University of Alberta Department of Chemistry
X-Ray Crystallography Laboratory

STRUCTURE REPORT for Compound 7a

Compound: [{(5,10,15,20-tetra-*p*-tolylporphyrinato)Ru(CO)}$_2$(μ–{C_5H_3N-3,5-(C≡CC-{=CMe_2}C≡C-)$_2$}$_2$)] – [({ 5,10,15,20-tetra-*p*-tolylporphyrinato)Ru(CO)-(HOEt)] cocrystallite

Formula: $C_{191}H_{144}N_{14}O_4Ru_3$ ($C_{140}H_{102}N_{10}O_2Ru_2$ + $C_{51}H_{42}N_4O_2Ru$)

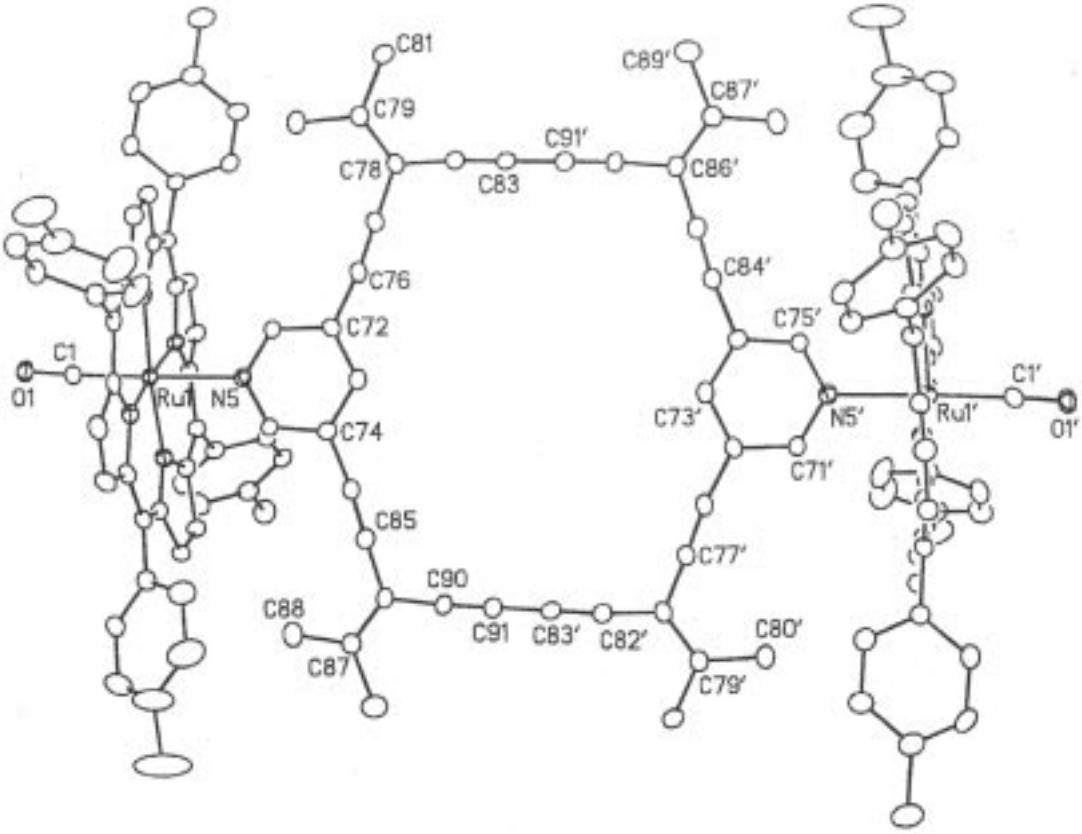


Figure Legends

Figure 1. Perspective view of the [{(5,10,15,20-tetra-*p*-tolylporphyrinato)Ru(CO)}$_2$(μ–{C_5H_3N-3,5-(C≡CC{=CMe_2}C≡C-)$_2$}$_2$)] complex molecule showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 20% probability level. Hydrogen atoms are not shown. Primed atoms are related to unprimed ones via the crystallographic inversion center (0, 0, 0) at the center of the macrocyclic ligand.

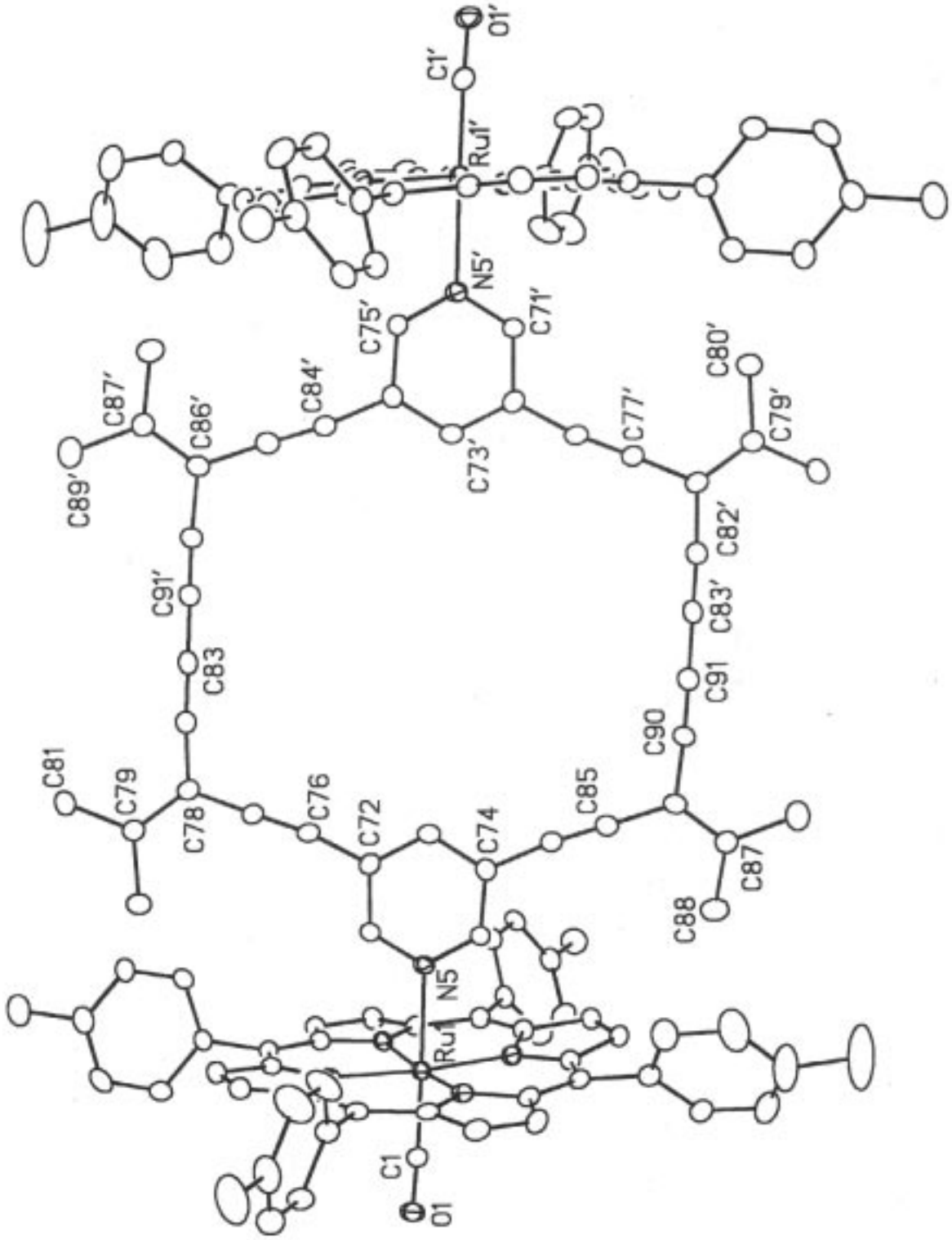
Figure 2. Alternate view of the complex with a closer to side-on view of the macrocycle.

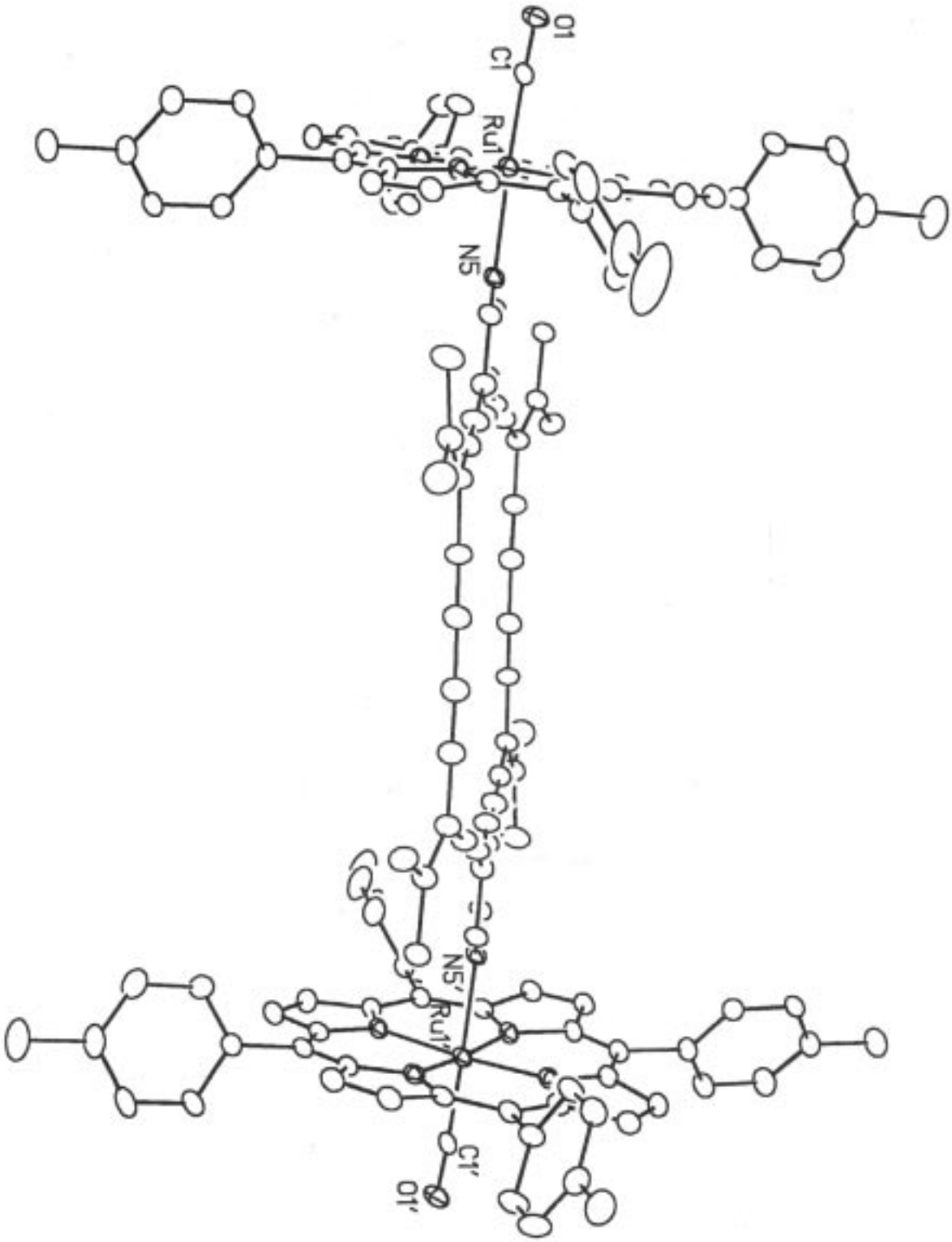
Figure 3. Perspective view of the [({ 5,10,15,20-tetra-*p*-tolylporphyrinato)Ru(CO)(HOEt)] complex molecule. The hydrogen atoms attached to C3 and C4 are shown with arbitarily small thermal parameters; all other hydrogens are not shown. Double-primed atoms are related to unprimed ones via the crystallographic inversion center ($^1/_2$, 0, 0) upon which the Ru2 atom is situated (thus the CO and EtOH ligands are inversion-disordered).

