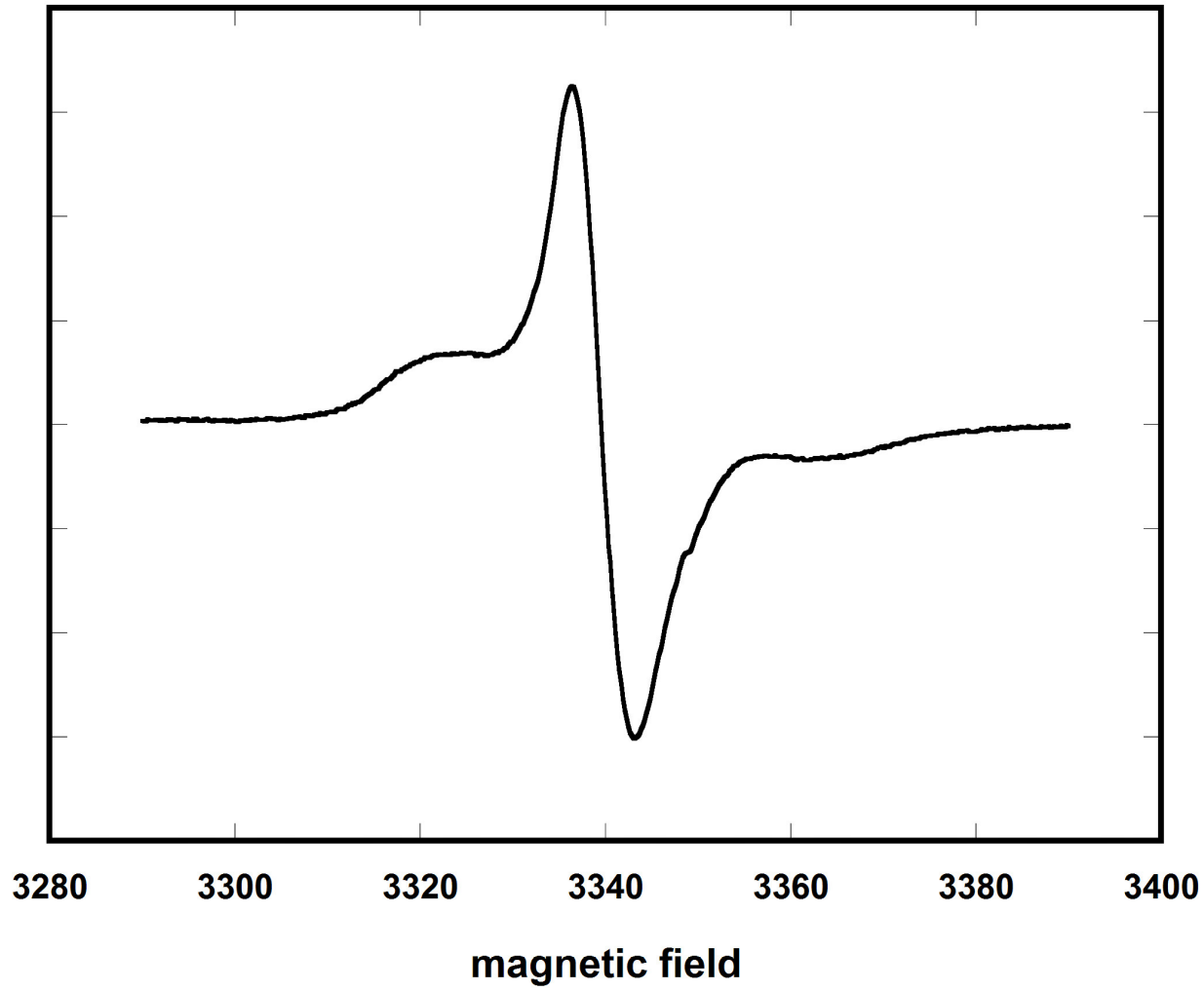
Supporting Information for

Excited-State Dynamics of *fac*-[$Re^{I}(L)(CO)_3(phen)]^+$ and *fac*-[$Re^{I}(L)(CO)_3(5\text{-}NO_2\text{-}phen)]^+$ (L = imidazole, 4-ethyl-pyridine; phen = 1,10-phenanthroline) Complexes

