-C(27)-C(26)          127.7(8)
N(2)-C(27)-C(26)          107.2(7)
C(34)-C(28)-C(19)         110.9(5)
C(30)-C(29)-C(34)         121.6(7)
C(29)-C(30)-C(31)         121.3(8)
C(32)-C(31)-C(30)         120.4(7)
C(31)-C(32)-C(33)         118.9(8)
C(34)-C(33)-C(32)         119.6(8)
C(33)-C(34)-C(29)         118.1(6)
C(33)-C(34)-C(28)         119.8(7)
C(29)-C(34)-C(28)         122.0(6)
O(9)-C(35)-O(10)          127.8(5)
O(9)-C(35)-C(36)          115.3(4)
O(10)-C(35)-C(36)         116.9(4)
N(3)-C(36)-C(45)          111.9(5)
N(3)-C(36)-C(35)          112.3(4)
C(45)-C(36)-C(35)         113.2(5)
O(11)-C(37)-N(3)          124.0(5)
O(11)-C(37)-C(38)         130.7(5)
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N(3)-C(37)-C(38)           105.2(5)
C(43)-C(38)-C(39)          121.5(6)
C(43)-C(38)-C(37)          109.4(5)
C(39)-C(38)-C(37)          129.0(6)
C(40)-C(39)-C(38)          118.0(6)
C(39)-C(40)-C(41)          120.2(6)
C(40)-C(41)-C(42)          123.0(6)
C(43)-C(42)-C(41)          115.3(7)
C(38)-C(43)-C(42)          121.8(5)
C(38)-C(43)-C(44)          107.8(5)
C(42)-C(43)-C(44)          130.3(6)
O(12)-C(44)-N(3)           124.4(5)
O(12)-C(44)-C(43)          129.6(6)
N(3)-C(44)-C(43)           106.0(4)
C(51)-C(45)-C(36)          110.6(6)
C(51)-C(46)-C(47)          118.4(11)
C(46)-C(47)-C(48)          123.0(12)
C(49)-C(48)-C(47)          116.6(10)
C(48)-C(49)-C(50)          122.6(11)
C(51)-C(50)-C(49)          117.5(10)
C(50)-C(51)-C(46)          121.7(8)
C(50)-C(51)-C(45)          120.5(9)
C(46)-C(51)-C(45)          117.8(8)
O(13)-C(52)-O(14)          127.4(5)
O(13)-C(52)-C(53)          117.0(4)
O(14)-C(52)-C(53)          115.4(4)
N(4)-C(53)-C(52)           110.8(4)
N(4)-C(53)-C(62)           112.1(4)
C(52)-C(53)-C(62)          112.6(4)
O(15)-C(54)-N(4)           124.2(5)
O(15)-C(54)-C(55)          130.4(4)
N(4)-C(54)-C(55)           105.4(4)
C(56)-C(55)-C(60)          120.4(5)
C(56)-C(55)-C(54)          130.9(5)
C(60)-C(55)-C(54)          108.6(4)
C(55)-C(56)-C(57)          118.1(5)
C(58)-C(57)-C(56)          121.7(5)
C(57)-C(58)-C(59)          120.8(6)
C(60)-C(59)-C(58)          117.0(6)
C(59)-C(60)-C(55)          121.9(5)
C(59)-C(60)-C(61)          130.2(5)
C(55)-C(60)-C(61)          107.8(5)
O(16)-C(61)-N(4)           124.3(5)
O(16)-C(61)-C(60)          130.1(6)
N(4)-C(61)-C(60)           105.5(4)
C(68)-C(62)-C(53)          113.3(4)
C(68)-C(63)-C(64)          122.1(8)
C(65)-C(64)-C(63)          120.0(9)
C(64)-C(65)-C(66)          120.9(7)
C(67)-C(66)-C(65)          117.0(9)
C(68)-C(67)-C(66)          122.1(8)
C(63)-C(68)-C(67)          117.8(6)
C(63)-C(68)-C(62)          124.3(6)
C(67)-C(68)-C(62)          117.9(6)
N(5)-C(69)-C(70)           176.9(7)
N(6)-C(71)-C(72)           176.7(8)
N(7)-C(73)-C(74)           167.1(15)
N(8)-C(75)-C(76)           126(3)
N(9)-C(77)-C(78)           134(3)
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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for joef099a.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Rh(1)	36(1)	35(1)	31(1)	0(1)	19(1)	2(1)
Rh(2)	36(1)	36(1)	31(1)	0(1)	19(1)	3(1)
N(1)	36(2)	48(2)	54(2)	-2(2)	25(2)	-3(2)
N(2)	64(3)	46(2)	43(2)	4(2)	32(2)	6(2)
N(3)	36(2)	50(2)	49(2)	-3(2)	22(2)	-8(2)
N(4)	47(2)	48(2)	40(2)	7(2)	25(2)	2(2)
N(5)	34(2)	35(2)	45(2)	0(2)	30(2)	-4(2)
N(6)	46(2)	43(3)	46(2)	-5(2)	25(2)	-1(2)
O(1)	35(2)	42(2)	45(2)	-4(2)	21(1)	1(1)
O(2)	40(2)	41(2)	43(2)	-4(2)	18(2)	1(2)
O(3)	57(2)	85(3)	68(3)	-1(2)	42(2)	-6(2)
O(4)	81(3)	112(4)	57(3)	5(3)	35(2)	10(3)
O(5)	47(2)	44(2)	33(2)	2(1)	23(1)	8(2)
O(6)	36(2)	43(2)	38(2)	3(1)	20(1)	6(1)
O(7)	139(5)	99(5)	50(3)	-20(3)	22(3)	9(4)
O(8)	70(3)	68(3)	93(4)	-14(3)	17(3)	-4(2)
O(9)	38(2)	46(2)	44(2)	-10(2)	25(2)	-4(2)
O(10)	36(2)	43(2)	46(2)	-7(1)	26(1)	-5(1)
O(11)	53(2)	99(4)	60(3)	7(2)	18(2)	7(2)
O(12)	43(2)	70(3)	76(3)	9(2)	18(2)	7(2)
O(13)	49(2)	40(2)	34(2)	3(1)	27(1)	6(1)
O(14)	57(2)	42(2)	33(2)	5(1)	25(2)	9(2)
O(15)	51(2)	72(3)	63(2)	-5(2)	39(2)	-3(2)
O(16)	54(2)	124(4)	65(3)	-12(3)	43(2)	-10(2)
C(1)	33(2)	45(3)	37(2)	4(2)	14(2)	3(2)
C(2)	40(2)	41(3)	46(3)	0(2)	13(2)	-1(2)
C(3)	42(3)	45(3)	66(3)	-8(3)	21(2)	-11(2)
C(4)	41(3)	45(3)	94(4)	1(3)	26(3)	-7(2)
C(5)	41(3)	50(4)	149(7)	5(4)	23(4)	-5(3)
C(6)	47(4)	63(5)	189(12)	15(6)	3(6)	-2(3)
C(7)	79(7)	100(8)	140(10)	39(7)	-36(6)	-14(5)
C(8)	73(5)	110(7)	94(6)	34(6)	1(4)	-8(5)
C(9)	49(3)	62(4)	73(4)	12(3)	7(3)	-9(3)
C(10)	51(3)	65(4)	50(3)	1(3)	17(2)	-3(3)
C(11)	45(3)	43(3)	74(4)	-8(3)	10(3)	-2(2)
C(12)	199(12)	85(6)	104(7)	-23(5)	86(8)	-73(8)
C(13)	210(13)	121(10)	166(11)	-30(8)	149(11)	-85(10)
C(14)	69(5)	82(6)	147(9)	-21(6)	48(6)	-25(4)
C(15)	79(5)	54(4)	88(5)	2(4)	6(4)	-12(3)
C(16)	68(4)	54(4)	81(5)	12(3)	-3(4)	-11(3)
C(17)	52(3)	38(3)	73(4)	-3(3)	21(3)	2(2)
C(18)	35(2)	43(3)	33(2)	2(2)	16(2)	-2(2)
C(19)	44(2)	46(3)	37(2)	3(2)	19(2)	8(2)
C(20)	134(7)	50(3)	47(3)	12(3)	50(4)	29(4)
C(21)	158(9)	61(4)	134(8)	46(5)	128(8)	38(5)
C(22)	430(30)	111(8)	213(14)	93(9)	290(19)	126(13)
C(23)	430(40)	110(11)	310(30)	114(14)	340(30)	131(17)
C(24)	340(30)	127(14)	510(50)	100(20)	390(40)	54(16)
C(25)	117(8)	81(6)	282(18)	26(9)	121(11)	5(6)
C(26)	103(6)	56(4)	137(8)	22(5)	84(6)	12(4)
C(27)	61(4)	43(3)	100(5)	16(3)	47(4)	9(3)

C(28)	61(3)	55(3)	46(3)	10(2)	29(3)	17(3)
C(29)	58(4)	77(4)	65(4)	18(3)	24(3)	20(3)
C(30)	81(5)	89(5)	70(4)	28(4)	30(4)	36(4)
C(31)	154(9)	76(5)	64(5)	28(4)	43(5)	43(6)
C(32)	130(7)	56(4)	76(5)	9(3)	63(5)	-11(4)
C(33)	124(6)	56(4)	63(4)	6(3)	46(4)	17(4)
C(34)	81(4)	42(3)	60(3)	9(2)	44(3)	18(3)
C(35)	37(2)	49(3)	34(2)	-4(2)	20(2)	-2(2)
C(36)	38(2)	54(3)	62(3)	-12(3)	26(2)	-8(2)
C(37)	36(2)	54(3)	55(3)	-6(2)	15(2)	-5(2)
C(38)	43(3)	46(3)	59(3)	-1(2)	27(2)	-4(2)
C(39)	43(3)	57(3)	98(5)	-8(3)	32(3)	2(2)
C(40)	58(3)	81(5)	94(5)	7(4)	60(4)	5(3)
C(41)	99(5)	71(4)	96(5)	22(4)	75(5)	9(4)
C(42)	80(4)	67(4)	65(4)	14(3)	40(3)	-1(3)
C(43)	51(3)	44(3)	68(3)	3(2)	34(3)	-6(2)
C(44)	44(3)	48(3)	60(3)	6(2)	16(2)	-4(2)
C(45)	66(4)	58(4)	131(7)	-43(4)	70(4)	-24(3)
C(46)	134(9)	157(10)	120(8)	-76(8)	80(7)	-92(8)
C(47)	121(9)	132(9)	166(12)	-69(9)	78(9)	-56(8)
C(48)	79(6)	125(8)	132(9)	-34(7)	46(6)	-41(6)
C(49)	122(8)	81(7)	165(11)	-15(7)	75(8)	-35(6)
C(50)	81(5)	70(5)	133(8)	-17(5)	65(5)	-24(4)
C(51)	91(5)	66(5)	113(7)	-35(5)	58(5)	-28(4)
C(52)	37(2)	39(3)	28(2)	-2(2)	13(2)	2(2)
C(53)	52(3)	41(3)	35(2)	5(2)	24(2)	3(2)
C(54)	51(3)	43(3)	38(2)	8(2)	23(2)	15(2)
C(55)	53(3)	43(3)	42(2)	9(2)	29(2)	7(2)
C(56)	73(3)	51(3)	44(3)	3(2)	32(3)	11(3)
C(57)	88(4)	61(4)	36(3)	2(2)	23(3)	9(3)
C(58)	74(4)	65(4)	50(3)	0(3)	14(3)	-8(3)
C(59)	73(4)	86(5)	53(3)	3(3)	19(3)	3(4)
C(60)	57(3)	60(3)	40(2)	6(3)	20(2)	8(3)
C(61)	54(3)	70(4)	39(2)	3(2)	26(2)	14(3)
C(62)	70(4)	45(3)	44(3)	6(2)	36(3)	11(3)
C(63)	93(5)	57(4)	62(4)	12(3)	20(4)	4(3)
C(64)	157(9)	69(5)	64(5)	19(4)	52(5)	23(6)
C(65)	146(8)	52(4)	95(6)	23(4)	88(6)	19(5)
C(66)	105(6)	74(5)	125(8)	21(5)	62(6)	-11(5)
C(67)	79(5)	93(6)	81(5)	21(4)	21(4)	-21(4)
C(68)	69(3)	41(3)	53(3)	12(2)	36(3)	10(3)
C(69)	55(3)	45(3)	56(3)	1(2)	33(3)	-2(2)
C(70)	129(8)	69(5)	114(7)	-18(5)	82(7)	-3(5)
C(71)	83(4)	42(3)	57(3)	-12(3)	42(3)	-2(3)
C(72)	159(8)	53(4)	103(6)	-11(4)	95(6)	28(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic
displacement parameters (A^2 x 10^3) for joef099a.

