Coordination-Driven Self-Assembly of M_3L_2 Trigonal Cages from Pre-organized Metalloligands Incorporating Octahedral Metal Centers and Fluorescent Detection of Nitroaromatics

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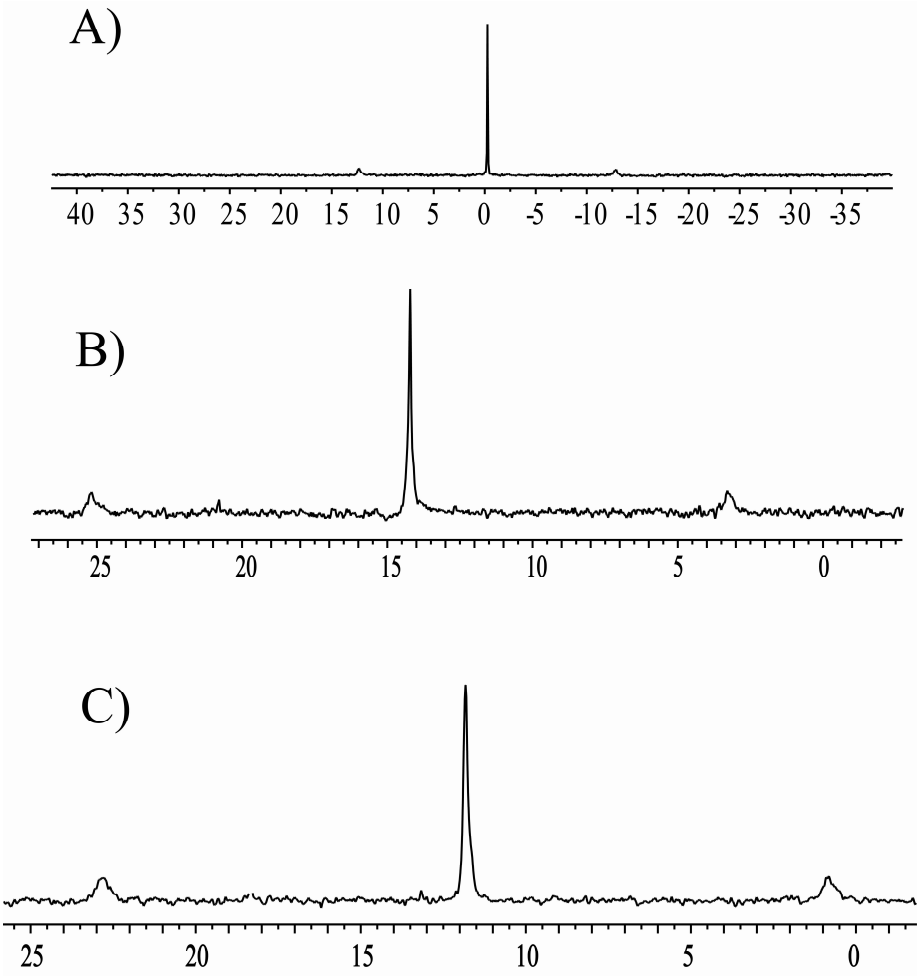

Figure S1. $^{31}P\{^{1}H\}$ NMR of trigonal-bipyramidal cages **6 – 8**: A) cage **6** in CD_2Cl_2/CD_3NO_2 (v:v = 2:1); B) cage **7** in acetone-d6/D_2O (v:v = 1:1); C) cage **8** in acetone-d6/D_2O (v:v = 1:1).

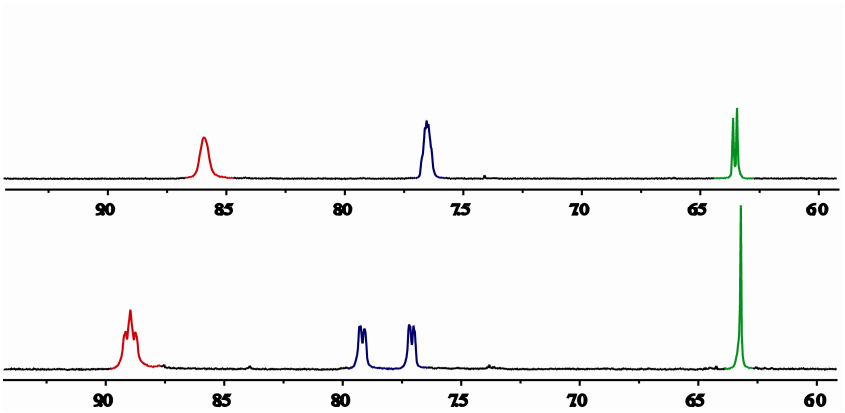

Figure S2. Partial ^{1}H NMR (300 MHz, 298 K) of donor **2** (*top*) and trigonal bipyramid **6** (*bottom*)in CD_2Cl_2/CD_3NO_2 (v:v = 2:1).

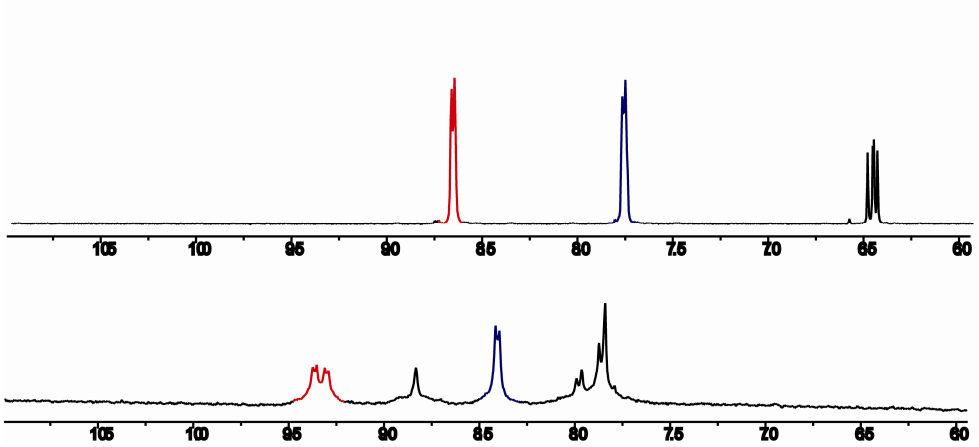

Figure S3. Partial ^{1}H NMR (300 MHz, 298 K) of donor **1** (*top*) and trigonal-bipyramidal cage **7** (*bottom*)in acetone-d6/D_2O (v:v = 1:1).

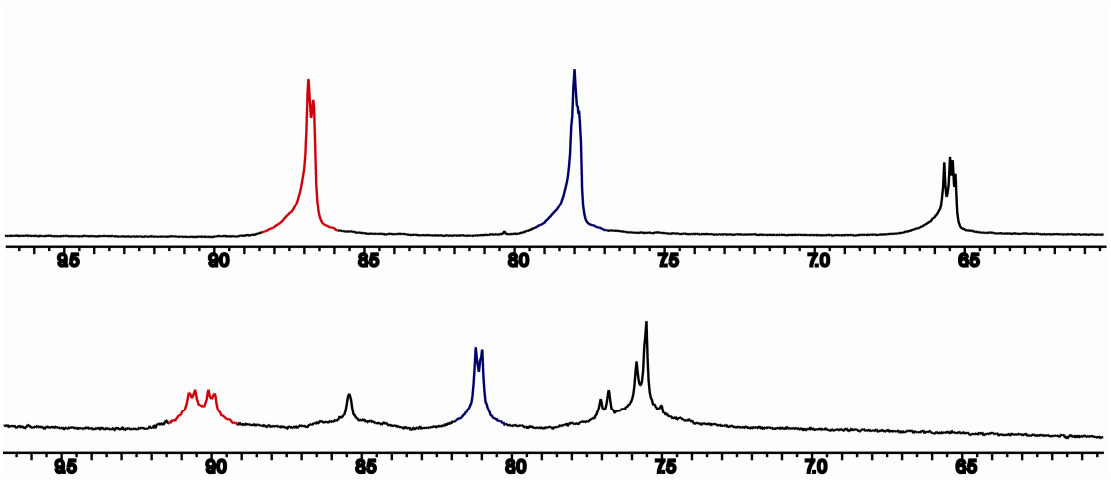

Figure S4. Partial ^{1}H NMR (300 MHz, 298 K) of donor **2** (*top*) and trigonal-bipyramid cage **8** (*bottom*)in acetone-d6/D_2O (v:v = 1:1).

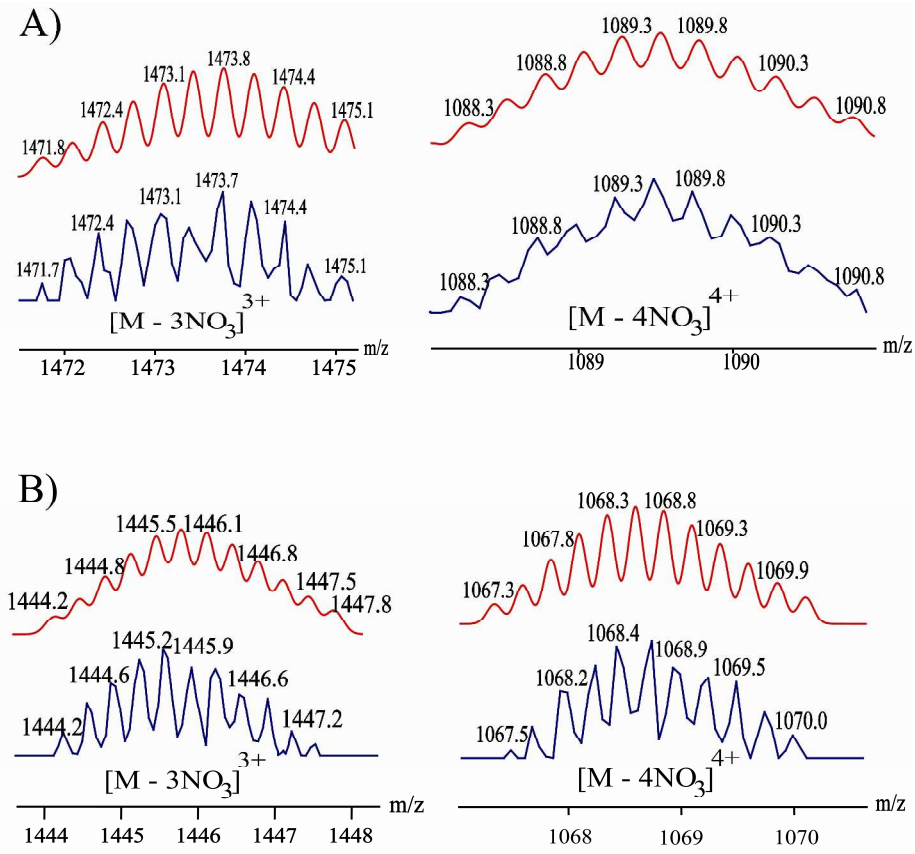

Figure S5. Calculated (red) and experimental (blue) ESI mass spectra of trigonal-bipyramidal cages **7** (A) and **8** (B).

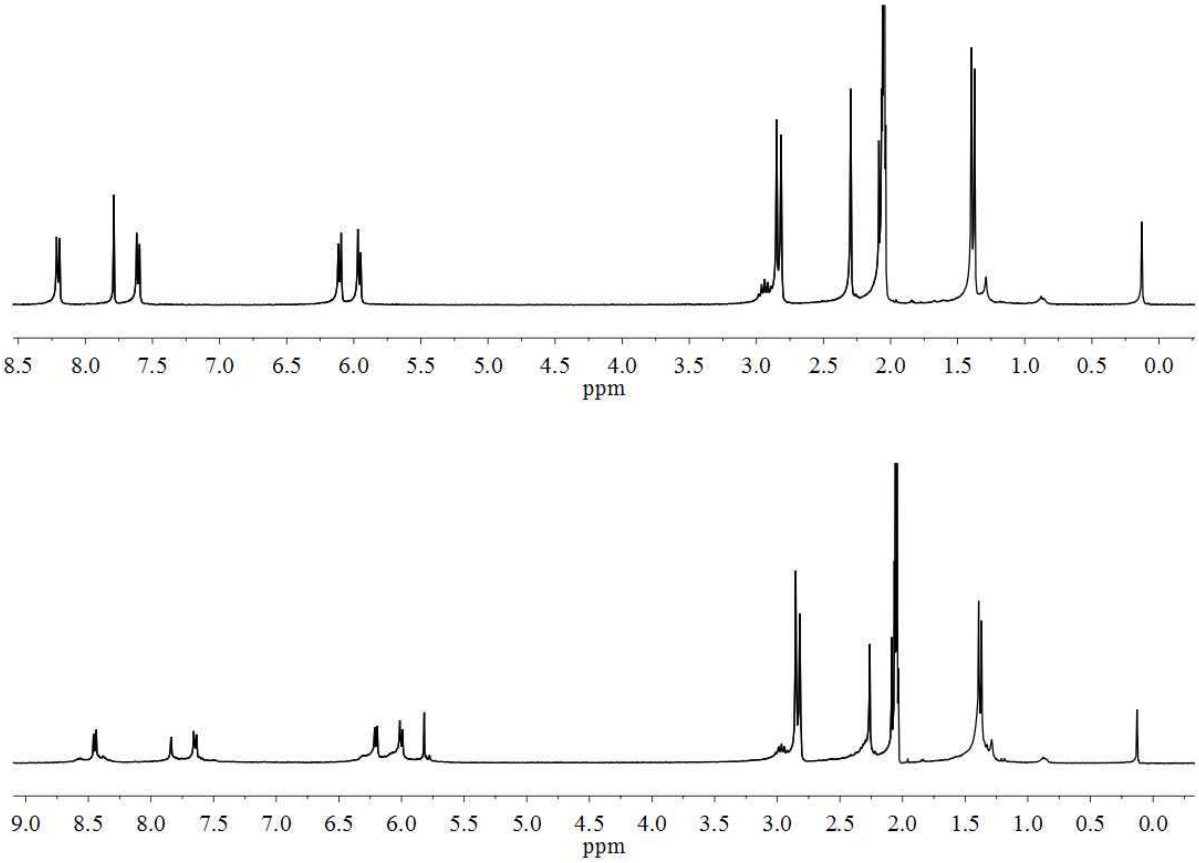

Figure S6. ^{1}H NMR (500 MHz) of trigonal prismatic cages **12** (*top*) and **13** (*bottom*). ^{1}H NMR were recorded in acetone-*d*6.

