Supporting Information Available: Tables of crystallographic data, and bond lengths and angles

Sequential Protonation and Methylation of a Hydride-Osmium Complex Containing a Cyclopentadienyl Ligand with a Pendant Amine Group

Miguel A. Esteruelas, Ana M. López, Enrique Oñate, Eva Royo*

Departamento de Química Inorgánica, Instituto de Ciencia de Materiales de Aragón, Universidad de Zaragoza-CSIC, 50009 Zaragoza, Spain

Table 1. Crystal data and structure refinement for 4.

Identification code	4
Empirical formula	C29 H60 F3 N O3 Os P2 S
Formula weight	811.98
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	triclinic, P-1
Unit cell dimensions	a = 8.5873(4) A alpha = 77.9920(10) deg. b = 10.3482(5) A beta = 83.5540(10) deg. c = 20.1959(10) A gamma = 83.3500(10) deg.
Volume	1736.39(14) A^3
Z, Calculated density	2, 1.553 Mg/m^3
Absorption coefficient	3.869 mm^-1
F(000)	828
Crystal size	0.20 x 0.12 x 0.08 mm
Theta range for data collection	2.02 to 28.80 deg.
Limiting indices	-11<=h<=11, -13<=k<=13, -27<=l<=26
Reflections collected / unique	21900 / 8307 [R(int) = 0.0323]
Completeness to theta = 27.50	98.9 %
Max. and min. transmission	0.685 and 0.571
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8307 / 0 / 380
Goodness-of-fit on F^2	0.842
Final R indices [I>2sigma(I)]	R1 = 0.0261, wR2 = 0.0442
R indices (all data)	R1 = 0.0321, wR2 = 0.0451
Largest diff. peak and hole	1.122 and -0.792 e.A^-3

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

	x	y	z	U(eq)
Os	7361(1)	7038(1)	7350(1)	14(1)
S	7368(1)	7165(1)	589(1)	26(1)
P(1)	7489(1)	6198(1)	6374(1)	14(1)
P(2)	8545(1)	8973(1)	7011(1)	15(1)
F(1)	7676(3)	6660(3)	1884(1)	81(1)
F(2)	6828(2)	8657(2)	1496(1)	50(1)
F(3)	9248(3)	7971(3)	1303(2)	98(1)
O(1)	5756(3)	6885(3)	744(1)	46(1)
O(2)	8450(3)	6023(2)	537(1)	40(1)
O(3)	7649(4)	8300(3)	84(1)	62(1)
N	2619(3)	7220(2)	9696(1)	18(1)
C(1)	6133(4)	6667(3)	8390(1)	18(1)
C(2)	7695(3)	6884(3)	8451(1)	18(1)
C(3)	8735(4)	5867(3)	8214(1)	20(1)
C(4)	7796(4)	5032(3)	8003(1)	19(1)
C(5)	6189(4)	5497(3)	8117(1)	20(1)
C(6)	4657(3)	7404(3)	8661(2)	22(1)
C(7)	4094(3)	6623(3)	9350(1)	16(1)
C(8)	2836(4)	8547(3)	9830(2)	29(1)
C(9)	2271(3)	6303(3)	10363(1)	21(1)
C(10)	1258(3)	7328(3)	9284(2)	29(1)
C(11)	6872(3)	7291(3)	5570(1)	16(1)
C(12)	5175(3)	7939(3)	5623(2)	23(1)
C(13)	7172(4)	6759(3)	4905(1)	22(1)
C(14)	9401(3)	5379(3)	6053(1)	15(1)
C(15)	10606(3)	6359(3)	5732(2)	19(1)
C(16)	10125(3)	4317(3)	6611(2)	21(1)
C(17)	6260(3)	4762(3)	6539(2)	16(1)
C(18)	4498(3)	5154(3)	6678(2)	27(1)
C(19)	6482(4)	3832(3)	6028(2)	26(1)
C(20)	9032(3)	9701(3)	6093(1)	16(1)
C(21)	7576(3)	10369(3)	5732(1)	20(1)
C(22)	10307(4)	10658(3)	5910(2)	23(1)
C(23)	7454(4)	10448(3)	7326(2)	21(1)
C(24)	5694(3)	10623(3)	7216(2)	26(1)
C(25)	7562(4)	10433(3)	8081(2)	28(1)
C(26)	10458(3)	8856(3)	7400(2)	20(1)
C(27)	11239(4)	10118(3)	7406(2)	27(1)
C(28)	11678(3)	7831(3)	7138(2)	23(1)
C(29)	7790(4)	7608(5)	1361(2)	43(1)

Table 3. Bond lengths [A] and angles [deg] for 4.

