

Supporting Information for:

**Synthesis, structure, and luminescence of a molecular Europium tetracyanoplatinate incorporating 4,5-diazafluoren-9-one**

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Table S1. Crystal data and structure refinement for  $[(\text{Eu}(\text{H}_2\text{O})_6)_2(\text{Pt}(\text{CN})_4)_3] \cdot 4\text{C}_{11}\text{H}_6\text{N}_2\text{O} \cdot 4\text{H}_2\text{O}$ .

Identification code	xc197	
Empirical formula	$\text{C}_{56} \text{H}_{60} \text{Eu}_2 \text{N}_{20} \text{O}_{22} \text{Pt}_3$	
Formula weight	2254.43	
Temperature	290(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	$a = 10.9678(3)$ Å	$\alpha = 90^\circ$ .
	$b = 25.1612(6)$ Å	$\beta = 91.400(2)^\circ$ .
	$c = 13.3381(3)$ Å	$\gamma = 90^\circ$ .
Volume	$3679.72(16)$ Å <sup>3</sup>	
Z	2	
Density (calculated)	2.035 Mg/m <sup>3</sup>	
Absorption coefficient	7.446 mm <sup>-1</sup>	
F(000)	2144	
Crystal size	0.15 x 0.07 x 0.05 mm <sup>3</sup>	
Theta range for data collection	3.06 to 25.35°.	
Index ranges	$-13 \leq h \leq 13, -30 \leq k \leq 30, -15 \leq l \leq 16$	
Reflections collected	27552	
Independent reflections	6722 [R(int) = 0.0414]	
Completeness to theta = 25.35°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00 and 0.67827	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	6722 / 0 / 466	
Goodness-of-fit on F <sup>2</sup>	0.855	

Final R indices [ $I > 2\sigma(I)$ ]

R1 = 0.0261, wR2 = 0.0455

R indices (all data)

R1 = 0.0461, wR2 = 0.0476

Largest diff. peak and hole

1.241 and -1.257 e.Å<sup>-3</sup>

Table S2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $[(\text{Eu}(\text{H}_2\text{O})_6)_2(\text{Pt}(\text{CN})_4)_3] \cdot 4\text{C}_{11}\text{H}_6\text{N}_2\text{O} \cdot 4\text{H}_2\text{O}$ .  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	$U(\text{eq})$
Eu(1)	1332(1)	1433(1)	1082(1)	27(1)
Pt(1)	5000	0	0	59(1)
Pt(2)	1343(1)	1693(1)	-3122(1)	34(1)
C(1)	1330(4)	1593(2)	-1642(4)	33(1)
C(2)	2070(5)	2414(2)	-2967(4)	42(1)
C(3)	1302(4)	1789(2)	-4616(4)	44(1)
C(4)	719(5)	956(3)	-3331(4)	46(1)
C(5)	3754(5)	518(2)	444(4)	53(2)
C(6)	3712(7)	-376(3)	-862(5)	65(2)
C(7)	-318(5)	3287(3)	-1359(4)	60(2)
C(8)	-621(6)	3794(3)	-1684(5)	78(2)
C(9)	-838(6)	4187(3)	-1007(6)	83(2)
C(10)	-768(5)	4049(2)	-16(5)	57(2)
C(11)	-452(4)	3534(2)	251(4)	42(1)
C(12)	-938(6)	4362(3)	922(6)	73(2)
C(13)	-418(4)	3502(2)	1370(4)	38(1)
C(14)	-714(5)	3995(2)	1770(5)	50(2)
C(15)	-742(6)	4054(3)	2783(5)	71(2)
C(16)	-464(5)	3620(3)	3360(5)	63(2)
C(17)	-183(5)	3150(2)	2922(4)	51(2)
C(18)	2791(5)	3203(3)	-373(4)	56(2)
C(19)	2609(5)	3721(3)	-671(4)	62(2)
C(20)	2514(5)	4117(2)	22(5)	56(2)
C(21)	2602(4)	3966(2)	1009(4)	39(1)
C(22)	2784(4)	3436(2)	1255(4)	34(1)
C(23)	2570(4)	4284(2)	1950(4)	44(1)
C(24)	2850(4)	3382(2)	2357(4)	36(1)
C(25)	2762(4)	3886(2)	2773(4)	38(1)
C(26)	2810(5)	3949(2)	3794(4)	51(2)
C(27)	2945(5)	3488(2)	4354(4)	54(2)