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	x	y	z	U(eq)
H(2A)	2261	-1036	2664	51
H(5A)	-1775	-217	1489	98
H(6A)	-3012	79	-271	129
H(7A)	-2562	-61	-1903	147
H(8A)	-835	-326	-1862	118
H(11A)	2587	-1487	702	67
H(11B)	3151	-1708	1937	67
H(12A)	1299	-1817	2807	144
H(13A)	-146	-2471	2528	174
H(14A)	-876	-2874	844	115
H(15A)	-71	-2779	-517	94
H(16A)	1329	-2137	-286	89
H(19A)	6573	-834	5906	49
H(22A)	4078	-916	8616	252
H(23A)	2367	-1216	8477	279
H(24A)	1240	-1513	6860	319
H(25A)	1774	-1635	5296	176
H(28A)	5701	-1759	4510	62
H(28B)	6948	-1536	4780	62
H(29A)	8053	-1505	6948	79
H(30A)	8540	-2019	8526	94
H(31A)	7536	-2770	8694	115
H(32A)	5881	-2976	7321	96
H(33A)	5347	-2443	5663	92
H(36A)	8359	859	4231	58
H(39A)	11706	639	2670	76
H(40A)	11934	715	923	83
H(41A)	10493	1024	-556	94
H(42A)	8677	1154	-424	80
H(45A)	7017	1703	2934	91
H(45B)	7277	1611	4242	91
H(46A)	9125	1808	5504	153
H(47A)	10727	2332	5869	158
H(48A)	11253	2758	4443	131
H(49A)	10101	2661	2657	139
H(50A)	8372	2182	2255	105
H(53A)	5213	1127	-98	48
H(56A)	4479	258	-4072	63
H(57A)	2923	-116	-5375	73
H(58A)	1282	-231	-4988	77
H(59A)	1134	23	-3244	85
H(62A)	3037	1473	-172	58
H(62B)	4122	1676	778	58
H(63A)	2693	1866	-2070	86
H(64A)	2970	2588	-3152	111
H(65A)	4474	3152	-2503	103
H(66A)	5678	3050	-681	114
H(67A)	5381	2300	371	102
H(70A)	2460	1851	4389	141
H(70B)	3226	1639	5573	141
H(70C)	2126	1309	4921	141
H(72A)	7845	-1648	460	139

H(72B)	7152	-1321	-628	139
H(72C)	6618	-1845	-226	139
H(74A)	9405	-769	3818	209
H(74B)	8076	-746	3386	209
H(74C)	8696	-1270	4057	209
H(76A)	-3683	654	-3594	331
H(76B)	-2760	249	-3775	331
H(76C)	-3194	754	-4602	331
H(78A)	7745	1927	-1829	362
H(78B)	6782	1502	-1828	362
H(78C)	6604	2143	-1683	362

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Table 6.  Torsion angles [deg] for joef099a.
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O(1)-Rh(1)-Rh(2)-O(14)                                88.29(15)
O(9)-Rh(1)-Rh(2)-O(14)                               -91.20(16)
O(13)-Rh(1)-Rh(2)-O(14)                               -5.14(15)
O(5)-Rh(1)-Rh(2)-O(14)                               175.72(17)
N(5)-Rh(1)-Rh(2)-O(14)                                  -56(5)
O(1)-Rh(1)-Rh(2)-O(2)                                 -4.65(14)
O(9)-Rh(1)-Rh(2)-O(2)                                175.85(16)
O(13)-Rh(1)-Rh(2)-O(2)                               -98.09(14)
O(5)-Rh(1)-Rh(2)-O(2)                                 82.77(14)
N(5)-Rh(1)-Rh(2)-O(2)                                  -149(5)
O(1)-Rh(1)-Rh(2)-O(6)                                -91.87(15)
O(9)-Rh(1)-Rh(2)-O(6)                                 88.64(14)
O(13)-Rh(1)-Rh(2)-O(6)                               174.70(15)
O(5)-Rh(1)-Rh(2)-O(6)                                 -4.44(14)
N(5)-Rh(1)-Rh(2)-O(6)                                   124(5)
O(1)-Rh(1)-Rh(2)-O(10)                               175.60(16)
O(9)-Rh(1)-Rh(2)-O(10)                                -3.89(14)
O(13)-Rh(1)-Rh(2)-O(10)                               82.17(15)
O(5)-Rh(1)-Rh(2)-O(10)                               -96.97(14)
N(5)-Rh(1)-Rh(2)-O(10)                                   31(5)
O(1)-Rh(1)-Rh(2)-N(6)                                   130(6)
O(9)-Rh(1)-Rh(2)-N(6)                                   -49(6)
O(13)-Rh(1)-Rh(2)-N(6)                                   37(6)
O(5)-Rh(1)-Rh(2)-N(6)                                  -143(6)
N(5)-Rh(1)-Rh(2)-N(6)                                   -14(7)
O(1)-Rh(1)-N(5)-C(69)                                    17(5)
O(9)-Rh(1)-N(5)-C(69)                                  -163(5)
O(13)-Rh(1)-N(5)-C(69)                                  111(5)
O(5)-Rh(1)-N(5)-C(69)                                   -70(5)
Rh(2)-Rh(1)-N(5)-C(69)                                  161(4)
O(14)-Rh(2)-N(6)-C(71)                                  -45(4)
O(2)-Rh(2)-N(6)-C(71)                                    48(4)
O(6)-Rh(2)-N(6)-C(71)                                   135(4)
O(10)-Rh(2)-N(6)-C(71)                                 -132(4)
Rh(1)-Rh(2)-N(6)-C(71)                                  -86(7)
O(9)-Rh(1)-O(1)-C(1)                                     18(3)
O(13)-Rh(1)-O(1)-C(1)                                  98.4(4)
O(5)-Rh(1)-O(1)-C(1)                                   -76.9(3)
N(5)-Rh(1)-O(1)-C(1)                                  -170.1(3)
Rh(2)-Rh(1)-O(1)-C(1)                                   10.7(3)
O(14)-Rh(2)-O(2)-C(1)                                  -88.2(4)
O(6)-Rh(2)-O(2)-C(1)                                    88.2(4)
O(10)-Rh(2)-O(2)-C(1)                                     3(2)
N(6)-Rh(2)-O(2)-C(1)                                  -179.0(4)
Rh(1)-Rh(2)-O(2)-C(1)                                   0.2(3)
O(1)-Rh(1)-O(5)-C(18)                                  90.2(4)
O(9)-Rh(1)-O(5)-C(18)                                  -86.0(4)
O(13)-Rh(1)-O(5)-C(18)                                   -8(2)
N(5)-Rh(1)-O(5)-C(18)                                 -176.8(4)
Rh(2)-Rh(1)-O(5)-C(18)                                  2.2(3)
O(14)-Rh(2)-O(6)-C(18)                                   11(3)
O(2)-Rh(2)-O(6)-C(18)                                  -79.7(4)
O(10)-Rh(2)-O(6)-C(18)                                 95.8(4)
N(6)-Rh(2)-O(6)-C(18)                                 -172.4(4)
Rh(1)-Rh(2)-O(6)-C(18)                                  8.4(4)
O(1)-Rh(1)-O(9)-C(35)                                    0(3)
O(13)-Rh(1)-O(9)-C(35)                                 -80.7(4)
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O(5)-Rh(1)-O(9)-C(35)           94.7(4)
N(5)-Rh(1)-O(9)-C(35)         -172.0(4)
Rh(2)-Rh(1)-O(9)-C(35)           7.3(4)
O(14)-Rh(2)-O(10)-C(35)         90.5(4)
O(2)-Rh(2)-O(10)-C(35)           -1(2)
O(6)-Rh(2)-O(10)-C(35)         -86.0(4)
N(6)-Rh(2)-O(10)-C(35)        -179.0(4)
Rh(1)-Rh(2)-O(10)-C(35)          1.9(3)
O(1)-Rh(1)-O(13)-C(52)         -85.1(4)
O(9)-Rh(1)-O(13)-C(52)          91.1(4)
O(5)-Rh(1)-O(13)-C(52)           13(2)
N(5)-Rh(1)-O(13)-C(52)        -178.4(4)
Rh(2)-Rh(1)-O(13)-C(52)          2.6(3)
O(2)-Rh(2)-O(14)-C(52)          97.1(4)
O(6)-Rh(2)-O(14)-C(52)            7(3)
O(10)-Rh(2)-O(14)-C(52)        -78.3(4)
N(6)-Rh(2)-O(14)-C(52)        -170.0(4)
Rh(1)-Rh(2)-O(14)-C(52)          9.2(3)
Rh(2)-O(2)-C(1)-O(1)             8.9(7)
Rh(2)-O(2)-C(1)-C(2)          -169.5(3)
Rh(1)-O(1)-C(1)-O(2)           -14.6(7)
Rh(1)-O(1)-C(1)-C(2)           163.9(3)
C(3)-N(1)-C(2)-C(1)           -113.4(5)
C(10)-N(1)-C(2)-C(1)            75.9(6)
C(3)-N(1)-C(2)-C(11)           118.5(6)
C(10)-N(1)-C(2)-C(11)          -52.2(7)
O(2)-C(1)-C(2)-N(1)           -125.3(5)
O(1)-C(1)-C(2)-N(1)             56.1(6)
O(2)-C(1)-C(2)-C(11)             2.5(7)
O(1)-C(1)-C(2)-C(11)          -176.1(5)
C(10)-N(1)-C(3)-O(3)           179.0(6)
C(2)-N(1)-C(3)-O(3)              7.0(9)
C(10)-N(1)-C(3)-C(4)            -1.5(6)
C(2)-N(1)-C(3)-C(4)           -173.4(4)
O(3)-C(3)-C(4)-C(9)           -178.2(6)
N(1)-C(3)-C(4)-C(9)              2.3(6)
O(3)-C(3)-C(4)-C(5)             -0.4(10)
N(1)-C(3)-C(4)-C(5)           -179.9(6)
C(9)-C(4)-C(5)-C(6)             -3.5(9)
C(3)-C(4)-C(5)-C(6)            179.0(6)
C(4)-C(5)-C(6)-C(7)             5.1(12)
C(5)-C(6)-C(7)-C(8)            -5.7(16)
C(6)-C(7)-C(8)-C(9)             4.0(16)
C(5)-C(4)-C(9)-C(8)             2.3(10)
C(3)-C(4)-C(9)-C(8)           -179.8(7)
C(5)-C(4)-C(9)-C(10)           179.8(6)
C(3)-C(4)-C(9)-C(10)            -2.3(7)
C(7)-C(8)-C(9)-C(4)             -2.4(13)
C(7)-C(8)-C(9)-C(10)          -179.3(8)
C(3)-N(1)-C(10)-O(4)          -177.9(6)
C(2)-N(1)-C(10)-O(4)            -6.2(10)
C(3)-N(1)-C(10)-C(9)             0.1(7)
C(2)-N(1)-C(10)-C(9)           171.8(5)
C(4)-C(9)-C(10)-O(4)           179.3(7)
C(8)-C(9)-C(10)-O(4)            -3.5(13)
C(4)-C(9)-C(10)-N(1)             1.4(7)
C(8)-C(9)-C(10)-N(1)           178.6(8)
N(1)-C(2)-C(11)-C(17)          -52.3(7)
C(1)-C(2)-C(11)-C(17)         -180.0(5)
C(17)-C(12)-C(13)-C(14)          -4(2)
C(12)-C(13)-C(14)-C(15)           5(2)
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C(13)-C(14)-C(15)-C(16)	-5.0(17)
C(14)-C(15)-C(16)-C(17)	4.3(12)
C(13)-C(12)-C(17)-C(16)	2.7(16)
C(13)-C(12)-C(17)-C(11)	-178.0(11)
C(15)-C(16)-C(17)-C(12)	-3.2(12)
C(15)-C(16)-C(17)-C(11)	177.6(7)
C(2)-C(11)-C(17)-C(12)	-48.6(11)
C(2)-C(11)-C(17)-C(16)	130.6(6)
Rh(2)-O(6)-C(18)-O(5)	-9.6(7)
Rh(2)-O(6)-C(18)-C(19)	172.9(3)
Rh(1)-O(5)-C(18)-O(6)	4.1(7)
Rh(1)-O(5)-C(18)-C(19)	-178.3(3)
C(20)-N(2)-C(19)-C(18)	-124.5(6)
C(27)-N(2)-C(19)-C(18)	63.2(6)
C(20)-N(2)-C(19)-C(28)	108.4(6)
C(27)-N(2)-C(19)-C(28)	-64.0(6)
O(6)-C(18)-C(19)-N(2)	-143.8(5)
O(5)-C(18)-C(19)-N(2)	38.4(6)
O(6)-C(18)-C(19)-C(28)	-18.0(7)
O(5)-C(18)-C(19)-C(28)	164.3(5)
C(19)-N(2)-C(20)-O(7)	5.0(10)
C(27)-N(2)-C(20)-O(7)	178.1(7)
C(19)-N(2)-C(20)-C(21)	-173.2(5)
C(27)-N(2)-C(20)-C(21)	-0.1(6)
O(7)-C(20)-C(21)-C(26)	-177.5(8)
N(2)-C(20)-C(21)-C(26)	0.5(8)
O(7)-C(20)-C(21)-C(22)	6.5(13)
N(2)-C(20)-C(21)-C(22)	-175.6(7)
C(26)-C(21)-C(22)-C(23)	2.3(15)
C(20)-C(21)-C(22)-C(23)	178.0(10)
C(21)-C(22)-C(23)-C(24)	-3(2)
C(22)-C(23)-C(24)-C(25)	3(3)
C(23)-C(24)-C(25)-C(26)	-2(3)
C(24)-C(25)-C(26)-C(21)	1.3(16)
C(24)-C(25)-C(26)-C(27)	-174.5(12)
C(22)-C(21)-C(26)-C(25)	-1.4(12)
C(20)-C(21)-C(26)-C(25)	-177.6(7)
C(22)-C(21)-C(26)-C(27)	175.6(7)
C(20)-C(21)-C(26)-C(27)	-0.7(8)
C(20)-N(2)-C(27)-O(8)	179.4(6)
C(19)-N(2)-C(27)-O(8)	-7.3(9)
C(20)-N(2)-C(27)-C(26)	-0.2(7)
C(19)-N(2)-C(27)-C(26)	173.1(5)
C(25)-C(26)-C(27)-O(8)	-3.0(15)
C(21)-C(26)-C(27)-O(8)	-179.0(7)
C(25)-C(26)-C(27)-N(2)	176.6(10)
C(21)-C(26)-C(27)-N(2)	0.5(7)
N(2)-C(19)-C(28)-C(34)	-56.9(7)
C(18)-C(19)-C(28)-C(34)	176.1(5)
C(34)-C(29)-C(30)-C(31)	0.7(11)
C(29)-C(30)-C(31)-C(32)	-3.3(13)
C(30)-C(31)-C(32)-C(33)	3.1(13)
C(31)-C(32)-C(33)-C(34)	-0.4(11)
C(32)-C(33)-C(34)-C(29)	-2.0(10)
C(32)-C(33)-C(34)-C(28)	-178.7(6)
C(30)-C(29)-C(34)-C(33)	2.0(10)
C(30)-C(29)-C(34)-C(28)	178.5(6)
C(19)-C(28)-C(34)-C(33)	108.4(7)
C(19)-C(28)-C(34)-C(29)	-68.1(7)
Rh(1)-O(9)-C(35)-O(10)	-8.4(7)
Rh(1)-O(9)-C(35)-C(36)	172.8(3)

