Supporting Information

Title: Syntheses, Structures, Photoluminescence of A Novel Class of d^{10} Metal Complexes Constructed by Pydrine-3,4-dicarboxylic Acid with Different Coordination Architectures

Authors: Xinlong Wang, Chao Qin, and Enbo Wang, Yangguang Li, Na Hao, Changwen Hu and Lin Xu

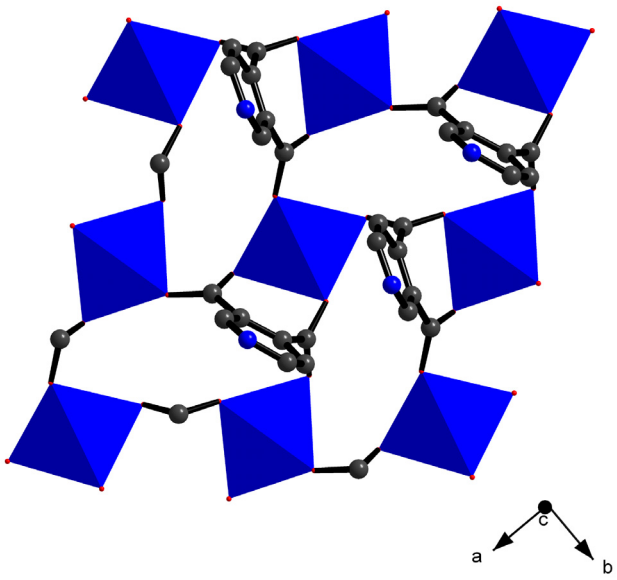

Figure S1. The coordination environment of PDB ligand normal to the direction of Zn-O-C layer.

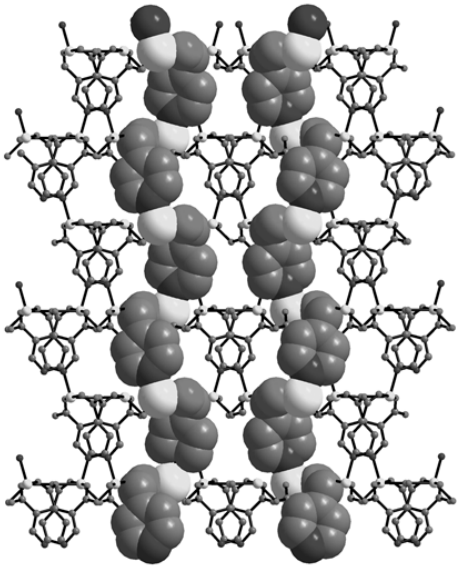

Figure S2 two representative helical chains in the three-dimensional structure.