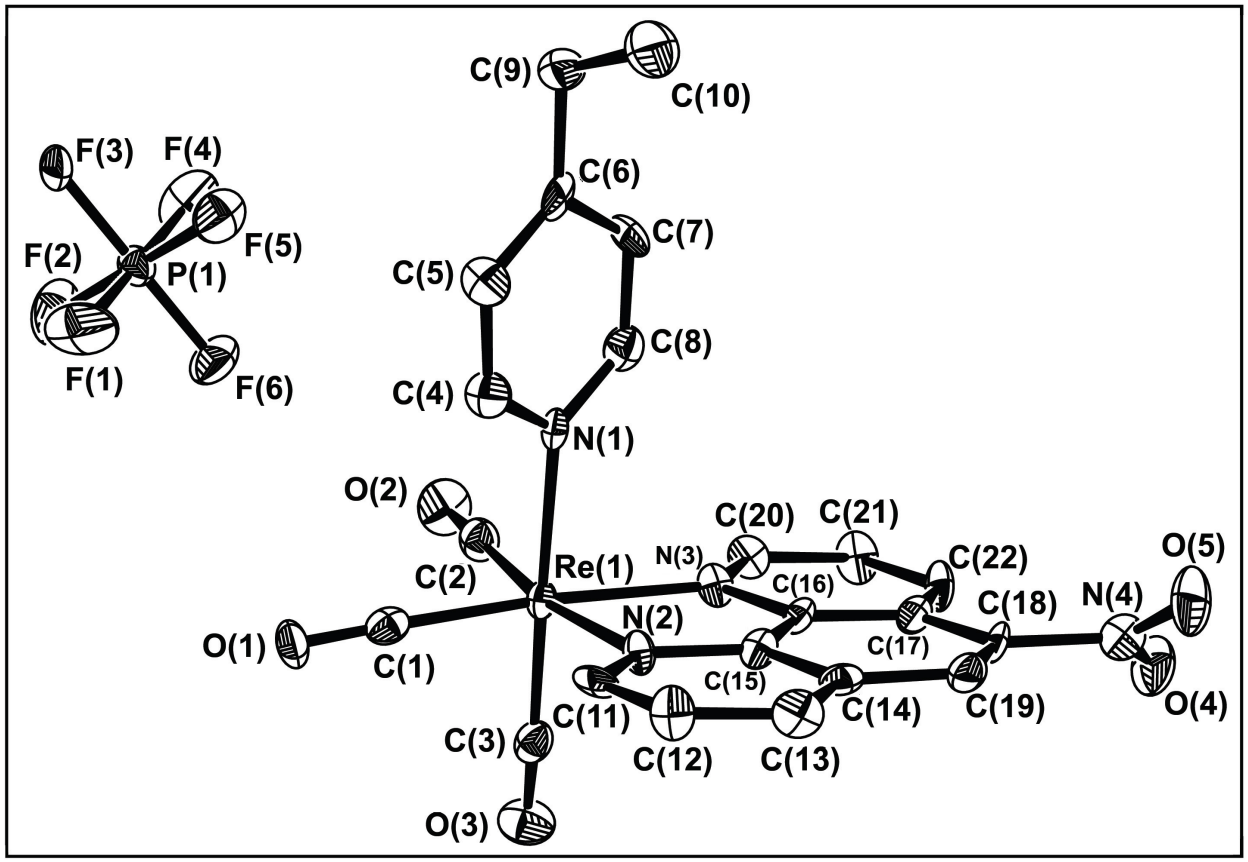
Michael Busby, Anders Gabrielsson, Pavel Matousek, Michael Towrie, Angel J. DiBilio, Harry B. Gray, and Antonín Vlček, Jr.



EPR spectrum of a frozen solution of ~2 mM $[Re^{I}(imH)(CO)_3(5\text{-}NO_2\text{-}phen)]^+$ and ~12 mM $[Co(NH_3)_5Cl]Cl$ in D_2O. The sample was irradiated while freezing. Data were collected at 60 K. The modulation amplitude was 2 G (100 KHz) and the microwave power 50 μWatts.