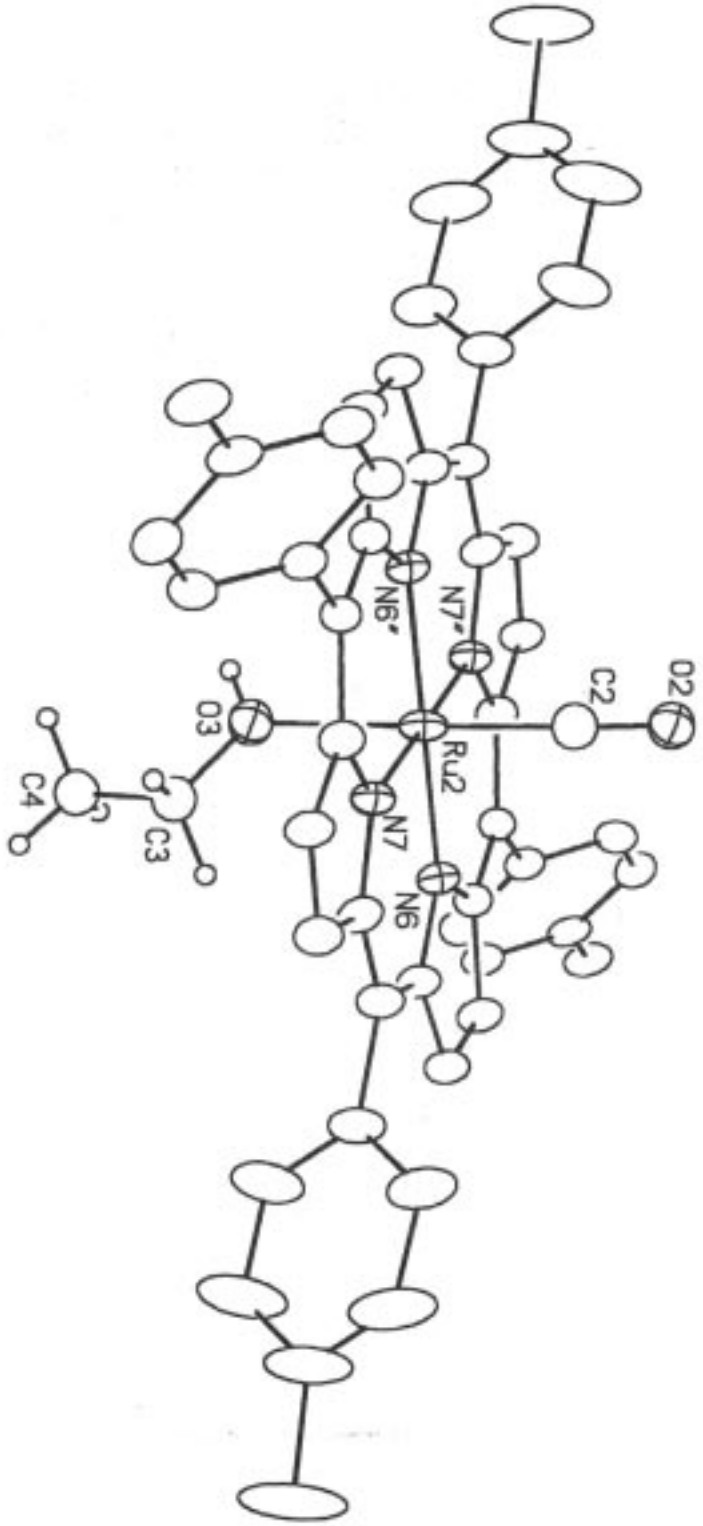
Figure 4. Illustration of the relative positions of adjacent [({5,10,15,20-tetra-*p*-tolyl-porphyrinato)Ru(CO)(HOEt)] and [{(5,10,15,20-tetra-*p*-tolylporphyrinato)Ru-(CO)}$_2$(μ–{C_5H_3N-3,5-(C≡CC{=CMe_2}C≡C-)$_2$}$_2$)] molecules.

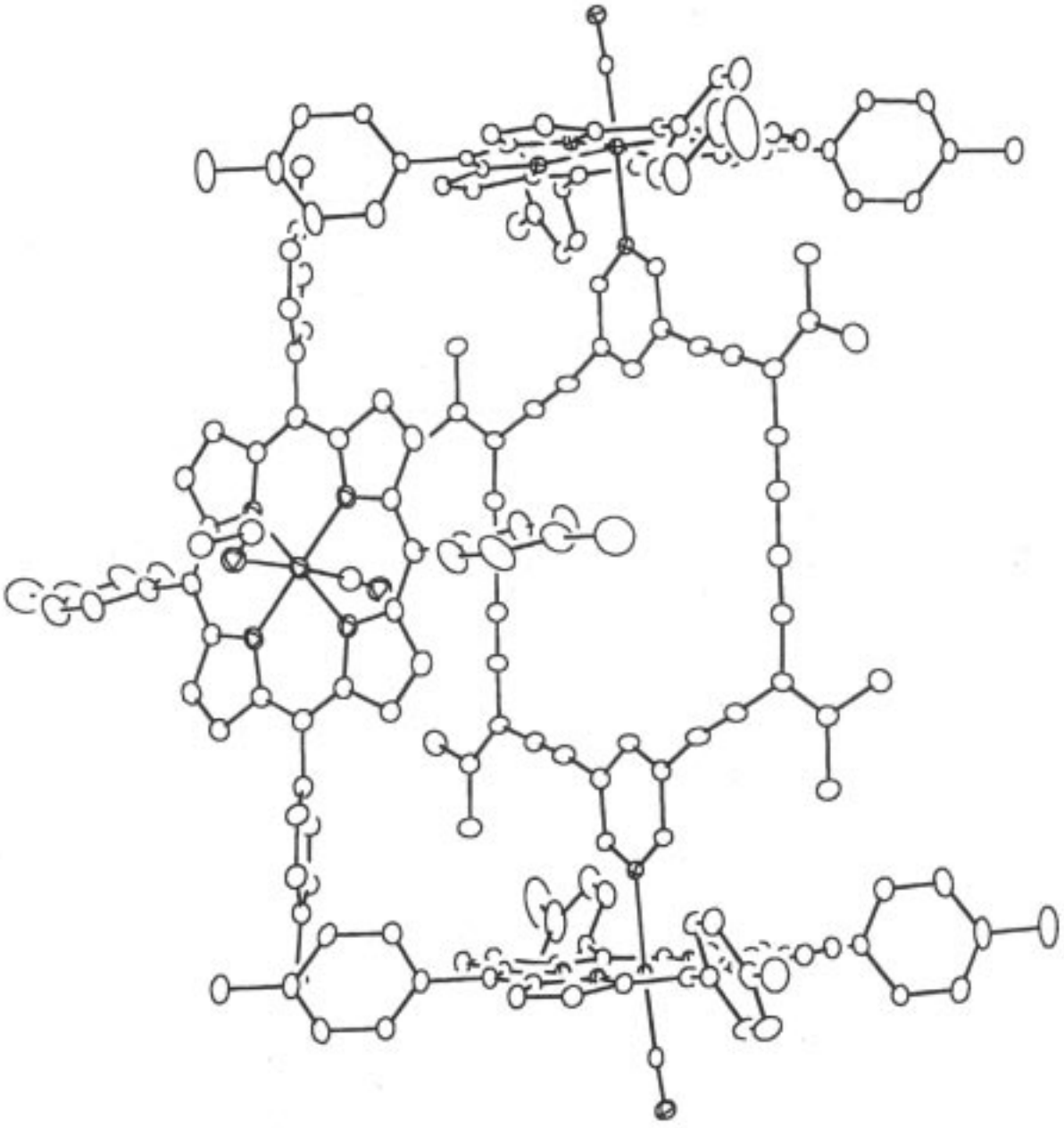
Figure 5. Packing plot with view direction along the crystallographic *b* axis. This view shows the diruthenium-macrocycle complex molecules, omitting the mono-ruthenium-carbonyl-ethanol complex molecules. Note the ‘channels’ through the centers of adjacent macrocycles.

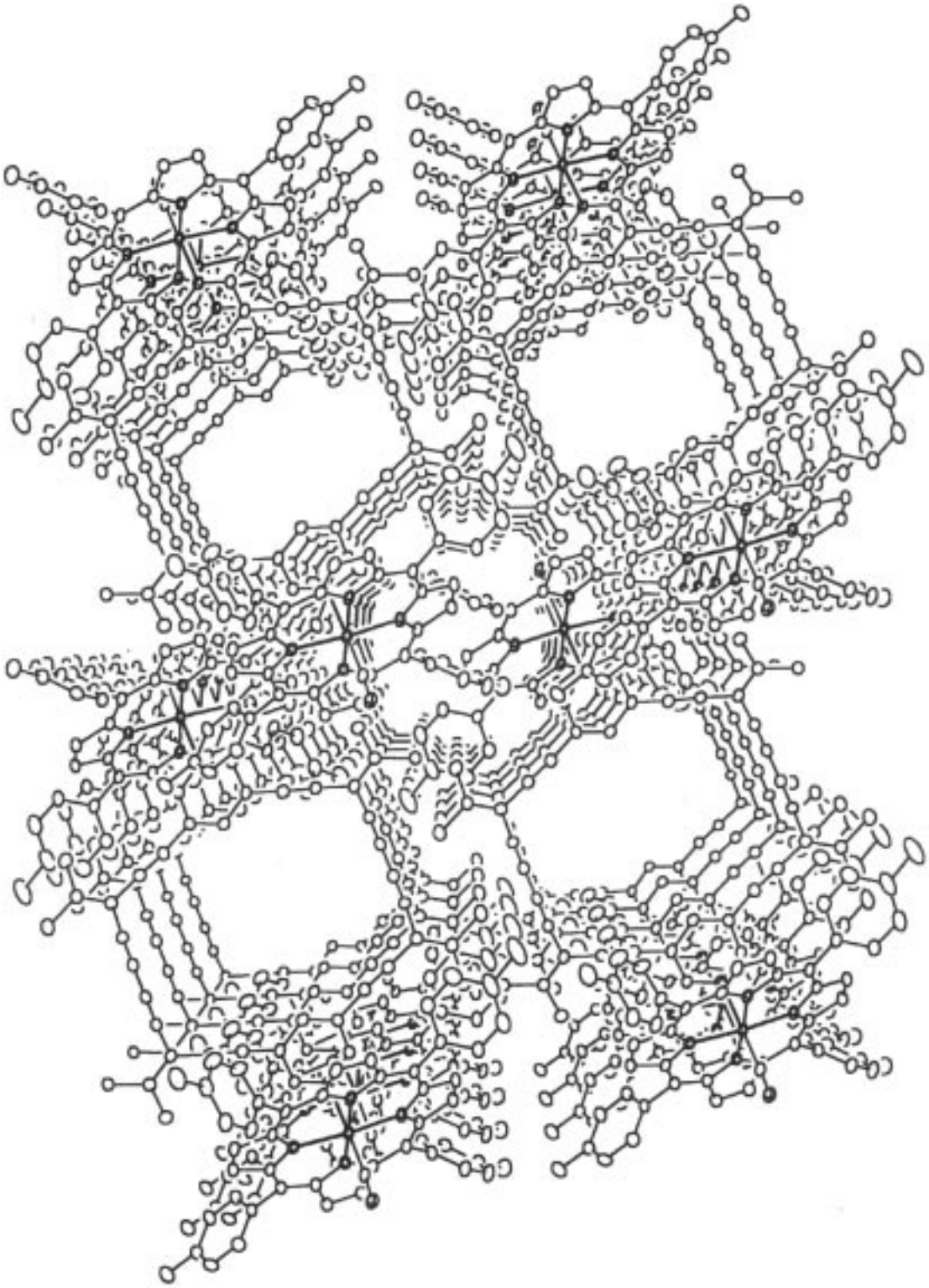
Figure 6. Similar to Figure 5 (packing plot along the *b* axis) but with both types of complex molecules shown. Note that the macrocycle channels are now occupied by *p*-tolyl groups from the monoruthenium complex molecules.