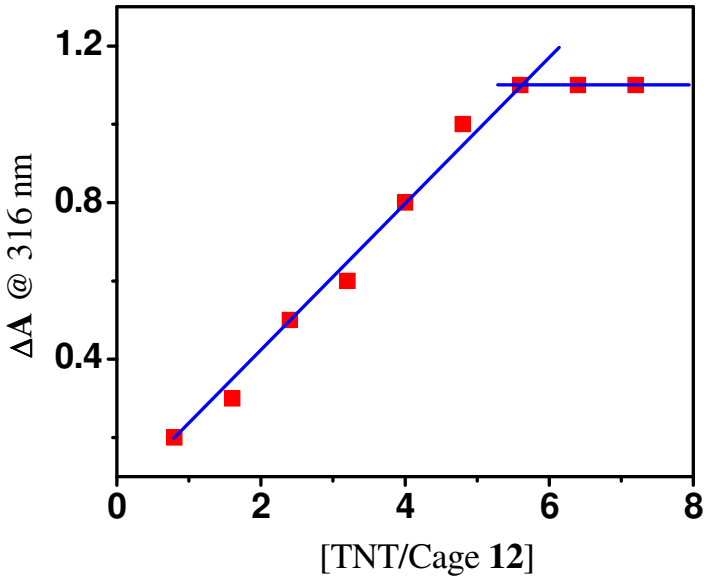

Figure S7. The stiochiometry plot of TNA/Cage **12**

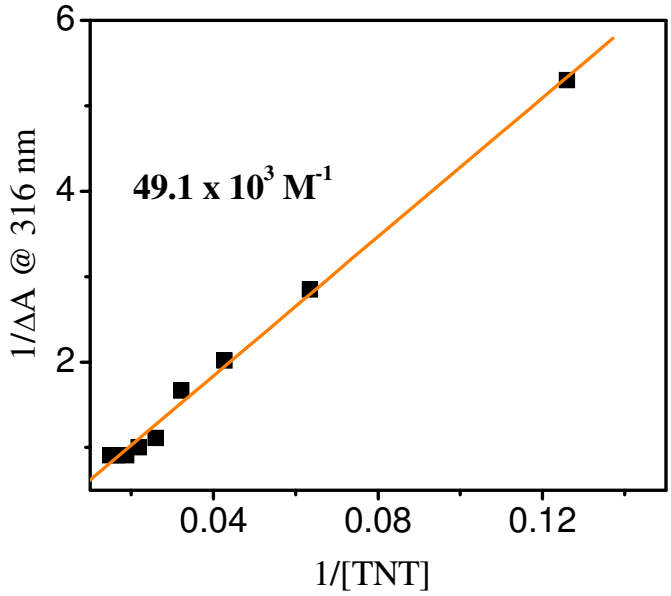

Figure S8. The binding constant of TNT/Cage **12**.

Table S1. Crystal data and structure refinement for **12**.

Empirical formula	$C_{120.79}H_{121.37}Cl_{5.02}N_{6.79}O_{36.16}Ru_6$	
Formula weight	3031.10	
Temperature	100(2) K	
Wavelength	0.90000 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.181(3) Å	α= 107.76(3)°.
	b = 23.307(5) Å	β= 102.02(3)°.
	c = 25.698(5) Å	γ = 98.37(3)°.
Volume	7166(2) $Å^3$	
Z	2	
Density (calculated)	1.405 mg/m^3	
Absorption coefficient	1.462 mm^{-1}	
F(000)	3065	
Crystal size	0.24 x 0.07 x 0.07 mm^3	
Theta range for data collection	2.05 to 29.74°.	
Index ranges	-11<=h<=11, -25<=k<=25, -25<=l<=25	
Reflections collected	20268	
Independent reflections	11062 [R(int) = 0.0553]	
Completeness to theta = 25.00°	81.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9046 and 0.7205	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11062 / 1254 / 1738	
Goodness-of-fit on F^2	1.163	
Final R indices [I>2sigma(I)]	R1 = 0.0904, wR2 = 0.2681	
R indices (all data)	R1 = 0.1085, wR2 = 0.2847	
Largest diff. peak and hole	1.102 and -0.841 $e.Å^{-3}$	

Table S2. Spectral and Photophysical Data of **12** and **13** in Methanol

M_3L_2 Cages	Absorption maxima λ_{max} (nm)	Molar extinction co-efficient $\varepsilon \times 10^3\ M^{-1}\ cm^{-1}$ [λ_{max}(nm)]	Fluorescence emission maxima λ_{max} (nm)	Quantum Yield (Φ) at 298 K
12	310, 502 (sh)	220 (310)	349, 361, 380	0.12
13	315	240 (315)	349, 361, 380	0.22

Determination of quantum yields of M_3L_2 cages **12** and **13**.

Fluorescence quantum yields of both the cages **12** and **13** were determined in the reference of anthracene (Φ = 0.27) in ethanol at 298 K.

The quantum yields are calculated according to the following equation

$$\Phi_{unk} = \Phi_{std} * (I_{unk}/A_{unk}) * (I_{std}/A_{std}) * (\eta_{unk}/\eta_{std})^2$$

Where, Φ is the quantum yield, I_{unk} and I_{std} is the integrated emission intensity of cages **12** or **13** and standard respectively, A_{unk} and A_{std} is the absorbance of the cages **12** or **13** and standard respectively, η is the refractive index of the solvent (ethanol).

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3)for **12**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	10969(1)	9635(1)	3382(1)	106(1)
Ru(2)	7312(1)	3580(1)	-3943(1)	110(1)
Ru(3)	10776(1)	2145(1)	2362(1)	119(1)
Ru(4)	3148(1)	2759(1)	-4062(1)	118(1)
Ru(5)	7330(1)	2894(1)	2981(1)	126(1)
Ru(6)	6992(1)	9816(1)	2344(1)	123(1)
O(1)	5870(9)	3849(4)	-4053(4)	113(3)
O(2)	6307(10)	2803(4)	-3938(4)	109(3)
O(3)	4102(10)	3478(4)	-4185(4)	117(3)
O(4)	4585(8)	2475(4)	-3998(4)	110(3)
O(5)	9119(9)	1816(4)	2172(5)	119(3)
O(6)	10441(11)	2812(5)	3008(5)	125(3)
O(7)	8958(9)	3162(4)	3210(4)	118(3)
O(8)	7669(10)	2153(4)	2410(4)	111(3)
O(9)	9370(8)	9451(4)	3411(4)	105(3)
O(10)	10209(10)	9954(4)	2746(4)	111(3)
O(11)	7751(10)	9528(4)	2992(4)	113(3)
O(12)	8557(9)	9999(4)	2303(5)	118(3)
N(1)	10513(11)	8782(5)	2693(5)	110(4)
N(2)	7399(10)	3895(5)	-3060(5)	108(3)
N(3)	10403(12)	2714(5)	1906(6)	119(4)
N(4)	3848(11)	3301(5)	-3208(5)	120(4)
N(5)	6921(12)	8902(6)	1841(6)	132(5)
N(6)	7395(10)	3330(5)	2394(6)	122(4)
C(1)	10921(14)	8718(6)	2253(8)	122(5)
C(2)	9949(16)	8285(6)	2713(8)	150(7)
C(3)	10671(15)	8146(7)	1800(7)	136(6)
C(4)	9672(19)	7741(7)	2292(8)	167(8)
C(5)	10031(14)	7642(6)	1829(7)	117(5)
C(6)	9767(13)	7050(6)	1398(6)	118(5)
C(7)	9511(14)	6498(5)	1028(6)	126(5)
C(8)	9292(13)	5898(6)	713(6)	113(5)
C(9)	8885(12)	5692(6)	150(6)	104(4)

C(10)	8619(12)	5064(6)	-190(6)	108(4)
C(11)	8789(11)	4641(6)	79(6)	98(4)
C(12)	9198(12)	4839(6)	655(6)	101(4)
C(13)	9422(12)	5453(6)	970(6)	107(4)
C(14)	8266(12)	4838(6)	-784(7)	99(4)
C(15)	7962(11)	4611(6)	-1296(7)	98(4)
C(16)	7718(11)	4352(6)	-1913(6)	98(4)
C(17)	7305(11)	4673(6)	-2238(6)	103(4)
C(18)	7897(14)	3784(6)	-2165(7)	124(5)
C(19)	7130(12)	4436(6)	-2818(7)	106(4)
C(20)	7748(14)	3575(6)	-2746(7)	125(5)
C(22)	9397(12)	4378(6)	928(6)	108(4)
C(23)	9562(13)	3998(6)	1123(6)	112(5)
C(24)	9878(14)	3574(6)	1401(7)	118(5)
C(25)	9241(13)	2971(7)	1180(7)	122(5)
C(26)	10701(14)	3737(7)	1861(7)	124(5)
C(27)	11009(15)	3297(7)	2106(8)	140(6)
C(28)	9537(15)	2561(6)	1451(8)	124(5)
C(29)	3763(12)	3907(6)	-3038(6)	106(4)
C(30)	4424(13)	3041(7)	-2847(7)	113(4)
C(31)	4201(13)	4242(7)	-2486(7)	121(5)
C(32)	4844(13)	3377(7)	-2288(7)	121(5)
C(33)	4792(13)	4019(7)	-2070(7)	116(4)
C(34)	5214(16)	4375(7)	-1490(8)	130(6)
C(35)	5608(14)	4637(7)	-1002(8)	118(5)
C(36)	5979(11)	4947(7)	-406(7)	106(4)
C(37)	6157(13)	5586(7)	-175(7)	121(5)
C(38)	6509(13)	5883(7)	426(7)	123(5)
C(39)	6750(12)	5521(7)	742(7)	117(5)
C(40)	6601(14)	4901(7)	517(7)	120(5)
C(41)	6659(14)	6506(6)	657(6)	121(5)
C(42)	6747(15)	7090(7)	908(7)	131(5)
C(43)	6836(16)	7689(7)	1226(9)	134(5)
C(44)	6421(17)	7810(8)	1676(8)	155(7)
C(45)	7325(13)	8181(7)	1092(7)	122(5)
C(46)	7338(16)	8768(8)	1419(8)	138(6)
C(47)	6792(14)	4546(7)	895(7)	129(5)
C(48)	6961(16)	4257(8)	1200(8)	141(6)