Crystal data, refinement details, atomic coordinates, bond lengths and angles for $[Re^{I}(4\text{-Etpy})(CO)_3(5\text{-}NO_2\text{-phen})]PF_6$.

Empirical formula	$C_{22}H_{16}F_6N_4O_5PRe$
Formula weight	747.56
Temperature	160(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 17.139(8) Å α= 90°.
	b = 11.904(6) Åβ= 109.43(8)°.
	c = 12.566(6) Åγ = 90°.
Volume	2418(2) $Å^3$
Z	4
Density (calculated)	2.054 Mg/m^3
Absorption coefficient	5.182 mm^{-1}
F(000)	1440
Crystal size	0.40 x 0.30 x 0.20 mm^3
Theta range for data collection	2.12 to 24.98°.
Index ranges	-20<=h<=19, 0<=k<=14, 0<=l<=14
Reflections collected	4576
Independent reflections	4229 [R(int) = 0.0118]
Completeness to theta = 24.98°	99.8 %
Max. and min. transmission	0.4238 and 0.2310
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4229 / 0 / 353
Goodness-of-fit on F^2	0.790
Final R indices [I > 2sigma(I)]	R1 = 0.0323, wR2 = 0.0807
R indices (all data)	R1 = 0.0738, wR2 = 0.0976
Largest diff. peak and hole	1.590 and -0.869 $e.Å^{-3}$



Ortep diagram showing 40% probability ellipsoids.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	2393(1)	671(1)	3726(1)	16(1)
P(1)	6944(1)	523(2)	1102(2)	27(1)
F(1)	6417(4)	1611(5)	625(6)	74(2)
F(2)	7018(5)	272(7)	-100(5)	78(2)
F(3)	7777(3)	1273(4)	1425(4)	32(1)
F(4)	7496(4)	-550(4)	1614(6)	55(2)
F(5)	6884(3)	775(5)	2313(4)	45(1)
F(6)	6129(3)	-224(5)	785(5)	44(1)
N(1)	3365(4)	1331(5)	5215(5)	18(1)
N(2)	1602(4)	1601(5)	4461(5)	19(1)
N(3)	2087(4)	-536(5)	4811(5)	19(1)
N(4)	505(4)	-957(6)	7444(6)	29(2)
O(1)	2649(3)	2454(4)	2107(5)	29(1)
O(2)	3613(4)	-811(5)	3049(6)	40(2)
O(3)	1078(4)	-358(5)	1667(5)	37(2)
O(4)	313(4)	-1950(5)	7241(5)	40(2)
O(5)	488(4)	-470(5)	8288(5)	41(2)
C(1)	2558(5)	1811(6)	2738(6)	22(2)
C(2)	3165(5)	-262(7)	3304(7)	27(2)
C(3)	1550(5)	57(6)	2450(7)	25(2)
C(4)	3609(5)	2417(6)	5288(7)	26(2)
C(5)	4243(5)	2859(6)	6147(7)	27(2)
C(6)	4684(5)	2188(7)	7045(7)	24(2)
C(7)	4423(5)	1076(7)	7011(7)	27(2)
C(8)	3784(5)	685(7)	6099(7)	27(2)
C(9)	5368(5)	2649(7)	8023(7)	28(2)
C(10)	5052(6)	3152(9)	8900(8)	42(2)
C(11)	1406(4)	2701(6)	4334(6)	20(2)
C(12)	924(5)	3213(6)	4881(7)	26(2)
C(13)	624(5)	2616(7)	5582(7)	26(2)
C(14)	830(4)	1482(6)	5764(6)	19(2)
C(15)	1329(5)	1004(6)	5202(6)	17(2)
C(16)	1560(4)	-149(6)	5374(6)	17(2)
C(17)	1284(4)	-853(6)	6065(6)	19(2)
C(18)	789(4)	-314(6)	6644(6)	17(2)
C(19)	575(5)	775(7)	6519(6)	23(2)
C(20)	2317(5)	-1613(6)	4947(7)	23(2)
C(21)	2044(5)	-2359(6)	5599(7)	27(2)
C(22)	1527(5)	-1981(6)	6153(6)	24(2)

Table 3. Bond lengths [Å] and angles [°].