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Rh(2)-O(10)-C(35)-O(9)              3.6(7)
Rh(2)-O(10)-C(35)-C(36)          -177.6(4)
C(44)-N(3)-C(36)-C(45)            -61.5(7)
C(37)-N(3)-C(36)-C(45)            105.2(7)
C(44)-N(3)-C(36)-C(35)            67.1(7)
C(37)-N(3)-C(36)-C(35)          -126.2(6)
O(9)-C(35)-C(36)-N(3)            -159.3(5)
O(10)-C(35)-C(36)-N(3)            21.8(7)
O(9)-C(35)-C(36)-C(45)           -31.4(8)
O(10)-C(35)-C(36)-C(45)          149.7(6)
C(44)-N(3)-C(37)-O(11)           174.6(6)
C(36)-N(3)-C(37)-O(11)             6.2(9)
C(44)-N(3)-C(37)-C(38)            -4.1(6)
C(36)-N(3)-C(37)-C(38)          -172.4(5)
O(11)-C(37)-C(38)-C(43)         -176.3(7)
N(3)-C(37)-C(38)-C(43)             2.2(6)
O(11)-C(37)-C(38)-C(39)            7.0(11)
N(3)-C(37)-C(38)-C(39)          -174.4(6)
C(43)-C(38)-C(39)-C(40)            0.4(9)
C(37)-C(38)-C(39)-C(40)          176.7(6)
C(38)-C(39)-C(40)-C(41)            1.6(10)
C(39)-C(40)-C(41)-C(42)           -4.3(12)
C(40)-C(41)-C(42)-C(43)            4.7(11)
C(39)-C(38)-C(43)-C(42)            0.3(9)
C(37)-C(38)-C(43)-C(42)         -176.7(6)
C(39)-C(38)-C(43)-C(44)          177.2(5)
C(37)-C(38)-C(43)-C(44)            0.2(6)
C(41)-C(42)-C(43)-C(38)           -2.7(9)
C(41)-C(42)-C(43)-C(44)         -178.8(6)
C(37)-N(3)-C(44)-O(12)          -177.6(6)
C(36)-N(3)-C(44)-O(12)            -9.6(9)
C(37)-N(3)-C(44)-C(43)             4.2(6)
C(36)-N(3)-C(44)-C(43)           172.2(5)
C(38)-C(43)-C(44)-O(12)          179.3(6)
C(42)-C(43)-C(44)-O(12)           -4.2(11)
C(38)-C(43)-C(44)-N(3)            -2.7(6)
C(42)-C(43)-C(44)-N(3)           173.9(6)
N(3)-C(36)-C(45)-C(51)           -47.5(9)
C(35)-C(36)-C(45)-C(51)         -175.6(6)
C(51)-C(46)-C(47)-C(48)           -2(2)
C(46)-C(47)-C(48)-C(49)            1(2)
C(47)-C(48)-C(49)-C(50)            1.5(19)
C(48)-C(49)-C(50)-C(51)           -3.7(18)
C(49)-C(50)-C(51)-C(46)            3.3(15)
C(49)-C(50)-C(51)-C(45)         -175.1(8)
C(47)-C(46)-C(51)-C(50)           -0.8(17)
C(47)-C(46)-C(51)-C(45)          177.6(10)
C(36)-C(45)-C(51)-C(50)           93.9(10)
C(36)-C(45)-C(51)-C(46)          -84.5(10)
Rh(1)-O(13)-C(52)-O(14)            4.4(7)
Rh(1)-O(13)-C(52)-C(53)         -169.8(3)
Rh(2)-O(14)-C(52)-O(13)          -10.5(7)
Rh(2)-O(14)-C(52)-C(53)          163.8(3)
C(61)-N(4)-C(53)-C(52)            62.7(6)
C(54)-N(4)-C(53)-C(52)          -112.2(5)
C(61)-N(4)-C(53)-C(62)           -64.1(6)
C(54)-N(4)-C(53)-C(62)           121.0(5)
O(13)-C(52)-C(53)-N(4)          -136.1(4)
O(14)-C(52)-C(53)-N(4)            49.0(6)
O(13)-C(52)-C(53)-C(62)           -9.6(7)
O(14)-C(52)-C(53)-C(62)          175.5(5)
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C(61)-N(4)-C(54)-O(15)        -176.3(5)
C(53)-N(4)-C(54)-O(15)          -0.9(8)
C(61)-N(4)-C(54)-C(55)           4.8(6)
C(53)-N(4)-C(54)-C(55)        -179.8(4)
O(15)-C(54)-C(55)-C(56)         -1.7(10)
N(4)-C(54)-C(55)-C(56)         177.1(5)
O(15)-C(54)-C(55)-C(60)        178.9(6)
N(4)-C(54)-C(55)-C(60)          -2.3(6)
C(60)-C(55)-C(56)-C(57)          0.8(8)
C(54)-C(55)-C(56)-C(57)       -178.5(5)
C(55)-C(56)-C(57)-C(58)         -1.7(9)
C(56)-C(57)-C(58)-C(59)          0.0(10)
C(57)-C(58)-C(59)-C(60)          2.6(10)
C(58)-C(59)-C(60)-C(55)         -3.5(10)
C(58)-C(59)-C(60)-C(61)        179.0(6)
C(56)-C(55)-C(60)-C(59)          1.9(9)
C(54)-C(55)-C(60)-C(59)       -178.6(6)
C(56)-C(55)-C(60)-C(61)        179.8(5)
C(54)-C(55)-C(60)-C(61)         -0.7(6)
C(54)-N(4)-C(61)-O(16)         176.9(6)
C(53)-N(4)-C(61)-O(16)           1.6(9)
C(54)-N(4)-C(61)-C(60)          -5.2(6)
C(53)-N(4)-C(61)-C(60)         179.5(5)
C(59)-C(60)-C(61)-O(16)         -1.1(12)
C(55)-C(60)-C(61)-O(16)       -178.8(7)
C(59)-C(60)-C(61)-N(4)        -178.8(7)
C(55)-C(60)-C(61)-N(4)           3.5(6)
N(4)-C(53)-C(62)-C(68)         -69.1(6)
C(52)-C(53)-C(62)-C(68)        165.1(5)
C(68)-C(63)-C(64)-C(65)          0.8(13)
C(63)-C(64)-C(65)-C(66)         -2.3(13)
C(64)-C(65)-C(66)-C(67)          2.9(13)
C(65)-C(66)-C(67)-C(68)         -2.1(14)
C(64)-C(63)-C(68)-C(67)          0.0(11)
C(64)-C(63)-C(68)-C(62)        179.3(7)
C(66)-C(67)-C(68)-C(63)          0.7(12)
C(66)-C(67)-C(68)-C(62)       -178.6(7)
C(53)-C(62)-C(68)-C(63)         90.7(8)
C(53)-C(62)-C(68)-C(67)        -90.0(7)
Rh(1)-N(5)-C(69)-C(70)            6(18)
Rh(2)-N(6)-C(71)-C(72)         135(12)
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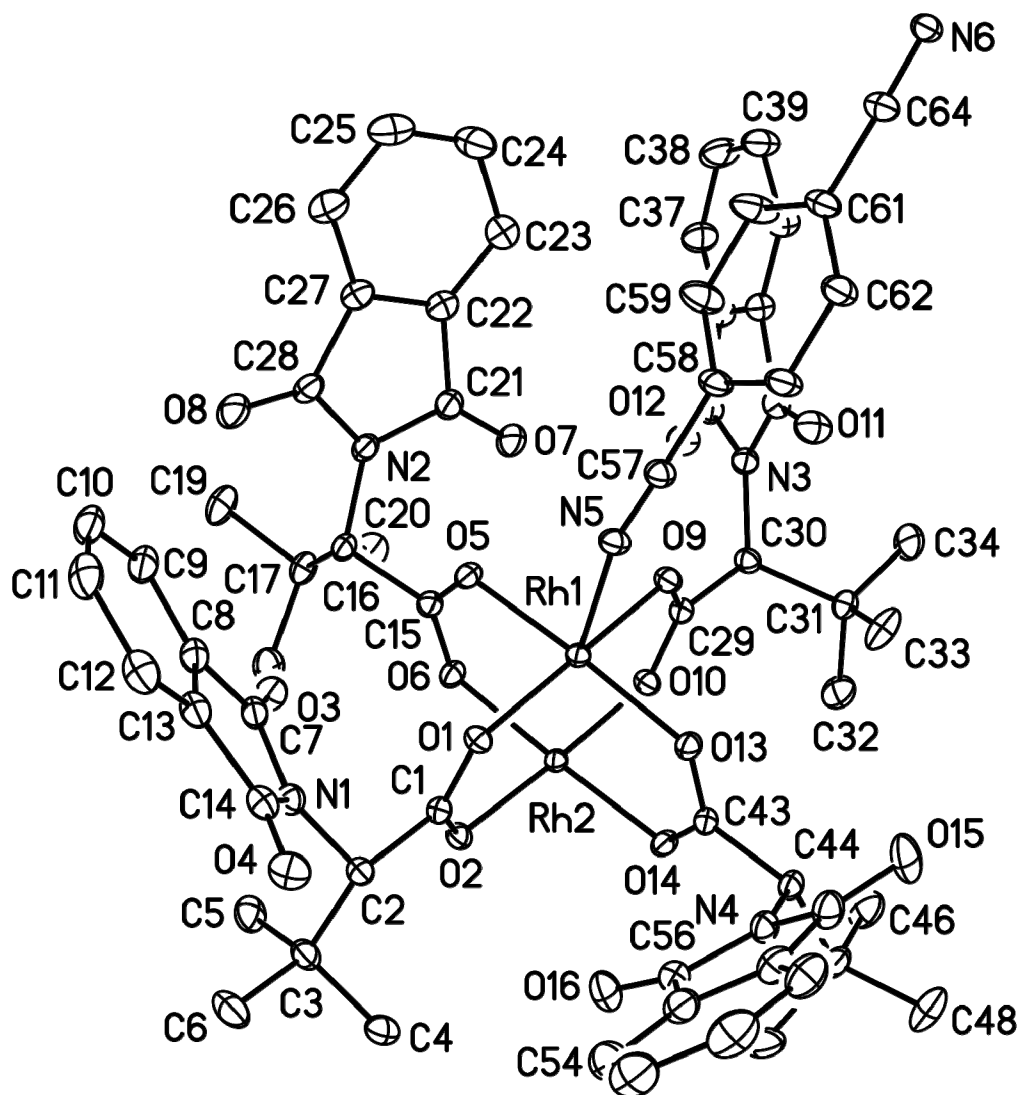Symmetry transformations used to generate equivalent atoms:

Figure 4. Molecular diagram of **5** monomer with ellipsoids at 30% probability. Three cocrystallized toluene solvent molecules and H-atoms deleted for clarity.

Table 1. Crystal data and structure refinement for joef086.

Identification code	joef086
Empirical formula	C85 H84 N6 O16 Rh2
Formula weight	1651.40
Temperature	170(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 13.412(3) A alpha = 90 deg. b = 21.783(5) A beta = 90 deg. c = 27.323(6) A gamma = 90 deg.
Volume	7982(3) A^3
Z, Calculated density	4, 1.374 Mg/m^3
Absorption coefficient	0.483 mm^-1
F(000)	3416
Crystal size	0.23 x 0.21 x 0.17 mm
Theta range for data collection	1.49 to 28.31 deg.
Limiting indices	-17<=h<=17, -28<=k<=28, -36<=l<=36
Reflections collected / unique	94308 / 19746 [R(int) = 0.0469]
Completeness to theta = 25.00	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9206 and 0.8986
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	19746 / 0 / 997
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0297, wR2 = 0.0748
R indices (all data)	R1 = 0.0317, wR2 = 0.0772
Absolute structure parameter	-0.043(11)
Largest diff. peak and hole	0.917 and -0.348 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for joef086.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

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	x	y	z	U(eq)
Rh(1)	6607(1)	402(1)	248(1)	18(1)
Rh(2)	6557(1)	-154(1)	1004(1)	18(1)
N(1)	4447(1)	1823(1)	963(1)	25(1)
N(2)	3679(1)	-547(1)	-258(1)	27(1)
N(3)	7530(1)	-1499(1)	-531(1)	25(1)
N(4)	9244(1)	1523(1)	993(1)	28(1)
N(5)	6759(1)	826(1)	-490(1)	26(1)
N(6)	8400(2)	620(1)	-3266(1)	25(1)
O(1)	5963(1)	1122(1)	611(1)	22(1)
O(2)	5892(1)	585(1)	1318(1)	24(1)
O(3)	3719(1)	891(1)	766(1)	32(1)
O(4)	4896(2)	2848(1)	951(1)	38(1)
O(5)	5232(1)	84(1)	90(1)	24(1)
O(6)	5184(1)	-458(1)	796(1)	25(1)
O(7)	5040(1)	-1198(1)	-356(1)	40(1)
O(8)	2454(1)	172(1)	-432(1)	42(1)
O(9)	7199(1)	-366(1)	-65(1)	24(1)
O(10)	7185(1)	-875(1)	655(1)	24(1)
O(11)	8221(1)	-697(1)	-988(1)	39(1)
O(12)	6680(1)	-2402(1)	-344(1)	36(1)
O(13)	7977(1)	724(1)	451(1)	24(1)
O(14)	7937(1)	200(1)	1161(1)	25(1)
O(15)	10379(2)	1737(1)	378(1)	49(1)
O(16)	7907(2)	1632(1)	1521(1)	41(1)
C(1)	5733(2)	1050(1)	1056(1)	22(1)
C(2)	5230(2)	1609(1)	1297(1)	24(1)
C(3)	4867(2)	1551(1)	1835(1)	30(1)
C(4)	5776(2)	1420(1)	2162(1)	39(1)
C(5)	4066(2)	1057(1)	1900(1)	39(1)
C(6)	4433(2)	2175(1)	1991(1)	43(1)
C(7)	3779(2)	1443(1)	709(1)	27(1)
C(8)	3209(2)	1852(1)	380(1)	28(1)
C(9)	2468(2)	1714(1)	47(1)	34(1)
C(10)	2071(2)	2209(1)	-212(1)	39(1)
C(11)	2395(2)	2802(1)	-143(1)	42(1)
C(12)	3149(2)	2937(1)	187(1)	38(1)
C(13)	3547(2)	2449(1)	449(1)	30(1)
C(14)	4373(2)	2436(1)	808(1)	29(1)
C(15)	4817(2)	-264(1)	398(1)	23(1)
C(16)	3728(2)	-426(1)	273(1)	26(1)
C(17)	3187(2)	-912(1)	590(1)	32(1)
C(18)	3122(2)	-676(2)	1116(1)	43(1)
C(19)	2118(2)	-967(2)	389(1)	46(1)
C(20)	3687(2)	-1544(1)	564(1)	43(1)
C(21)	4361(2)	-900(1)	-526(1)	31(1)
C(22)	4068(2)	-827(1)	-1050(1)	34(1)
C(23)	4441(2)	-1109(2)	-1462(1)	47(1)
C(24)	3984(3)	-955(2)	-1909(1)	54(1)

C(25)	3206(3)	-548(2)	-1931(1)	52(1)
C(26)	2829(2)	-264(1)	-1512(1)	43(1)
C(27)	3278(2)	-419(1)	-1072(1)	33(1)
C(28)	3050(2)	-209(1)	-565(1)	31(1)
C(29)	7357(2)	-829(1)	200(1)	23(1)
C(30)	7848(2)	-1398(1)	-23(1)	23(1)
C(31)	8999(2)	-1409(1)	68(1)	29(1)
C(32)	9180(2)	-1586(2)	604(1)	46(1)
C(33)	9489(2)	-782(1)	-24(1)	49(1)
C(34)	9468(2)	-1898(2)	-253(1)	52(1)
C(35)	6953(2)	-2026(1)	-637(1)	29(1)
C(36)	6788(2)	-2017(1)	-1178(1)	33(1)
C(37)	6289(2)	-2430(1)	-1477(1)	45(1)
C(38)	6297(3)	-2300(2)	-1979(1)	53(1)
C(39)	6782(2)	-1795(2)	-2169(1)	50(1)
C(40)	7277(2)	-1385(1)	-1862(1)	41(1)
C(41)	7262(2)	-1509(1)	-1367(1)	31(1)
C(42)	7739(2)	-1162(1)	-954(1)	28(1)
C(43)	8329(2)	564(1)	861(1)	23(1)
C(44)	9356(2)	854(1)	967(1)	27(1)
C(45)	9991(2)	584(1)	1391(1)	34(1)
C(46)	10140(2)	-104(1)	1294(1)	44(1)
C(47)	9516(2)	681(2)	1895(1)	46(1)
C(48)	11019(2)	895(2)	1382(1)	53(1)
C(49)	9803(2)	1913(1)	683(1)	35(1)
C(50)	9490(2)	2548(1)	808(1)	36(1)
C(51)	9803(2)	3107(1)	618(1)	45(1)
C(52)	9331(3)	3632(1)	794(1)	52(1)
C(53)	8580(3)	3596(1)	1137(1)	52(1)
C(54)	8268(2)	3033(1)	1328(1)	44(1)
C(55)	8740(2)	2513(1)	1153(1)	35(1)
C(56)	8544(2)	1854(1)	1262(1)	31(1)
C(57)	7028(2)	820(1)	-887(1)	27(1)
C(58)	7333(2)	801(1)	-1394(1)	29(1)
C(59)	6925(2)	351(1)	-1694(1)	43(1)
C(60)	7206(2)	324(1)	-2181(1)	44(1)
C(61)	7892(2)	744(1)	-2361(1)	30(1)
C(62)	8305(2)	1193(1)	-2062(1)	32(1)
C(63)	8020(2)	1218(1)	-1572(1)	32(1)
C(64)	8191(2)	692(1)	-2867(1)	29(1)
C(65)	4751(4)	1866(2)	3442(1)	68(1)
C(66)	3962(5)	1610(2)	3676(2)	86(1)
C(67)	3260(5)	1974(4)	3902(2)	115(2)
C(68)	3376(6)	2582(5)	3903(3)	143(4)
C(69)	4134(5)	2842(2)	3678(2)	96(2)
C(70)	4860(4)	2495(2)	3432(1)	75(1)
C(71)	5714(5)	2758(3)	3182(2)	124(3)
C(72)	5021(2)	4904(2)	1614(1)	55(1)
C(73)	5254(3)	4931(2)	2103(2)	63(1)
C(74)	5807(3)	4484(2)	2321(1)	64(1)
C(75)	6129(3)	3990(2)	2045(1)	54(1)
C(76)	5901(2)	3956(1)	1553(1)	44(1)
C(77)	5341(2)	4413(1)	1329(1)	42(1)
C(78)	5092(3)	4381(2)	790(1)	53(1)
C(79)	10679(3)	3092(2)	2082(2)	65(1)
C(80)	11359(5)	2608(3)	2156(3)	113(2)
C(81)	11776(4)	2551(3)	2658(3)	101(2)

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C(82)	11462(4)	2973(3)	2987(2)	94(2)
C(83)	10801(5)	3418(3)	2902(2)	101(2)
C(84)	10422(4)	3475(2)	2448(2)	78(1)
C(85)	9674(5)	3986(3)	2353(3)	119(2)

Table 3. Bond lengths [A] and angles [deg] for joef086.