C(28)	2992(5)	3003(2)	3888(4)	51(2)
N(1)	1303(4)	1540(2)	-791(3)	41(1)
N(2)	2511(4)	2820(2)	-2899(3)	56(1)
N(3)	1261(5)	1834(2)	-5454(4)	85(2)
N(4)	416(5)	527(2)	-3495(4)	69(2)
N(5)	3049(4)	821(2)	676(3)	51(1)
N(6)	3006(7)	-587(3)	-1313(5)	93(2)
N(7)	-240(4)	3143(2)	-394(3)	45(1)
N(8)	-133(3)	3080(2)	1916(3)	39(1)
N(9)	2871(4)	3046(2)	589(3)	42(1)
N(10)	2950(4)	2937(2)	2887(3)	41(1)
O(1)	1649(3)	1949(1)	2567(2)	49(1)
O(2)	1556(3)	770(1)	2379(2)	47(1)
O(3)	3080(3)	1972(1)	854(3)	46(1)
O(4)	-648(3)	1373(1)	1895(3)	59(1)
O(5)	306(3)	681(1)	349(2)	52(1)
O(6)	323(3)	2232(1)	740(2)	40(1)
O(7)	-826(4)	-110(2)	1387(3)	65(1)
O(8)	456(4)	3329(2)	5868(5)	125(2)
O(9)	223(5)	560(2)	3948(3)	113(2)
O(10)	-1222(5)	4831(2)	978(4)	112(2)
O(11)	2399(4)	4755(2)	2038(3)	64(1)

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Table S3. Bond lengths [Å] and angles [°] for [(Eu(H<sub>2</sub>O)<sub>6</sub>)<sub>2</sub>(Pt(CN)<sub>4</sub>)<sub>3</sub>]·4C<sub>11</sub>H<sub>6</sub>N<sub>2</sub>O·4H<sub>2</sub>O.

Eu(1)-O(6)	2.335(3)
Eu(1)-O(3)	2.373(3)
Eu(1)-O(1)	2.386(3)
Eu(1)-O(5)	2.397(3)
Eu(1)-O(2)	2.411(3)
Eu(1)-O(4)	2.456(3)
Eu(1)-N(5)	2.501(4)
Eu(1)-N(1)	2.513(4)
Pt(1)-C(5)	1.989(5)
Pt(1)-C(5)#1	1.989(5)
Pt(1)-C(6)#1	2.034(8)
Pt(1)-C(6)	2.034(8)
Pt(2)-C(1)	1.989(5)
Pt(2)-C(2)	1.989(6)
Pt(2)-C(4)	1.994(6)
Pt(2)-C(3)	2.007(5)
C(1)-N(1)	1.144(5)
C(2)-N(2)	1.133(6)
C(3)-N(3)	1.123(6)
C(4)-N(4)	1.148(6)
C(5)-N(5)	1.135(6)
C(6)-N(6)	1.104(8)
C(7)-N(7)	1.339(7)
C(7)-C(8)	1.385(8)
C(7)-H(7)	0.9300
C(8)-C(9)	1.365(9)
C(8)-H(8)	0.9300
C(9)-C(10)	1.366(9)
C(9)-H(9)	0.9300
C(10)-C(11)	1.386(7)
C(10)-C(12)	1.493(9)
C(11)-N(7)	1.331(6)
C(11)-C(13)	1.494(7)
C(12)-O(10)	1.223(7)