Re(1)-C(3)	1.912(9)	C(1)-Re(1)-C(2)	88.1(3)
Re(1)-C(1)	1.924(8)	C(3)-Re(1)-N(3)	90.1(3)
Re(1)-C(2)	1.932(9)	C(1)-Re(1)-N(3)	174.3(3)
Re(1)-N(3)	2.161(6)	C(2)-Re(1)-N(3)	97.1(3)
Re(1)-N(2)	2.180(6)	C(3)-Re(1)-N(2)	98.4(3)
Re(1)-N(1)	2.196(7)	C(1)-Re(1)-N(2)	99.3(3)
P(1)-F(1)	1.578(6)	C(2)-Re(1)-N(2)	171.1(3)
P(1)-F(2)	1.585(6)	N(3)-Re(1)-N(2)	75.8(2)
P(1)-F(5)	1.588(5)	C(3)-Re(1)-N(1)	178.4(3)
P(1)-F(6)	1.590(5)	C(1)-Re(1)-N(1)	93.7(3)
P(1)-F(4)	1.593(6)	C(2)-Re(1)-N(1)	92.6(3)
P(1)-F(3)	1.617(5)	N(3)-Re(1)-N(1)	88.6(2)
N(1)-C(8)	1.344(10)	N(2)-Re(1)-N(1)	81.9(2)
N(1)-C(4)	1.353(9)	F(1)-P(1)-F(2)	90.6(4)
N(2)-C(11)	1.348(9)	F(1)-P(1)-F(5)	89.9(4)
N(2)-C(15)	1.371(9)	F(2)-P(1)-F(5)	179.2(4)
N(3)-C(20)	1.335(9)	F(1)-P(1)-F(6)	91.2(3)
N(3)-C(16)	1.399(9)	F(2)-P(1)-F(6)	89.9(3)
N(4)-O(5)	1.218(9)	F(5)-P(1)-F(6)	90.8(3)
N(4)-O(4)	1.231(8)	F(1)-P(1)-F(4)	178.1(4)
N(4)-C(18)	1.469(10)	F(2)-P(1)-F(4)	90.5(4)
O(1)-C(1)	1.148(9)	F(5)-P(1)-F(4)	89.1(4)
O(2)-C(2)	1.132(10)	F(6)-P(1)-F(4)	90.4(3)
O(3)-C(3)	1.156(10)	F(1)-P(1)-F(3)	89.3(3)
C(4)-C(5)	1.358(11)	F(2)-P(1)-F(3)	89.9(3)
C(4)-H(4)	0.9500	F(5)-P(1)-F(3)	89.4(3)
C(5)-C(6)	1.384(11)	F(6)-P(1)-F(3)	179.5(3)
C(5)-H(5)	0.9500	F(4)-P(1)-F(3)	89.1(3)
C(6)-C(7)	1.393(11)	C(8)-N(1)-C(4)	115.0(7)
C(6)-C(9)	1.493(11)	C(8)-N(1)-Re(1)	123.0(5)
C(7)-C(8)	1.376(12)	C(4)-N(1)-Re(1)	121.9(5)
C(7)-H(7)	0.9500	C(11)-N(2)-C(15)	117.1(6)
C(8)-H(8)	0.9500	C(11)-N(2)-Re(1)	127.5(5)
C(9)-C(10)	1.504(11)	C(15)-N(2)-Re(1)	115.2(5)
C(9)-H(9A)	0.9900	C(20)-N(3)-C(16)	117.6(6)
C(9)-H(9B)	0.9900	C(20)-N(3)-Re(1)	126.6(5)
C(10)-H(10A)	0.9800	C(16)-N(3)-Re(1)	115.7(5)
C(10)-H(10B)	0.9800	O(5)-N(4)-O(4)	123.7(7)
C(10)-H(10C)	0.9800	O(5)-N(4)-C(18)	117.2(7)
C(11)-C(12)	1.380(11)	O(4)-N(4)-C(18)	119.1(7)
C(11)-H(11)	0.9500	O(1)-C(1)-Re(1)	176.7(6)
C(12)-C(13)	1.359(11)	O(2)-C(2)-Re(1)	179.5(9)
C(12)-H(12)	0.9500	O(3)-C(3)-Re(1)	175.7(7)
C(13)-C(14)	1.395(10)	N(1)-C(4)-C(5)	124.8(8)
C(13)-H(13)	0.9500	N(1)-C(4)-H(4)	117.6
C(14)-C(15)	1.398(10)	C(5)-C(4)-H(4)	117.6
C(14)-C(19)	1.440(10)	C(4)-C(5)-C(6)	120.0(7)
C(15)-C(16)	1.426(10)	C(4)-C(5)-H(5)	120.0
C(16)-C(17)	1.398(10)	C(6)-C(5)-H(5)	120.0
C(17)-C(22)	1.399(10)	C(5)-C(6)-C(7)	116.2(7)
C(17)-C(18)	1.440(10)	C(5)-C(6)-C(9)	121.7(7)
C(18)-C(19)	1.342(10)	C(7)-C(6)-C(9)	122.1(7)
C(19)-H(19)	0.9500	C(8)-C(7)-C(6)	120.3(7)
C(20)-C(21)	1.390(11)	C(8)-C(7)-H(7)	119.8
C(20)-H(20)	0.9500	C(6)-C(7)-H(7)	119.8
C(21)-C(22)	1.373(11)	N(1)-C(8)-C(7)	123.6(8)
C(21)-H(21)	0.9500	N(1)-C(8)-H(8)	118.2
C(22)-H(22)	0.9500	C(7)-C(8)-H(8)	118.2
C(3)-Re(1)-C(1)	87.7(3)	C(6)-C(9)-C(10)	112.0(7)
C(3)-Re(1)-C(2)	86.9(3)	C(6)-C(9)-H(9A)	109.2