Os-C(1)	2.222(3)	C(13)-H(13C)	0.9800
Os-C(5)	2.225(3)	C(14)-C(15)	1.529(4)
Os-C(4)	2.231(3)	C(14)-C(16)	1.532(4)
Os-C(2)	2.246(3)	C(14)-H(14)	1.0000
Os-C(3)	2.271(3)	C(15)-H(15A)	0.9800
Os-P(2)	2.2928(8)	C(15)-H(15B)	0.9800
Os-P(1)	2.3002(8)	C(15)-H(15C)	0.9800
Os-H(01)	1.45(3)	C(16)-H(16A)	0.9800
S-O(3)	1.410(3)	C(16)-H(16B)	0.9800
S-O(2)	1.430(2)	C(16)-H(16C)	0.9800
S-O(1)	1.433(2)	C(17)-C(18)	1.530(4)
S-C(29)	1.799(4)	C(17)-C(19)	1.534(4)
P(1)-C(11)	1.867(3)	C(17)-H(17)	1.0000
P(1)-C(14)	1.872(3)	C(18)-H(18A)	0.9800
P(1)-C(17)	1.875(3)	C(18)-H(18B)	0.9800
P(2)-C(20)	1.871(3)	C(18)-H(18C)	0.9800
P(2)-C(26)	1.880(3)	C(19)-H(19A)	0.9800
P(2)-C(23)	1.885(3)	C(19)-H(19B)	0.9800
F(1)-C(29)	1.286(5)	C(19)-H(19C)	0.9800
F(2)-C(29)	1.342(4)	C(20)-C(22)	1.525(4)
F(3)-C(29)	1.334(4)	C(20)-C(21)	1.538(4)
N-C(8)	1.489(4)	C(20)-H(20)	1.0000
N-C(10)	1.489(4)	C(21)-H(21A)	0.9800
N-C(9)	1.500(3)	C(21)-H(21B)	0.9800
N-C(7)	1.508(3)	C(21)-H(21C)	0.9800
C(1)-C(2)	1.409(4)	C(22)-H(22A)	0.9800
C(1)-C(5)	1.425(4)	C(22)-H(22B)	0.9800
C(1)-C(6)	1.510(4)	C(22)-H(22C)	0.9800
C(2)-C(3)	1.425(4)	C(23)-C(25)	1.533(4)
C(2)-H(2)	0.9500	C(23)-C(24)	1.537(4)
C(3)-C(4)	1.403(4)	C(23)-H(23)	1.0000
C(3)-H(3)	0.9500	C(24)-H(24A)	0.9800
C(4)-C(5)	1.417(4)	C(24)-H(24B)	0.9800
C(4)-H(4)	0.9500	C(24)-H(24C)	0.9800
C(5)-H(5)	0.9500	C(25)-H(25A)	0.9800
C(6)-C(7)	1.515(4)	C(25)-H(25B)	0.9800
C(6)-H(6A)	0.9900	C(25)-H(25C)	0.9800
C(6)-H(6B)	0.9900	C(26)-C(28)	1.533(4)
C(7)-H(7A)	0.9900	C(26)-C(27)	1.538(4)
C(7)-H(7B)	0.9900	C(26)-H(26)	1.0000
C(8)-H(8A)	0.9800	C(27)-H(27A)	0.9800
C(8)-H(8B)	0.9800	C(27)-H(27B)	0.9800
C(8)-H(8C)	0.9800	C(27)-H(27C)	0.9800
C(9)-H(9A)	0.9800	C(28)-H(28A)	0.9800
C(9)-H(9B)	0.9800	C(28)-H(28B)	0.9800
C(9)-H(9C)	0.9800	C(28)-H(28C)	0.9800
C(10)-H(10A)	0.9800		
C(10)-H(10B)	0.9800	C(1)-Os-C(5)	37.39(10)
C(10)-H(10C)	0.9800	C(1)-Os-C(4)	61.98(11)
C(11)-C(12)	1.534(4)	C(5)-Os-C(4)	37.10(10)
C(11)-C(13)	1.540(4)	C(1)-Os-C(2)	36.76(10)
C(11)-H(11)	1.0000	C(5)-Os-C(2)	61.45(11)
C(12)-H(12A)	0.9800	C(4)-Os-C(2)	61.04(11)
C(12)-H(12B)	0.9800	C(1)-Os-C(3)	61.78(11)
C(12)-H(12C)	0.9800	C(5)-Os-C(3)	61.49(11)
C(13)-H(13A)	0.9800	C(4)-Os-C(3)	36.32(10)
C(13)-H(13B)	0.9800	C(2)-Os-C(3)	36.79(10)