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Rh(1)-O(5)	2.0173(15)
Rh(1)-O(9)	2.0393(15)
Rh(1)-O(13)	2.0431(15)
Rh(1)-O(1)	2.0477(15)
Rh(1)-N(5)	2.2292(18)
Rh(1)-Rh(2)	2.3949(5)
Rh(2)-O(10)	2.0208(15)
Rh(2)-O(2)	2.0310(15)
Rh(2)-O(6)	2.0383(15)
Rh(2)-O(14)	2.0497(15)
Rh(2)-N(6)#1	2.2380(17)
N(1)-C(7)	1.404(3)
N(1)-C(14)	1.405(3)
N(1)-C(2)	1.468(3)
N(2)-C(28)	1.400(3)
N(2)-C(21)	1.402(3)
N(2)-C(16)	1.474(3)
N(3)-C(42)	1.396(3)
N(3)-C(35)	1.415(3)
N(3)-C(30)	1.470(3)
N(4)-C(56)	1.394(3)
N(4)-C(49)	1.414(3)
N(4)-C(44)	1.467(3)
N(5)-C(57)	1.143(3)
N(6)-C(64)	1.136(3)
N(6)-Rh(2)#2	2.2380(17)
O(1)-C(1)	1.264(3)
O(2)-C(1)	1.259(3)
O(3)-C(7)	1.215(3)
O(4)-C(14)	1.205(3)
O(5)-C(15)	1.263(3)
O(6)-C(15)	1.265(2)
O(7)-C(21)	1.210(3)
O(8)-C(28)	1.209(3)
O(9)-C(29)	1.259(3)
O(10)-C(29)	1.269(3)
O(11)-C(42)	1.205(3)
O(12)-C(35)	1.202(3)
O(13)-C(43)	1.265(2)
O(14)-C(43)	1.256(2)
O(15)-C(49)	1.198(3)
O(16)-C(56)	1.211(3)
C(1)-C(2)	1.539(3)
C(2)-C(3)	1.554(3)
C(3)-C(5)	1.530(4)
C(3)-C(4)	1.537(3)
C(3)-C(6)	1.538(3)
C(7)-C(8)	1.478(3)
C(8)-C(9)	1.381(3)
C(8)-C(13)	1.390(3)
C(9)-C(10)	1.396(4)
C(10)-C(11)	1.376(4)
C(11)-C(12)	1.386(4)
C(12)-C(13)	1.389(3)
C(13)-C(14)	1.480(3)

C(15)-C(16)	1.540(3)
C(16)-C(17)	1.549(3)
C(17)-C(18)	1.529(4)
C(17)-C(20)	1.532(4)
C(17)-C(19)	1.539(3)
C(21)-C(22)	1.493(3)
C(22)-C(23)	1.377(4)
C(22)-C(27)	1.385(3)
C(23)-C(24)	1.407(4)
C(24)-C(25)	1.371(5)
C(25)-C(26)	1.396(4)
C(26)-C(27)	1.387(3)
C(27)-C(28)	1.488(3)
C(29)-C(30)	1.530(3)
C(30)-C(31)	1.563(3)
C(31)-C(34)	1.515(4)
C(31)-C(32)	1.535(4)
C(31)-C(33)	1.536(4)
C(35)-C(36)	1.495(3)
C(36)-C(41)	1.378(4)
C(36)-C(37)	1.387(4)
C(37)-C(38)	1.401(4)
C(38)-C(39)	1.378(5)
C(39)-C(40)	1.393(4)
C(40)-C(41)	1.382(3)
C(41)-C(42)	1.500(3)
C(43)-C(44)	1.543(3)
C(44)-C(45)	1.554(3)
C(45)-C(47)	1.530(4)
C(45)-C(46)	1.534(4)
C(45)-C(48)	1.538(4)
C(49)-C(50)	1.486(4)
C(50)-C(55)	1.382(4)
C(50)-C(51)	1.388(4)
C(51)-C(52)	1.393(5)
C(52)-C(53)	1.377(5)
C(53)-C(54)	1.398(4)
C(54)-C(55)	1.383(4)
C(55)-C(56)	1.490(3)
C(57)-C(58)	1.446(3)
C(58)-C(63)	1.383(3)
C(58)-C(59)	1.388(4)
C(59)-C(60)	1.384(3)
C(60)-C(61)	1.386(4)
C(61)-C(62)	1.390(3)
C(61)-C(64)	1.446(3)
C(62)-C(63)	1.392(3)
C(65)-C(66)	1.358(7)
C(65)-C(70)	1.377(6)
C(66)-C(67)	1.375(8)
C(67)-C(68)	1.335(10)
C(68)-C(69)	1.317(10)
C(69)-C(70)	1.403(8)
C(70)-C(71)	1.452(7)
C(72)-C(73)	1.373(5)
C(72)-C(77)	1.390(4)
C(73)-C(74)	1.362(6)
C(74)-C(75)	1.384(5)
C(75)-C(76)	1.380(5)
C(76)-C(77)	1.390(4)
C(77)-C(78)	1.512(4)

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C(79)-C(84)              1.347(6)
C(79)-C(80)              1.408(8)
C(80)-C(81)              1.486(9)
C(81)-C(82)              1.354(8)
C(82)-C(83)              1.334(8)
C(83)-C(84)              1.348(7)
C(84)-C(85)              1.521(8)

O(5)-Rh(1)-O(9)          89.10(6)
O(5)-Rh(1)-O(13)         176.64(6)
O(9)-Rh(1)-O(13)         92.63(6)
O(5)-Rh(1)-O(1)          88.90(6)
O(9)-Rh(1)-O(1)          174.83(6)
O(13)-Rh(1)-O(1)         89.14(6)
O(5)-Rh(1)-N(5)          91.80(6)
O(9)-Rh(1)-N(5)          85.69(6)
O(13)-Rh(1)-N(5)         91.20(6)
O(1)-Rh(1)-N(5)          99.14(6)
O(5)-Rh(1)-Rh(2)         89.17(4)
O(9)-Rh(1)-Rh(2)         87.59(4)
O(13)-Rh(1)-Rh(2)        88.03(4)
O(1)-Rh(1)-Rh(2)         87.61(4)
N(5)-Rh(1)-Rh(2)         173.19(5)
O(10)-Rh(2)-O(2)         176.79(6)
O(10)-Rh(2)-O(6)         89.58(6)
O(2)-Rh(2)-O(6)          88.78(6)
O(10)-Rh(2)-O(14)        90.82(7)
O(2)-Rh(2)-O(14)         90.58(6)
O(6)-Rh(2)-O(14)         175.01(6)
O(10)-Rh(2)-N(6)#1       93.30(6)
O(2)-Rh(2)-N(6)#1        89.65(6)
O(6)-Rh(2)-N(6)#1        97.17(7)
O(14)-Rh(2)-N(6)#1       87.77(7)
O(10)-Rh(2)-Rh(1)        88.55(4)
O(2)-Rh(2)-Rh(1)         88.61(4)
O(6)-Rh(2)-Rh(1)         87.07(4)
O(14)-Rh(2)-Rh(1)        87.97(4)
N(6)#1-Rh(2)-Rh(1)       175.39(5)
C(7)-N(1)-C(14)          111.49(19)
C(7)-N(1)-C(2)           125.27(18)
C(14)-N(1)-C(2)          122.68(19)
C(28)-N(2)-C(21)         111.55(19)
C(28)-N(2)-C(16)         121.59(18)
C(21)-N(2)-C(16)         125.63(18)
C(42)-N(3)-C(35)         111.63(19)
C(42)-N(3)-C(30)         130.12(18)
C(35)-N(3)-C(30)         118.19(18)
C(56)-N(4)-C(49)         111.29(19)
C(56)-N(4)-C(44)         127.41(19)
C(49)-N(4)-C(44)         120.9(2)
C(57)-N(5)-Rh(1)         151.96(18)
C(64)-N(6)-Rh(2)#2       157.51(19)
C(1)-O(1)-Rh(1)          118.26(13)
C(1)-O(2)-Rh(2)          118.20(13)
C(15)-O(5)-Rh(1)         117.83(13)
C(15)-O(6)-Rh(2)         118.91(14)
C(29)-O(9)-Rh(1)         118.77(13)
C(29)-O(10)-Rh(2)        118.46(14)
C(43)-O(13)-Rh(1)        118.69(13)
C(43)-O(14)-Rh(2)        118.61(13)
O(2)-C(1)-O(1)           127.25(19)
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O(2)-C(1)-C(2)	117.89(18)
O(1)-C(1)-C(2)	114.84(18)
N(1)-C(2)-C(1)	107.35(16)
N(1)-C(2)-C(3)	113.03(18)
C(1)-C(2)-C(3)	118.50(18)
C(5)-C(3)-C(4)	111.0(2)
C(5)-C(3)-C(6)	108.8(2)
C(4)-C(3)-C(6)	107.7(2)
C(5)-C(3)-C(2)	112.76(19)
C(4)-C(3)-C(2)	108.44(19)
C(6)-C(3)-C(2)	107.97(19)
O(3)-C(7)-N(1)	124.2(2)
O(3)-C(7)-C(8)	129.8(2)
N(1)-C(7)-C(8)	105.97(19)
C(9)-C(8)-C(13)	121.8(2)
C(9)-C(8)-C(7)	129.9(2)
C(13)-C(8)-C(7)	108.3(2)
C(8)-C(9)-C(10)	116.2(2)
C(11)-C(10)-C(9)	122.3(3)
C(10)-C(11)-C(12)	121.3(2)
C(11)-C(12)-C(13)	117.0(3)
C(12)-C(13)-C(8)	121.4(2)
C(12)-C(13)-C(14)	130.1(2)
C(8)-C(13)-C(14)	108.41(19)
O(4)-C(14)-N(1)	124.7(2)
O(4)-C(14)-C(13)	129.6(2)
N(1)-C(14)-C(13)	105.71(19)
O(5)-C(15)-O(6)	126.9(2)
O(5)-C(15)-C(16)	114.00(18)
O(6)-C(15)-C(16)	118.97(19)
N(2)-C(16)-C(15)	107.57(17)
N(2)-C(16)-C(17)	113.99(18)
C(15)-C(16)-C(17)	118.40(18)
C(18)-C(17)-C(20)	111.7(2)
C(18)-C(17)-C(19)	107.9(2)
C(20)-C(17)-C(19)	108.8(2)
C(18)-C(17)-C(16)	108.8(2)
C(20)-C(17)-C(16)	112.6(2)
C(19)-C(17)-C(16)	106.9(2)
O(7)-C(21)-N(2)	125.9(2)
O(7)-C(21)-C(22)	128.4(2)
N(2)-C(21)-C(22)	105.7(2)
C(23)-C(22)-C(27)	121.9(2)
C(23)-C(22)-C(21)	129.9(2)
C(27)-C(22)-C(21)	108.1(2)
C(22)-C(23)-C(24)	116.4(3)
C(25)-C(24)-C(23)	121.6(3)
C(24)-C(25)-C(26)	121.7(3)
C(27)-C(26)-C(25)	116.6(3)
C(22)-C(27)-C(26)	121.7(2)
C(22)-C(27)-C(28)	108.3(2)
C(26)-C(27)-C(28)	130.0(2)
O(8)-C(28)-N(2)	125.3(2)
O(8)-C(28)-C(27)	128.8(2)
N(2)-C(28)-C(27)	105.9(2)
O(9)-C(29)-O(10)	126.6(2)
O(9)-C(29)-C(30)	119.50(18)
O(10)-C(29)-C(30)	113.87(18)
N(3)-C(30)-C(29)	111.84(17)
N(3)-C(30)-C(31)	115.76(18)
C(29)-C(30)-C(31)	112.01(19)

C(34)-C(31)-C(32)	108.0(2)
C(34)-C(31)-C(33)	110.7(2)
C(32)-C(31)-C(33)	108.1(2)
C(34)-C(31)-C(30)	109.3(2)
C(32)-C(31)-C(30)	108.2(2)
C(33)-C(31)-C(30)	112.5(2)
O(12)-C(35)-N(3)	125.7(2)
O(12)-C(35)-C(36)	128.5(2)
N(3)-C(35)-C(36)	105.8(2)
C(41)-C(36)-C(37)	121.6(2)
C(41)-C(36)-C(35)	108.2(2)
C(37)-C(36)-C(35)	130.2(3)
C(36)-C(37)-C(38)	116.2(3)
C(39)-C(38)-C(37)	122.2(3)
C(38)-C(39)-C(40)	120.8(3)
C(41)-C(40)-C(39)	117.2(3)
C(36)-C(41)-C(40)	122.0(2)
C(36)-C(41)-C(42)	108.7(2)
C(40)-C(41)-C(42)	129.2(2)
O(11)-C(42)-N(3)	127.8(2)
O(11)-C(42)-C(41)	126.5(2)
N(3)-C(42)-C(41)	105.73(19)
O(14)-C(43)-O(13)	126.6(2)
O(14)-C(43)-C(44)	120.61(18)
O(13)-C(43)-C(44)	112.74(18)
N(4)-C(44)-C(43)	108.93(17)
N(4)-C(44)-C(45)	113.35(19)
C(43)-C(44)-C(45)	118.36(19)
C(47)-C(45)-C(46)	110.2(2)
C(47)-C(45)-C(48)	109.2(2)
C(46)-C(45)-C(48)	108.0(2)
C(47)-C(45)-C(44)	113.0(2)
C(46)-C(45)-C(44)	108.1(2)
C(48)-C(45)-C(44)	108.2(2)
O(15)-C(49)-N(4)	124.5(2)
O(15)-C(49)-C(50)	129.7(2)
N(4)-C(49)-C(50)	105.8(2)
C(55)-C(50)-C(51)	121.5(3)
C(55)-C(50)-C(49)	108.2(2)
C(51)-C(50)-C(49)	130.2(3)
C(50)-C(51)-C(52)	117.1(3)
C(53)-C(52)-C(51)	121.3(3)
C(52)-C(53)-C(54)	121.6(3)
C(55)-C(54)-C(53)	116.9(3)
C(50)-C(55)-C(54)	121.6(3)
C(50)-C(55)-C(56)	108.5(2)
C(54)-C(55)-C(56)	129.8(3)
O(16)-C(56)-N(4)	125.3(2)
O(16)-C(56)-C(55)	128.8(2)
N(4)-C(56)-C(55)	105.9(2)
N(5)-C(57)-C(58)	177.9(3)
C(63)-C(58)-C(59)	121.3(2)
C(63)-C(58)-C(57)	120.4(2)
C(59)-C(58)-C(57)	118.2(2)
C(60)-C(59)-C(58)	119.2(2)
C(59)-C(60)-C(61)	119.6(2)
C(60)-C(61)-C(62)	121.3(2)
C(60)-C(61)-C(64)	118.2(2)
C(62)-C(61)-C(64)	120.4(2)
C(61)-C(62)-C(63)	118.9(2)
C(58)-C(63)-C(62)	119.6(2)