C(10)-C(9)-H(9A)	109.2	N(2)-C(15)-C(16)	117.5(6)
C(6)-C(9)-H(9B)	109.2	C(14)-C(15)-C(16)	120.1(7)
C(10)-C(9)-H(9B)	109.2	C(17)-C(16)-N(3)	121.8(7)
H(9A)-C(9)-H(9B)	107.9	C(17)-C(16)-C(15)	122.5(7)
C(9)-C(10)-H(10A)	109.5	N(3)-C(16)-C(15)	115.7(6)
C(9)-C(10)-H(10B)	109.5	C(16)-C(17)-C(22)	118.1(7)
H(10A)-C(10)-H(10B)	109.5	C(16)-C(17)-C(18)	115.1(6)
C(9)-C(10)-H(10C)	109.5	C(22)-C(17)-C(18)	126.7(7)
H(10A)-C(10)-H(10C)	109.5	C(19)-C(18)-C(17)	123.7(7)
H(10B)-C(10)-H(10C)	109.5	C(19)-C(18)-N(4)	116.4(7)
N(2)-C(11)-C(12)	122.5(7)	C(17)-C(18)-N(4)	119.9(6)
N(2)-C(11)-H(11)	118.8	C(18)-C(19)-C(14)	120.7(7)
C(12)-C(11)-H(11)	118.8	C(18)-C(19)-H(19)	119.6
C(13)-C(12)-C(11)	120.7(7)	C(14)-C(19)-H(19)	119.6
C(13)-C(12)-H(12)	119.7	N(3)-C(20)-C(21)	123.2(7)
C(11)-C(12)-H(12)	119.7	N(3)-C(20)-H(20)	118.4
C(12)-C(13)-C(14)	118.9(7)	C(21)-C(20)-H(20)	118.4
C(12)-C(13)-H(13)	120.6	C(22)-C(21)-C(20)	119.3(7)
C(14)-C(13)-H(13)	120.6	C(22)-C(21)-H(21)	120.3
C(13)-C(14)-C(15)	118.4(7)	C(20)-C(21)-H(21)	120.3
C(13)-C(14)-C(19)	123.9(7)	C(21)-C(22)-C(17)	120.0(7)
C(15)-C(14)-C(19)	117.7(7)	C(21)-C(22)-H(22)	120.0
N(2)-C(15)-C(14)	122.4(7)	C(17)-C(22)-H(22)	120.0