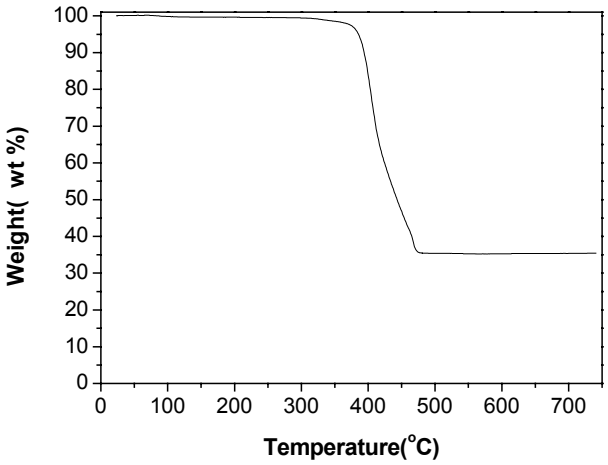

Figure S3a TGA Curve of compound **1**

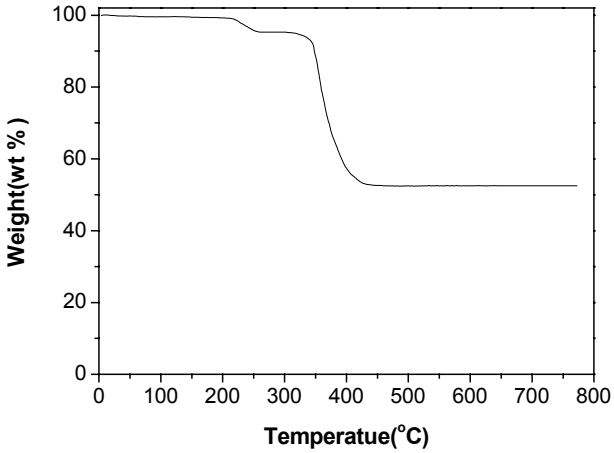

Figure S3b TGA Curve of compound **2**

Thermogravimetric analysis (TGA) was performed in air at a heating rate of 10℃ /min on a polycrystalline sample of compound **1**. The result showed that a total weight loss of 64.33% occurred between 385℃ and 468℃, corresponding to the removal of the organic component (Calcd 64.72%). The remaining weight of 35.15% corresponds to the percentage (35.28%) of Zn and O components, indicating that the final product is ZnO (Figure S2a). The TG curve of compound **2** exhibits two continuous weight loss steps (Figure S2b). The first weight loss starts at ca. 220℃ to 260℃ to give a total weight loss of ca. 4.65%, corresponding to the loss of coordinated water (4.88%). The second weight loss starts at ca. 340℃ up to 425℃ (42.85%), corresponding to the release of PDB ligand and hydroxyl group. The residue is CdO. The whole weight loss (47.5%) is in good agreement with the calculated value (47.77%).

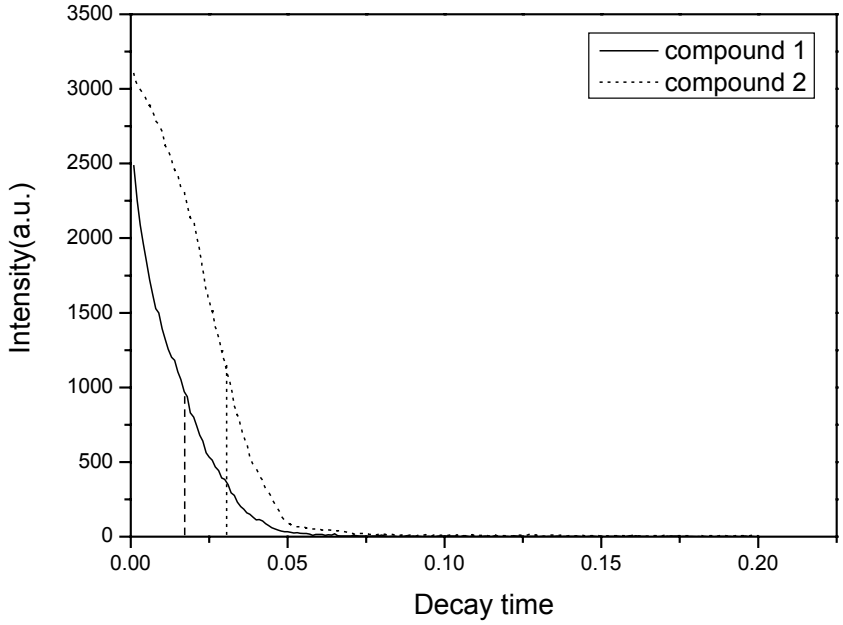

Figure S4. Decay curves of **1** and **2** luminescence at room temperature.

Table 1. Crystal data and structure refinement for **1**.