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N(6)-C(64)-C(61)              176.0(3)
C(66)-C(65)-C(70)             120.0(4)
C(65)-C(66)-C(67)             120.6(5)
C(68)-C(67)-C(66)             119.5(7)
C(69)-C(68)-C(67)             121.0(6)
C(68)-C(69)-C(70)             121.9(5)
C(65)-C(70)-C(69)             116.9(5)
C(65)-C(70)-C(71)             119.1(5)
C(69)-C(70)-C(71)             124.0(6)
C(73)-C(72)-C(77)             120.5(3)
C(74)-C(73)-C(72)             121.3(3)
C(73)-C(74)-C(75)             119.1(3)
C(76)-C(75)-C(74)             120.3(3)
C(75)-C(76)-C(77)             120.7(3)
C(72)-C(77)-C(76)             118.1(3)
C(72)-C(77)-C(78)             120.9(3)
C(76)-C(77)-C(78)             121.1(3)
C(84)-C(79)-C(80)             121.5(5)
C(79)-C(80)-C(81)             116.1(6)
C(82)-C(81)-C(80)             116.0(6)
C(83)-C(82)-C(81)             125.9(6)
C(82)-C(83)-C(84)             118.4(7)
C(79)-C(84)-C(83)             122.1(6)
C(79)-C(84)-C(85)             119.7(5)
C(83)-C(84)-C(85)             118.2(6)
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Symmetry transformations used to generate equivalent atoms:
#1 -x+3/2,-y,z+1/2   #2 -x+3/2,-y,z-1/2

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for joef086.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

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	U11	U22	U33	U23	U13	U12
Rh(1)	18(1)	21(1)	16(1)	1(1)	0(1)	0(1)
Rh(2)	18(1)	22(1)	16(1)	2(1)	-1(1)	0(1)
N(1)	25(1)	24(1)	27(1)	1(1)	0(1)	4(1)
N(2)	23(1)	28(1)	31(1)	-4(1)	-7(1)	2(1)
N(3)	25(1)	24(1)	25(1)	-2(1)	0(1)	0(1)
N(4)	23(1)	28(1)	33(1)	-1(1)	2(1)	-4(1)
N(5)	30(1)	29(1)	19(1)	-1(1)	1(1)	-4(1)
N(6)	28(1)	29(1)	20(1)	-2(1)	1(1)	3(1)
O(1)	24(1)	22(1)	20(1)	0(1)	3(1)	1(1)
O(2)	25(1)	27(1)	20(1)	1(1)	2(1)	3(1)
O(3)	32(1)	25(1)	40(1)	1(1)	-3(1)	0(1)
O(4)	48(1)	26(1)	40(1)	-1(1)	0(1)	-1(1)
O(5)	21(1)	27(1)	23(1)	1(1)	-4(1)	-2(1)
O(6)	20(1)	29(1)	26(1)	3(1)	-2(1)	-3(1)
O(7)	33(1)	43(1)	45(1)	-7(1)	-8(1)	14(1)
O(8)	37(1)	42(1)	45(1)	-6(1)	-12(1)	15(1)
O(9)	27(1)	25(1)	21(1)	-1(1)	1(1)	3(1)
O(10)	27(1)	24(1)	21(1)	0(1)	1(1)	3(1)
O(11)	47(1)	38(1)	33(1)	3(1)	3(1)	-12(1)
O(12)	40(1)	30(1)	38(1)	1(1)	1(1)	-8(1)
O(13)	20(1)	29(1)	22(1)	2(1)	0(1)	-3(1)
O(14)	20(1)	30(1)	24(1)	1(1)	-4(1)	-4(1)
O(15)	36(1)	47(1)	63(1)	0(1)	23(1)	-5(1)
O(16)	37(1)	43(1)	44(1)	-1(1)	14(1)	0(1)
C(1)	18(1)	25(1)	23(1)	-1(1)	1(1)	-1(1)
C(2)	24(1)	25(1)	23(1)	-2(1)	1(1)	0(1)
C(3)	32(1)	35(1)	24(1)	-3(1)	5(1)	5(1)
C(4)	41(2)	50(2)	25(1)	-5(1)	-2(1)	7(1)
C(5)	34(1)	51(2)	32(1)	8(1)	8(1)	2(1)
C(6)	54(2)	44(2)	33(1)	-5(1)	8(1)	17(1)
C(7)	23(1)	31(1)	28(1)	0(1)	4(1)	5(1)
C(8)	25(1)	30(1)	30(1)	4(1)	4(1)	5(1)
C(9)	24(1)	41(1)	36(1)	6(1)	1(1)	3(1)
C(10)	25(1)	59(2)	34(1)	12(1)	0(1)	9(1)
C(11)	39(1)	47(2)	41(1)	18(1)	5(1)	18(1)
C(12)	46(2)	32(1)	38(1)	9(1)	9(1)	11(1)
C(13)	32(1)	31(1)	29(1)	4(1)	6(1)	7(1)
C(14)	33(1)	26(1)	28(1)	0(1)	5(1)	4(1)
C(15)	22(1)	23(1)	24(1)	-2(1)	-2(1)	1(1)
C(16)	18(1)	29(1)	30(1)	-5(1)	-3(1)	-1(1)
C(17)	21(1)	34(1)	40(1)	2(1)	-2(1)	-7(1)
C(18)	32(1)	55(2)	41(1)	4(1)	8(1)	-8(1)
C(19)	24(1)	54(2)	61(2)	6(1)	-5(1)	-10(1)
C(20)	45(2)	31(1)	54(2)	6(1)	-4(1)	-6(1)
C(21)	26(1)	33(1)	35(1)	-5(1)	-3(1)	1(1)
C(22)	31(1)	39(1)	33(1)	-3(1)	-5(1)	-2(1)
C(23)	41(2)	58(2)	41(1)	-5(1)	0(1)	4(1)
C(24)	60(2)	69(2)	32(1)	-6(1)	3(1)	-2(2)
C(25)	66(2)	57(2)	34(1)	4(1)	-12(1)	-7(2)
C(26)	47(2)	43(2)	40(1)	3(1)	-13(1)	2(1)
C(27)	33(1)	33(1)	34(1)	-1(1)	-7(1)	-2(1)

C(28)	27(1)	31(1)	35(1)	-3(1)	-10(1)	-1(1)
C(29)	19(1)	26(1)	24(1)	-3(1)	0(1)	-1(1)
C(30)	26(1)	21(1)	22(1)	-2(1)	0(1)	3(1)
C(31)	23(1)	34(1)	31(1)	-1(1)	-4(1)	6(1)
C(32)	38(2)	61(2)	38(1)	7(1)	-9(1)	8(1)
C(33)	28(1)	49(2)	70(2)	9(2)	-17(1)	-9(1)
C(34)	35(1)	61(2)	61(2)	-22(2)	-4(1)	20(1)
C(35)	24(1)	29(1)	32(1)	-7(1)	-1(1)	0(1)
C(36)	31(1)	35(1)	33(1)	-7(1)	-3(1)	1(1)
C(37)	46(2)	45(2)	43(1)	-13(1)	-7(1)	-6(1)
C(38)	55(2)	60(2)	45(2)	-20(1)	-17(1)	-2(2)
C(39)	54(2)	67(2)	29(1)	-10(1)	-8(1)	11(2)
C(40)	42(2)	50(2)	31(1)	1(1)	-3(1)	6(1)
C(41)	30(1)	38(1)	26(1)	-3(1)	-2(1)	2(1)
C(42)	27(1)	31(1)	26(1)	-2(1)	1(1)	2(1)
C(43)	18(1)	25(1)	25(1)	-2(1)	0(1)	1(1)
C(44)	18(1)	29(1)	33(1)	-5(1)	0(1)	-3(1)
C(45)	23(1)	39(1)	41(1)	-4(1)	-10(1)	-1(1)
C(46)	36(1)	38(1)	58(2)	-2(1)	-13(1)	9(1)
C(47)	53(2)	54(2)	32(1)	-3(1)	-15(1)	4(1)
C(48)	28(1)	54(2)	76(2)	3(2)	-19(1)	-5(1)
C(49)	26(1)	35(1)	43(1)	0(1)	2(1)	-6(1)
C(50)	33(1)	32(1)	44(1)	0(1)	-6(1)	-6(1)
C(51)	38(2)	41(1)	56(2)	7(1)	-7(1)	-11(1)
C(52)	54(2)	34(1)	69(2)	5(1)	-17(2)	-8(1)
C(53)	56(2)	33(1)	68(2)	-9(1)	-15(2)	7(1)
C(54)	43(2)	41(1)	48(1)	-7(1)	-4(1)	5(1)
C(55)	32(1)	35(1)	38(1)	-3(1)	-6(1)	0(1)
C(56)	27(1)	33(1)	32(1)	-3(1)	-1(1)	0(1)
C(57)	30(1)	30(1)	22(1)	1(1)	0(1)	2(1)
C(58)	36(1)	34(1)	18(1)	1(1)	1(1)	2(1)
C(59)	60(2)	42(1)	27(1)	-2(1)	9(1)	-18(1)
C(60)	70(2)	39(1)	23(1)	-8(1)	4(1)	-20(1)
C(61)	38(1)	33(1)	18(1)	-2(1)	2(1)	4(1)
C(62)	36(1)	36(1)	24(1)	-4(1)	5(1)	-7(1)
C(63)	40(1)	37(1)	21(1)	-6(1)	2(1)	-5(1)
C(64)	35(1)	31(1)	21(1)	-3(1)	0(1)	2(1)
C(65)	85(3)	74(2)	45(2)	-21(2)	-6(2)	12(2)
C(66)	122(4)	69(3)	65(3)	-7(2)	-13(3)	-7(3)
C(67)	95(4)	175(7)	74(3)	-34(4)	-8(3)	-13(5)
C(68)	79(4)	224(9)	126(5)	-105(6)	-36(4)	52(5)
C(69)	118(4)	64(2)	106(4)	-36(3)	-72(4)	41(3)
C(70)	90(3)	90(3)	46(2)	12(2)	-28(2)	-21(3)
C(71)	160(6)	146(5)	66(3)	9(3)	-26(4)	-63(5)
C(72)	42(2)	40(2)	82(2)	-8(2)	-6(2)	3(1)
C(73)	51(2)	58(2)	79(2)	-26(2)	3(2)	-1(2)
C(74)	60(2)	78(2)	54(2)	-15(2)	-1(2)	-17(2)
C(75)	49(2)	53(2)	60(2)	9(2)	-13(2)	-5(1)
C(76)	41(2)	37(1)	55(2)	-3(1)	-3(1)	-3(1)
C(77)	36(1)	33(1)	58(2)	4(1)	-3(1)	-7(1)
C(78)	51(2)	46(2)	63(2)	12(2)	-7(2)	-5(1)
C(79)	63(2)	67(2)	65(2)	-5(2)	-4(2)	-22(2)
C(80)	87(4)	95(4)	157(6)	-17(4)	38(4)	-34(3)
C(81)	73(3)	94(4)	135(5)	42(4)	-5(3)	-23(3)
C(82)	78(3)	103(4)	101(4)	38(3)	-4(3)	-10(3)
C(83)	99(4)	119(5)	86(3)	15(3)	-18(3)	-36(4)
C(84)	82(3)	81(3)	71(3)	4(2)	-7(2)	-38(2)
C(85)	140(6)	93(4)	125(5)	-12(4)	-22(4)	-1(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic
displacement parameters (A^2 x 10^3) for joef086.