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$). 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}
Re(1)	19(1)	15(1)	18(1)	0(1)	11(1)	0(1)
P(1)	33(1)	22(1)	24(1)	2(1)	7(1)	-4(1)
F(1)	56(4)	33(3)	102(6)	27(3)	-17(4)	2(3)
F(2)	100(6)	108(6)	36(4)	-24(4)	35(4)	-60(5)
F(3)	39(3)	28(3)	29(3)	8(2)	11(2)	-10(2)
F(4)	47(3)	24(3)	100(5)	2(3)	32(3)	9(2)
F(5)	44(3)	58(4)	40(3)	-17(3)	25(3)	-9(3)
F(6)	39(3)	42(3)	51(3)	-9(3)	16(3)	-18(3)
N(1)	20(3)	19(3)	20(3)	3(3)	13(3)	-1(3)
N(2)	26(4)	18(3)	16(3)	-1(3)	12(3)	0(3)
N(3)	29(3)	14(3)	18(3)	-4(3)	11(3)	0(3)
N(4)	27(4)	29(4)	31(4)	-1(3)	11(3)	-1(3)
O(1)	36(3)	30(3)	21(3)	8(2)	11(3)	-6(3)
O(2)	42(4)	41(4)	47(4)	-4(3)	26(3)	17(3)
O(3)	39(4)	28(3)	36(4)	-7(3)	2(3)	-4(3)
O(4)	48(4)	36(4)	41(4)	-7(3)	23(3)	-22(3)
O(5)	57(4)	43(4)	38(4)	-8(3)	36(3)	-4(3)
C(1)	20(4)	25(4)	21(4)	-9(3)	6(3)	-4(3)
C(2)	29(5)	23(4)	28(5)	4(4)	10(4)	1(4)
C(3)	22(4)	21(4)	34(5)	6(4)	12(4)	2(3)
C(4)	29(4)	21(4)	29(5)	1(3)	9(4)	1(4)
C(5)	36(5)	16(4)	27(4)	-2(3)	8(4)	-1(3)
C(6)	20(4)	32(5)	28(4)	-5(4)	21(4)	-3(3)
C(7)	30(5)	31(4)	17(4)	12(4)	3(4)	5(4)
C(8)	27(4)	25(4)	31(4)	2(4)	12(4)	-3(4)
C(9)	21(4)	36(5)	26(5)	1(4)	6(3)	1(4)
C(10)	41(5)	59(6)	29(5)	-7(5)	16(4)	-2(5)
C(11)	19(4)	14(4)	20(4)	7(3)	-3(3)	5(3)
C(12)	34(5)	19(4)	30(5)	1(3)	16(4)	3(3)
C(13)	25(4)	27(4)	28(5)	-5(3)	13(3)	14(4)
C(14)	14(4)	23(4)	18(4)	-6(3)	1(3)	-3(3)
C(15)	20(4)	15(4)	20(4)	-7(3)	9(3)	-5(3)
C(16)	15(4)	19(4)	19(4)	-6(3)	9(3)	-6(3)
C(17)	18(4)	22(4)	21(4)	-4(3)	9(3)	-4(3)
C(18)	17(4)	18(4)	21(4)	-1(3)	13(3)	-7(3)
C(19)	17(4)	33(5)	21(4)	-3(4)	9(3)	0(3)
C(20)	29(4)	16(4)	24(4)	-3(3)	11(4)	6(3)
C(21)	46(5)	7(3)	31(5)	-8(3)	18(4)	-5(3)
C(22)	37(5)	17(4)	26(4)	1(3)	19(4)	-9(4)

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

	x	y	z	U(eq)
H(4)	3314	2908	4694	31
H(5)	4385	3629	6131	32
H(7)	4686	586	7621	33
H(8)	3630	-82	6093	33
H(9A)	5668	3232	7751	34
H(9B)	5764	2040	8371	34
H(10A)	4680	3778	8567	63
H(10B)	5520	3428	9534	63
H(10C)	4752	2579	9168	63
H(11)	1607	3140	3849	24
H(12)	800	3991	4765	32
H(13)	280	2965	5942	31
H(19)	252	1083	6932	28
H(20)	2684	-1882	4581	27
H(21)	2214	-3123	5660	32
H(22)	1334	-2485	6597	29