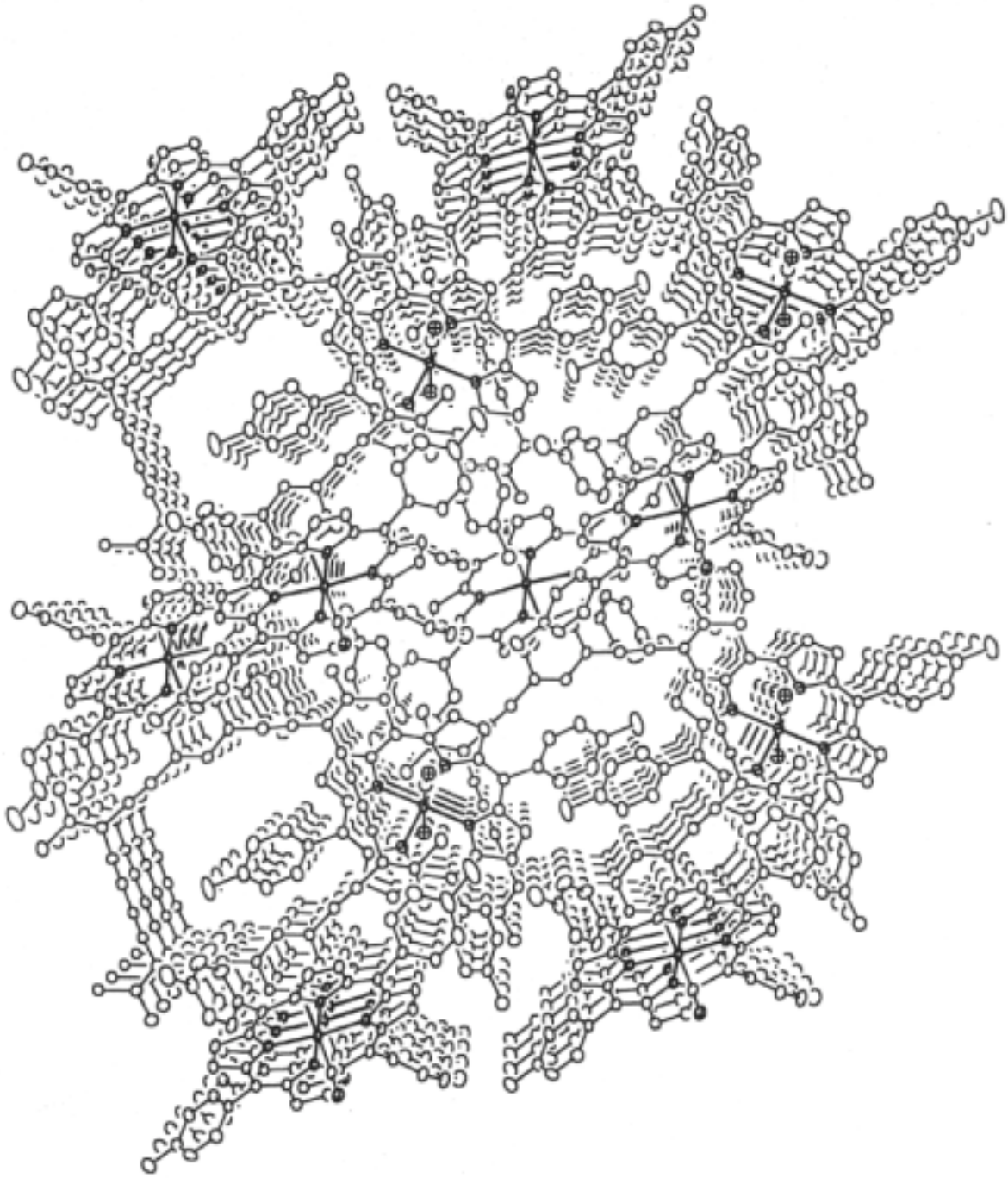

C1'
O1'
Ru1'
N5'
C75'
C71'
C80'
C87'
C84'
C86'
C73'
C77'
C79'
C89'
C82'
C91'
C83'
C83
C91
C90
C81
C79
C78
C76
C72
C74
C85
C87
C88
N5
Ru1
C1
O1


O1
C1
Ru1
N5
N5'
Ru1'
C1'
O1'


N6*
N7*
O3
C2
O2
Ru2
C4
C3
N7
N6







List of Tables

Table 1. Crystallographic Experimental Details

A. Crystal Data	
formula	$C_{191}H_{144}N_{14}O_4Ru_3$
formula weight	3002.41
crystal dimensions (mm)	$0.36 \times 0.35 \times 0.30$
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	16.1421 (11)
b (Å)	17.1025 (11)
c (Å)	17.5359 (12)
α (deg)	90.3641 (14)
β (deg)	100.8011 (13)
γ (deg)	114.5012 (14)
V (Å^3)	4308.0 (5)
Z	1
ρ_{calcd} (g cm^{-3})	1.157
μ (mm^{-1})	0.316
B. Data Collection and Refinement Conditions	
diffractometer	Bruker P4/RA/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ϕ rotations (0.3°) / ω scans (0.3°) (30 s exposures)
data collection 2θ limit (deg)	53.00
total data collected	22653 ($-15 \le h \le 20$, $-19 \le k \le 21$, $-21 \le l \le 17$)
independent reflections	17506
number of observations (*NO*)	10363 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–86*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.9180–0.8460
data/restraints/parameters	17506 [$F_o^2 \ge -3\sigma(F_o^2)$] / 6[e] / 960
goodness-of-fit (S)[f]	1.055 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[g]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0887
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.2941
largest difference peak and hole	1.212 and –1.212 e Å^{-3}

[a]Obtained from least-squares refinement of 8192 centered reflections.

(continued)

Table 1. Crystallographic Experimental Details (continued)

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

[c]Sheldrick, G. M. *Acta Crystallogr.* **1990**, *A46*, 467–473.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted *R*-factors wR_2 and all goodnesses of fit *S* are based on F_o^2; conventional *R*-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. *R*-factors based on F_o^2 are statistically about twice as large as those based on F_o, and *R*-factors based on ALL data will be even larger.

[e]An idealized geometry was imposed as follows upon the inversion-disordered CO and EtOH groups attached to Ru2: d(Ru2–C2) = 1.85 Å; d(O2–C2) = 1.15 Å; d(Ru2···O2) = 3.00 Å; d(Ru2–O3) = 2.22 Å; d(O3–C3) = 1.40 Å; d(C3–C4) = 1.50 Å.

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.1854P)^2]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[g]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters

(a) atoms of [{(5,10,15,20-tetra-p-tolylporphyrinato)Ru(CO)}$_2$(μ–{C_5H_3N-3,5-(C≡CC{=CMe_2}-C≡C-)$_2$}$_2$)]

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Ru1	0.22042(3)	0.34612(3)	0.45606(3)	0.03779(18)*
O1	0.2805(3)	0.4735(3)	0.5949(3)	0.0570(12)*
N1	0.2094(3)	0.2447(3)	0.5214(3)	0.0405(11)*
N2	0.0841(3)	0.3208(3)	0.4567(3)	0.0417(12)*
N3	0.2277(3)	0.4409(3)	0.3815(3)	0.0403(11)*
N4	0.3521(3)	0.3633(3)	0.4464(3)	0.0416(12)*
N5	0.1686(3)	0.2535(3)	0.3505(3)	0.0408(11)*
C1	0.2602(4)	0.4249(4)	0.5420(4)	0.0420(14)*
C11	0.2775(4)	0.2170(4)	0.5460(4)	0.0417(14)*
C12	0.2476(4)	0.1534(4)	0.6002(4)	0.0478(15)*
C13	0.1613(4)	0.1412(4)	0.6060(4)	0.0472(15)*
C14	0.1355(4)	0.1977(4)	0.5550(4)	0.0446(15)*
C15	0.0500(4)	0.2021(4)	0.5420(4)	0.0433(14)*
C16	0.0250(4)	0.2577(4)	0.4949(4)	0.0421(14)*
C17	-0.0647(4)	0.2598(4)	0.4762(4)	0.0496(16)*
C18	-0.0592(4)	0.3219(4)	0.4302(4)	0.0505(16)*
C19	0.0348(4)	0.3628(4)	0.4182(4)	0.0406(14)*
C20	0.0695(4)	0.4324(4)	0.3746(4)	0.0438(15)*
C21	0.1597(4)	0.4689(4)	0.3587(4)	0.0425(14)*
C22	0.1950(4)	0.5407(4)	0.3121(4)	0.0536(17)*
C23	0.2795(4)	0.5526(4)	0.3089(4)	0.0490(16)*
C24	0.3017(4)	0.4901(4)	0.3501(4)	0.0428(14)*
C25	0.3850(4)	0.4789(4)	0.3578(4)	0.0418(14)*
C26	0.4074(4)	0.4201(4)	0.4018(4)	0.0437(14)*
C27	0.4876(4)	0.4020(4)	0.4027(4)	0.0451(15)*
C28	0.4807(4)	0.3377(4)	0.4456(4)	0.0464(15)*
C29	0.3950(4)	0.3105(4)	0.4749(4)	0.0422(14)*
C30	0.3626(4)	0.2453(4)	0.5214(4)	0.0440(14)*
C31	-0.0254(4)	0.1385(4)	0.5774(4)	0.0478(16)*
C32	-0.0674(4)	0.0515(4)	0.5498(4)	0.0525(17)*
C33	-0.1360(5)	-0.0072(5)	0.5823(4)	0.0564(18)*
C34	-0.1667(5)	0.0176(5)	0.6431(4)	0.0585(19)*
C35	-0.1276(6)	0.1040(6)	0.6690(4)	0.071(2)*
C36	-0.0566(5)	0.1642(5)	0.6374(4)	0.064(2)*
C37	-0.2440(6)	-0.0458(6)	0.6776(5)	0.078(2)*
C41	0.0051(4)	0.4717(4)	0.3402(4)	0.0493(16)*
C42	-0.0423(6)	0.4518(7)	0.2646(5)	0.086(3)*