C(49)	7124(12)	3950(7)	1592(7)	122(5)
C(50)	7589(12)	4246(8)	2175(8)	132(5)
C(51)	6798(12)	3298(7)	1423(7)	120(5)
C(52)	7716(12)	3935(7)	2528(7)	130(6)
C(53)	6966(13)	3012(8)	1819(8)	134(6)
C(54)	11060(14)	1236(7)	1982(8)	124(5)
C(55)	11149(14)	1337(7)	2559(8)	125(5)
C(56)	11663(14)	1674(7)	1804(8)	127(5)
C(57)	12345(14)	2210(8)	2217(8)	128(5)
C(58)	11839(13)	1888(7)	2956(8)	120(5)
C(59)	12418(14)	2347(8)	2818(8)	129(5)
C(60)	10255(16)	675(7)	1557(8)	137(5)
C(61)	9798(16)	695(8)	969(8)	150(6)
C(62)	2165(14)	1947(8)	-4075(9)	137(5)
C(63)	2246(15)	1867(7)	-4642(8)	137(5)
C(64)	2083(11)	2272(6)	-4905(7)	113(4)
C(65)	1733(16)	2441(7)	-3849(8)	144(6)
C(66)	1527(15)	2896(8)	-4114(8)	136(5)
C(67)	1755(16)	2798(7)	-4656(8)	139(5)
C(68)	1672(17)	3323(8)	-4931(8)	143(5)
C(69)	510(18)	3347(9)	-5119(9)	169(7)
C(70)	9766(18)	5232(8)	-3861(12)	198(10)
C(71)	7455(14)	3364(7)	-4820(7)	128(5)
C(72)	7976(13)	2986(6)	-4559(7)	107(4)
C(73)	8779(14)	3273(7)	-4019(7)	126(5)
C(74)	9072(15)	3911(7)	-3746(7)	131(5)
C(75)	8575(15)	4309(7)	-3976(7)	127(5)
C(76)	7708(14)	4010(6)	-4526(7)	126(5)
C(77)	7691(16)	2309(6)	-4829(7)	141(6)
C(78)	8884(16)	4998(7)	-3682(9)	148(6)
C(79)	7963(16)	5329(8)	-3809(9)	164(7)
C(80)	8633(17)	2187(7)	2460(7)	107(4)
C(81)	7220(20)	3419(8)	3794(8)	156(7)
C(82)	6439(18)	3494(9)	3374(9)	151(6)
C(83)	5885(17)	2400(8)	2990(9)	138(5)
C(84)	6638(15)	2330(7)	3398(8)	130(5)
C(85)	7234(15)	2834(7)	3756(9)	139(5)
C(86)	5715(16)	2957(8)	2949(9)	145(6)

C(87)	5233(15)	1747(8)	2456(8)	139(5)
C(88)	4639(16)	1888(10)	1912(9)	175(8)
C(89)	4411(13)	1368(8)	2648(8)	140(6)
C(90)	9501(18)	2777(7)	2968(8)	116(5)
C(91)	10725(19)	81(8)	1482(9)	179(8)
C(92)	13082(14)	2945(7)	3257(8)	143(6)
C(93)	6233(13)	4595(7)	-62(7)	118(5)
C(94)	6427(15)	8435(7)	1983(8)	144(6)
C(95)	12104(11)	9374(6)	3949(7)	105(4)
C(96)	11564(14)	9746(7)	4268(7)	123(5)
C(97)	11512(13)	10311(6)	4219(6)	108(4)
C(98)	11995(13)	10533(6)	3880(6)	112(4)
C(99)	12592(12)	10168(6)	3527(7)	108(4)
C(100)	12670(13)	9577(6)	3601(7)	116(4)
C(101)	13041(13)	10388(7)	3134(7)	120(5)
C(102)	10921(15)	9503(7)	4635(7)	131(5)
C(103)	10604(15)	8805(7)	4484(9)	155(7)
C(104)	6825(13)	10647(7)	2208(8)	127(5)
C(105)	6167(16)	10196(7)	1759(8)	140(6)
C(106)	5350(14)	9765(7)	1888(8)	131(5)
C(107)	5440(18)	9808(10)	2421(10)	156(6)
C(108)	6132(18)	10263(10)	2877(9)	149(6)
C(109)	6853(17)	10715(9)	2790(9)	154(6)
C(110)	6181(19)	10259(11)	3492(9)	191(7)
C(111)	5384(17)	2837(6)	-4000(6)	104(4)
C(112)	5056(16)	3448(7)	-4092(6)	105(4)
C(113)	2461(16)	1496(8)	-3764(8)	155(6)
C(114)	7150(20)	10337(10)	1070(10)	188(8)
C(115)	8763(17)	9603(6)	3072(7)	112(5)
C(116)	9181(18)	9886(7)	2662(7)	118(5)
C(117)	6145(19)	10095(8)	1130(9)	156(6)
C(118)	5220(20)	10424(12)	904(11)	222(10)
C(119)	11670(17)	9771(10)	5265(8)	168(6)
C(120)	2250(16)	3241(8)	-5369(8)	151(6)
C(121)	8035(17)	3997(8)	4184(8)	169(7)
Cl(1)	-441(4)	1518(2)	-6153(2)	113(1)
O(1S)	-854(8)	879(4)	-6349(4)	127(3)
O(2S)	-498(10)	1759(6)	-5580(5)	171(5)

O(3S)	-1018(10)	1805(6)	-6480(6)	184(5)
O(4S)	655(8)	1656(5)	-6135(4)	129(4)
Cl(2)	5783(5)	5948(2)	-2365(3)	142(2)
O(5S)	6007(12)	6613(4)	-2134(6)	168(5)
O(6S)	5894(10)	5710(5)	-1911(5)	152(4)
O(7S)	6523(9)	5772(5)	-2685(5)	130(4)
O(8S)	4724(9)	5741(6)	-2710(6)	163(5)
Cl(3)	1185(5)	3817(2)	-2605(2)	130(2)
O(9S)	527(18)	4187(10)	-2342(10)	164(10)
O(9')	1880(20)	3413(12)	-2550(14)	146(9)
O(10S)	1965(14)	3721(10)	-2188(8)	134(9)
O(10')	137(14)	3737(16)	-2561(13)	154(10)
O(11S)	1668(19)	4114(11)	-2929(9)	118(13)
O(11')	1260(30)	4095(14)	-3020(11)	116(11)
O(12S)	516(15)	3230(6)	-2979(7)	120(7)
O(12')	1810(20)	4273(10)	-2073(7)	143(8)
Cl(4)	13807(5)	8227(2)	2669(2)	148(2)
O(13S)	14933(11)	8374(12)	2915(11)	175(10)
O(14S)	13501(16)	8679(7)	2453(8)	102(9)
O(15S)	13490(20)	7628(6)	2262(7)	164(9)
O(16S)	13301(16)	8218(9)	3123(7)	127(7)
O(17S)	12812(15)	7829(12)	2535(13)	192(12)
O(18S)	14500(20)	7916(11)	2397(11)	160(9)
O(19S)	13650(30)	8720(12)	2452(15)	250(30)
O(20S)	14260(30)	8488(14)	3259(7)	241(17)
Cl(5)	7170(20)	6983(14)	-708(14)	267(13)
O(21S)	7660(40)	7200(20)	-1077(18)	178(17)
O(22S)	6060(20)	6930(13)	-786(12)	100(8)
O(23S)	7760(40)	6520(20)	-820(20)	187(18)
O(24S)	7820(20)	7552(13)	-287(13)	112(10)
Cl(6)	6309(8)	1757(3)	268(3)	215(3)
O(25S)	5774(17)	1829(10)	704(8)	268(10)
O(26S)	6220(20)	2246(9)	56(11)	384(19)
O(27S)	7391(13)	1762(13)	486(12)	440(30)
O(28S)	5820(14)	1181(7)	-179(7)	212(7)
N(1N)	7670(20)	9033(11)	-58(12)	177(8)
O(1N)	7920(20)	9085(11)	-500(11)	225(9)
O(2N)	8224(18)	9168(10)	427(10)	192(7)

C(1N)	6640(30)	8759(18)	-199(16)	237(16)
O(1WA)	6470(30)	5108(14)	4453(16)	138(10)
O(1WB)	6020(30)	4810(20)	4719(17)	162(12)
O(1WC)	5050(30)	4941(13)	4040(13)	120(9)
O(2WA)	9100(50)	7900(20)	90(20)	203(16)
O(2WB)	9690(40)	8180(20)	-280(20)	198(14)
O(2WC)	9810(50)	7530(30)	60(20)	212(15)
O(3W)	12018(19)	7890(9)	3521(9)	129(6)

Table 3. Bond lengths [Å] and angles [°] for p-1.

Ru(1)-O(10)	2.122(9)
Ru(1)-O(9)	2.111(10)
Ru(1)-N(1)	2.123(11)
Ru(1)-C(95)	2.153(14)
Ru(1)-C(97)	2.141(13)
Ru(1)-C(98)	2.162(14)
Ru(1)-C(96)	2.169(17)
Ru(1)-C(99)	2.207(15)
Ru(1)-C(100)	2.230(16)
Ru(2)-O(1)	2.078(11)
Ru(2)-O(2)	2.086(9)
Ru(2)-N(2)	2.133(12)
Ru(2)-C(76)	2.148(15)
Ru(2)-C(72)	2.187(14)
Ru(2)-C(73)	2.183(17)
Ru(2)-C(71)	2.210(17)
Ru(2)-C(75)	2.235(15)
Ru(2)-C(74)	2.233(18)
Ru(3)-N(3)	2.069(12)
Ru(3)-O(6)	2.073(12)
Ru(3)-O(5)	2.107(11)
Ru(3)-C(58)	2.135(15)
Ru(3)-C(55)	2.188(15)
Ru(3)-C(54)	2.167(15)
Ru(3)-C(57)	2.168(19)
Ru(3)-C(59)	2.142(18)
Ru(3)-C(56)	2.177(18)
Ru(4)-N(4)	2.095(12)
Ru(4)-O(4)	2.087(10)
Ru(4)-O(3)	2.090(10)
Ru(4)-C(62)	2.117(16)
Ru(4)-C(65)	2.143(19)
Ru(4)-C(67)	2.16(2)
Ru(4)-C(63)	2.146(16)
Ru(4)-C(64)	2.174(15)
Ru(4)-C(66)	2.19(2)

Ru(5)-O(7)	2.049(11)
Ru(5)-C(85)	2.07(2)
Ru(5)-O(8)	2.071(10)
Ru(5)-N(6)	2.067(12)
Ru(5)-C(83)	2.087(19)
Ru(5)-C(81)	2.12(2)
Ru(5)-C(84)	2.152(16)
Ru(5)-C(82)	2.114(19)
Ru(5)-C(86)	2.14(2)
Ru(6)-C(107)	2.09(2)
Ru(6)-C(108)	2.09(2)
Ru(6)-O(11)	2.098(10)
Ru(6)-O(12)	2.076(11)
Ru(6)-C(104)	2.106(16)
Ru(6)-N(5)	2.103(14)
Ru(6)-C(109)	2.116(19)
Ru(6)-C(106)	2.203(17)
Ru(6)-C(105)	2.156(16)
O(1)-C(112)	1.281(18)
O(2)-C(111)	1.212(18)
O(3)-C(112)	1.246(18)
O(4)-C(111)	1.252(18)
O(5)-C(80)	1.294(19)
O(6)-C(90)	1.211(19)
O(7)-C(90)	1.32(2)
O(8)-C(80)	1.239(18)
O(9)-C(115)	1.227(19)
O(10)-C(116)	1.30(2)
O(11)-C(115)	1.285(19)
O(12)-C(116)	1.22(2)
N(1)-C(2)	1.301(17)
N(1)-C(1)	1.327(18)
N(2)-C(20)	1.316(17)
N(2)-C(19)	1.359(17)
N(3)-C(27)	1.354(18)
N(3)-C(28)	1.367(19)
N(4)-C(29)	1.374(17)
N(4)-C(30)	1.411(19)

N(5)-C(46)	1.29(2)
N(5)-C(94)	1.370(19)
N(6)-C(52)	1.326(17)
N(6)-C(53)	1.38(2)
C(1)-C(3)	1.42(2)
C(2)-C(4)	1.33(2)
C(3)-C(5)	1.38(2)
C(4)-C(5)	1.34(2)
C(5)-C(6)	1.422(19)
C(6)-C(7)	1.291(13)
C(7)-C(8)	1.338(13)
C(8)-C(9)	1.337(18)
C(8)-C(13)	1.401(18)
C(9)-C(10)	1.404(17)
C(10)-C(14)	1.402(19)
C(10)-C(11)	1.385(18)
C(11)-C(12)	1.369(18)
C(12)-C(13)	1.366(17)
C(12)-C(22)	1.476(19)
C(14)-C(15)	1.212(17)
C(15)-C(16)	1.46(2)
C(16)-C(18)	1.363(19)
C(16)-C(17)	1.364(18)
C(17)-C(19)	1.378(18)
C(18)-C(20)	1.38(2)
C(22)-C(23)	1.167(17)
C(23)-C(24)	1.44(2)
C(24)-C(26)	1.34(2)
C(24)-C(25)	1.405(19)
C(25)-C(28)	1.40(2)
C(26)-C(27)	1.42(2)
C(29)-C(31)	1.344(19)
C(30)-C(32)	1.36(2)
C(31)-C(33)	1.46(2)
C(32)-C(33)	1.45(2)
C(33)-C(34)	1.41(2)
C(34)-C(35)	1.175(19)
C(35)-C(36)	1.42(2)