C(1)-Os-P(2)	117.03(8)	C(3)-C(4)-Os	73.38(17)
C(5)-Os-P(2)	153.60(8)	C(5)-C(4)-Os	71.21(17)
C(4)-Os-P(2)	139.13(8)	C(3)-C(4)-H(4)	125.4
C(2)-Os-P(2)	93.53(8)	C(5)-C(4)-H(4)	125.4
C(3)-Os-P(2)	104.23(8)	Os-C(4)-H(4)	121.6
C(1)-Os-P(1)	137.81(8)	C(4)-C(5)-C(1)	107.5(3)
C(5)-Os-P(1)	102.24(8)	C(4)-C(5)-Os	71.69(17)
C(4)-Os-P(1)	93.04(8)	C(1)-C(5)-Os	71.20(17)
C(2)-Os-P(1)	153.39(8)	C(4)-C(5)-H(5)	126.2
C(3)-Os-P(1)	117.95(8)	C(1)-C(5)-H(5)	126.2
P(2)-Os-P(1)	104.14(3)	Os-C(5)-H(5)	122.6
C(1)-Os-H(01)	94.8(10)	C(1)-C(6)-C(7)	108.7(2)
C(5)-Os-H(01)	106.1(11)	C(1)-C(6)-H(6A)	109.9
C(4)-Os-H(01)	141.8(11)	C(7)-C(6)-H(6A)	109.9
C(2)-Os-H(01)	118.6(10)	C(1)-C(6)-H(6B)	109.9
C(3)-Os-H(01)	154.9(10)	C(7)-C(6)-H(6B)	109.9
P(2)-Os-H(01)	77.4(11)	H(6A)-C(6)-H(6B)	108.3
P(1)-Os-H(01)	85.1(10)	N-C(7)-C(6)	115.8(2)
O(3)-S-O(2)	114.87(16)	N-C(7)-H(7A)	108.3
O(3)-S-O(1)	115.92(18)	C(6)-C(7)-H(7A)	108.3
O(2)-S-O(1)	114.20(15)	N-C(7)-H(7B)	108.3
O(3)-S-C(29)	104.1(2)	C(6)-C(7)-H(7B)	108.3
O(2)-S-C(29)	103.55(17)	H(7A)-C(7)-H(7B)	107.4
O(1)-S-C(29)	101.78(16)	N-C(8)-H(8A)	109.5
C(11)-P(1)-C(14)	100.48(12)	N-C(8)-H(8B)	109.5
C(11)-P(1)-C(17)	105.87(13)	H(8A)-C(8)-H(8B)	109.5
C(14)-P(1)-C(17)	99.63(13)	N-C(8)-H(8C)	109.5
C(11)-P(1)-Os	120.08(9)	H(8A)-C(8)-H(8C)	109.5
C(14)-P(1)-Os	119.40(9)	H(8B)-C(8)-H(8C)	109.5
C(17)-P(1)-Os	108.84(9)	N-C(9)-H(9A)	109.5
C(20)-P(2)-C(26)	104.10(13)	N-C(9)-H(9B)	109.5
C(20)-P(2)-C(23)	101.36(14)	H(9A)-C(9)-H(9B)	109.5
C(26)-P(2)-C(23)	100.61(13)	N-C(9)-H(9C)	109.5
C(20)-P(2)-Os	121.84(10)	H(9A)-C(9)-H(9C)	109.5
C(26)-P(2)-Os	111.32(10)	H(9B)-C(9)-H(9C)	109.5
C(23)-P(2)-Os	114.99(10)	N-C(10)-H(10A)	109.5
C(8)-N-C(10)	109.9(2)	N-C(10)-H(10B)	109.5
C(8)-N-C(9)	108.5(2)	H(10A)-C(10)-H(10B)	109.5
C(10)-N-C(9)	108.4(2)	N-C(10)-H(10C)	109.5
C(8)-N-C(7)	111.5(2)	H(10A)-C(10)-H(10C)	109.5
C(10)-N-C(7)	111.1(2)	H(10B)-C(10)-H(10C)	109.5
C(9)-N-C(7)	107.3(2)	C(12)-C(11)-C(13)	108.6(2)
C(2)-C(1)-C(5)	107.4(3)	C(12)-C(11)-P(1)	114.40(19)
C(2)-C(1)-C(6)	126.5(3)	C(13)-C(11)-P(1)	118.9(2)
C(5)-C(1)-C(6)	125.5(3)	C(12)-C(11)-H(11)	104.4
C(2)-C(1)-Os	72.55(16)	C(13)-C(11)-H(11)	104.4
C(5)-C(1)-Os	71.41(16)	P(1)-C(11)-H(11)	104.4
C(6)-C(1)-Os	128.4(2)	C(11)-C(12)-H(12A)	109.5
C(1)-C(2)-C(3)	109.0(3)	C(11)-C(12)-H(12B)	109.5
C(1)-C(2)-Os	70.69(16)	H(12A)-C(12)-H(12B)	109.5
C(3)-C(2)-Os	72.54(16)	C(11)-C(12)-H(12C)	109.5
C(1)-C(2)-H(2)	125.5	H(12A)-C(12)-H(12C)	109.5
C(3)-C(2)-H(2)	125.5	H(12B)-C(12)-H(12C)	109.5
Os-C(2)-H(2)	122.9	C(11)-C(13)-H(13A)	109.5
C(4)-C(3)-C(2)	107.0(3)	C(11)-C(13)-H(13B)	109.5
C(4)-C(3)-Os	70.30(17)	H(13A)-C(13)-H(13B)	109.5
C(2)-C(3)-Os	70.67(16)	C(11)-C(13)-H(13C)	109.5
C(4)-C(3)-H(3)	126.5	H(13A)-C(13)-H(13C)	109.5
C(2)-C(3)-H(3)	126.5	H(13B)-C(13)-H(13C)	109.5
Os-C(3)-H(3)	124.2	C(15)-C(14)-C(16)	109.7(2)
C(3)-C(4)-C(5)	109.1(3)	C(15)-C(14)-P(1)	113.3(2)