Table 2. Atomic Coordinates and Displacement Parameters (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C43	-0.1024(7)	0.4868(8)	0.2336(6)	0.108(4)*
C44	-0.1158(6)	0.5462(6)	0.2792(6)	0.078(3)*
C45	-0.0690(5)	0.5661(5)	0.3558(5)	0.065(2)*
C46	-0.0092(4)	0.5297(4)	0.3857(5)	0.0582(18)*
C47	-0.1818(7)	0.5872(8)	0.2455(7)	0.119(4)*
C51	0.4509(4)	0.5295(4)	0.3081(4)	0.0468(15)*
C52	0.4197(6)	0.5239(6)	0.2287(5)	0.070(2)*
C53	0.4817(7)	0.5711(8)	0.1811(6)	0.103(4)*
C54	0.5757(7)	0.6239(8)	0.2152(8)	0.113(4)*
C55	0.6055(6)	0.6280(5)	0.2958(6)	0.076(3)*
C56	0.5441(4)	0.5824(4)	0.3400(5)	0.0535(17)*
C57	0.6398(9)	0.6697(11)	0.1583(9)	0.186(9)*
C61	0.4264(4)	0.2018(4)	0.5513(4)	0.0464(15)*
C62	0.4008(4)	0.1157(4)	0.5285(4)	0.0483(15)*
C63	0.4599(5)	0.0765(4)	0.5535(4)	0.0493(16)*
C64	0.5462(5)	0.1242(5)	0.6031(4)	0.0545(17)*
C65	0.5711(5)	0.2093(5)	0.6236(5)	0.063(2)*
C66	0.5107(4)	0.2480(5)	0.5981(4)	0.0551(17)*
C67	0.6118(6)	0.0823(6)	0.6328(5)	0.076(2)*
C71	0.0836(4)	0.1922(4)	0.3362(4)	0.0442(14)*
C72	0.0461(4)	0.1341(4)	0.2674(4)	0.0474(15)*
C73	0.1026(4)	0.1451(4)	0.2147(4)	0.0534(17)*
C74	0.1918(4)	0.2096(4)	0.2303(4)	0.0502(16)*
C75	0.2210(4)	0.2626(4)	0.2990(4)	0.0434(14)*
C76	-0.0488(5)	0.0749(4)	0.2527(4)	0.0548(17)*
C77	-0.1320(4)	0.0320(4)	0.2449(4)	0.0487(15)*
C78	-0.2300(4)	-0.0171(4)	0.2310(4)	0.0498(16)*
C79	-0.2825(5)	-0.0054(4)	0.2783(4)	0.0496(16)*
C80	-0.2385(5)	0.0591(4)	0.3491(4)	0.0548(17)*
C81	-0.3865(4)	-0.0566(5)	0.2599(4)	0.0568(18)*
C82	-0.2694(4)	-0.0735(5)	0.1619(4)	0.0518(16)*
C83	-0.2978(4)	-0.1192(5)	0.1017(4)	0.0532(17)*
C84	0.2586(5)	0.2238(4)	0.1811(4)	0.0546(18)*
C85	0.3186(5)	0.2419(4)	0.1467(4)	0.0514(16)*
C86	0.3906(5)	0.2623(4)	0.1028(4)	0.0515(16)*
C87	0.4797(5)	0.3198(4)	0.1310(4)	0.0530(16)*
C88	0.5098(5)	0.3663(5)	0.2101(5)	0.074(2)*
C89	0.5529(6)	0.3384(6)	0.0815(5)	0.079(3)*
C90	0.3600(4)	0.2129(4)	0.0280(4)	0.0495(16)*
C91	0.3317(5)	0.1702(5)	-0.0317(4)	0.0545(17)*

Table 2. Atomic Coordinates and Displacement Parameters (continued)

(b) atoms of [({ 5,10,15,20-tetra-p-tolylporphyrinato)Ru(CO)(HOEt)]

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Ru2	0.5000	0.0000	0.0000	0.0551(3)*
O2[a]	0.5136(8)	0.1613(4)	-0.0742(6)	0.0717(16)
O3[a]	0.5016(8)	-0.1114(5)	0.0634(7)	0.0717(16)
N6	0.4415(4)	0.0307(4)	0.0825(3)	0.0531(14)*
N7	0.3700(4)	-0.0780(4)	-0.0653(3)	0.0521(14)*
C2[a]	0.5055(13)	0.0975(6)	-0.0482(11)	0.0717(16)
C3[a]	0.4166(8)	-0.1791(8)	0.0683(9)	0.0717(16)
C4[a]	0.4384(12)	-0.2344(10)	0.1275(9)	0.0717(16)
C101	0.4871(5)	0.0873(5)	0.1497(4)	0.0502(16)*
C102	0.4185(5)	0.0951(5)	0.1872(4)	0.0598(19)*
C103	0.3326(5)	0.0417(5)	0.1441(4)	0.0626(19)*
C104	0.3470(4)	0.0008(5)	0.0800(4)	0.0541(17)*
C105	0.2755(5)	-0.0579(5)	0.0219(4)	0.0588(19)*
C106	0.2875(5)	-0.0928(5)	-0.0456(4)	0.0567(17)*
C107	0.2120(5)	-0.1528(5)	-0.1068(4)	0.0623(19)*
C108	0.2492(5)	-0.1709(5)	-0.1618(4)	0.0589(18)*
C109	0.3506(5)	-0.1260(5)	-0.1356(4)	0.0544(17)*
C110	0.4172(5)	-0.1299(4)	-0.1753(4)	0.0515(16)*
C111	0.1789(5)	-0.0849(6)	0.0343(5)	0.071(2)*
C112	0.1162(7)	-0.0610(8)	-0.0100(6)	0.100(3)*
C113	0.0268(7)	-0.0897(10)	0.0062(8)	0.135(5)*
C114	0.0006(7)	-0.1351(10)	0.0670(8)	0.131(5)*
C115	0.0631(7)	-0.1621(11)	0.1097(7)	0.141(6)*
C116	0.1491(6)	-0.1367(8)	0.0934(6)	0.108(4)*
C117	-0.0964(8)	-0.1549(12)	0.0833(10)	0.207(9)*
C121	0.3817(5)	-0.1848(5)	-0.2527(4)	0.0534(17)*
C122	0.4084(5)	-0.1508(5)	-0.3197(4)	0.0613(19)*
C123	0.3742(5)	-0.1996(5)	-0.3907(5)	0.066(2)*
C124	0.3123(5)	-0.2852(5)	-0.3991(4)	0.0587(19)*
C125	0.2868(5)	-0.3204(5)	-0.3309(5)	0.0628(19)*
C126	0.3199(5)	-0.2723(5)	-0.2607(4)	0.0591(18)*
C127	0.2707(6)	-0.3371(6)	-0.4777(5)	0.076(2)*

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$. [a]Atoms of the inversion-disordered CO and EtOH groups attached to Ru2 were refined with an occupancy factor of 0.5 and a common isotropic displacement parameter.

Table 3. Selected Interatomic Distances (Å)

(a) within [{(5,10,15,20-tetra-p-tolylporphyrinato)Ru(CO)}$_2$(μ–{C_5H_3N-3,5-(C≡CC{=CMe_2}-C≡C)$_2$}$_2$)]

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Ru1	N1	2.049(5)	C28	C29	1.460(8)
Ru1	N2	2.061(5)	C29	C30	1.367(9)
Ru1	N3	2.069(5)	C30	C61	1.526(8)
Ru1	N4	2.062(5)	C31	C32	1.393(9)
Ru1	N5	2.218(5)	C31	C36	1.388(9)
Ru1	C1	1.841(6)	C32	C33	1.371(9)
O1	C1	1.144(7)	C33	C34	1.389(10)
N1	C11	1.371(7)	C34	C35	1.378(11)
N1	C14	1.374(7)	C34	C37	1.506(10)
N2	C16	1.385(8)	C35	C36	1.395(10)
N2	C19	1.373(8)	C41	C42	1.362(10)
N3	C21	1.368(8)	C41	C46	1.387(9)
N3	C24	1.362(7)	C42	C43	1.373(11)
N4	C26	1.380(8)	C43	C44	1.397(13)
N4	C29	1.391(7)	C44	C45	1.376(12)
N5	C71	1.312(7)	C44	C47	1.538(11)
N5	C75	1.316(7)	C45	C46	1.380(10)
C11	C12	1.438(8)	C51	C52	1.379(10)
C11	C30	1.407(8)	C51	C56	1.394(9)
C12	C13	1.344(8)	C52	C53	1.415(11)
C13	C14	1.453(9)	C53	C54	1.411(15)
C14	C15	1.390(8)	C54	C55	1.395(15)
C15	C16	1.397(9)	C54	C57	1.551(13)
C15	C31	1.498(8)	C55	C56	1.358(10)
C16	C17	1.439(8)	C61	C62	1.387(9)
C17	C18	1.322(9)	C61	C66	1.354(9)
C18	C19	1.440(8)	C62	C63	1.389(9)
C19	C20	1.391(9)	C63	C64	1.399(10)
C20	C21	1.411(8)	C64	C65	1.365(10)
C20	C41	1.498(9)	C64	C67	1.526(10)
C21	C22	1.450(9)	C65	C66	1.401(9)
C22	C23	1.306(9)	C71	C72	1.421(8)
C23	C24	1.422(9)	C72	C73	1.376(9)
C24	C25	1.416(8)	C72	C76	1.414(9)
C25	C26	1.394(9)	C73	C74	1.377(9)
C25	C51	1.495(8)	C74	C75	1.384(9)
C26	C27	1.447(8)			
C27	C28	1.315(9)			

Table 3. Selected Interatomic Distances (continued)

Atom1	Atom2	Distance	Atom1	Atom2	Distance
C74	C84	1.448(9)	C83	C91’	1.380(9)
C76	C77	1.214(9)	C84	C85	1.171(9)
C77	C78	1.420(8)	C85	C86	1.438(9)
C78	C79	1.361(9)	C86	C87	1.354(9)
C78	C82	1.411(9)	C86	C90	1.441(8)
C79	C80	1.504(9)	C87	C88	1.484(10)
C79	C81	1.504(9)	C87	C89	1.525(10)
C82	C83	1.203(9)	C90	C91	1.172(9)

Primed atoms are related to unprimed ones via the inversion center (0, 0, 0).