C(36)-C(37)	1.388(19)
C(36)-C(93)	1.402(19)
C(37)-C(38)	1.43(2)
C(38)-C(41)	1.357(13)
C(38)-C(39)	1.36(2)
C(39)-C(40)	1.349(19)
C(40)-C(93)	1.38(2)
C(40)-C(47)	1.46(2)
C(41)-C(42)	1.291(13)
C(42)-C(43)	1.36(2)
C(43)-C(44)	1.35(2)
C(43)-C(45)	1.40(2)
C(44)-C(94)	1.43(2)
C(45)-C(46)	1.37(2)
C(47)-C(48)	1.19(2)
C(48)-C(49)	1.40(2)
C(49)-C(51)	1.42(2)
C(49)-C(50)	1.40(2)
C(50)-C(52)	1.32(2)
C(51)-C(53)	1.38(2)
C(54)-C(55)	1.41(2)
C(54)-C(56)	1.44(2)
C(54)-C(60)	1.51(2)
C(55)-C(58)	1.41(2)
C(56)-C(57)	1.40(2)
C(57)-C(59)	1.46(2)
C(58)-C(59)	1.40(2)
C(59)-C(92)	1.50(2)
C(60)-C(91)	1.57(2)
C(60)-C(61)	1.53(2)
C(62)-C(65)	1.38(2)
C(62)-C(63)	1.44(2)
C(62)-C(113)	1.55(2)
C(63)-C(64)	1.34(2)
C(64)-C(67)	1.37(2)
C(65)-C(66)	1.45(2)
C(66)-C(67)	1.44(2)
C(67)-C(68)	1.59(2)

C(68)-C(120)	1.47(2)
C(68)-C(69)	1.52(3)
C(70)-C(78)	1.43(2)
C(71)-C(72)	1.43(2)
C(71)-C(76)	1.415(19)
C(72)-C(73)	1.45(2)
C(72)-C(77)	1.470(18)
C(73)-C(74)	1.39(2)
C(74)-C(75)	1.41(2)
C(75)-C(76)	1.51(2)
C(75)-C(78)	1.50(2)
C(78)-C(79)	1.56(3)
C(80)-C(90)	1.65(2)
C(81)-C(85)	1.34(2)
C(81)-C(82)	1.40(3)
C(81)-C(121)	1.51(2)
C(82)-C(86)	1.43(3)
C(83)-C(84)	1.35(2)
C(83)-C(86)	1.38(2)
C(83)-C(87)	1.67(2)
C(84)-C(85)	1.27(2)
C(87)-C(89)	1.55(2)
C(87)-C(88)	1.60(2)
C(95)-C(96)	1.38(2)
C(95)-C(100)	1.42(2)
C(96)-C(97)	1.372(19)
C(96)-C(102)	1.56(2)
C(97)-C(98)	1.36(2)
C(98)-C(99)	1.48(2)
C(99)-C(101)	1.45(2)
C(99)-C(100)	1.463(18)
C(102)-C(103)	1.52(2)
C(102)-C(119)	1.59(2)
C(104)-C(105)	1.33(2)
C(104)-C(109)	1.45(3)
C(105)-C(106)	1.52(2)
C(105)-C(117)	1.55(3)
C(106)-C(107)	1.32(2)

C(107)-C(108)	1.36(3)
C(108)-C(109)	1.42(3)
C(108)-C(110)	1.57(3)
C(111)-C(112)	1.62(2)
C(114)-C(117)	1.41(3)
C(115)-C(116)	1.55(3)
C(117)-C(118)	1.63(3)
Cl(1)-O(3S)	1.400(10)
Cl(1)-O(4S)	1.421(9)
Cl(1)-O(2S)	1.430(10)
Cl(1)-O(1S)	1.401(8)
Cl(2)-O(8S)	1.413(10)
Cl(2)-O(7S)	1.428(9)
Cl(2)-O(6S)	1.429(10)
Cl(2)-O(5S)	1.439(10)
Cl(3)-O(10')	1.400(14)
Cl(3)-O(10S)	1.418(13)
Cl(3)-O(9S)	1.435(13)
Cl(3)-O(11')	1.419(14)
Cl(3)-O(9')	1.426(14)
Cl(3)-O(12')	1.434(14)
Cl(3)-O(11S)	1.424(13)
Cl(3)-O(12S)	1.438(12)
O(9S)-O(10')	1.02(3)
O(9S)-O(12')	1.64(3)
O(9')-O(10S)	0.96(3)
O(9')-O(12S)	1.82(3)
O(10S)-O(12')	1.29(3)
O(10')-O(12S)	1.56(3)
O(11S)-O(11')	0.53(5)
Cl(4)-O(20S)	1.406(14)
Cl(4)-O(17S)	1.401(14)
Cl(4)-O(14S)	1.403(11)
Cl(4)-O(13S)	1.431(13)
Cl(4)-O(15S)	1.405(12)
Cl(4)-O(19S)	1.445(14)
Cl(4)-O(18S)	1.415(13)
Cl(4)-O(16S)	1.464(12)

O(13S)-O(18S)	1.37(3)
O(13S)-O(20S)	1.37(3)
O(15S)-O(17S)	1.30(3)
O(15S)-O(18S)	1.32(3)
O(16S)-O(20S)	1.25(3)
O(16S)-O(17S)	1.45(3)
Cl(5)-O(21S)	1.419(15)
Cl(5)-O(23S)	1.408(15)
Cl(5)-O(22S)	1.423(15)
Cl(5)-O(24S)	1.438(15)
O(21S)-O(24S)	1.89(5)
O(24S)-O(2WA)	1.70(6)
Cl(6)-O(27S)	1.417(14)
Cl(6)-O(25S)	1.424(13)
Cl(6)-O(26S)	1.415(14)
Cl(6)-O(28S)	1.427(12)
N(1N)-C(1N)	1.33(4)
N(1N)-O(2N)	1.23(3)
N(1N)-O(1N)	1.29(3)
O(2WB)-O(2WC)	1.98(7)

O(10)-Ru(1)-O(9)	78.4(4)
O(10)-Ru(1)-N(1)	82.0(4)
O(9)-Ru(1)-N(1)	85.1(5)
O(10)-Ru(1)-C(95)	164.7(5)
O(9)-Ru(1)-C(95)	116.9(5)
N(1)-Ru(1)-C(95)	97.6(5)
O(10)-Ru(1)-C(97)	114.9(5)
O(9)-Ru(1)-C(97)	94.0(5)
N(1)-Ru(1)-C(97)	162.5(5)
C(95)-Ru(1)-C(97)	67.3(6)
O(10)-Ru(1)-C(98)	93.1(5)
O(9)-Ru(1)-C(98)	119.7(5)
N(1)-Ru(1)-C(98)	153.4(6)
C(95)-Ru(1)-C(98)	80.4(5)
C(97)-Ru(1)-C(98)	36.7(5)
O(10)-Ru(1)-C(96)	150.5(5)
O(9)-Ru(1)-C(96)	92.3(6)

N(1)-Ru(1)-C(96)	125.4(5)
C(95)-Ru(1)-C(96)	37.4(6)
C(97)-Ru(1)-C(96)	37.1(5)
C(98)-Ru(1)-C(96)	67.1(6)
O(10)-Ru(1)-C(99)	96.6(5)
O(9)-Ru(1)-C(99)	159.0(5)
N(1)-Ru(1)-C(99)	114.7(6)
C(95)-Ru(1)-C(99)	69.6(5)
C(97)-Ru(1)-C(99)	69.4(6)
C(98)-Ru(1)-C(99)	39.6(6)
C(96)-Ru(1)-C(99)	82.1(6)
O(10)-Ru(1)-C(100)	127.0(5)
O(9)-Ru(1)-C(100)	154.2(5)
N(1)-Ru(1)-C(100)	93.3(5)
C(95)-Ru(1)-C(100)	37.7(5)
C(97)-Ru(1)-C(100)	79.9(6)
C(98)-Ru(1)-C(100)	68.7(6)
C(96)-Ru(1)-C(100)	67.7(6)
C(99)-Ru(1)-C(100)	38.5(5)
O(1)-Ru(2)-O(2)	79.8(4)
O(1)-Ru(2)-N(2)	85.8(4)
O(2)-Ru(2)-N(2)	82.3(4)
O(1)-Ru(2)-C(76)	88.7(5)
O(2)-Ru(2)-C(76)	140.2(5)
N(2)-Ru(2)-C(76)	135.0(5)
O(1)-Ru(2)-C(72)	130.3(5)
O(2)-Ru(2)-C(72)	90.3(5)
N(2)-Ru(2)-C(72)	141.4(5)
C(76)-Ru(2)-C(72)	68.6(6)
O(1)-Ru(2)-C(73)	167.7(5)
O(2)-Ru(2)-C(73)	103.5(5)
N(2)-Ru(2)-C(73)	106.3(6)
C(76)-Ru(2)-C(73)	81.3(7)
C(72)-Ru(2)-C(73)	38.9(6)
O(1)-Ru(2)-C(71)	98.6(5)
O(2)-Ru(2)-C(71)	106.2(5)
N(2)-Ru(2)-C(71)	171.0(5)
C(76)-Ru(2)-C(71)	37.9(5)

C(72)-Ru(2)-C(71)	37.9(5)
C(73)-Ru(2)-C(71)	69.2(6)
O(1)-Ru(2)-C(75)	109.2(5)
O(2)-Ru(2)-C(75)	170.5(6)
N(2)-Ru(2)-C(75)	100.8(5)
C(76)-Ru(2)-C(75)	40.3(6)
C(72)-Ru(2)-C(75)	81.7(6)
C(73)-Ru(2)-C(75)	67.1(6)
C(71)-Ru(2)-C(75)	70.3(6)
O(1)-Ru(2)-C(74)	144.1(5)
O(2)-Ru(2)-C(74)	135.0(6)
N(2)-Ru(2)-C(74)	90.4(5)
C(76)-Ru(2)-C(74)	69.3(6)
C(72)-Ru(2)-C(74)	68.5(6)
C(73)-Ru(2)-C(74)	36.7(6)
C(71)-Ru(2)-C(74)	81.4(6)
C(75)-Ru(2)-C(74)	36.8(6)
N(3)-Ru(3)-O(6)	83.6(5)
N(3)-Ru(3)-O(5)	85.6(5)
O(6)-Ru(3)-O(5)	80.3(5)
N(3)-Ru(3)-C(58)	152.5(6)
O(6)-Ru(3)-C(58)	91.8(6)
O(5)-Ru(3)-C(58)	120.4(5)
N(3)-Ru(3)-C(55)	160.7(6)
O(6)-Ru(3)-C(55)	115.4(6)
O(5)-Ru(3)-C(55)	93.8(5)
C(58)-Ru(3)-C(55)	38.0(6)
N(3)-Ru(3)-C(54)	123.0(6)
O(6)-Ru(3)-C(54)	152.4(6)
O(5)-Ru(3)-C(54)	93.8(5)
C(58)-Ru(3)-C(54)	67.9(7)
C(55)-Ru(3)-C(54)	37.7(6)
N(3)-Ru(3)-C(57)	91.2(6)
O(6)-Ru(3)-C(57)	122.3(6)
O(5)-Ru(3)-C(57)	156.7(6)
C(58)-Ru(3)-C(57)	68.5(6)
C(55)-Ru(3)-C(57)	81.8(6)
C(54)-Ru(3)-C(57)	68.8(6)

N(3)-Ru(3)-C(59)	114.7(6)
O(6)-Ru(3)-C(59)	92.2(6)
O(5)-Ru(3)-C(59)	157.6(5)
C(58)-Ru(3)-C(59)	38.2(6)
C(55)-Ru(3)-C(59)	70.3(6)
C(54)-Ru(3)-C(59)	83.1(7)
C(57)-Ru(3)-C(59)	39.5(6)
N(3)-Ru(3)-C(56)	94.1(6)
O(6)-Ru(3)-C(56)	159.9(6)
O(5)-Ru(3)-C(56)	119.6(6)
C(58)-Ru(3)-C(56)	81.0(7)
C(55)-Ru(3)-C(56)	69.4(6)
C(54)-Ru(3)-C(56)	38.8(6)
C(57)-Ru(3)-C(56)	37.6(6)
C(59)-Ru(3)-C(56)	70.5(7)
N(4)-Ru(4)-O(4)	83.5(5)
N(4)-Ru(4)-O(3)	81.9(4)
O(4)-Ru(4)-O(3)	79.2(4)
N(4)-Ru(4)-C(62)	107.0(7)
O(4)-Ru(4)-C(62)	98.7(6)
O(3)-Ru(4)-C(62)	170.7(7)
N(4)-Ru(4)-C(65)	89.8(6)
O(4)-Ru(4)-C(65)	130.9(6)
O(3)-Ru(4)-C(65)	147.7(6)
C(62)-Ru(4)-C(65)	37.8(6)
N(4)-Ru(4)-C(67)	130.5(6)
O(4)-Ru(4)-C(67)	143.7(6)
O(3)-Ru(4)-C(67)	92.2(6)
C(62)-Ru(4)-C(67)	84.2(7)
C(65)-Ru(4)-C(67)	69.8(8)
N(4)-Ru(4)-C(63)	145.4(6)
O(4)-Ru(4)-C(63)	93.0(6)
O(3)-Ru(4)-C(63)	131.4(6)
C(62)-Ru(4)-C(63)	39.4(7)
C(65)-Ru(4)-C(63)	66.7(7)
C(67)-Ru(4)-C(63)	66.5(6)
N(4)-Ru(4)-C(64)	166.2(6)
O(4)-Ru(4)-C(64)	110.2(5)