C(16)-C(14)-P(1)	111.76(19)	C(20)-C(22)-H(22B)	109.5
C(15)-C(14)-H(14)	107.3	H(22A)-C(22)-H(22B)	109.5
C(16)-C(14)-H(14)	107.3	C(20)-C(22)-H(22C)	109.5
P(1)-C(14)-H(14)	107.3	H(22A)-C(22)-H(22C)	109.5
C(14)-C(15)-H(15A)	109.5	H(22B)-C(22)-H(22C)	109.5
C(14)-C(15)-H(15B)	109.5	C(25)-C(23)-C(24)	106.8(2)
H(15A)-C(15)-H(15B)	109.5	C(25)-C(23)-P(2)	114.6(2)
C(14)-C(15)-H(15C)	109.5	C(24)-C(23)-P(2)	113.0(2)
H(15A)-C(15)-H(15C)	109.5	C(25)-C(23)-H(23)	107.4
H(15B)-C(15)-H(15C)	109.5	C(24)-C(23)-H(23)	107.4
C(14)-C(16)-H(16A)	109.5	P(2)-C(23)-H(23)	107.4
C(14)-C(16)-H(16B)	109.5	C(23)-C(24)-H(24A)	109.5
H(16A)-C(16)-H(16B)	109.5	C(23)-C(24)-H(24B)	109.5
C(14)-C(16)-H(16C)	109.5	H(24A)-C(24)-H(24B)	109.5
H(16A)-C(16)-H(16C)	109.5	C(23)-C(24)-H(24C)	109.5
H(16B)-C(16)-H(16C)	109.5	H(24A)-C(24)-H(24C)	109.5
C(18)-C(17)-C(19)	108.7(2)	H(24B)-C(24)-H(24C)	109.5
C(18)-C(17)-P(1)	113.6(2)	C(23)-C(25)-H(25A)	109.5
C(19)-C(17)-P(1)	118.0(2)	C(23)-C(25)-H(25B)	109.5
C(18)-C(17)-H(17)	105.1	H(25A)-C(25)-H(25B)	109.5
C(19)-C(17)-H(17)	105.1	C(23)-C(25)-H(25C)	109.5
P(1)-C(17)-H(17)	105.1	H(25A)-C(25)-H(25C)	109.5
C(17)-C(18)-H(18A)	109.5	H(25B)-C(25)-H(25C)	109.5
C(17)-C(18)-H(18B)	109.5	C(28)-C(26)-C(27)	109.8(2)
H(18A)-C(18)-H(18B)	109.5	C(28)-C(26)-P(2)	111.4(2)
C(17)-C(18)-H(18C)	109.5	C(27)-C(26)-P(2)	120.5(2)
H(18A)-C(18)-H(18C)	109.5	C(28)-C(26)-H(26)	104.5
H(18B)-C(18)-H(18C)	109.5	C(27)-C(26)-H(26)	104.5
C(17)-C(19)-H(19A)	109.5	P(2)-C(26)-H(26)	104.5
C(17)-C(19)-H(19B)	109.5	C(26)-C(27)-H(27A)	109.5
H(19A)-C(19)-H(19B)	109.5	C(26)-C(27)-H(27B)	109.5
C(17)-C(19)-H(19C)	109.5	H(27A)-C(27)-H(27B)	109.5
H(19A)-C(19)-H(19C)	109.5	C(26)-C(27)-H(27C)	109.5
H(19B)-C(19)-H(19C)	109.5	H(27A)-C(27)-H(27C)	109.5
C(22)-C(20)-C(21)	107.7(2)	H(27B)-C(27)-H(27C)	109.5
C(22)-C(20)-P(2)	118.2(2)	C(26)-C(28)-H(28A)	109.5
C(21)-C(20)-P(2)	112.87(19)	C(26)-C(28)-H(28B)	109.5
C(22)-C(20)-H(20)	105.7	H(28A)-C(28)-H(28B)	109.5
C(21)-C(20)-H(20)	105.7	C(26)-C(28)-H(28C)	109.5
P(2)-C(20)-H(20)	105.7	H(28A)-C(28)-H(28C)	109.5
C(20)-C(21)-H(21A)	109.5	H(28B)-C(28)-H(28C)	109.5