(b) within [({ 5,10,15,20-tetra-p-tolylporphyrinato)Ru(CO)(HOEt)]

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Ru2	O3	2.22†	C107	C108	1.325(10)
Ru2	N6	2.042(5)	C108	C109	1.466(9)
Ru2	N7	2.062(5)	C109	C110	1.409(9)
Ru2	C2	1.85†	C110	C121	1.517(10)
O2	C2	1.15†	C111	C112	1.359(12)
O3	C3	1.40†	C111	C116	1.391(13)
N6	C101	1.392(9)	C112	C113	1.405(13)
N6	C104	1.385(8)	C113	C114	1.351(17)
N7	C106	1.361(8)	C114	C115	1.378(19)
N7	C109	1.386(9)	C114	C117	1.542(13)
C3	C4	1.50†	C115	C116	1.359(12)
C101	C102	1.439(9)	C121	C122	1.375(9)
C101	C110”	1.387(9)	C121	C126	1.400(10)
C102	C103	1.370(10)	C122	C123	1.378(10)
C103	C104	1.424(10)	C123	C124	1.377(11)
C104	C105	1.401(10)	C124	C125	1.396(11)
C105	C106	1.403(10)	C124	C127	1.511(10)
C105	C111	1.492(9)	C125	C126	1.361(10)
C106	C107	1.465(10)			

Double-primed atoms are related to unprimed ones via the inversion center ($^1/_2$, 0, 0).

†Distance fixed during refinement.

Table 4. Selected Interatomic Angles (deg)

(a) within [{(5,10,15,20-tetra-p-tolylporphyrinato)Ru(CO)}$_2$(μ–{C_5H_3N-3,5-(C≡CC{=CMe_2}-C≡C)$_2$}$_2$)]

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
N1	Ru1	N2	89.77(19)	N1	C14	C13	108.4(5)
N1	Ru1	N3	174.93(18)	N1	C14	C15	126.2(6)
N1	Ru1	N4	89.97(19)	C13	C14	C15	125.3(6)
N1	Ru1	N5	87.89(19)	C14	C15	C16	126.1(6)
N1	Ru1	C1	93.7(2)	C14	C15	C31	118.1(6)
N2	Ru1	N3	90.25(19)	C16	C15	C31	115.7(5)
N2	Ru1	N4	174.65(19)	N2	C16	C15	124.9(5)
N2	Ru1	N5	88.21(18)	N2	C16	C17	107.8(6)
N2	Ru1	C1	90.2(2)	C15	C16	C17	127.3(6)
N3	Ru1	N4	89.54(19)	C16	C17	C18	108.4(6)
N3	Ru1	N5	87.04(19)	C17	C18	C19	108.1(6)
N3	Ru1	C1	91.3(2)	N2	C19	C18	108.3(6)
N4	Ru1	N5	86.44(18)	N2	C19	C20	125.8(5)
N4	Ru1	C1	95.2(2)	C18	C19	C20	125.9(6)
N5	Ru1	C1	177.7(2)	C19	C20	C21	126.0(6)
Ru1	N1	C11	126.3(4)	C19	C20	C41	117.4(5)
Ru1	N1	C14	125.9(4)	C21	C20	C41	116.7(6)
C11	N1	C14	107.4(5)	N3	C21	C20	126.2(6)
Ru1	N2	C16	126.5(4)	N3	C21	C22	108.1(5)
Ru1	N2	C19	126.2(4)	C20	C21	C22	125.7(6)
C16	N2	C19	107.4(5)	C21	C22	C23	106.7(6)
Ru1	N3	C21	125.3(4)	C22	C23	C24	109.7(6)
Ru1	N3	C24	127.1(4)	N3	C24	C23	107.9(5)
C21	N3	C24	107.6(5)	N3	C24	C25	124.8(6)
Ru1	N4	C26	126.5(4)	C23	C24	C25	127.2(6)
Ru1	N4	C29	125.2(4)	C24	C25	C26	126.4(5)
C26	N4	C29	107.8(5)	C24	C25	C51	116.4(6)
Ru1	N5	C71	120.5(4)	C26	C25	C51	117.0(5)
Ru1	N5	C75	120.3(4)	N4	C26	C25	125.5(5)
C71	N5	C75	119.1(5)	N4	C26	C27	108.1(6)
Ru1	C1	O1	176.6(5)	C25	C26	C27	126.2(6)
N1	C11	C12	109.1(5)	C26	C27	C28	108.6(5)
N1	C11	C30	125.4(6)	C27	C28	C29	108.5(5)
C12	C11	C30	125.5(6)	N4	C29	C28	107.1(5)
C11	C12	C13	107.7(6)	N4	C29	C30	126.4(5)
C12	C13	C14	107.3(5)	C28	C29	C30	126.5(5)

Table 4. Selected Interatomic Angles (continued)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C11	C30	C29	125.9(6)	C61	C62	C63	121.0(6)
C11	C30	C61	117.4(6)	C62	C63	C64	119.6(6)
C29	C30	C61	116.6(5)	C63	C64	C65	118.5(6)
C15	C31	C32	120.4(6)	C63	C64	C67	120.8(7)
C15	C31	C36	121.5(6)	C65	C64	C67	120.7(7)
C32	C31	C36	118.1(6)	C64	C65	C66	121.2(7)
C31	C32	C33	120.8(6)	C61	C66	C65	120.5(7)
C32	C33	C34	121.7(7)	N5	C71	C72	122.3(5)
C33	C34	C35	117.9(6)	C71	C72	C73	117.3(6)
C33	C34	C37	122.1(8)	C71	C72	C76	118.9(6)
C35	C34	C37	119.9(7)	C73	C72	C76	123.4(6)
C34	C35	C36	121.1(7)	C72	C73	C74	120.0(6)
C31	C36	C35	120.5(7)	C73	C74	C75	117.8(6)
C20	C41	C42	122.4(6)	C73	C74	C84	124.6(6)
C20	C41	C46	120.3(6)	C75	C74	C84	117.6(6)
C42	C41	C46	117.4(7)	N5	C75	C74	123.5(6)
C41	C42	C43	122.2(8)	C72	C76	C77	171.8(7)
C42	C43	C44	120.4(9)	C76	C77	C78	176.5(7)
C43	C44	C45	117.9(7)	C77	C78	C79	121.8(6)
C43	C44	C47	121.3(10)	C77	C78	C82	115.5(6)
C45	C44	C47	120.8(9)	C79	C78	C82	122.5(6)
C44	C45	C46	120.6(8)	C78	C79	C80	121.1(6)
C41	C46	C45	121.5(7)	C78	C79	C81	120.1(6)
C25	C51	C52	119.7(6)	C80	C79	C81	118.8(6)
C25	C51	C56	121.7(6)	C78	C82	C83	176.0(7)
C52	C51	C56	118.6(6)	C82	C83	C91’	178.2(9)
C51	C52	C53	120.1(8)	C74	C84	C85	173.4(7)
C52	C53	C54	119.8(10)	C84	C85	C86	178.5(8)
C53	C54	C55	118.9(8)	C85	C86	C87	122.9(6)
C53	C54	C57	116.3(12)	C85	C86	C90	113.7(6)
C55	C54	C57	124.8(11)	C87	C86	C90	123.4(6)
C54	C55	C56	120.0(8)	C86	C87	C88	121.9(6)
C51	C56	C55	122.6(8)	C86	C87	C89	120.3(6)
C30	C61	C62	120.8(6)	C88	C87	C89	117.8(6)
C30	C61	C66	120.2(6)	C86	C90	C91	177.0(7)
C62	C61	C66	119.0(6)	C83’	C91	C90	179.5(9)

Primed atoms are related to unprimed ones via the inversion center (0, 0, 0).

Table 4. Selected Interatomic Angles (continued)

(b) within [({ 5,10,15,20-tetra-p-tolylporphyrinato)Ru(CO)(HOEt)]

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
O3	Ru2	N6	89.5(4)	C106	C105	C111	118.2(7)
O3	Ru2	N6”	90.5(4)	N7	C106	C105	126.4(7)
O3	Ru2	N7	89.9(3)	N7	C106	C107	108.4(6)
O3	Ru2	N7”	90.1(3)	C105	C106	C107	125.2(6)
O3	Ru2	C2	176.3(7)	C106	C107	C108	108.4(6)
N6	Ru2	N6”	180.0	C107	C108	C109	107.1(7)
N6	Ru2	N7	90.8(2)	N7	C109	C108	108.4(6)
N6	Ru2	N7”	89.2(2)	N7	C109	C110	125.6(6)
N6	Ru2	C2	89.7(7)	C108	C109	C110	126.0(7)
N6”	Ru2	C2	90.3(7)	C101”	C110	C109	125.5(7)
N7	Ru2	N7”	180.0	C101”	C110	C121	117.0(6)
N7	Ru2	C2	93.7(5)	C109	C110	C121	117.5(6)
N7”	Ru2	C2	86.3(5)	C105	C111	C112	122.9(8)
Ru2	O3	C3	118.6(7)	C105	C111	C116	120.3(8)
Ru2	N6	C101	127.6(4)	C112	C111	C116	116.8(8)
Ru2	N6	C104	125.7(5)	C111	C112	C113	118.7(10)
C101	N6	C104	106.6(5)	C112	C113	C114	124.0(11)
Ru2	N7	C106	125.6(5)	C113	C114	C115	116.8(10)
Ru2	N7	C109	126.7(4)	C113	C114	C117	118.9(14)
C106	N7	C109	107.7(6)	C115	C114	C117	124.3(14)
Ru2	C2	O2	175.5(14)	C114	C115	C116	119.7(13)
O3	C3	C4	106.6(9)	C111	C116	C115	123.8(11)
N6	C101	C102	108.8(6)	C110	C121	C122	121.5(6)
N6	C101	C110”	125.3(6)	C110	C121	C126	122.5(6)
C102	C101	C110”	125.9(7)	C122	C121	C126	116.1(7)
C101	C102	C103	107.4(6)	C121	C122	C123	121.8(7)
C102	C103	C104	107.4(6)	C122	C123	C124	122.3(7)
N6	C104	C103	109.7(6)	C123	C124	C125	115.9(7)
N6	C104	C105	125.8(6)	C123	C124	C127	122.2(7)
C103	C104	C105	124.5(6)	C125	C124	C127	121.8(7)
C104	C105	C106	125.7(6)	C124	C125	C126	121.9(7)
C104	C105	C111	116.1(6)	C121	C126	C125	121.9(7)

Double-primed atoms are related to unprimed ones via the inversion center ($^1/_2$, 0, 0).