O(3)-Ru(4)-C(64)	102.1(5)
C(62)-Ru(4)-C(64)	69.9(7)
C(65)-Ru(4)-C(64)	79.8(6)
C(67)-Ru(4)-C(64)	36.9(6)
C(63)-Ru(4)-C(64)	36.0(6)
N(4)-Ru(4)-C(66)	98.4(6)
O(4)-Ru(4)-C(66)	169.6(5)
O(3)-Ru(4)-C(66)	111.2(6)
C(62)-Ru(4)-C(66)	70.9(7)
C(65)-Ru(4)-C(66)	39.2(7)
C(67)-Ru(4)-C(66)	38.8(6)
C(63)-Ru(4)-C(66)	79.6(7)
C(64)-Ru(4)-C(66)	67.8(6)
O(7)-Ru(5)-C(85)	94.9(6)
O(7)-Ru(5)-O(8)	80.4(4)
C(85)-Ru(5)-O(8)	117.7(5)
O(7)-Ru(5)-N(6)	85.0(5)
C(85)-Ru(5)-N(6)	155.7(6)
O(8)-Ru(5)-N(6)	86.3(4)
O(7)-Ru(5)-C(83)	153.8(6)
C(85)-Ru(5)-C(83)	64.1(8)
O(8)-Ru(5)-C(83)	95.1(6)
N(6)-Ru(5)-C(83)	120.8(7)
O(7)-Ru(5)-C(81)	93.1(7)
C(85)-Ru(5)-C(81)	37.3(6)
O(8)-Ru(5)-C(81)	154.1(6)
N(6)-Ru(5)-C(81)	118.3(6)
C(83)-Ru(5)-C(81)	79.7(8)
O(7)-Ru(5)-C(84)	116.9(6)
C(85)-Ru(5)-C(84)	35.0(6)
O(8)-Ru(5)-C(84)	93.2(5)
N(6)-Ru(5)-C(84)	157.8(7)
C(83)-Ru(5)-C(84)	37.2(7)
C(81)-Ru(5)-C(84)	67.2(7)
O(7)-Ru(5)-C(82)	119.5(7)
C(85)-Ru(5)-C(82)	67.5(8)
O(8)-Ru(5)-C(82)	159.6(7)
N(6)-Ru(5)-C(82)	91.4(7)

C(83)-Ru(5)-C(82)	68.8(8)
C(81)-Ru(5)-C(82)	38.5(7)
C(84)-Ru(5)-C(82)	81.4(7)
O(7)-Ru(5)-C(86)	158.8(6)
C(85)-Ru(5)-C(86)	79.2(8)
O(8)-Ru(5)-C(86)	120.5(6)
N(6)-Ru(5)-C(86)	92.2(6)
C(83)-Ru(5)-C(86)	38.1(6)
C(81)-Ru(5)-C(86)	69.8(9)
C(84)-Ru(5)-C(86)	69.0(7)
C(82)-Ru(5)-C(86)	39.4(7)
C(107)-Ru(6)-C(108)	37.9(7)
C(107)-Ru(6)-O(11)	105.7(7)
C(108)-Ru(6)-O(11)	89.5(6)
C(107)-Ru(6)-O(12)	169.3(6)
C(108)-Ru(6)-O(12)	134.4(7)
O(11)-Ru(6)-O(12)	79.3(5)
C(107)-Ru(6)-C(104)	81.3(7)
C(108)-Ru(6)-C(104)	71.1(8)
O(11)-Ru(6)-C(104)	138.6(5)
O(12)-Ru(6)-C(104)	88.7(6)
C(107)-Ru(6)-N(5)	104.3(7)
C(108)-Ru(6)-N(5)	136.7(8)
O(11)-Ru(6)-N(5)	82.2(5)
O(12)-Ru(6)-N(5)	85.7(5)
C(104)-Ru(6)-N(5)	136.7(7)
C(107)-Ru(6)-C(109)	69.3(8)
C(108)-Ru(6)-C(109)	39.3(8)
O(11)-Ru(6)-C(109)	103.1(6)
O(12)-Ru(6)-C(109)	100.5(7)
C(104)-Ru(6)-C(109)	40.1(7)
N(5)-Ru(6)-C(109)	172.4(7)
C(107)-Ru(6)-C(106)	35.6(7)
C(108)-Ru(6)-C(106)	67.0(7)
O(11)-Ru(6)-C(106)	137.6(6)
O(12)-Ru(6)-C(106)	142.3(6)
C(104)-Ru(6)-C(106)	68.1(6)
N(5)-Ru(6)-C(106)	91.4(6)

C(109)-Ru(6)-C(106)	81.0(7)
C(107)-Ru(6)-C(105)	70.3(8)
C(108)-Ru(6)-C(105)	84.0(8)
O(11)-Ru(6)-C(105)	173.0(6)
O(12)-Ru(6)-C(105)	103.7(6)
C(104)-Ru(6)-C(105)	36.3(6)
N(5)-Ru(6)-C(105)	104.2(6)
C(109)-Ru(6)-C(105)	70.2(7)
C(106)-Ru(6)-C(105)	40.9(7)
C(112)-O(1)-Ru(2)	115.7(10)
C(111)-O(2)-Ru(2)	114.1(9)
C(112)-O(3)-Ru(4)	112.3(10)
C(111)-O(4)-Ru(4)	118.0(11)
C(80)-O(5)-Ru(3)	115.0(12)
C(90)-O(6)-Ru(3)	114.3(12)
C(90)-O(7)-Ru(5)	118.7(11)
C(80)-O(8)-Ru(5)	113.8(10)
C(115)-O(9)-Ru(1)	113.6(12)
C(116)-O(10)-Ru(1)	115.3(11)
C(115)-O(11)-Ru(6)	114.4(11)
C(116)-O(12)-Ru(6)	113.5(13)
C(2)-N(1)-C(1)	117.2(13)
C(2)-N(1)-Ru(1)	122.4(11)
C(1)-N(1)-Ru(1)	119.9(9)
C(20)-N(2)-C(19)	120.0(13)
C(20)-N(2)-Ru(2)	119.8(10)
C(19)-N(2)-Ru(2)	120.2(9)
C(27)-N(3)-C(28)	118.2(13)
C(27)-N(3)-Ru(3)	117.1(11)
C(28)-N(3)-Ru(3)	124.4(9)
C(29)-N(4)-C(30)	123.5(13)
C(29)-N(4)-Ru(4)	117.5(11)
C(30)-N(4)-Ru(4)	119.0(10)
C(46)-N(5)-C(94)	119.4(15)
C(46)-N(5)-Ru(6)	123.0(11)
C(94)-N(5)-Ru(6)	117.5(12)
C(52)-N(6)-C(53)	114.1(13)
C(52)-N(6)-Ru(5)	124.1(12)

C(53)-N(6)-Ru(5)	121.3(10)
N(1)-C(1)-C(3)	121.2(14)
N(1)-C(2)-C(4)	123.6(17)
C(1)-C(3)-C(5)	119.2(16)
C(2)-C(4)-C(5)	122.6(16)
C(6)-C(5)-C(4)	121.8(14)
C(6)-C(5)-C(3)	122.4(16)
C(4)-C(5)-C(3)	115.9(14)
C(7)-C(6)-C(5)	176.4(16)
C(6)-C(7)-C(8)	171.2(17)
C(9)-C(8)-C(7)	122.2(14)
C(9)-C(8)-C(13)	117.2(12)
C(7)-C(8)-C(13)	120.4(14)
C(8)-C(9)-C(10)	123.5(12)
C(14)-C(10)-C(9)	124.8(12)
C(14)-C(10)-C(11)	117.6(12)
C(9)-C(10)-C(11)	117.4(13)
C(10)-C(11)-C(12)	120.2(12)
C(13)-C(12)-C(11)	120.3(12)
C(13)-C(12)-C(22)	120.8(13)
C(11)-C(12)-C(22)	118.9(12)
C(8)-C(13)-C(12)	121.2(14)
C(15)-C(14)-C(10)	176.4(14)
C(14)-C(15)-C(16)	173.7(15)
C(18)-C(16)-C(17)	120.0(14)
C(18)-C(16)-C(15)	119.6(13)
C(17)-C(16)-C(15)	120.3(13)
C(19)-C(17)-C(16)	119.6(14)
C(16)-C(18)-C(20)	118.3(14)
N(2)-C(19)-C(17)	119.8(13)
N(2)-C(20)-C(18)	122.0(14)
C(23)-C(22)-C(12)	177.2(17)
C(22)-C(23)-C(24)	173.8(18)
C(26)-C(24)-C(25)	120.0(14)
C(26)-C(24)-C(23)	123.3(13)
C(25)-C(24)-C(23)	116.6(16)
C(24)-C(25)-C(28)	116.8(16)
C(24)-C(26)-C(27)	121.3(14)

N(3)-C(27)-C(26)	119.7(16)
N(3)-C(28)-C(25)	123.7(14)
C(31)-C(29)-N(4)	116.3(15)
C(32)-C(30)-N(4)	119.8(14)
C(29)-C(31)-C(33)	125.1(14)
C(30)-C(32)-C(33)	120.3(16)
C(32)-C(33)-C(34)	121.2(15)
C(32)-C(33)-C(31)	114.8(14)
C(34)-C(33)-C(31)	123.8(14)
C(35)-C(34)-C(33)	175(2)
C(34)-C(35)-C(36)	174(2)
C(37)-C(36)-C(35)	120.8(14)
C(37)-C(36)-C(93)	120.9(15)
C(35)-C(36)-C(93)	118.1(14)
C(36)-C(37)-C(38)	119.5(14)
C(41)-C(38)-C(39)	122.8(15)
C(41)-C(38)-C(37)	120.0(15)
C(39)-C(38)-C(37)	117.1(14)
C(40)-C(39)-C(38)	123.4(16)
C(93)-C(40)-C(39)	121.0(15)
C(93)-C(40)-C(47)	119.5(14)
C(39)-C(40)-C(47)	119.4(15)
C(42)-C(41)-C(38)	174.6(18)
C(41)-C(42)-C(43)	173.5(17)
C(44)-C(43)-C(42)	118.7(16)
C(44)-C(43)-C(45)	119.5(16)
C(42)-C(43)-C(45)	121.8(18)
C(43)-C(44)-C(94)	119.2(16)
C(43)-C(45)-C(46)	118.0(17)
N(5)-C(46)-C(45)	124.4(17)
C(48)-C(47)-C(40)	179(2)
C(47)-C(48)-C(49)	175(2)
C(51)-C(49)-C(48)	121.5(16)
C(51)-C(49)-C(50)	114.1(14)
C(48)-C(49)-C(50)	124.4(15)
C(52)-C(50)-C(49)	122.1(16)
C(53)-C(51)-C(49)	120.0(16)
N(6)-C(52)-C(50)	126.2(16)

C(51)-C(53)-N(6)	123.4(15)
C(55)-C(54)-C(56)	121.3(16)
C(55)-C(54)-C(60)	117.2(15)
C(56)-C(54)-C(60)	121.3(16)
C(55)-C(54)-Ru(3)	72.0(9)
C(56)-C(54)-Ru(3)	71.0(9)
C(60)-C(54)-Ru(3)	126.8(13)
C(58)-C(55)-C(54)	117.2(15)
C(58)-C(55)-Ru(3)	68.9(9)
C(54)-C(55)-Ru(3)	70.4(9)
C(57)-C(56)-C(54)	118.8(17)
C(57)-C(56)-Ru(3)	70.8(11)
C(54)-C(56)-Ru(3)	70.2(10)
C(59)-C(57)-C(56)	121.5(16)
C(59)-C(57)-Ru(3)	69.3(10)
C(56)-C(57)-Ru(3)	71.5(11)
C(55)-C(58)-C(59)	125.0(17)
C(55)-C(58)-Ru(3)	73.0(9)
C(59)-C(58)-Ru(3)	71.2(9)
C(58)-C(59)-C(57)	115.9(16)
C(58)-C(59)-C(92)	122.7(17)
C(57)-C(59)-C(92)	121.5(15)
C(58)-C(59)-Ru(3)	70.6(10)
C(57)-C(59)-Ru(3)	71.2(10)
C(92)-C(59)-Ru(3)	128.3(13)
C(54)-C(60)-C(91)	110.4(17)
C(54)-C(60)-C(61)	117.5(14)
C(91)-C(60)-C(61)	107.9(15)
C(65)-C(62)-C(63)	113.7(18)
C(65)-C(62)-C(113)	123.0(19)
C(63)-C(62)-C(113)	123.1(18)
C(65)-C(62)-Ru(4)	72.1(11)
C(63)-C(62)-Ru(4)	71.4(9)
C(113)-C(62)-Ru(4)	128.3(13)
C(64)-C(63)-C(62)	124.8(18)
C(64)-C(63)-Ru(4)	73.1(9)
C(62)-C(63)-Ru(4)	69.2(10)
C(63)-C(64)-C(67)	121.1(18)