C(20)-C(21)-H(21B)	109.5	F(1)-C(29)-F(3)	107.1(4)
H(21A)-C(21)-H(21B)	109.5	F(1)-C(29)-F(2)	108.0(3)
C(20)-C(21)-H(21C)	109.5	F(3)-C(29)-F(2)	106.0(3)
H(21A)-C(21)-H(21C)	109.5	F(1)-C(29)-S	113.5(3)
H(21B)-C(21)-H(21C)	109.5	F(3)-C(29)-S	110.7(3)
C(20)-C(22)-H(22A)	109.5	F(2)-C(29)-S	111.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 4.
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
Os	13(1)	16(1)	12(1)	-2(1)	0(1)	-2(1)
S	23(1)	31(1)	25(1)	-10(1)	0(1)	-5(1)
P(1)	12(1)	15(1)	14(1)	-3(1)	-1(1)	-1(1)
P(2)	14(1)	17(1)	14(1)	-5(1)	0(1)	-2(1)
F(1)	100(2)	105(2)	31(1)	-5(2)	-22(1)	20(2)
F(2)	40(1)	64(2)	55(2)	-41(1)	10(1)	-8(1)
F(3)	25(1)	175(3)	137(3)	-131(2)	6(2)	-20(2)
O(1)	21(1)	72(2)	54(2)	-29(2)	-6(1)	-9(1)
O(2)	34(2)	37(2)	55(2)	-26(1)	-1(1)	-1(1)
O(3)	94(2)	37(2)	42(2)	-1(1)	25(2)	-1(2)
N	16(1)	20(2)	16(1)	-3(1)	0(1)	-1(1)
C(1)	19(2)	20(2)	11(2)	1(1)	1(1)	0(1)
C(2)	23(2)	21(2)	12(2)	-3(1)	0(1)	-6(1)
C(3)	17(2)	26(2)	14(2)	4(1)	-1(1)	0(1)
C(4)	26(2)	16(2)	11(2)	-1(1)	1(1)	0(1)
C(5)	23(2)	22(2)	12(2)	1(1)	-2(1)	-6(1)
C(6)	20(2)	26(2)	18(2)	-1(1)	2(1)	0(2)
C(7)	15(2)	18(2)	17(2)	-5(1)	0(1)	0(1)
C(8)	33(2)	18(2)	35(2)	-10(2)	8(2)	-2(2)
C(9)	18(2)	27(2)	15(2)	1(1)	4(1)	0(1)
C(10)	15(2)	48(2)	20(2)	0(2)	-3(1)	0(2)
C(11)	15(2)	15(2)	17(2)	-4(1)	-1(1)	-2(1)
C(12)	19(2)	24(2)	23(2)	-1(2)	-7(1)	1(1)
C(13)	28(2)	20(2)	19(2)	-3(1)	-9(1)	-2(1)
C(14)	16(2)	17(2)	14(2)	-7(1)	-1(1)	-1(1)
C(15)	16(2)	21(2)	21(2)	-6(1)	0(1)	-2(1)
C(16)	16(2)	24(2)	23(2)	-7(2)	-1(1)	3(1)
C(17)	16(2)	15(2)	17(2)	-2(1)	1(1)	-2(1)
C(18)	18(2)	24(2)	39(2)	-5(2)	1(2)	-7(2)
C(19)	27(2)	21(2)	32(2)	-7(2)	-1(2)	-8(2)
C(20)	17(2)	16(2)	15(2)	-3(1)	1(1)	-1(1)
C(21)	25(2)	18(2)	16(2)	-1(1)	-1(1)	0(1)
C(22)	26(2)	22(2)	20(2)	-1(1)	4(1)	-9(2)
C(23)	22(2)	17(2)	25(2)	-7(1)	2(1)	-1(1)
C(24)	22(2)	25(2)	29(2)	-6(2)	3(2)	1(2)
C(25)	28(2)	30(2)	27(2)	-14(2)	4(2)	-3(2)
C(26)	17(2)	26(2)	17(2)	-6(1)	-3(1)	-5(1)
C(27)	21(2)	36(2)	30(2)	-13(2)	-2(2)	-10(2)
C(28)	15(2)	32(2)	24(2)	-9(2)	-5(1)	-2(2)
C(29)	27(2)	65(3)	46(3)	-31(2)	-2(2)	-3(2)