Table 5. Torsional Angles (deg)

(a) within [{(5,10,15,20-tetra-p-tolylporphyrinato)Ru(CO)}$_2$(μ–{C_5H_3N-3,5-(C≡CC{=CMe_2}-C≡C)$_2$}$_2$)]

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
N2	Ru1	N1	C11	178.9(5)	C1	Ru1	N4	C26	-92.1(5)
N2	Ru1	N1	C14	-8.2(5)	C1	Ru1	N4	C29	97.8(5)
N3	Ru1	N1	C11	89(2)	N1	Ru1	N5	C71	65.7(5)
N3	Ru1	N1	C14	-98(2)	N1	Ru1	N5	C75	-118.4(5)
N4	Ru1	N1	C11	4.2(5)	N2	Ru1	N5	C71	-24.1(5)
N4	Ru1	N1	C14	177.2(5)	N2	Ru1	N5	C75	151.8(5)
N5	Ru1	N1	C11	90.7(5)	N3	Ru1	N5	C71	-114.5(5)
N5	Ru1	N1	C14	-96.4(5)	N3	Ru1	N5	C75	61.4(5)
C1	Ru1	N1	C11	-90.9(5)	N4	Ru1	N5	C71	155.8(5)
C1	Ru1	N1	C14	82.0(5)	N4	Ru1	N5	C75	-28.3(5)
N1	Ru1	N2	C16	2.6(5)	C1	Ru1	N5	C71	-70(6)
N1	Ru1	N2	C19	-176.4(5)	C1	Ru1	N5	C75	106(6)
N3	Ru1	N2	C16	177.5(5)	N1	Ru1	C1	O1	-99(10)
N3	Ru1	N2	C19	-1.4(5)	N2	Ru1	C1	O1	-9(10)
N4	Ru1	N2	C16	90(2)	N3	Ru1	C1	O1	81(10)
N4	Ru1	N2	C19	-89(2)	N4	Ru1	C1	O1	170(10)
N5	Ru1	N2	C16	90.5(5)	N5	Ru1	C1	O1	36(14)
N5	Ru1	N2	C19	-88.5(5)	Ru1	N1	C11	C12	171.0(4)
C1	Ru1	N2	C16	-91.1(5)	Ru1	N1	C11	C30	-9.8(9)
C1	Ru1	N2	C19	89.9(5)	C14	N1	C11	C12	-3.0(7)
N1	Ru1	N3	C21	96(2)	C14	N1	C11	C30	176.1(6)
N1	Ru1	N3	C24	-88(2)	Ru1	N1	C14	C13	-171.1(4)
N2	Ru1	N3	C21	6.2(5)	Ru1	N1	C14	C15	9.7(9)
N2	Ru1	N3	C24	-178.1(5)	C11	N1	C14	C13	3.0(7)
N4	Ru1	N3	C21	-179.1(5)	C11	N1	C14	C15	-176.2(6)
N4	Ru1	N3	C24	-3.5(5)	Ru1	N2	C16	C15	2.3(8)
N5	Ru1	N3	C21	94.4(5)	Ru1	N2	C16	C17	-177.0(4)
N5	Ru1	N3	C24	-89.9(5)	C19	N2	C16	C15	-178.6(5)
C1	Ru1	N3	C21	-84.0(5)	C19	N2	C16	C17	2.1(6)
C1	Ru1	N3	C24	91.7(5)	Ru1	N2	C19	C18	176.6(4)
N1	Ru1	N4	C26	174.1(5)	Ru1	N2	C19	C20	-2.8(8)
N1	Ru1	N4	C29	4.0(5)	C16	N2	C19	C18	-2.6(6)
N2	Ru1	N4	C26	87(2)	C16	N2	C19	C20	178.0(5)
N2	Ru1	N4	C29	-83(2)	Ru1	N3	C21	C20	-7.5(8)
N3	Ru1	N4	C26	-0.8(5)	Ru1	N3	C21	C22	175.0(4)
N3	Ru1	N4	C29	-170.9(5)	C24	N3	C21	C20	176.1(6)
N5	Ru1	N4	C26	86.2(5)					
N5	Ru1	N4	C29	-83.9(5)					

Table 5. Torsional Angles (continued)

Atom1	Atom2	Atom3	Atom4	Angle
C24	N3	C21	C22	-1.3(7)
Ru1	N3	C24	C23	-174.1(4)
Ru1	N3	C24	C25	6.2(9)
C21	N3	C24	C23	2.1(7)
C21	N3	C24	C25	-177.5(6)
Ru1	N4	C26	C25	2.9(9)
Ru1	N4	C26	C27	-171.5(4)
C29	N4	C26	C25	174.5(6)
C29	N4	C26	C27	0.0(7)
Ru1	N4	C29	C28	171.7(4)
Ru1	N4	C29	C30	-8.0(9)
C26	N4	C29	C28	0.0(7)
C26	N4	C29	C30	-179.7(6)
Ru1	N5	C71	C72	176.9(5)
C75	N5	C71	C72	1.0(10)
Ru1	N5	C75	C74	-177.1(5)
C71	N5	C75	C74	-1.2(10)
N1	C11	C12	C13	1.9(7)
C30	C11	C12	C13	-177.2(6)
N1	C11	C30	C29	6.6(11)
N1	C11	C30	C61	-175.7(6)
C12	C11	C30	C29	-174.3(6)
C12	C11	C30	C61	3.3(10)
C11	C12	C13	C14	-0.1(7)
C12	C13	C14	N1	-1.8(7)
C12	C13	C14	C15	177.4(6)
N1	C14	C15	C16	-2.8(10)
N1	C14	C15	C31	173.3(6)
C13	C14	C15	C16	178.1(6)
C13	C14	C15	C31	-5.8(9)
C14	C15	C16	N2	-3.7(10)
C14	C15	C16	C17	175.5(6)
C31	C15	C16	N2	-179.8(5)
C31	C15	C16	C17	-0.7(9)
C14	C15	C31	C32	-69.5(8)
C14	C15	C31	C36	111.5(8)
C16	C15	C31	C32	107.0(7)
C16	C15	C31	C36	-72.0(8)
N2	C16	C17	C18	-0.8(7)
C15	C16	C17	C18	179.9(6)
C16	C17	C18	C19	-0.7(7)
C17	C18	C19	N2	2.1(7)
C17	C18	C19	C20	-178.5(6)
N2	C19	C20	C21	3.7(10)
N2	C19	C20	C41	-177.3(5)
C18	C19	C20	C21	-175.6(6)
C18	C19	C20	C41	3.4(9)
C19	C20	C21	N3	2.0(10)
C19	C20	C21	C22	179.0(6)
C41	C20	C21	N3	-177.1(6)
C41	C20	C21	C22	-0.1(9)
C19	C20	C41	C42	-98.4(9)
C19	C20	C41	C46	80.7(8)
C21	C20	C41	C42	80.7(9)
C21	C20	C41	C46	-100.2(8)
N3	C21	C22	C23	-0.1(7)
C20	C21	C22	C23	-177.6(6)
C21	C22	C23	C24	1.4(8)
C22	C23	C24	N3	-2.3(8)
C22	C23	C24	C25	177.4(6)
N3	C24	C25	C26	-3.9(10)
N3	C24	C25	C51	170.0(6)
C23	C24	C25	C26	176.4(6)
C23	C24	C25	C51	-9.6(9)
C24	C25	C26	N4	-1.0(10)
C24	C25	C26	C27	172.5(6)
C51	C25	C26	N4	-174.8(5)
C51	C25	C26	C27	-1.4(9)
C24	C25	C51	C52	-53.6(9)
C24	C25	C51	C56	126.7(7)
C26	C25	C51	C52	120.9(7)
C26	C25	C51	C56	-58.8(8)
N4	C26	C27	C28	0.0(7)
C25	C26	C27	C28	-174.4(6)
C26	C27	C28	C29	0.0(7)
C27	C28	C29	N4	0.0(7)
C27	C28	C29	C30	179.7(6)
N4	C29	C30	C11	3.0(11)
N4	C29	C30	C61	-174.6(6)
C28	C29	C30	C11	-176.6(6)

Table 5. Torsional Angles (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C28	C29	C30	C61	5.7(10)	C61	C62	C63	C64	0.7(10)
C11	C30	C61	C62	67.1(8)	C62	C63	C64	C65	-2.1(10)
C11	C30	C61	C66	-115.6(7)	C62	C63	C64	C67	178.8(7)
C29	C30	C61	C62	-115.1(7)	C63	C64	C65	C66	2.3(12)
C29	C30	C61	C66	62.3(9)	C67	C64	C65	C66	-178.6(7)
C15	C31	C32	C33	179.5(7)	C64	C65	C66	C61	-1.1(12)
C36	C31	C32	C33	-1.5(11)	N5	C71	C72	C73	-0.8(10)
C15	C31	C36	C35	179.4(7)	N5	C71	C72	C76	-174.3(6)
C32	C31	C36	C35	0.3(12)	C71	C72	C73	C74	0.9(10)
C31	C32	C33	C34	0.6(11)	C76	C72	C73	C74	174.0(7)
C32	C33	C34	C35	1.4(11)	C71	C72	C76	C77	32(6)
C32	C33	C34	C37	178.2(7)	C73	C72	C76	C77	-141(5)
C33	C34	C35	C36	-2.6(12)	C72	C73	C74	C75	-1.1(11)
C37	C34	C35	C36	-179.3(8)	C72	C73	C74	C84	176.5(7)
C34	C35	C36	C31	1.7(13)	C73	C74	C75	N5	1.2(11)
C20	C41	C42	C43	178.9(10)	C84	C74	C75	N5	-176.5(6)
C46	C41	C42	C43	-0.2(15)	C73	C74	C84	C85	-179(100)
C20	C41	C46	C45	-179.2(7)	C75	C74	C84	C85	-1(8)
C42	C41	C46	C45	-0.1(12)	C72	C76	C77	C78	104(12)
C41	C42	C43	C44	1.1(18)	C76	C77	C78	C79	-130(12)
C42	C43	C44	C45	-1.7(16)	C76	C77	C78	C82	46(13)
C42	C43	C44	C47	179.2(11)	C77	C78	C79	C80	-1.5(11)
C43	C44	C45	C46	1.4(13)	C77	C78	C79	C81	178.0(7)
C47	C44	C45	C46	-179.5(8)	C82	C78	C79	C80	-176.5(7)
C44	C45	C46	C41	-0.5(12)	C82	C78	C79	C81	3.0(11)
C25	C51	C52	C53	-179.6(8)	C77	C78	C82	C83	-9(13)
C56	C51	C52	C53	0.1(12)	C79	C78	C82	C83	166(12)
C25	C51	C56	C55	179.1(7)	C78	C82	C83	C91’	-100(26)
C52	C51	C56	C55	-0.7(11)	C82	C83	C91’	C90’	64(100)
C51	C52	C53	C54	0.0(15)	C74	C84	C85	C86	-177(100)
C52	C53	C54	C55	0.4(16)	C84	C85	C86	C87	-174(100)
C52	C53	C54	C57	177.0(11)	C84	C85	C86	C90	3(33)
C53	C54	C55	C56	-1.0(15)	C85	C86	C87	C88	0.2(12)
C57	C54	C55	C56	-177.2(11)	C85	C86	C87	C89	179.8(7)
C54	C55	C56	C51	1.1(12)	C90	C86	C87	C88	-176.7(7)
C30	C61	C62	C63	177.9(6)	C90	C86	C87	C89	3.0(12)
C66	C61	C62	C63	0.5(10)	C85	C86	C90	C91	-16(17)
C30	C61	C66	C65	-177.7(7)	C87	C86	C90	C91	162(16)
C62	C61	C66	C65	-0.3(11)	C86	C90	C91	C83’	-21(100)

Primed atoms are related to unprimed ones via the inversion center (0, 0, 0).