Empirical formula	C7 H3 N O4 Zn
Formula weight	230.47
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pna2(1)
Unit cell dimensions	a = 8.4225(17) A alpha = 90 deg.
	b = 6.5742(13) A beta = 90 deg.
	c = 12.899(3) A gamma = 90 deg.
Volume	714.2(2) A^3
Z, Calculated density	4, 2.143 Mg/m^3
Absorption coefficient	3.412 mm^-1
F(000)	456
Crystal size	0.342 x 0.276 x 0.159 mm
Theta range for data collection	3.48 to 27.47 deg.
Limiting indices	-10<=h<=10, -8<=k<=8, -16<=l<=16
Reflections collected / unique	1513 / 1513 [R(int) = 0.0000]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.581 and 0.337
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1513 / 1 / 118
Goodness-of-fit on F^2	0.883
Final R indices [I>2sigma(I)]	R1 = 0.0263, wR2 = 0.0457
R indices (all data)	R1 = 0.0308, wR2 = 0.0465
Absolute structure parameter	0.00
Largest diff. peak and hole	0.302 and -0.354 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zn(1)	8333(1)	567(1)	9330(1)	17(1)
O(2)	9033(2)	-2330(3)	9350(4)	29(1)
C(7)	10868(4)	-2394(5)	10764(3)	16(1)
C(2)	10332(4)	-3027(5)	9694(3)	17(1)
C(1)	11459(4)	-469(5)	11023(2)	17(1)
C(3)	10707(4)	-3830(5)	11551(3)	22(1)
C(5)	11030(4)	-3273(5)	12557(3)	22(1)
N(1)	11549(3)	-1400(4)	12818(2)	18(1)
C(6)	11752(4)	1132(5)	10211(2)	17(1)
C(4)	11788(4)	-54(5)	12053(3)	19(1)
O(6)	10898(3)	1237(3)	9430(3)	26(1)
O(5)	12929(3)	2332(4)	10385(2)	24(1)
O(1)	11099(3)	-4327(3)	9199(3)	22(1)

Table 3. Bond lengths [A] and angles [deg] for **1**.

Zn(1)-O(5)#1	1.968(2)	O(2)-Zn(1)-O(6)	84.29(9)
Zn(1)-O(2)	1.9934(19)	N(1)#2-Zn(1)-O(6)	87.36(13)
Zn(1)-N(1)#2	2.029(3)	O(1)#3-Zn(1)-O(6)	168.06(8)
Zn(1)-O(1)#3	2.057(2)	C(2)-O(2)-Zn(1)	127.3(2)
Zn(1)-O(6)	2.209(2)	C(3)-C(7)-C(1)	118.2(3)
O(2)-C(2)	1.267(4)	C(3)-C(7)-C(2)	116.7(3)
C(7)-C(3)	1.393(5)	C(1)-C(7)-C(2)	125.0(3)
C(7)-C(1)	1.400(4)	O(1)-C(2)-O(2)	121.1(4)
C(7)-C(2)	1.510(4)	O(1)-C(2)-C(7)	120.1(3)
C(2)-O(1)	1.247(4)	O(2)-C(2)-C(7)	118.6(3)
C(1)-C(4)	1.384(4)	C(4)-C(1)-C(7)	118.6(3)
C(1)-C(6)	1.505(4)	C(4)-C(1)-C(6)	119.9(3)
C(3)-C(5)	1.375(5)	C(7)-C(1)-C(6)	121.6(3)
C(5)-N(1)	1.349(4)	C(5)-C(3)-C(7)	119.2(3)
N(1)-C(4)	1.341(4)	N(1)-C(5)-C(3)	122.8(3)
N(1)-Zn(1)#4	2.029(3)	C(4)-N(1)-C(5)	117.9(3)
C(6)-O(6)	1.239(5)	C(4)-N(1)-Zn(1)#4	121.5(2)
C(6)-O(5)	1.287(4)	C(5)-N(1)-Zn(1)#4	120.2(2)
O(5)-Zn(1)#5	1.968(2)	O(6)-C(6)-O(5)	123.7(3)
O(1)-Zn(1)#6	2.057(2)	O(6)-C(6)-C(1)	120.6(3)
O(5)#1-Zn(1)-O(2)	135.41(17)	O(5)-C(6)-C(1)	115.7(3)
O(5)#1-Zn(1)-N(1)#2	118.92(11)	N(1)-C(4)-C(1)	123.1(3)
O(2)-Zn(1)-N(1)#2	104.84(17)	C(6)-O(6)-Zn(1)	127.2(3)
O(5)#1-Zn(1)-O(1)#3	100.19(11)	C(6)-O(5)-Zn(1)#5	116.3(2)
O(2)-Zn(1)-O(1)#3	83.86(8)	C(2)-O(1)-Zn(1)#6	134.7(3)
N(1)#2-Zn(1)-O(1)#3	94.20(12)	O(5)#1-Zn(1)-O(6)	89.34(11)