C(63)-C(64)-Ru(4)	70.9(10)
C(67)-C(64)-Ru(4)	71.1(10)
C(62)-C(65)-C(66)	123.8(18)
C(62)-C(65)-Ru(4)	70.1(11)
C(66)-C(65)-Ru(4)	72.1(10)
C(67)-C(66)-C(65)	116.5(17)
C(67)-C(66)-Ru(4)	69.7(11)
C(65)-C(66)-Ru(4)	68.7(11)
C(64)-C(67)-C(66)	119.3(17)
C(64)-C(67)-C(68)	122.2(17)
C(66)-C(67)-C(68)	118.5(15)
C(64)-C(67)-Ru(4)	71.9(11)
C(66)-C(67)-Ru(4)	71.6(11)
C(68)-C(67)-Ru(4)	125.6(12)
C(120)-C(68)-C(67)	110.1(16)
C(120)-C(68)-C(69)	115.8(18)
C(67)-C(68)-C(69)	109.5(15)
C(72)-C(71)-C(76)	118.2(16)
C(72)-C(71)-Ru(2)	70.1(9)
C(76)-C(71)-Ru(2)	68.7(9)
C(71)-C(72)-C(73)	119.7(13)
C(71)-C(72)-C(77)	120.5(15)
C(73)-C(72)-C(77)	119.8(14)
C(71)-C(72)-Ru(2)	71.9(9)
C(73)-C(72)-Ru(2)	70.4(9)
C(77)-C(72)-Ru(2)	129.0(11)
C(74)-C(73)-C(72)	121.9(15)
C(74)-C(73)-Ru(2)	73.6(10)
C(72)-C(73)-Ru(2)	70.7(9)
C(73)-C(74)-C(75)	121.3(16)
C(73)-C(74)-Ru(2)	69.7(10)
C(75)-C(74)-Ru(2)	71.7(11)
C(76)-C(75)-C(78)	121.6(16)
C(76)-C(75)-C(74)	116.9(14)
C(78)-C(75)-C(74)	121.4(17)
C(76)-C(75)-Ru(2)	66.7(8)
C(78)-C(75)-Ru(2)	132.1(12)
C(74)-C(75)-Ru(2)	71.5(10)

C(75)-C(76)-C(71)	121.8(15)
C(75)-C(76)-Ru(2)	73.0(9)
C(71)-C(76)-Ru(2)	73.4(9)
C(75)-C(78)-C(79)	113.6(16)
C(75)-C(78)-C(70)	107.7(15)
C(79)-C(78)-C(70)	109.6(19)
O(8)-C(80)-O(5)	130.1(16)
O(8)-C(80)-C(90)	119.4(17)
O(5)-C(80)-C(90)	110.5(18)
C(85)-C(81)-C(82)	116.0(19)
C(85)-C(81)-C(121)	127(2)
C(82)-C(81)-C(121)	116.2(17)
C(85)-C(81)-Ru(5)	69.1(12)
C(82)-C(81)-Ru(5)	70.4(12)
C(121)-C(81)-Ru(5)	122.9(15)
C(81)-C(82)-C(86)	119.1(19)
C(81)-C(82)-Ru(5)	71.1(13)
C(86)-C(82)-Ru(5)	71.3(11)
C(84)-C(83)-C(86)	125.6(19)
C(84)-C(83)-C(87)	114.9(16)
C(86)-C(83)-C(87)	119.0(19)
C(84)-C(83)-Ru(5)	74.0(12)
C(86)-C(83)-Ru(5)	73.1(11)
C(87)-C(83)-Ru(5)	120.7(12)
C(85)-C(84)-C(83)	114.5(18)
C(85)-C(84)-Ru(5)	68.9(11)
C(83)-C(84)-Ru(5)	68.8(11)
C(84)-C(85)-C(81)	130(2)
C(84)-C(85)-Ru(5)	76.1(13)
C(81)-C(85)-Ru(5)	73.5(13)
C(83)-C(86)-C(82)	115(2)
C(83)-C(86)-Ru(5)	68.8(11)
C(82)-C(86)-Ru(5)	69.3(12)
C(83)-C(87)-C(89)	110.0(14)
C(83)-C(87)-C(88)	111.2(15)
C(89)-C(87)-C(88)	109.7(16)
O(6)-C(90)-O(7)	133.2(17)
O(6)-C(90)-C(80)	118.9(18)

O(7)-C(90)-C(80)	107.3(17)
C(40)-C(93)-C(36)	117.8(14)
N(5)-C(94)-C(44)	119.3(17)
C(96)-C(95)-C(100)	121.9(13)
C(96)-C(95)-Ru(1)	72.0(9)
C(100)-C(95)-Ru(1)	74.1(9)
C(97)-C(96)-C(95)	119.3(15)
C(97)-C(96)-C(102)	119.6(16)
C(95)-C(96)-C(102)	120.8(13)
C(97)-C(96)-Ru(1)	70.3(9)
C(95)-C(96)-Ru(1)	70.7(10)
C(102)-C(96)-Ru(1)	126.1(12)
C(96)-C(97)-C(98)	122.7(16)
C(96)-C(97)-Ru(1)	72.6(9)
C(98)-C(97)-Ru(1)	72.4(9)
C(97)-C(98)-C(99)	121.5(13)
C(97)-C(98)-Ru(1)	70.8(8)
C(99)-C(98)-Ru(1)	71.9(8)
C(101)-C(99)-C(100)	123.9(15)
C(101)-C(99)-C(98)	121.3(13)
C(100)-C(99)-C(98)	114.8(14)
C(101)-C(99)-Ru(1)	128.3(11)
C(100)-C(99)-Ru(1)	71.6(8)
C(98)-C(99)-Ru(1)	68.6(9)
C(95)-C(100)-C(99)	119.4(14)
C(95)-C(100)-Ru(1)	68.2(9)
C(99)-C(100)-Ru(1)	69.9(9)
C(103)-C(102)-C(96)	117.2(15)
C(103)-C(102)-C(119)	106.5(15)
C(96)-C(102)-C(119)	106.1(15)
C(105)-C(104)-C(109)	124.3(18)
C(105)-C(104)-Ru(6)	73.9(9)
C(109)-C(104)-Ru(6)	70.3(11)
C(104)-C(105)-C(106)	115.4(17)
C(104)-C(105)-C(117)	125.6(18)
C(106)-C(105)-C(117)	119.0(15)
C(104)-C(105)-Ru(6)	69.8(10)
C(106)-C(105)-Ru(6)	71.2(9)

C(117)-C(105)-Ru(6)	130.5(14)
C(107)-C(106)-C(105)	118.8(17)
C(107)-C(106)-Ru(6)	67.7(12)
C(105)-C(106)-Ru(6)	67.9(9)
C(106)-C(107)-C(108)	125(2)
C(106)-C(107)-Ru(6)	76.7(13)
C(108)-C(107)-Ru(6)	70.9(14)
C(107)-C(108)-C(109)	119(2)
C(107)-C(108)-C(110)	120(2)
C(109)-C(108)-C(110)	121(2)
C(107)-C(108)-Ru(6)	71.2(14)
C(109)-C(108)-Ru(6)	71.3(13)
C(110)-C(108)-Ru(6)	125.9(14)
C(104)-C(109)-C(108)	116.8(18)
C(104)-C(109)-Ru(6)	69.6(10)
C(108)-C(109)-Ru(6)	69.4(12)
O(4)-C(111)-O(2)	131.3(15)
O(4)-C(111)-C(112)	110.2(17)
O(2)-C(111)-C(112)	118.5(14)
O(3)-C(112)-O(1)	128.9(15)
O(3)-C(112)-C(111)	119.4(15)
O(1)-C(112)-C(111)	111.7(17)
O(11)-C(115)-O(9)	126.3(17)
O(11)-C(115)-C(116)	112.8(17)
O(9)-C(115)-C(116)	120.8(19)
O(12)-C(116)-O(10)	128.0(18)
O(12)-C(116)-C(115)	120(2)
O(10)-C(116)-C(115)	112.0(17)
C(114)-C(117)-C(105)	112.3(18)
C(114)-C(117)-C(118)	112.5(19)
C(105)-C(117)-C(118)	105.4(18)
O(3S)-Cl(1)-O(4S)	110.5(7)
O(3S)-Cl(1)-O(2S)	109.7(8)
O(4S)-Cl(1)-O(2S)	106.3(7)
O(3S)-Cl(1)-O(1S)	111.7(7)
O(4S)-Cl(1)-O(1S)	111.3(6)
O(2S)-Cl(1)-O(1S)	107.2(6)
O(8S)-Cl(2)-O(7S)	111.5(8)

O(8S)-Cl(2)-O(6S)	109.8(7)
O(7S)-Cl(2)-O(6S)	110.2(7)
O(8S)-Cl(2)-O(5S)	107.7(9)
O(7S)-Cl(2)-O(5S)	108.4(7)
O(6S)-Cl(2)-O(5S)	109.2(7)
O(10')-Cl(3)-O(10S)	117.7(16)
O(10')-Cl(3)-O(9S)	42.3(13)
O(10S)-Cl(3)-O(9S)	110.4(10)
O(10')-Cl(3)-O(11')	109(2)
O(10S)-Cl(3)-O(11')	132.4(19)
O(9S)-Cl(3)-O(11')	97(2)
O(10')-Cl(3)-O(9')	126.4(18)
O(10S)-Cl(3)-O(9')	39.4(12)
O(9S)-Cl(3)-O(9')	146.1(14)
O(11')-Cl(3)-O(9')	116(2)
O(10')-Cl(3)-O(12')	105.2(18)
O(10S)-Cl(3)-O(12')	53.7(12)
O(9S)-Cl(3)-O(12')	69.8(14)
O(11')-Cl(3)-O(12')	105.7(17)
O(9')-Cl(3)-O(12')	90.7(17)
O(10')-Cl(3)-O(11S)	129.7(17)
O(10S)-Cl(3)-O(11S)	111.0(11)
O(9S)-Cl(3)-O(11S)	109.3(10)
O(11')-Cl(3)-O(11S)	21(2)
O(9')-Cl(3)-O(11S)	98.9(16)
O(12')-Cl(3)-O(11S)	93.4(14)
O(10')-Cl(3)-O(12S)	66.5(14)
O(10S)-Cl(3)-O(12S)	109.2(9)
O(9S)-Cl(3)-O(12S)	108.1(10)
O(11')-Cl(3)-O(12S)	97.7(16)
O(9')-Cl(3)-O(12S)	78.8(14)
O(12')-Cl(3)-O(12S)	156.6(12)
O(11S)-Cl(3)-O(12S)	108.8(10)
O(10')-O(9S)-Cl(3)	67.0(12)
O(10')-O(9S)-O(12')	113.3(19)
Cl(3)-O(9S)-O(12')	55.1(9)
O(10S)-O(9')-Cl(3)	69.8(12)
O(10S)-O(9')-O(12S)	110.0(19)