Table 5. Torsional Angles (continued)

(b) within [({ 5,10,15,20-tetra-p-tolylporphyrinato)Ru(CO)(HOEt)]

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
N6	Ru2	O3	C3	65.4(12)	Ru2	N7	C106	C105	0.3(11)
N6”	Ru2	O3	C3	-114.6(12)	Ru2	N7	C106	C107	-179.0(5)
N7	Ru2	O3	C3	-25.4(12)	C109	N7	C106	C105	178.9(7)
N7”	Ru2	O3	C3	154.6(12)	C109	N7	C106	C107	-0.3(8)
C2	Ru2	O3	C3	144(15)	Ru2	N7	C109	C108	-179.4(5)
O3	Ru2	N6	C101	92.6(6)	Ru2	N7	C109	C110	-0.1(10)
O3	Ru2	N6	C104	-90.2(6)	C106	N7	C109	C108	2.0(8)
N6”	Ru2	N6	C101	97(100)	C106	N7	C109	C110	-178.7(7)
N6”	Ru2	N6	C104	-86(100)	N6	C101	C102	C103	1.7(8)
N7	Ru2	N6	C101	-177.5(6)	C110”	C101	C102	C103	-179.1(7)
N7	Ru2	N6	C104	-0.3(6)	C101	C102	C103	C104	-0.1(9)
N7”	Ru2	N6	C101	2.5(6)	C102	C103	C104	N6	-1.6(9)
N7”	Ru2	N6	C104	179.7(6)	C102	C103	C104	C105	-179.1(7)
C2	Ru2	N6	C101	-83.7(8)	N6	C104	C105	C106	-3.6(13)
C2	Ru2	N6	C104	93.4(7)	N6	C104	C105	C111	176.2(7)
O3	Ru2	N7	C106	88.6(7)	C103	C104	C105	C106	173.6(7)
O3	Ru2	N7	C109	-89.8(7)	C103	C104	C105	C111	-6.6(12)
N6	Ru2	N7	C106	-1.0(6)	C104	C105	C106	N7	2.1(13)
N6	Ru2	N7	C109	-179.4(6)	C104	C105	C106	C107	-178.7(7)
N6”	Ru2	N7	C106	179.0(6)	C111	C105	C106	N7	-177.7(7)
N6”	Ru2	N7	C109	0.6(6)	C111	C105	C106	C107	1.5(12)
N7”	Ru2	N7	C106	67(100)	C104	C105	C111	C112	110.6(10)
N7”	Ru2	N7	C109	-112(100)	C104	C105	C111	C116	-69.3(12)
C2	Ru2	N7	C106	-90.8(9)	C106	C105	C111	C112	-69.6(12)
C2	Ru2	N7	C109	90.8(9)	C106	C105	C111	C116	110.5(10)
O3	Ru2	C2	O2	-4(40)	N7	C106	C107	C108	-1.6(9)
N6	Ru2	C2	O2	75(25)	C105	C106	C107	C108	179.1(7)
N6”	Ru2	C2	O2	-105(25)	C106	C107	C108	C109	2.8(9)
N7	Ru2	C2	O2	165(25)	C107	C108	C109	N7	-3.1(9)
N7”	Ru2	C2	O2	-15(25)	C107	C108	C109	C110	177.7(7)
Ru2	O3	C3	C4	-168.2(11)	N7	C109	C110	C101”	1.1(12)
Ru2	N6	C101	C102	175.0(5)	N7	C109	C110	C121	-178.6(7)
Ru2	N6	C101	C110”	-4.2(10)	C108	C109	C110	C101”	-179.8(7)
C104	N6	C101	C102	-2.6(8)	C108	C109	C110	C121	0.5(11)
C104	N6	C101	C110”	178.2(7)	C101”	C110	C121	C122	-55.6(10)
Ru2	N6	C104	C103	-175.1(5)	C101”	C110	C121	C126	124.7(7)
Ru2	N6	C104	C105	2.5(10)	C109	C110	C121	C122	124.1(8)
C101	N6	C104	C103	2.6(8)	C109	C110	C121	C126	-55.6(10)
C101	N6	C104	C105	-179.9(7)	C105	C111	C112	C113	-180.0(9)

Table 5. Torsional Angles (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C116	C111	C112	C113	-0.1(16)	C126	C121	C122	C123	1.7(11)
C105	C111	C116	C115	178.2(11)	C110	C121	C126	C125	178.5(7)
C112	C111	C116	C115	-1.8(17)	C122	C121	C126	C125	-1.3(11)
C111	C112	C113	C114	5(2)	C121	C122	C123	C124	-0.8(12)
C112	C113	C114	C115	-7(2)	C122	C123	C124	C125	-0.7(11)
C112	C113	C114	C117	173.9(12)	C122	C123	C124	C127	176.3(7)
C113	C114	C115	C116	5(2)	C123	C124	C125	C126	1.2(11)
C117	C114	C115	C116	-176.0(12)	C127	C124	C125	C126	-175.9(7)
C114	C115	C116	C111	-1(2)	C124	C125	C126	C121	-0.2(12)
C110	C121	C122	C123	-178.0(7)					

Double-primed atoms are related to unprimed ones via the inversion center ($^1/_2$, 0, 0).

Table 6. Anisotropic Displacement Parameters (U_{ij}, Å^2)

(a) atoms of [{(5,10,15,20-tetra-p-tolylporphyrinato)Ru(CO)}$_2$(μ–{C_5H_3N-3,5-(C≡CC{=CMe_2}-C≡C-)$_2$}$_2$)]

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	0.0262(2)	0.0422(3)	0.0463(3)	-0.0085(2)	0.00124(19)	0.0186(2)
O1	0.046(3)	0.058(3)	0.065(3)	-0.023(2)	0.000(2)	0.025(2)
N1	0.032(2)	0.046(3)	0.047(3)	-0.004(2)	0.006(2)	0.021(2)
N2	0.036(3)	0.046(3)	0.043(3)	-0.011(2)	-0.001(2)	0.021(2)
N3	0.030(2)	0.043(3)	0.048(3)	-0.009(2)	-0.005(2)	0.022(2)
N4	0.028(2)	0.043(3)	0.054(3)	-0.004(2)	0.003(2)	0.018(2)
N5	0.034(3)	0.042(3)	0.049(3)	-0.009(2)	0.002(2)	0.021(2)
C1	0.032(3)	0.039(3)	0.058(4)	-0.003(3)	0.001(3)	0.021(3)
C11	0.035(3)	0.041(3)	0.050(4)	-0.002(3)	0.003(3)	0.019(3)
C12	0.045(4)	0.053(4)	0.056(4)	0.007(3)	0.010(3)	0.030(3)
C13	0.043(3)	0.047(4)	0.053(4)	0.000(3)	0.012(3)	0.019(3)
C14	0.034(3)	0.047(4)	0.053(4)	-0.008(3)	0.005(3)	0.020(3)
C15	0.034(3)	0.041(3)	0.053(4)	-0.007(3)	0.009(3)	0.014(3)
C16	0.029(3)	0.046(4)	0.049(4)	-0.016(3)	0.001(2)	0.017(3)
C17	0.031(3)	0.056(4)	0.060(4)	-0.009(3)	0.008(3)	0.018(3)
C18	0.033(3)	0.058(4)	0.060(4)	-0.012(3)	-0.001(3)	0.024(3)
C19	0.027(3)	0.050(4)	0.047(3)	-0.012(3)	-0.003(2)	0.022(3)
C20	0.033(3)	0.048(4)	0.049(4)	-0.019(3)	-0.009(3)	0.023(3)
C21	0.041(3)	0.037(3)	0.046(3)	-0.013(3)	-0.004(3)	0.019(3)
C22	0.044(4)	0.046(4)	0.067(4)	-0.010(3)	-0.005(3)	0.023(3)
C23	0.035(3)	0.043(4)	0.063(4)	0.005(3)	0.004(3)	0.014(3)
C24	0.031(3)	0.039(3)	0.054(4)	-0.006(3)	-0.002(3)	0.015(3)
C25	0.028(3)	0.040(3)	0.053(4)	-0.008(3)	0.000(2)	0.014(2)
C26	0.027(3)	0.049(4)	0.053(4)	-0.012(3)	0.000(3)	0.017(3)
C27	0.027(3)	0.045(4)	0.062(4)	-0.004(3)	0.009(3)	0.014(3)
C28	0.031(3)	0.052(4)	0.060(4)	-0.001(3)	0.008(3)	0.022(3)
C29	0.028(3)	0.049(4)	0.056(4)	-0.002(3)	0.001(3)	0.025(3)
C30	0.031(3)	0.048(4)	0.057(4)	-0.003(3)	0.002(3)	0.023(3)
C31	0.029(3)	0.060(4)	0.054(4)	-0.010(3)	0.006(3)	0.020(3)
C32	0.042(4)	0.057(4)	0.064(4)	-0.010(3)	0.012(3)	0.026(3)
C33	0.042(4)	0.059(4)	0.073(5)	0.005(4)	0.018(3)	0.023(3)
C34	0.046(4)	0.083(6)	0.054(4)	0.012(4)	0.010(3)	0.034(4)
C35	0.072(5)	0.094(6)	0.055(4)	-0.008(4)	0.029(4)	0.036(5)
C36	0.057(4)	0.060(5)	0.068(5)	-0.020(4)	0.015(4)	0.019(4)
C37	0.069(5)	0.092(6)	0.083(6)	0.033(5)	0.035(5)	0.037(5)
C41	0.036(3)	0.053(4)	0.058(4)	-0.007(3)	-0.004(3)	0.025(3)
C42	0.091(6)	0.143(9)	0.056(5)	-0.012(5)	-0.003(4)	0.089(6)