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+1/2,z #2 -x+2,-y,z-1/2

#3 x-1/2,-y-1/2,z #4 -x+2,-y,z+1/2

#5 x+1/2,-y+1/2,z #6 x+1/2,-y-1/2,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **1**.
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
Zn(1)	23(1)	16(1)	13(1)	-1(1)	-1(1)	2(1)
O(2)	22(1)	21(1)	42(1)	-7(2)	-12(2)	4(1)
C(7)	17(2)	17(1)	13(2)	-5(1)	3(1)	-1(1)
C(2)	21(2)	13(1)	18(2)	0(1)	-1(1)	-3(1)
C(1)	21(2)	15(2)	16(2)	1(1)	1(1)	-2(1)
C(3)	34(2)	13(1)	19(2)	1(1)	0(2)	-3(1)
C(5)	31(2)	17(2)	19(2)	3(1)	2(1)	-4(1)
N(1)	25(2)	19(1)	11(1)	1(1)	2(1)	-1(1)
C(6)	20(2)	19(1)	13(2)	-3(1)	3(1)	-2(1)
C(4)	20(2)	19(2)	18(2)	-3(1)	0(1)	-4(1)
O(6)	28(1)	27(1)	23(2)	8(2)	-8(1)	-5(1)
O(5)	26(1)	24(1)	21(1)	8(1)	-5(1)	-8(1)
O(1)	24(1)	23(1)	19(2)	-7(1)	-2(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1**.

	x	y	z	U(eq)
H(3A)	10386	-5150	11398	26
H(5AA)	10884	-4229	13080	27
H(4A)	12194	1219	12222	23

Table 1. Crystal data and structure refinement for **2**.

Empirical formula	C14 H12 Cd3 N2 O12
Formula weight	737.46
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 20.130(4) A alpha = 90 deg. b = 6.6921(13) A beta = 102.78(3) deg. c = 13.081(3) A gamma = 90 deg.
Volume	1718.5(6) A^3
Z, Calculated density	4, 2.850 Mg/m^3
Absorption coefficient	3.756 mm^-1
F(000)	1400
Crystal size	0.334 x 0.242 x 0.233 mm
Theta range for data collection	3.22 to 27.48 deg.
Limiting indices	-25<=h<=26, -8<=k<=8, -16<=l<=16
Reflections collected / unique	3695 / 1961 [R(int) = 0.0401]
Completeness to theta = 27.48	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.550 and 0.295
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1961 / 0 / 153
Goodness-of-fit on F^2	0.993
Final R indices [I>2sigma(I)]	R1 = 0.0241, wR2 = 0.0666
R indices (all data)	R1 = 0.0259, wR2 = 0.0681
Largest diff. peak and hole	0.543 and -1.051 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cd(1)	808(1)	5780(1)	416(1)	15(1)
Cd(2)	0	3553(1)	2500	13(1)
O(1)	129(1)	3442(3)	846(1)	13(1)
N(1)	1880(1)	4402(3)	1020(2)	16(1)
C(4)	2586(1)	1537(4)	1509(2)	18(1)
O(2)	444(1)	8860(4)	1085(2)	26(1)
C(1)	2442(1)	5478(4)	1024(2)	16(1)
C(2)	3095(1)	4675(4)	1267(2)	14(1)
C(5)	1956(1)	2462(4)	1266(2)	20(1)
C(3)	3168(1)	2637(4)	1505(2)	14(1)
C(6)	3859(1)	1622(4)	1647(2)	16(1)
O(4)	4043(1)	539(4)	2437(2)	27(1)
C(7)	3686(1)	6057(4)	1263(2)	16(1)
O(5)	4194(1)	5920(3)	2014(2)	20(1)
O(6)	3601(1)	7266(4)	521(2)	30(1)
O(3)	4178(1)	1927(3)	946(2)	22(1)