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	x	y	z	U(eq)
H(2A)	5746	1940	1299	29
H(4A)	5569	1415	2506	58
H(4B)	6279	1740	2113	58
H(4C)	6060	1020	2075	58
H(5A)	3882	1029	2247	58
H(5B)	4327	661	1789	58
H(5C)	3477	1166	1707	58
H(6A)	4245	2158	2338	65
H(6B)	3844	2267	1793	65
H(6C)	4935	2496	1943	65
H(9A)	2241	1306	-3	41
H(10A)	1558	2134	-445	47
H(11A)	2097	3125	-325	51
H(12A)	3383	3345	231	46
H(16A)	3346	-37	323	31
H(18A)	2700	-952	1309	64
H(18B)	2831	-263	1116	64
H(18C)	3791	-661	1259	64
H(19A)	1736	-1250	595	69
H(19B)	2140	-1122	53	69
H(19C)	1800	-562	393	69
H(20A)	3329	-1831	777	65
H(20B)	4381	-1509	674	65
H(20C)	3671	-1694	227	65
H(23A)	4978	-1393	-1445	56
H(24A)	4220	-1138	-2203	64
H(25A)	2917	-455	-2240	63
H(26A)	2292	19	-1528	52
H(30A)	7577	-1754	166	28
H(32A)	9892	-1549	679	68
H(32B)	8966	-2011	658	68
H(32C)	8798	-1312	818	68
H(33A)	10209	-814	33	73
H(33B)	9204	-478	200	73
H(33C)	9368	-655	-362	73
H(34A)	10181	-1929	-177	78
H(34B)	9383	-1787	-598	78
H(34C)	9145	-2294	-190	78
H(37A)	5959	-2781	-1348	53
H(38A)	5957	-2569	-2196	64
H(39A)	6779	-1727	-2512	60
H(40A)	7610	-1034	-1989	49
H(44A)	9757	778	665	32
H(46A)	10617	-271	1531	66
H(46B)	10399	-161	962	66
H(46C)	9501	-317	1327	66
H(47A)	9489	1121	1968	69
H(47B)	9916	472	2144	69
H(47C)	8839	512	1895	69
H(48A)	10943	1334	1450	79
H(48B)	11321	840	1058	79
H(48C)	11449	709	1631	79

H(51A)	10316	3130	379	54
H(52A)	9532	4023	676	63
H(53A)	8267	3963	1245	63
H(54A)	7755	3009	1567	53
H(59A)	6459	64	-1566	51
H(60A)	6930	21	-2390	53
H(62A)	8774	1478	-2189	39
H(63A)	8296	1521	-1361	39
H(65A)	5228	1612	3284	82
H(66A)	3893	1176	3685	103
H(67A)	2697	1793	4056	138
H(68A)	2905	2832	4070	171
H(69A)	4192	3276	3681	115
H(71A)	5591	3195	3119	186
H(71B)	5819	2544	2871	186
H(71C)	6308	2714	3388	186
H(72A)	4637	5222	1470	66
H(73A)	5026	5269	2292	75
H(74A)	5970	4511	2659	77
H(75A)	6509	3673	2194	65
H(76A)	6129	3616	1366	53
H(78A)	4448	4581	731	80
H(78B)	5055	3951	687	80
H(78C)	5612	4591	601	80
H(79A)	10396	3149	1767	78
H(80A)	11540	2334	1901	135
H(81A)	12236	2236	2743	121
H(82A)	11737	2951	3307	113
H(83A)	10601	3689	3157	121
H(85A)	9674	4089	2004	179
H(85B)	9859	4349	2544	179
H(85C)	9007	3848	2450	179

Table 6. Torsion angles [deg] for joef086.

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O(5)-Rh(1)-Rh(2)-O(10)	90.75(6)
O(9)-Rh(1)-Rh(2)-O(10)	1.61(6)
O(13)-Rh(1)-Rh(2)-O(10)	-91.10(6)
O(1)-Rh(1)-Rh(2)-O(10)	179.68(6)
N(5)-Rh(1)-Rh(2)-O(10)	-7.5(4)
O(5)-Rh(1)-Rh(2)-O(2)	-87.76(6)
O(9)-Rh(1)-Rh(2)-O(2)	-176.89(6)
O(13)-Rh(1)-Rh(2)-O(2)	90.39(6)
O(1)-Rh(1)-Rh(2)-O(2)	1.17(6)
N(5)-Rh(1)-Rh(2)-O(2)	174.0(4)
O(5)-Rh(1)-Rh(2)-O(6)	1.09(6)
O(9)-Rh(1)-Rh(2)-O(6)	-88.04(6)
O(13)-Rh(1)-Rh(2)-O(6)	179.24(6)
O(1)-Rh(1)-Rh(2)-O(6)	90.02(6)
N(5)-Rh(1)-Rh(2)-O(6)	-97.2(4)
O(5)-Rh(1)-Rh(2)-O(14)	-178.38(6)
O(9)-Rh(1)-Rh(2)-O(14)	92.48(6)
O(13)-Rh(1)-Rh(2)-O(14)	-0.23(6)
O(1)-Rh(1)-Rh(2)-O(14)	-89.45(6)
N(5)-Rh(1)-Rh(2)-O(14)	83.4(4)
O(5)-Rh(1)-Rh(2)-N(6)#1	-155.6(6)
O(9)-Rh(1)-Rh(2)-N(6)#1	115.3(6)
O(13)-Rh(1)-Rh(2)-N(6)#1	22.5(6)
O(1)-Rh(1)-Rh(2)-N(6)#1	-66.7(6)
N(5)-Rh(1)-Rh(2)-N(6)#1	106.1(8)
O(5)-Rh(1)-N(5)-C(57)	-96.5(4)
O(9)-Rh(1)-N(5)-C(57)	-7.5(4)
O(13)-Rh(1)-N(5)-C(57)	85.0(4)
O(1)-Rh(1)-N(5)-C(57)	174.3(4)
Rh(2)-Rh(1)-N(5)-C(57)	1.6(7)
O(5)-Rh(1)-O(1)-C(1)	86.69(15)
O(9)-Rh(1)-O(1)-C(1)	19.5(8)
O(13)-Rh(1)-O(1)-C(1)	-90.58(15)
N(5)-Rh(1)-O(1)-C(1)	178.35(15)
Rh(2)-Rh(1)-O(1)-C(1)	-2.52(14)
O(10)-Rh(2)-O(2)-C(1)	-27.9(12)
O(6)-Rh(2)-O(2)-C(1)	-87.32(15)
O(14)-Rh(2)-O(2)-C(1)	87.73(15)
N(6)#1-Rh(2)-O(2)-C(1)	175.50(16)
Rh(1)-Rh(2)-O(2)-C(1)	-0.23(15)
O(9)-Rh(1)-O(5)-C(15)	87.79(15)
O(13)-Rh(1)-O(5)-C(15)	-33.2(11)
O(1)-Rh(1)-O(5)-C(15)	-87.44(15)
N(5)-Rh(1)-O(5)-C(15)	173.45(15)
Rh(2)-Rh(1)-O(5)-C(15)	0.19(14)
O(10)-Rh(2)-O(6)-C(15)	-91.31(15)
O(2)-Rh(2)-O(6)-C(15)	85.92(15)
O(14)-Rh(2)-O(6)-C(15)	3.3(8)
N(6)#1-Rh(2)-O(6)-C(15)	175.42(15)
Rh(1)-Rh(2)-O(6)-C(15)	-2.75(15)
O(5)-Rh(1)-O(9)-C(29)	-90.64(16)
O(13)-Rh(1)-O(9)-C(29)	86.47(16)
O(1)-Rh(1)-O(9)-C(29)	-23.4(8)
N(5)-Rh(1)-O(9)-C(29)	177.48(16)
Rh(2)-Rh(1)-O(9)-C(29)	-1.44(15)

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O(2)-Rh(2)-O(10)-C(29)         25.4(12)
O(6)-Rh(2)-O(10)-C(29)         84.74(16)
O(14)-Rh(2)-O(10)-C(29)        -90.29(16)
N(6)#1-Rh(2)-O(10)-C(29)       -178.10(16)
Rh(1)-Rh(2)-O(10)-C(29)        -2.33(15)
O(5)-Rh(1)-O(13)-C(43)         32.4(11)
O(9)-Rh(1)-O(13)-C(43)         -88.59(15)
O(1)-Rh(1)-O(13)-C(43)         86.55(15)
N(5)-Rh(1)-O(13)-C(43)         -174.32(15)
Rh(2)-Rh(1)-O(13)-C(43)        -1.09(15)
O(10)-Rh(2)-O(14)-C(43)        90.17(15)
O(2)-Rh(2)-O(14)-C(43)         -86.93(15)
O(6)-Rh(2)-O(14)-C(43)         -4.4(8)
N(6)#1-Rh(2)-O(14)-C(43)       -176.56(16)
Rh(1)-Rh(2)-O(14)-C(43)        1.65(15)
Rh(2)-O(2)-C(1)-O(1)           -1.9(3)
Rh(2)-O(2)-C(1)-C(2)           -179.92(14)
Rh(1)-O(1)-C(1)-O(2)           3.3(3)
Rh(1)-O(1)-C(1)-C(2)           -178.62(13)
C(7)-N(1)-C(2)-C(1)            42.9(3)
C(14)-N(1)-C(2)-C(1)           -127.8(2)
C(7)-N(1)-C(2)-C(3)            -89.6(2)
C(14)-N(1)-C(2)-C(3)           99.7(2)
O(2)-C(1)-C(2)-N(1)            -134.52(19)
O(1)-C(1)-C(2)-N(1)            47.2(2)
O(2)-C(1)-C(2)-C(3)            -5.0(3)
O(1)-C(1)-C(2)-C(3)            176.69(19)
N(1)-C(2)-C(3)-C(5)            65.0(3)
C(1)-C(2)-C(3)-C(5)            -61.8(3)
N(1)-C(2)-C(3)-C(4)            -171.6(2)
C(1)-C(2)-C(3)-C(4)            61.5(3)
N(1)-C(2)-C(3)-C(6)            -55.2(3)
C(1)-C(2)-C(3)-C(6)            177.9(2)
C(14)-N(1)-C(7)-O(3)           177.8(2)
C(2)-N(1)-C(7)-O(3)            6.2(4)
C(14)-N(1)-C(7)-C(8)           -2.5(2)
C(2)-N(1)-C(7)-C(8)            -174.03(19)
O(3)-C(7)-C(8)-C(9)            -1.1(4)
N(1)-C(7)-C(8)-C(9)            179.1(2)
O(3)-C(7)-C(8)-C(13)           179.7(2)
N(1)-C(7)-C(8)-C(13)           -0.1(2)
C(13)-C(8)-C(9)-C(10)          -0.7(4)
C(7)-C(8)-C(9)-C(10)           -179.8(2)
C(8)-C(9)-C(10)-C(11)          0.1(4)
C(9)-C(10)-C(11)-C(12)         0.8(4)
C(10)-C(11)-C(12)-C(13)        -1.1(4)
C(11)-C(12)-C(13)-C(8)         0.5(4)
C(11)-C(12)-C(13)-C(14)        177.1(2)
C(9)-C(8)-C(13)-C(12)          0.4(4)
C(7)-C(8)-C(13)-C(12)          179.7(2)
C(9)-C(8)-C(13)-C(14)          -176.9(2)
C(7)-C(8)-C(13)-C(14)          2.4(3)
C(7)-N(1)-C(14)-O(4)           -176.4(2)
C(2)-N(1)-C(14)-O(4)           -4.6(3)
C(7)-N(1)-C(14)-C(13)          3.9(2)
C(2)-N(1)-C(14)-C(13)          175.70(18)
C(12)-C(13)-C(14)-O(4)         -0.5(4)
C(8)-C(13)-C(14)-O(4)          176.5(2)
C(12)-C(13)-C(14)-N(1)         179.2(2)
C(8)-C(13)-C(14)-N(1)          -3.8(2)
Rh(1)-O(5)-C(15)-O(6)          -2.6(3)
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Rh(1)-O(5)-C(15)-C(16)            173.63(13)
Rh(2)-O(6)-C(15)-O(5)                4.0(3)
Rh(2)-O(6)-C(15)-C(16)            -172.12(14)
C(28)-N(2)-C(16)-C(15)            -121.7(2)
C(21)-N(2)-C(16)-C(15)              44.5(3)
C(28)-N(2)-C(16)-C(17)             104.9(2)
C(21)-N(2)-C(16)-C(17)             -88.9(3)
O(5)-C(15)-C(16)-N(2)               41.6(2)
O(6)-C(15)-C(16)-N(2)             -141.81(19)
O(5)-C(15)-C(16)-C(17)            172.63(19)
O(6)-C(15)-C(16)-C(17)             -10.8(3)
N(2)-C(16)-C(17)-C(18)            -169.5(2)
C(15)-C(16)-C(17)-C(18)             62.5(3)
N(2)-C(16)-C(17)-C(20)              66.1(3)
C(15)-C(16)-C(17)-C(20)            -61.9(3)
N(2)-C(16)-C(17)-C(19)             -53.2(3)
C(15)-C(16)-C(17)-C(19)            178.7(2)
C(28)-N(2)-C(21)-O(7)              173.9(2)
C(16)-N(2)-C(21)-O(7)                6.5(4)