Cl(3)-O(9')-O(12S)	50.9(9)
O(9')-O(10S)-O(12')	129(2)
O(9')-O(10S)-Cl(3)	70.8(12)
O(12')-O(10S)-Cl(3)	63.8(9)
O(9S)-O(10')-Cl(3)	70.7(12)
O(9S)-O(10')-O(12S)	127.6(17)
Cl(3)-O(10')-O(12S)	57.9(10)
O(11')-O(11S)-Cl(3)	79(2)
O(11S)-O(11')-Cl(3)	80(2)
Cl(3)-O(12S)-O(10')	55.6(8)
Cl(3)-O(12S)-O(9')	50.3(8)
O(10')-O(12S)-O(9')	96.4(13)
O(10S)-O(12')-Cl(3)	62.5(9)
O(10S)-O(12')-O(9S)	105.6(15)
Cl(3)-O(12')-O(9S)	55.1(9)
O(20S)-Cl(4)-O(17S)	111.6(12)
O(20S)-Cl(4)-O(14S)	110.3(18)
O(17S)-Cl(4)-O(14S)	99.9(17)
O(20S)-Cl(4)-O(13S)	57.8(13)
O(17S)-Cl(4)-O(13S)	149.2(16)
O(14S)-Cl(4)-O(13S)	110.9(10)
O(20S)-Cl(4)-O(15S)	136.1(17)
O(17S)-Cl(4)-O(15S)	55.4(12)
O(14S)-Cl(4)-O(15S)	113.2(10)
O(13S)-Cl(4)-O(15S)	109.6(10)
O(20S)-Cl(4)-O(19S)	108.5(11)
O(17S)-Cl(4)-O(19S)	107.6(11)
O(14S)-Cl(4)-O(19S)	8.0(19)
O(13S)-Cl(4)-O(19S)	103.1(18)
O(15S)-Cl(4)-O(19S)	115.4(18)
O(20S)-Cl(4)-O(18S)	110.8(11)
O(17S)-Cl(4)-O(18S)	110.7(11)
O(14S)-Cl(4)-O(18S)	113.1(15)
O(13S)-Cl(4)-O(18S)	57.5(12)
O(15S)-Cl(4)-O(18S)	55.8(11)
O(19S)-Cl(4)-O(18S)	107.4(11)
O(20S)-Cl(4)-O(16S)	51.8(13)
O(17S)-Cl(4)-O(16S)	60.9(12)

O(14S)-Cl(4)-O(16S)	108.7(9)
O(13S)-Cl(4)-O(16S)	107.0(10)
O(15S)-Cl(4)-O(16S)	107.2(10)
O(19S)-Cl(4)-O(16S)	114.1(17)
O(18S)-Cl(4)-O(16S)	138.2(14)
O(18S)-O(13S)-O(20S)	115.8(15)
O(18S)-O(13S)-Cl(4)	60.7(9)
O(20S)-O(13S)-Cl(4)	60.2(10)
O(17S)-O(15S)-O(18S)	124.0(14)
O(17S)-O(15S)-Cl(4)	62.1(10)
O(18S)-O(15S)-Cl(4)	62.5(9)
O(20S)-O(16S)-Cl(4)	61.7(10)
O(20S)-O(16S)-O(17S)	118.0(14)
Cl(4)-O(16S)-O(17S)	57.4(8)
O(15S)-O(17S)-Cl(4)	62.5(9)
O(15S)-O(17S)-O(16S)	113.6(17)
Cl(4)-O(17S)-O(16S)	61.7(9)
O(13S)-O(18S)-O(15S)	119.0(15)
O(13S)-O(18S)-Cl(4)	61.8(9)
O(15S)-O(18S)-Cl(4)	61.7(9)
O(16S)-O(20S)-Cl(4)	66.5(10)
O(16S)-O(20S)-O(13S)	124.7(16)
Cl(4)-O(20S)-O(13S)	62.0(10)
O(21S)-Cl(5)-O(23S)	85(4)
O(21S)-Cl(5)-O(22S)	118(4)
O(23S)-Cl(5)-O(22S)	130(3)
O(21S)-Cl(5)-O(24S)	83(3)
O(23S)-Cl(5)-O(24S)	111(3)
O(22S)-Cl(5)-O(24S)	115(3)
Cl(5)-O(21S)-O(24S)	48.9(16)
Cl(5)-O(24S)-O(2WA)	142(3)
Cl(5)-O(24S)-O(21S)	48.0(15)
O(2WA)-O(24S)-O(21S)	113(3)
O(27S)-Cl(6)-O(25S)	110.1(11)
O(27S)-Cl(6)-O(26S)	111.0(11)
O(25S)-Cl(6)-O(26S)	108.1(11)
O(27S)-Cl(6)-O(28S)	108.7(11)
O(25S)-Cl(6)-O(28S)	109.5(10)

O(26S)-Cl(6)-O(28S)	109.4(10)
C(1N)-N(1N)-O(2N)	120(3)
C(1N)-N(1N)-O(1N)	109(3)
O(2N)-N(1N)-O(1N)	130(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for p-1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	124(1)	66(1)	126(1)	36(1)	29(1)	18(1)
Ru(2)	129(1)	80(1)	113(1)	32(1)	20(1)	15(1)
Ru(3)	132(1)	89(1)	143(1)	55(1)	34(1)	19(1)
Ru(4)	133(1)	79(1)	125(1)	24(1)	28(1)	8(1)
Ru(5)	152(2)	100(1)	150(1)	64(1)	52(1)	39(1)
Ru(6)	128(1)	95(1)	138(1)	46(1)	18(1)	9(1)
O(1)	146(8)	76(5)	101(6)	29(5)	17(6)	4(5)
O(2)	109(8)	87(5)	115(7)	34(5)	10(7)	5(5)
O(3)	136(8)	94(6)	124(8)	45(5)	28(8)	28(6)
O(4)	105(8)	85(5)	127(7)	23(5)	28(6)	14(5)
O(5)	122(9)	103(6)	148(8)	55(6)	49(7)	32(6)
O(6)	117(8)	116(7)	147(9)	58(6)	29(8)	26(6)
O(7)	127(9)	95(6)	141(8)	54(5)	29(6)	29(5)
O(8)	103(8)	97(6)	144(8)	54(5)	38(7)	25(5)
O(9)	112(8)	81(5)	124(7)	39(5)	30(6)	22(5)
O(10)	139(8)	74(5)	112(7)	45(5)	9(7)	8(6)
O(11)	123(8)	80(5)	127(7)	40(5)	14(7)	13(6)
O(12)	125(9)	93(6)	136(8)	52(6)	19(7)	18(5)
N(1)	143(12)	71(6)	123(9)	43(6)	36(8)	22(6)
N(2)	113(10)	79(6)	131(8)	46(6)	24(7)	14(6)
N(3)	139(12)	82(6)	131(10)	37(7)	32(7)	14(6)
N(4)	128(11)	87(6)	124(9)	28(6)	20(7)	0(6)
N(5)	159(14)	106(8)	125(10)	40(7)	36(9)	10(7)
N(6)	144(12)	87(6)	146(8)	55(7)	35(9)	32(7)
C(1)	158(16)	63(6)	159(13)	39(7)	66(11)	29(7)
C(2)	210(20)	74(7)	145(12)	23(7)	65(12)	-12(9)
C(3)	187(18)	95(7)	120(11)	36(7)	49(11)	10(9)
C(4)	280(30)	73(7)	132(13)	27(7)	76(14)	-8(10)
C(5)	153(15)	75(6)	110(9)	33(6)	13(9)	11(7)
C(6)	137(14)	100(6)	104(10)	33(6)	22(9)	8(8)
C(7)	177(17)	81(6)	139(11)	42(5)	70(11)	40(9)
C(8)	130(14)	81(5)	114(8)	34(5)	15(10)	7(8)
C(9)	126(13)	78(6)	117(7)	44(5)	34(9)	32(7)

C(10)	121(13)	79(6)	115(6)	37(5)	19(9)	10(7)
C(11)	107(12)	80(6)	109(7)	39(6)	32(8)	11(7)
C(12)	113(12)	82(6)	104(8)	34(6)	25(8)	8(7)
C(13)	112(12)	81(6)	113(9)	35(6)	7(8)	11(7)
C(14)	98(11)	80(7)	115(6)	39(6)	12(9)	17(7)
C(15)	85(11)	91(8)	116(6)	46(7)	20(9)	1(7)
C(16)	84(11)	88(7)	117(6)	39(6)	18(8)	8(7)
C(17)	103(12)	77(7)	117(7)	37(6)	12(9)	4(7)
C(18)	167(16)	69(7)	123(8)	37(7)	15(11)	10(8)
C(19)	125(13)	74(7)	122(8)	44(7)	32(9)	9(7)
C(20)	171(17)	82(8)	120(9)	41(7)	25(11)	28(8)
C(22)	115(13)	92(8)	118(10)	43(7)	26(9)	23(8)
C(23)	132(14)	92(8)	116(11)	40(7)	30(9)	28(8)
C(24)	124(14)	86(7)	147(13)	55(8)	25(8)	18(7)
C(25)	117(13)	105(8)	141(12)	51(8)	26(8)	8(7)
C(26)	128(14)	94(8)	147(13)	54(9)	19(8)	11(8)
C(27)	147(15)	102(9)	157(14)	66(9)	1(10)	1(8)
C(28)	134(14)	81(8)	151(14)	49(8)	25(8)	4(8)
C(29)	103(12)	82(7)	114(8)	20(7)	16(8)	13(7)
C(30)	112(14)	96(8)	135(10)	40(6)	44(9)	16(8)
C(31)	133(15)	91(8)	127(9)	32(6)	21(9)	20(8)
C(32)	115(14)	111(8)	134(9)	43(7)	25(10)	23(9)
C(33)	119(14)	107(8)	121(7)	44(6)	31(9)	16(8)
C(34)	163(18)	102(9)	122(7)	49(7)	29(12)	12(10)
C(35)	114(15)	116(10)	121(7)	45(7)	23(11)	15(9)
C(36)	81(11)	109(7)	124(7)	48(6)	20(8)	4(8)
C(37)	121(14)	104(7)	133(8)	48(6)	25(10)	11(9)
C(38)	120(14)	106(6)	129(9)	50(6)	9(10)	-5(9)
C(39)	109(13)	98(6)	130(10)	46(6)	17(9)	-9(8)
C(40)	129(14)	112(8)	125(8)	49(7)	29(10)	33(9)
C(41)	147(15)	115(6)	120(11)	53(7)	48(10)	41(10)
C(42)	163(16)	108(6)	127(12)	57(8)	35(11)	14(10)
C(43)	153(17)	104(6)	160(15)	58(8)	48(12)	40(10)
C(44)	200(20)	104(7)	134(14)	32(9)	46(12)	-14(11)
C(45)	126(14)	103(7)	148(13)	55(8)	41(10)	33(9)
C(46)	169(18)	102(7)	125(13)	32(9)	34(11)	-2(10)
C(47)	134(15)	104(9)	134(11)	52(8)	12(10)	-4(9)
C(48)	180(18)	121(11)	136(11)	60(9)	38(12)	47(11)

C(49)	132(15)	109(8)	132(9)	53(7)	26(10)	36(9)
C(50)	143(15)	113(9)	144(9)	61(7)	16(11)	34(9)
C(51)	97(12)	120(8)	146(10)	62(8)	20(9)	18(8)
C(52)	139(14)	93(7)	132(10)	47(7)	-9(10)	1(9)
C(53)	146(16)	100(9)	148(10)	51(7)	19(12)	11(9)
C(54)	138(14)	106(8)	150(9)	52(7)	63(9)	36(7)
C(55)	125(14)	115(9)	150(9)	63(8)	43(10)	25(7)
C(56)	125(15)	119(10)	156(11)	72(8)	35(10)	32(7)
C(57)	120(14)	123(10)	155(10)	84(8)	13(10)	29(8)
C(58)	110(14)	113(9)	151(10)	70(7)	24(9)	32(7)
C(59)	123(15)	123(10)	156(10)	72(8)	30(10)	29(8)
C(60)	184(17)	92(8)	150(10)	48(8)	70(10)	29(7)
C(61)	173(18)	127(12)	158(11)	55(10)	45(11)	43(11)
C(62)	116(15)	122(11)	171(13)	54(10)	48(12)	2(9)
C(63)	142(16)	98(9)	157(12)	39(9)	32(12)	7(9)
C(64)	76(11)	99(8)	139(11)	25(7)	17(9)	-6(7)
C(65)	175(18)	93(9)	125(11)	15(8)	27(11)	-19(8)
C(66)	139(16)	104(10)	142(12)	26(8)	36(11)	2(8)
C(67)	175(17)	84(8)	140(12)	28(8)	33(11)	13(8)
C(68)	166(15)	107(9)	140(13)	35(9)	33(11)	11(10)
C(69)	190(16)	140(14)	191(19)	51(13)	62(15)	75(14)
C(70)	164(17)	103(11)	300(30)	30(15)	102(18)	-12(10)
C(71)	143(15)	94(7)	147(12)	49(7)	33(9)	24(8)
C(72)	121(13)	81(6)	127(10)	33(6)	48(8)	30(7)
C(73)	143(15)	110(7)	131(11)	40(8)	42(8)	44(9)
C(74)	157(16)	111(7)	116(11)	43(7)	26(9)	7(9)
C(75)	151(15)	97(7)	139(11)	46(7)	52(9)	11(7)
C(76)	162(16)	87(6)	144(12)	55(7)	48(8)	33(8)
C(77)	188(18)	83(7)	154(14)	25(7)	60(12)	49(9)
C(78)	160(16)	99(7)	179(15)	27(8)	73(12)	17(8)
C(79)	169(16)	111(11)	220(20)	55(13)	67(15)	23(10)
C(80)	122(10)	100(8)	114(10)	51(6)	39(9)	25(8)
C(81)	220(20)	108(7)	141(15)	51(9)	46(10)	25(10)
C(82)	168(19)	134(9)	172(17)	53(10)	78(10)	54(9)
C(83)	146(16)	124(8)	173(13)	70(8)	71(9)	37(8)
C(84)	134(16)	97(7)	175(15)	64(8)	55(9)	24(8)
C(85)	121(14)	101(7)	194(15)	24(9)	68(9)	36(8)
C(86)	160(17)	128(9)	178(16)	79(9)	57(10)	48(9)