Table 3. Bond lengths [A] and angles [deg] for **2**

Cd(1)-O(1)	2.2295(18)	O(1)-Cd(1)-N(1)	102.20(7)
Cd(1)-O(1)#1	2.274(2)	O(1)#1-Cd(1)-N(1)	153.82(7)
Cd(1)-O(6)#2	2.297(2)	O(6)#2-Cd(1)-N(1)	81.63(8)
Cd(1)-N(1)	2.319(2)	O(1)-Cd(1)-O(2)	104.84(8)
Cd(1)-O(2)	2.415(2)	O(1)#1-Cd(1)-O(2)	78.40(8)
Cd(1)-O(3)#3	2.546(2)	O(6)#2-Cd(1)-O(2)	86.66(9)
Cd(1)-Cd(1)#1	3.3583(9)	N(1)-Cd(1)-O(2)	123.35(8)
Cd(2)-O(1)#4	2.2362(19)	O(1)-Cd(1)-O(3)#3	77.28(7)
Cd(2)-O(1)	2.2362(19)	O(1)#1-Cd(1)-O(3)#3	77.90(7)
Cd(2)-O(4)#5	2.327(2)	O(6)#2-Cd(1)-O(3)#3	86.78(8)
Cd(2)-O(4)#6	2.327(2)	N(1)-Cd(1)-O(3)#3	78.55(8)
Cd(2)-O(5)#7	2.3846(19)	O(2)-Cd(1)-O(3)#3	155.80(7)
Cd(2)-O(5)#8	2.3846(19)	O(1)-Cd(1)-Cd(1)#1	42.30(5)
O(1)-Cd(1)#1	2.274(2)	O(1)#1-Cd(1)-Cd(1)#1	41.28(5)
N(1)-C(5)	1.338(4)	O(6)#2-Cd(1)-Cd(1)#1	125.65(6)
N(1)-C(1)	1.340(3)	N(1)-Cd(1)-Cd(1)#1	138.43(6)
C(4)-C(5)	1.383(4)	O(2)-Cd(1)-Cd(1)#1	91.94(6)
C(4)-C(3)	1.385(4)	O(3)#3-Cd(1)-Cd(1)#1	73.25(5)
C(1)-C(2)	1.390(4)	O(1)#4-Cd(2)-O(1)	176.19(9)
C(2)-C(3)	1.400(4)	O(1)#4-Cd(2)-O(4)#5	77.36(7)
C(2)-C(7)	1.508(3)	O(1)-Cd(2)-O(4)#5	104.88(7)
C(3)-C(6)	1.521(4)	O(1)#4-Cd(2)-O(4)#6	104.88(7)
C(6)-O(3)	1.247(3)	O(1)-Cd(2)-O(4)#6	77.36(7)
C(6)-O(4)	1.249(3)	O(4)#5-Cd(2)-O(4)#6	110.37(12)
O(4)-Cd(2)#9	2.327(2)	O(1)#4-Cd(2)-O(5)#7	90.88(7)
C(7)-O(6)	1.246(3)	O(1)-Cd(2)-O(5)#7	86.30(7)
C(7)-O(5)	1.255(3)	O(4)#5-Cd(2)-O(5)#7	84.43(8)
O(5)-Cd(2)#10	2.3846(19)	O(4)#6-Cd(2)-O(5)#7	160.19(7)
O(6)-Cd(1)#2	2.297(2)	O(1)#4-Cd(2)-O(5)#8	86.30(7)
O(3)-Cd(1)#3	2.546(2)	O(1)-Cd(2)-O(5)#8	90.88(7)
O(1)-Cd(1)-O(1)#1	83.58(7)	O(4)#5-Cd(2)-O(5)#8	160.19(7)
O(1)-Cd(1)-O(6)#2	162.37(8)	O(4)#6-Cd(2)-O(5)#8	84.43(8)
O(1)#1-Cd(1)-O(6)#2	85.78(7)	O(5)#7-Cd(2)-O(5)#8	84.72(10)
Cd(1)-O(1)-Cd(2)	115.42(8)	C(4)-C(3)-C(6)	120.9(2)
Cd(1)-O(1)-Cd(1)#1	96.42(7)	C(2)-C(3)-C(6)	120.8(2)
Cd(2)-O(1)-Cd(1)#1	116.11(8)	O(3)-C(6)-O(4)	126.6(3)
C(5)-N(1)-C(1)	117.9(2)	O(3)-C(6)-C(3)	116.3(2)
C(5)-N(1)-Cd(1)	121.09(18)	O(4)-C(6)-C(3)	117.1(2)
C(1)-N(1)-Cd(1)	120.63(18)	C(6)-O(4)-Cd(2)#9	116.87(18)
C(5)-C(4)-C(3)	119.7(2)	O(6)-C(7)-O(5)	127.2(2)
N(1)-C(1)-C(2)	123.3(3)	O(6)-C(7)-C(2)	115.4(2)
C(1)-C(2)-C(3)	118.4(2)	O(5)-C(7)-C(2)	117.3(2)