C(28)-N(2)-C(21)-C(22)              -6.1(3)
C(16)-N(2)-C(21)-C(22)            -173.5(2)
O(7)-C(21)-C(22)-C(23)               5.3(5)
N(2)-C(21)-C(22)-C(23)            -174.7(3)
O(7)-C(21)-C(22)-C(27)            -177.0(3)
N(2)-C(21)-C(22)-C(27)               3.0(3)
C(27)-C(22)-C(23)-C(24)              0.7(4)
C(21)-C(22)-C(23)-C(24)            178.2(3)
C(22)-C(23)-C(24)-C(25)             -0.2(5)
C(23)-C(24)-C(25)-C(26)              0.0(5)
C(24)-C(25)-C(26)-C(27)             -0.3(5)
C(23)-C(22)-C(27)-C(26)             -1.0(4)
C(21)-C(22)-C(27)-C(26)           -179.0(2)
C(23)-C(22)-C(27)-C(28)            178.9(3)
C(21)-C(22)-C(27)-C(28)              0.9(3)
C(25)-C(26)-C(27)-C(22)              0.8(4)
C(25)-C(26)-C(27)-C(28)           -179.1(3)
C(21)-N(2)-C(28)-O(8)             -173.2(2)
C(16)-N(2)-C(28)-O(8)               -5.2(4)
C(21)-N(2)-C(28)-C(27)               6.6(3)
C(16)-N(2)-C(28)-C(27)            174.64(19)
C(22)-C(27)-C(28)-O(8)            175.3(3)
C(26)-C(27)-C(28)-O(8)              -4.8(5)
C(22)-C(27)-C(28)-N(2)              -4.5(3)
C(26)-C(27)-C(28)-N(2)            175.4(3)
Rh(1)-O(9)-C(29)-O(10)               0.0(3)
Rh(1)-O(9)-C(29)-C(30)            -176.97(14)
Rh(2)-O(10)-C(29)-O(9)               2.0(3)
Rh(2)-O(10)-C(29)-C(30)           179.06(13)
C(42)-N(3)-C(30)-C(29)              69.4(3)
C(35)-N(3)-C(30)-C(29)            -113.6(2)
C(42)-N(3)-C(30)-C(31)             -60.5(3)
C(35)-N(3)-C(30)-C(31)             116.5(2)
O(9)-C(29)-C(30)-N(3)              -35.7(3)
O(10)-C(29)-C(30)-N(3)            146.92(18)
O(9)-C(29)-C(30)-C(31)              96.1(2)
O(10)-C(29)-C(30)-C(31)            -81.2(2)
N(3)-C(30)-C(31)-C(34)             -37.7(3)
C(29)-C(30)-C(31)-C(34)           -167.5(2)
N(3)-C(30)-C(31)-C(32)            -155.0(2)
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C(29)-C(30)-C(31)-C(32)	75.1(3)
N(3)-C(30)-C(31)-C(33)	85.7(3)
C(29)-C(30)-C(31)-C(33)	-44.1(3)
C(42)-N(3)-C(35)-O(12)	178.8(2)
C(30)-N(3)-C(35)-O(12)	1.3(3)
C(42)-N(3)-C(35)-C(36)	0.1(3)
C(30)-N(3)-C(35)-C(36)	-177.44(19)
O(12)-C(35)-C(36)-C(41)	-178.1(3)
N(3)-C(35)-C(36)-C(41)	0.6(3)
O(12)-C(35)-C(36)-C(37)	0.0(5)
N(3)-C(35)-C(36)-C(37)	178.7(3)
C(41)-C(36)-C(37)-C(38)	0.1(4)
C(35)-C(36)-C(37)-C(38)	-177.8(3)
C(36)-C(37)-C(38)-C(39)	0.7(5)
C(37)-C(38)-C(39)-C(40)	-1.0(5)
C(38)-C(39)-C(40)-C(41)	0.4(4)
C(37)-C(36)-C(41)-C(40)	-0.7(4)
C(35)-C(36)-C(41)-C(40)	177.6(2)
C(37)-C(36)-C(41)-C(42)	-179.3(2)
C(35)-C(36)-C(41)-C(42)	-1.0(3)
C(39)-C(40)-C(41)-C(36)	0.5(4)
C(39)-C(40)-C(41)-C(42)	178.7(3)
C(35)-N(3)-C(42)-O(11)	-179.0(2)
C(30)-N(3)-C(42)-O(11)	-1.8(4)
C(35)-N(3)-C(42)-C(41)	-0.7(2)
C(30)-N(3)-C(42)-C(41)	176.5(2)
C(36)-C(41)-C(42)-O(11)	179.4(2)
C(40)-C(41)-C(42)-O(11)	0.9(4)
C(36)-C(41)-C(42)-N(3)	1.0(3)
C(40)-C(41)-C(42)-N(3)	-177.4(3)
Rh(2)-O(14)-C(43)-O(13)	-3.2(3)
Rh(2)-O(14)-C(43)-C(44)	178.68(14)
Rh(1)-O(13)-C(43)-O(14)	2.9(3)
Rh(1)-O(13)-C(43)-C(44)	-178.83(13)
C(56)-N(4)-C(44)-C(43)	49.5(3)
C(49)-N(4)-C(44)-C(43)	-122.8(2)
C(56)-N(4)-C(44)-C(45)	-84.5(3)
C(49)-N(4)-C(44)-C(45)	103.2(3)
O(14)-C(43)-C(44)-N(4)	-118.6(2)
O(13)-C(43)-C(44)-N(4)	63.0(2)
O(14)-C(43)-C(44)-C(45)	12.8(3)
O(13)-C(43)-C(44)-C(45)	-165.56(19)
N(4)-C(44)-C(45)-C(47)	63.5(3)
C(43)-C(44)-C(45)-C(47)	-65.9(3)
N(4)-C(44)-C(45)-C(46)	-174.2(2)
C(43)-C(44)-C(45)-C(46)	56.4(3)
N(4)-C(44)-C(45)-C(48)	-57.4(3)
C(43)-C(44)-C(45)-C(48)	173.2(2)
C(56)-N(4)-C(49)-O(15)	-172.1(3)
C(44)-N(4)-C(49)-O(15)	1.4(4)
C(56)-N(4)-C(49)-C(50)	6.0(3)
C(44)-N(4)-C(49)-C(50)	179.4(2)
O(15)-C(49)-C(50)-C(55)	174.4(3)
N(4)-C(49)-C(50)-C(55)	-3.4(3)
O(15)-C(49)-C(50)-C(51)	-2.6(5)
N(4)-C(49)-C(50)-C(51)	179.6(3)
C(55)-C(50)-C(51)-C(52)	0.3(4)
C(49)-C(50)-C(51)-C(52)	176.9(3)
C(50)-C(51)-C(52)-C(53)	-0.7(5)
C(51)-C(52)-C(53)-C(54)	1.0(5)
C(52)-C(53)-C(54)-C(55)	-0.8(5)

C(51)-C(50)-C(55)-C(54)	-0.1(4)
C(49)-C(50)-C(55)-C(54)	-177.4(2)
C(51)-C(50)-C(55)-C(56)	177.2(2)
C(49)-C(50)-C(55)-C(56)	-0.1(3)
C(53)-C(54)-C(55)-C(50)	0.3(4)
C(53)-C(54)-C(55)-C(56)	-176.3(3)
C(49)-N(4)-C(56)-O(16)	172.8(3)
C(44)-N(4)-C(56)-O(16)	-0.1(4)
C(49)-N(4)-C(56)-C(55)	-6.0(3)
C(44)-N(4)-C(56)-C(55)	-179.0(2)
C(50)-C(55)-C(56)-O(16)	-175.1(3)
C(54)-C(55)-C(56)-O(16)	1.9(5)
C(50)-C(55)-C(56)-N(4)	3.7(3)
C(54)-C(55)-C(56)-N(4)	-179.3(3)
Rh(1)-N(5)-C(57)-C(58)	89(7)
N(5)-C(57)-C(58)-C(63)	155(7)
N(5)-C(57)-C(58)-C(59)	-26(7)
C(63)-C(58)-C(59)-C(60)	-0.6(4)
C(57)-C(58)-C(59)-C(60)	179.9(3)
C(58)-C(59)-C(60)-C(61)	0.4(5)
C(59)-C(60)-C(61)-C(62)	0.0(5)
C(59)-C(60)-C(61)-C(64)	178.2(3)
C(60)-C(61)-C(62)-C(63)	0.0(4)
C(64)-C(61)-C(62)-C(63)	-178.2(2)
C(59)-C(58)-C(63)-C(62)	0.6(4)
C(57)-C(58)-C(63)-C(62)	-180.0(2)
C(61)-C(62)-C(63)-C(58)	-0.3(4)
Rh(2)#2-N(6)-C(64)-C(61)	4(4)
C(60)-C(61)-C(64)-N(6)	-11(4)
C(62)-C(61)-C(64)-N(6)	167(4)
C(70)-C(65)-C(66)-C(67)	0.6(7)
C(65)-C(66)-C(67)-C(68)	-2.2(8)
C(66)-C(67)-C(68)-C(69)	2.3(9)
C(67)-C(68)-C(69)-C(70)	-0.8(9)
C(66)-C(65)-C(70)-C(69)	0.8(6)
C(66)-C(65)-C(70)-C(71)	179.5(4)
C(68)-C(69)-C(70)-C(65)	-0.7(7)
C(68)-C(69)-C(70)-C(71)	-179.3(5)
C(77)-C(72)-C(73)-C(74)	0.4(6)
C(72)-C(73)-C(74)-C(75)	-0.7(6)
C(73)-C(74)-C(75)-C(76)	0.7(5)
C(74)-C(75)-C(76)-C(77)	-0.4(5)
C(73)-C(72)-C(77)-C(76)	-0.1(5)
C(73)-C(72)-C(77)-C(78)	-179.6(3)
C(75)-C(76)-C(77)-C(72)	0.1(4)
C(75)-C(76)-C(77)-C(78)	179.7(3)
C(84)-C(79)-C(80)-C(81)	-0.4(6)
C(79)-C(80)-C(81)-C(82)	-0.5(7)
C(80)-C(81)-C(82)-C(83)	1.8(8)
C(81)-C(82)-C(83)-C(84)	-2.2(9)
C(80)-C(79)-C(84)-C(83)	0.2(7)
C(80)-C(79)-C(84)-C(85)	-179.1(5)
C(82)-C(83)-C(84)-C(79)	1.1(8)
C(82)-C(83)-C(84)-C(85)	-179.6(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x+3/2,-y,z+1/2   #2 -x+3/2,-y,z-1/2