C(87)	151(16)	131(9)	159(12)	75(8)	58(9)	20(9)
C(88)	128(17)	220(20)	203(15)	125(14)	31(11)	24(13)
C(89)	112(14)	148(13)	179(16)	79(11)	52(11)	19(9)
C(90)	122(10)	87(8)	146(12)	58(6)	21(10)	26(7)
C(91)	260(30)	127(10)	197(19)	78(11)	95(17)	84(13)
C(92)	125(15)	125(10)	177(13)	67(9)	30(11)	4(9)
C(93)	122(13)	95(8)	130(8)	45(6)	19(10)	10(8)
C(94)	155(17)	97(8)	149(14)	18(8)	46(11)	-21(9)
C(95)	75(11)	73(7)	175(14)	58(8)	25(8)	21(6)
C(96)	129(15)	95(8)	151(11)	49(8)	36(9)	32(8)
C(97)	118(13)	71(7)	117(11)	14(7)	18(8)	26(7)
C(98)	140(15)	77(8)	109(11)	25(7)	18(8)	29(7)
C(99)	109(12)	79(7)	128(11)	38(7)	19(8)	13(7)
C(100)	119(13)	75(7)	153(13)	40(8)	32(9)	18(7)
C(101)	118(14)	105(10)	147(13)	52(9)	38(9)	31(9)
C(102)	145(16)	109(8)	145(11)	53(8)	39(8)	34(9)
C(103)	165(18)	97(8)	207(17)	51(9)	66(13)	26(9)
C(104)	102(13)	91(9)	164(10)	28(9)	17(10)	10(7)
C(105)	175(16)	87(9)	141(9)	52(8)	2(9)	6(8)
C(106)	121(14)	99(9)	146(9)	40(9)	-2(10)	2(8)
C(107)	165(15)	140(11)	168(9)	80(10)	24(10)	23(9)
C(108)	152(19)	159(15)	141(9)	51(9)	28(10)	68(10)
C(109)	146(18)	133(13)	148(9)	30(10)	-9(12)	33(9)
C(110)	196(12)	216(12)	167(8)	66(8)	44(8)	73(9)
C(111)	106(10)	72(7)	111(10)	28(7)	5(11)	-4(7)
C(112)	123(10)	83(7)	94(10)	18(7)	20(11)	16(7)
C(113)	175(19)	127(12)	154(14)	47(10)	46(13)	5(10)
C(114)	238(19)	147(16)	182(18)	79(15)	52(16)	10(15)
C(115)	121(10)	67(7)	125(11)	32(7)	4(9)	-5(9)
C(116)	130(11)	87(9)	104(11)	23(7)	4(9)	-10(10)
C(117)	201(18)	107(11)	154(9)	56(10)	24(13)	25(11)
C(118)	280(20)	230(20)	190(20)	123(19)	28(19)	100(20)
C(119)	172(11)	169(10)	150(8)	52(8)	38(7)	15(8)
C(120)	179(17)	121(12)	162(16)	56(11)	50(12)	38(12)
C(121)	220(20)	112(9)	170(16)	44(10)	64(12)	8(10)
Cl(1)	130(4)	76(2)	133(3)	43(2)	29(3)	20(2)
O(1S)	135(8)	95(6)	142(7)	39(5)	24(6)	20(5)
O(2S)	159(9)	170(8)	178(9)	47(7)	73(7)	10(6)

O(3S)	173(9)	170(8)	210(9)	87(8)	32(7)	23(7)
O(4S)	130(8)	120(6)	137(7)	49(5)	32(6)	29(6)
Cl(2)	160(5)	100(3)	191(5)	76(3)	52(4)	41(3)
O(5S)	188(9)	136(8)	186(9)	60(7)	56(7)	35(7)
O(6S)	164(9)	139(7)	172(8)	66(7)	60(7)	42(6)
O(7S)	139(8)	112(6)	147(7)	52(6)	48(6)	29(6)
O(8S)	165(9)	140(7)	191(9)	76(7)	34(7)	35(7)
Cl(3)	155(5)	115(3)	122(4)	43(3)	38(4)	29(3)
O(9S)	162(19)	155(17)	163(18)	64(14)	34(15)	-4(14)
O(9')	160(18)	127(15)	175(18)	57(13)	77(14)	54(13)
O(10S)	134(16)	117(14)	123(15)	17(13)	27(13)	12(12)
O(10')	120(17)	190(18)	155(17)	69(15)	46(14)	9(14)
O(11S)	120(20)	123(16)	115(18)	49(13)	29(14)	27(13)
O(11')	118(18)	121(15)	107(15)	59(12)	-7(12)	31(12)
O(12S)	131(15)	107(12)	113(12)	50(10)	14(11)	0(11)
O(12')	169(18)	145(15)	120(14)	62(12)	27(12)	37(13)
Cl(4)	160(5)	103(3)	174(5)	39(3)	38(4)	38(3)
O(13S)	177(19)	169(17)	182(18)	71(14)	35(15)	46(14)
O(14S)	101(13)	82(10)	120(13)	36(8)	18(8)	23(7)
O(15S)	193(19)	131(15)	161(16)	55(13)	29(14)	26(14)
O(16S)	109(14)	140(14)	115(13)	33(11)	24(11)	11(11)
O(17S)	177(19)	180(18)	210(20)	60(15)	67(16)	7(15)
O(18S)	144(17)	152(15)	195(18)	50(13)	67(14)	51(13)
O(19S)	250(30)	250(30)	250(30)	87(15)	58(13)	53(12)
O(20S)	240(20)	250(20)	230(20)	104(18)	33(18)	58(18)
Cl(5)	270(20)	250(20)	270(20)	84(16)	72(17)	64(17)
O(21S)	170(20)	200(20)	160(20)	51(18)	48(18)	30(18)
O(22S)	95(12)	99(11)	105(12)	41(9)	13(9)	26(9)
O(23S)	190(20)	190(20)	190(20)	62(11)	52(11)	42(11)
O(24S)	90(17)	109(16)	129(17)	27(13)	50(14)	-1(12)
Cl(6)	293(10)	128(4)	190(6)	32(4)	62(6)	0(5)
O(25S)	269(14)	272(14)	253(13)	77(9)	89(10)	31(9)
O(26S)	410(20)	370(20)	380(20)	135(12)	97(11)	91(11)
O(27S)	430(30)	440(30)	440(30)	134(13)	122(13)	94(12)
O(28S)	200(11)	204(10)	212(10)	52(8)	57(8)	24(8)
N(1N)	190(18)	182(15)	175(16)	89(13)	62(14)	15(12)
O(1N)	239(13)	232(12)	220(12)	98(9)	71(9)	48(9)
O(2N)	191(11)	189(11)	194(11)	71(8)	50(9)	33(8)

C(1N)	243(18)	240(18)	234(18)	91(11)	58(11)	55(11)
O(1WA)	138(13)	111(12)	160(13)	38(9)	30(9)	42(9)
O(1WB)	162(15)	169(14)	157(14)	47(10)	49(10)	50(10)
O(1WC)	121(13)	114(12)	132(12)	47(9)	32(9)	39(9)
O(2WA)	206(19)	204(18)	201(18)	76(11)	44(11)	56(11)
O(2WB)	193(17)	195(16)	202(17)	61(11)	49(10)	51(10)
O(2WC)	215(18)	216(17)	207(17)	76(11)	57(10)	47(10)
O(3W)	161(11)	105(9)	135(10)	54(8)	41(8)	42(8)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for p-1.

	x	y	z	U(eq)
H(1)	11388	9063	2243	147
H(2)	9723	8313	3045	179
H(3)	10943	8112	1480	163
H(4)	9201	7410	2322	200
H(9)	8769	5987	-30	124
H(11)	8621	4212	-137	118
H(13)	9672	5582	1372	128
H(17)	7138	5057	-2065	123
H(18)	8119	3539	-1947	149
H(19)	6823	4651	-3048	128
H(20)	7903	3188	-2924	150
H(25)	8639	2848	861	147
H(26)	11088	4155	2027	149
H(27)	11637	3412	2409	168
H(28)	9111	2152	1312	149
H(29)	3415	4080	-3296	127
H(30)	4518	2631	-2996	136
H(31)	4120	4656	-2357	146
H(32)	5173	3189	-2038	146
H(37)	6046	5823	-415	145
H(39)	7037	5715	1140	140
H(44)	6128	7483	1786	186
H(45)	7638	8108	784	146
H(46)	7676	9101	1330	166
H(50)	7821	4683	2321	159
H(51)	6464	3058	1035	144
H(52)	8070	4168	2914	155
H(53)	6777	2573	1692	161
H(55)	10632	1079	2678	150
H(56)	11482	1640	1396	153
H(57)	12624	2554	2093	153
H(58)	11756	2010	3350	144

H(60)	9641	615	1723	164
H(61A)	9303	301	731	225
H(61B)	10378	767	796	225
H(61C)	9419	1031	1001	225
H(63)	2667	1564	-4795	164
H(64)	2369	2245	-5241	136
H(65)	1769	2560	-3436	173
H(66)	1395	3301	-3895	163
H(68)	2043	3727	-4624	172
H(69A)	462	3685	-5269	254
H(69B)	205	3418	-4795	254
H(69C)	115	2955	-5416	254
H(70A)	10342	5023	-3783	297
H(70B)	10018	5677	-3655	297
H(70C)	9540	5155	-4269	297
H(71)	6806	3171	-5148	153
H(73)	9022	3004	-3803	151
H(74)	9496	4079	-3340	157
H(76)	7235	4266	-4656	151
H(77A)	7149	2193	-5190	212
H(77B)	7409	2124	-4578	212
H(77C)	8325	2159	-4898	212
H(78)	9120	5090	-3264	177
H(79A)	7362	5171	-3684	247
H(79B)	7732	5248	-4218	247
H(79C)	8215	5775	-3606	247
H(82)	6471	3908	3331	181
H(84)	6800	1918	3375	155
H(85)	7904	2785	3989	167
H(86)	5223	2982	2607	174
H(87)	5759	1495	2348	167
H(88A)	5163	2120	1788	262
H(88B)	4118	2132	2012	262
H(88C)	4273	1497	1604	262
H(89A)	4044	981	2335	210
H(89B)	3890	1609	2756	210
H(89C)	4779	1274	2974	210
H(91A)	10198	-278	1199	268

H(91B)	10898	13	1845	268
H(91C)	11371	138	1355	268
H(92A)	13045	2948	3635	215
H(92B)	12812	3291	3185	215
H(92C)	13823	2986	3239	215
H(93)	6154	4161	-222	142
H(94)	6094	8526	2283	173
H(95)	12001	8930	3918	126
H(97)	10985	10529	4377	129
H(98)	11804	10904	3801	135
H(100)	12927	9269	3323	140
H(10A)	12924	10803	3171	181
H(10B)	12695	10106	2745	181
H(10C)	13807	10404	3220	181
H(102)	10267	9674	4626	157
H(10D)	10125	8710	4706	232
H(10E)	11242	8645	4570	232
H(10F)	10240	8612	4079	232
H(104)	7451	10887	2143	152
H(106)	4941	9369	1580	157
H(107)	5063	9445	2489	187
H(109)	7453	11009	3111	185
H(11A)	6681	10632	3770	286
H(11B)	6421	9892	3534	286
H(11C)	5472	10249	3555	286
H(11D)	2319	1628	-3391	232
H(11E)	3219	1496	-3716	232
H(11F)	2034	1078	-3989	232
H(11G)	7092	10270	669	282
H(11H)	7675	10127	1212	282
H(11I)	7364	10781	1289	282
H(117)	5932	9642	908	187
H(11J)	4544	10243	955	333
H(11K)	5141	10359	501	333
H(11L)	5418	10869	1121	333
H(11M)	11304	9631	5515	252
H(11N)	11837	10223	5396	252
H(11O)	12330	9623	5274	252

H(12A)	2993	3248	-5202	227
H(12B)	2222	3577	-5522	227
H(12C)	1920	2844	-5674	227
H(12D)	8561	3889	4447	253
H(12E)	7682	4291	4399	253
H(12F)	8393	4185	3958	253
H(1N1)	6476	8656	121	356
H(1N2)	6491	8379	-528	356
H(1N3)	6208	9039	-292	356