C(1)-C(2)-C(7)	118.0(2)	C(7)-O(5)-Cd(2)#10	122.90(17)
C(3)-C(2)-C(7)	123.6(2)	C(7)-O(6)-Cd(1)#2	141.94(18)
N(1)-C(5)-C(4)	122.7(2)	C(6)-O(3)-Cd(1)#3	119.04(17)
C(4)-C(3)-C(2)	118.1(2)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z #2 -x+1/2,-y+3/2,-z

#3 -x+1/2,-y+1/2,-z #4 -x,y,-z+1/2

#5 x-1/2,y+1/2,z #6 -x+1/2,y+1/2,-z+1/2

#7 x-1/2,y-1/2,z #8 -x+1/2,y-1/2,-z+1/2

#9 x+1/2,y-1/2,z #10 x+1/2,y+1/2,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **2**

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
Cd(1)	9(1)	15(1)	20(1)	3(1)	2(1)	-1(1)
Cd(2)	12(1)	14(1)	14(1)	0	4(1)	0
O(1)	13(1)	12(1)	15(1)	1(1)	3(1)	0(1)
N(1)	10(1)	18(1)	19(1)	2(1)	3(1)	1(1)
C(4)	17(1)	10(1)	27(1)	4(1)	2(1)	-1(1)
O(2)	26(1)	29(1)	22(1)	-7(1)	4(1)	-1(1)
C(1)	13(1)	15(1)	17(1)	1(1)	1(1)	0(1)
C(2)	12(1)	13(1)	16(1)	-1(1)	2(1)	-2(1)
C(5)	13(1)	19(1)	28(1)	4(1)	3(1)	-3(1)
C(3)	12(1)	14(1)	16(1)	2(1)	1(1)	1(1)
C(6)	14(1)	12(1)	21(1)	-1(1)	2(1)	2(1)
O(4)	25(1)	29(1)	26(1)	11(1)	5(1)	15(1)
C(7)	10(1)	16(1)	21(1)	3(1)	4(1)	0(1)
O(5)	14(1)	18(1)	24(1)	4(1)	-2(1)	-5(1)
O(6)	16(1)	34(1)	36(1)	23(1)	1(1)	-5(1)
O(3)	17(1)	22(1)	28(1)	-3(1)	9(1)	1(1)

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

	x	y	z	U(eq)
H(4A)	2618	184	1673	22
H(1A)	2393	6828	857	19
H(5A)	1570	1705	1274	24
H(1)	209(16)	2350(60)	710(20)	9(7)
H(2)	646(18)	9270(50)	1650(30)	14(8)
H(3)	-10(30)	8650(80)	1090(40)	62(16)