Table 6. Anisotropic Displacement Parameters (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C43	0.104(8)	0.182(12)	0.075(6)	0.000(7)	-0.012(5)	0.111(8)
C44	0.057(5)	0.100(7)	0.102(7)	0.031(6)	0.020(5)	0.055(5)
C45	0.054(4)	0.054(4)	0.098(6)	-0.001(4)	0.008(4)	0.036(4)
C46	0.042(4)	0.057(4)	0.075(5)	-0.020(4)	-0.008(3)	0.030(3)
C47	0.092(7)	0.174(12)	0.145(10)	0.066(9)	0.041(7)	0.101(8)
C51	0.037(3)	0.046(4)	0.058(4)	-0.002(3)	0.002(3)	0.021(3)
C52	0.057(5)	0.085(6)	0.078(6)	0.019(4)	0.012(4)	0.041(4)
C53	0.098(8)	0.152(10)	0.091(7)	0.061(7)	0.032(6)	0.079(8)
C54	0.079(7)	0.127(9)	0.174(12)	0.098(9)	0.065(8)	0.064(7)
C55	0.058(5)	0.050(5)	0.132(8)	0.032(5)	0.031(5)	0.029(4)
C56	0.039(3)	0.043(4)	0.079(5)	-0.004(3)	0.010(3)	0.019(3)
C57	0.107(10)	0.266(19)	0.234(17)	0.190(16)	0.099(11)	0.097(11)
C61	0.036(3)	0.053(4)	0.060(4)	0.007(3)	0.011(3)	0.027(3)
C62	0.042(3)	0.056(4)	0.051(4)	0.004(3)	0.009(3)	0.025(3)
C63	0.054(4)	0.053(4)	0.057(4)	0.005(3)	0.018(3)	0.035(3)
C64	0.044(4)	0.064(5)	0.069(5)	0.010(4)	0.012(3)	0.035(3)
C65	0.036(4)	0.061(5)	0.088(6)	-0.006(4)	-0.008(3)	0.025(3)
C66	0.040(4)	0.053(4)	0.072(5)	-0.008(3)	-0.002(3)	0.026(3)
C67	0.066(5)	0.080(6)	0.099(6)	0.004(5)	0.005(5)	0.052(5)
C71	0.034(3)	0.050(4)	0.046(3)	-0.012(3)	0.004(3)	0.017(3)
C72	0.032(3)	0.050(4)	0.056(4)	-0.008(3)	0.001(3)	0.017(3)
C73	0.044(4)	0.060(4)	0.049(4)	-0.018(3)	0.002(3)	0.019(3)
C74	0.038(3)	0.059(4)	0.052(4)	-0.005(3)	0.010(3)	0.019(3)
C75	0.033(3)	0.044(4)	0.051(4)	-0.009(3)	0.007(3)	0.016(3)
C76	0.050(4)	0.050(4)	0.054(4)	-0.017(3)	0.007(3)	0.013(3)
C77	0.043(4)	0.051(4)	0.045(4)	-0.008(3)	0.005(3)	0.014(3)
C78	0.039(3)	0.051(4)	0.051(4)	-0.011(3)	0.002(3)	0.014(3)
C79	0.047(4)	0.047(4)	0.052(4)	-0.004(3)	0.008(3)	0.018(3)
C80	0.059(4)	0.051(4)	0.052(4)	-0.006(3)	0.008(3)	0.023(3)
C81	0.041(4)	0.079(5)	0.050(4)	-0.004(3)	0.010(3)	0.024(3)
C82	0.039(3)	0.060(4)	0.052(4)	-0.008(3)	0.010(3)	0.016(3)
C83	0.038(3)	0.064(4)	0.054(4)	-0.004(3)	0.015(3)	0.016(3)
C84	0.045(4)	0.053(4)	0.058(4)	-0.014(3)	0.010(3)	0.012(3)
C85	0.048(4)	0.054(4)	0.053(4)	-0.007(3)	0.007(3)	0.024(3)
C86	0.050(4)	0.053(4)	0.050(4)	-0.009(3)	0.009(3)	0.021(3)
C87	0.044(4)	0.053(4)	0.060(4)	-0.004(3)	0.009(3)	0.019(3)
C88	0.057(5)	0.074(5)	0.077(5)	-0.027(4)	0.003(4)	0.021(4)
C89	0.052(5)	0.097(7)	0.084(6)	0.001(5)	0.017(4)	0.026(4)
C90	0.045(4)	0.058(4)	0.040(3)	-0.010(3)	0.007(3)	0.018(3)
C91	0.042(4)	0.061(4)	0.056(4)	-0.009(3)	0.011(3)	0.018(3)

Table 6. Anisotropic Displacement Parameters (continued)

(b) atoms of [({ 5,10,15,20-tetra-p-tolylporphyrinato)Ru(CO)(HOEt)]

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru2	0.0369(4)	0.0838(6)	0.0473(5)	-0.0019(4)	0.0096(3)	0.0280(4)
N6	0.044(3)	0.068(4)	0.056(3)	0.003(3)	0.015(3)	0.030(3)
N7	0.038(3)	0.068(4)	0.054(3)	0.005(3)	0.012(2)	0.025(3)
C101	0.048(4)	0.059(4)	0.051(4)	0.008(3)	0.016(3)	0.027(3)
C102	0.053(4)	0.077(5)	0.056(4)	-0.006(4)	0.012(3)	0.035(4)
C103	0.051(4)	0.078(5)	0.070(5)	0.007(4)	0.022(4)	0.034(4)
C104	0.040(3)	0.072(5)	0.057(4)	0.006(3)	0.011(3)	0.029(3)
C105	0.042(4)	0.082(5)	0.057(4)	0.003(4)	0.010(3)	0.030(4)
C106	0.046(4)	0.069(5)	0.062(4)	0.000(4)	0.010(3)	0.033(3)
C107	0.042(4)	0.078(5)	0.070(5)	0.005(4)	0.011(3)	0.029(4)
C108	0.040(4)	0.074(5)	0.065(5)	-0.002(4)	0.010(3)	0.026(3)
C109	0.048(4)	0.067(5)	0.050(4)	0.001(3)	0.009(3)	0.027(3)
C110	0.049(4)	0.054(4)	0.057(4)	0.007(3)	0.019(3)	0.024(3)
C111	0.041(4)	0.109(7)	0.063(5)	-0.004(4)	0.009(3)	0.033(4)
C112	0.075(6)	0.173(11)	0.077(6)	0.007(6)	0.012(5)	0.077(7)
C113	0.061(6)	0.240(16)	0.115(9)	-0.031(10)	0.001(6)	0.083(9)
C114	0.054(6)	0.218(15)	0.102(9)	-0.047(9)	0.021(6)	0.041(7)
C115	0.050(6)	0.255(17)	0.089(8)	-0.014(9)	0.019(5)	0.036(8)
C116	0.053(5)	0.185(12)	0.078(6)	0.015(7)	0.018(5)	0.040(6)
C117	0.062(7)	0.31(2)	0.220(17)	-0.084(16)	0.058(9)	0.045(10)
C121	0.045(4)	0.063(5)	0.057(4)	0.002(3)	0.011(3)	0.028(3)
C122	0.059(4)	0.065(5)	0.062(5)	-0.006(4)	0.019(4)	0.026(4)
C123	0.060(5)	0.081(6)	0.069(5)	0.003(4)	0.020(4)	0.039(4)
C124	0.040(4)	0.079(5)	0.063(5)	-0.011(4)	0.005(3)	0.033(4)
C125	0.045(4)	0.061(5)	0.077(5)	-0.011(4)	0.003(4)	0.021(3)
C126	0.046(4)	0.072(5)	0.060(4)	0.003(4)	0.014(3)	0.024(4)
C127	0.065(5)	0.097(7)	0.074(5)	-0.015(5)	0.013(4)	0.044(5)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 7. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms

(a) hydrogens of [{(5,10,15,20-tetra-p-tolylporphyrinato)Ru(CO)}$_2$(μ–{C_5H_3N-3,5-(C≡CC{=CMe$_2$}C≡C-)$_2$}$_2$)]

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H12	0.2825	0.1252	0.6271	0.057
H13	0.1240	0.1028	0.6376	0.057
H17	-0.1186	0.2229	0.4940	0.060
H18	-0.1086	0.3369	0.4087	0.061
H22	0.1628	0.5728	0.2885	0.064
H23	0.3200	0.5963	0.2831	0.059
H27	0.5369	0.4317	0.3767	0.054
H28	0.5243	0.3131	0.4558	0.056
H32	-0.0483	0.0325	0.5080	0.063
H33	-0.1631	-0.0663	0.5628	0.068
H35	-0.1493	0.1229	0.7090	0.086
H36	-0.0294	0.2232	0.6571	0.076
H37A	-0.2703	-0.1023	0.6476	0.093
H37B	-0.2927	-0.0255	0.6759	0.093
H37C	-0.2192	-0.0510	0.7319	0.093
H42	-0.0335	0.4123	0.2323	0.103
H43	-0.1351	0.4706	0.1809	0.129
H45	-0.0778	0.6053	0.3884	0.078
H46	0.0228	0.5448	0.4386	0.070
H47A	-0.2447	0.5418	0.2269	0.143
H47B	-0.1600	0.6197	0.2019	0.143
H47C	-0.1826	0.6263	0.2861	0.143
H52	0.3564	0.4882	0.2058	0.084
H53	0.4602	0.5672	0.1263	0.123
H55	0.6687	0.6625	0.3196	0.091
H56	0.5656	0.5869	0.3948	0.064
H57A	0.6830	0.7283	0.1812	0.223
H57B	0.6018	0.6726	0.1088	0.223
H57C	0.6752	0.6372	0.1491	0.223
H62	0.3419	0.0830	0.4953	0.058
H63	0.4418	0.0177	0.5370	0.059
H65	0.6305	0.2430	0.6557	0.076
H66	0.5291	0.3071	0.6138	0.066
H67A	0.6695	0.1108	0.6136	0.091
H67B	0.5818	0.0210	0.6138	0.091
H67C	0.6261	0.0884	0.6899	0.091
H71	0.0457	0.1864	0.3731	0.053
H73	0.0800	0.1082	0.1677	0.064
H75	0.2821	0.3079	0.3096	0.052
H80A	-0.1709	0.0781	0.3599	0.066
H80B	-0.2632	0.0322	0.3940	0.066

Table 7. Derived Parameters for Hydrogen Atoms (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H80C	-0.2528	0.1090	0.3394	0.066
H81A	-0.4042	-0.0995	0.2155	0.068
H81B	-0.4166	-0.0177	0.2468	0.068
H81C	-0.4064	-0.0860	0.3054	0.068
H88A	0.4569	0.3472	0.2360	0.088
H88B	0.5330	0.4285	0.2057	0.088
H88C	0.5595	0.3537	0.2407	0.088
H89A	0.5225	0.3107	0.0285	0.095
H89B	0.5976	0.3156	0.1045	0.095
H89C	0.5858	0.4009	0.0798	0.095

(b) hydrogens of [({ 5,10,15,20-tetra-p-tolylporphyrinato)Ru(CO)(HOEt)]

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H3O[a]	0.5588	-0.1131	0.0867	0.086
H3A[a]	0.3854	-0.2130	0.0170	0.086
H3B[a]	0.3748	-0.1562	0.0848	0.086
H4A[a]	0.3806	-0.2831	0.1326	0.086
H4B[a]	0.4688	-0.2001	0.1780	0.086
H4C[a]	0.4801	-0.2561	0.1106	0.086
H102	0.4306	0.1307	0.2335	0.072
H103	0.2742	0.0335	0.1549	0.075
H107	0.1474	-0.1751	-0.1069	0.075
H108	0.2165	-0.2062	-0.2094	0.071
H112	0.1326	-0.0256	-0.0512	0.120
H113	-0.0180	-0.0765	-0.0277	0.162
H115	0.0461	-0.1983	0.1503	0.169
H116	0.1913	-0.1555	0.1241	0.130
H11A	-0.0920	-0.1082	0.1188	0.248
H11B	-0.1192	-0.2094	0.1074	0.248
H11C	-0.1396	-0.1598	0.0342	0.248
H122	0.4516	-0.0921	-0.3168	0.074
H123	0.3941	-0.1731	-0.4355	0.079
H125	0.2452	-0.3796	-0.3335	0.075
H126	0.3005	-0.2989	-0.2159	0.071
H12A	0.2421	-0.3071	-0.5134	0.091
H12B	0.2232	-0.3942	-0.4719	0.091
H12C	0.3197	-0.3437	-0.4988	0.091

[a]Included with an occupancy factor of 0.5.