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

	x	y	z	U(eq)
H(01)	6110(30)	7960(30)	7056(13)	23(8)
H(2)	8006	7594	8623	22
H(3)	9851	5772	8200	24
H(4)	8176	4277	7813	22
H(5)	5311	5101	8028	23
H(6A)	3831	7507	8344	27
H(6B)	4880	8299	8704	27
H(7A)	3909	5726	9296	20
H(7B)	4949	6515	9653	20
H(8A)	3070	9156	9398	44
H(8B)	3711	8463	10113	44
H(8C)	1869	8894	10067	44
H(9A)	1312	6659	10602	32
H(9B)	3155	6225	10642	32
H(9C)	2120	5426	10283	32
H(10A)	291	7610	9545	43
H(10B)	1160	6463	9175	43
H(10C)	1426	7983	8862	43
H(11)	7537	8050	5494	19
H(12A)	5056	8719	5255	34
H(12B)	4937	8213	6062	34
H(12C)	4448	7301	5585	34
H(13A)	6451	6086	4915	33
H(13B)	8262	6360	4860	33
H(13C)	6996	7490	4518	33
H(14)	9171	4919	5690	18
H(15A)	10832	6851	6070	29
H(15B)	10181	6981	5345	29
H(15C)	11579	5872	5576	29
H(16A)	11091	3876	6419	32
H(16B)	9373	3661	6797	32
H(16C)	10374	4735	6974	32
H(17)	6585	4195	6975	19
H(18A)	4030	5467	6245	41
H(18B)	4348	5863	6940	41
H(18C)	3988	4381	6937	41
H(19A)	5812	3103	6188	39
H(19B)	7587	3470	5986	39
H(19C)	6189	4328	5584	39
H(20)	9428	8931	5872	20
H(21A)	7297	11252	5840	30
H(21B)	6692	9827	5886	30
H(21C)	7811	10454	5240	30
H(22A)	10390	11007	5419	34
H(22B)	11318	10189	6042	34
H(22C)	10034	11394	6152	34
H(23)	7927	11258	7059	25
H(24A)	5169	9895	7513	39
H(24B)	5571	10613	6741	39
H(24C)	5221	11471	7324	39
H(25A)	7092	11282	8188	41
H(25B)	8669	10294	8177	41

H(25C)	6993	9711	8359	41
H(26)	10207	8462	7891	23
H(27A)	11829	9974	7807	41
H(27B)	10426	10861	7421	41
H(27C)	11959	10322	6994	41
H(28A)	11980	8145	6654	35
H(28B)	11222	6983	7202	35
H(28C)	12610	7710	7392	35