C(12)-C(14)	1.476(8)
C(13)-N(8)	1.320(6)
C(13)-C(14)	1.393(7)
C(14)-C(15)	1.360(8)
C(15)-C(16)	1.366(8)
C(15)-H(15)	0.9300
C(16)-C(17)	1.356(7)
C(16)-H(16)	0.9300
C(17)-N(8)	1.356(6)
C(17)-H(17)	0.9300
C(18)-N(9)	1.343(6)
C(18)-C(19)	1.378(8)
C(18)-H(18)	0.9300
C(19)-C(20)	1.364(8)
C(19)-H(19)	0.9300
C(20)-C(21)	1.370(7)
C(20)-H(20)	0.9300
C(21)-C(22)	1.387(6)
C(21)-C(23)	1.489(7)
C(22)-N(9)	1.329(6)
C(22)-C(24)	1.477(7)
C(23)-O(11)	1.206(6)
C(23)-C(25)	1.497(7)
C(24)-N(10)	1.328(6)
C(24)-C(25)	1.387(6)
C(25)-C(26)	1.371(7)
C(26)-C(27)	1.385(7)
C(26)-H(26)	0.9300
C(27)-C(28)	1.371(7)
C(27)-H(27)	0.9300
C(28)-N(10)	1.346(6)
C(28)-H(28)	0.9300
O(1)-H(1A)	0.8502
O(1)-H(1B)	0.8494
O(2)-H(2A)	0.8501
O(2)-H(2B)	0.8495

O(3)-H(3A)	0.8504
O(3)-H(3B)	0.8508
O(4)-H(4A)	0.8498
O(4)-H(4B)	0.8502
O(5)-H(5A)	0.8500
O(5)-H(5B)	0.8506
O(6)-H(6A)	0.8500
O(6)-H(6B)	0.8505
O(7)-H(7A)	0.8500
O(7)-H(7B)	0.8502
O(8)-H(8A)	0.8503
O(8)-H(8B)	0.8496
O(9)-H(9A)	0.8495
O(9)-H(9B)	0.8579

O(6)-Eu(1)-O(3)	82.14(11)
O(6)-Eu(1)-O(1)	75.66(11)
O(3)-Eu(1)-O(1)	72.17(12)
O(6)-Eu(1)-O(5)	112.59(12)
O(3)-Eu(1)-O(5)	140.45(11)
O(1)-Eu(1)-O(5)	145.61(11)
O(6)-Eu(1)-O(2)	140.81(11)
O(3)-Eu(1)-O(2)	114.74(12)
O(1)-Eu(1)-O(2)	76.71(11)
O(5)-Eu(1)-O(2)	77.64(12)
O(6)-Eu(1)-O(4)	73.64(11)
O(3)-Eu(1)-O(4)	144.79(12)
O(1)-Eu(1)-O(4)	77.25(13)
O(5)-Eu(1)-O(4)	73.77(12)
O(2)-Eu(1)-O(4)	73.55(12)
O(6)-Eu(1)-N(5)	147.47(13)
O(3)-Eu(1)-N(5)	73.07(13)
O(1)-Eu(1)-N(5)	114.78(14)
O(5)-Eu(1)-N(5)	77.01(14)
O(2)-Eu(1)-N(5)	70.51(12)
O(4)-Eu(1)-N(5)	137.49(13)

O(6)-Eu(1)-N(1)	73.64(12)
O(3)-Eu(1)-N(1)	78.57(12)
O(1)-Eu(1)-N(1)	139.87(12)
O(5)-Eu(1)-N(1)	71.64(12)
O(2)-Eu(1)-N(1)	141.91(12)
O(4)-Eu(1)-N(1)	117.09(13)
N(5)-Eu(1)-N(1)	80.94(14)
C(5)-Pt(1)-C(5)#1	180.0(4)
C(5)-Pt(1)-C(6)#1	90.0(3)
C(5)#1-Pt(1)-C(6)#1	90.0(3)
C(5)-Pt(1)-C(6)	90.0(3)
C(5)#1-Pt(1)-C(6)	90.0(3)
C(6)#1-Pt(1)-C(6)	180.0(6)
C(1)-Pt(2)-C(2)	91.40(19)
C(1)-Pt(2)-C(4)	90.61(19)
C(2)-Pt(2)-C(4)	175.9(2)
C(1)-Pt(2)-C(3)	178.25(19)
C(2)-Pt(2)-C(3)	89.6(2)
C(4)-Pt(2)-C(3)	88.5(2)
N(1)-C(1)-Pt(2)	178.8(5)
N(2)-C(2)-Pt(2)	177.8(5)
N(3)-C(3)-Pt(2)	178.5(5)
N(4)-C(4)-Pt(2)	175.6(5)
N(5)-C(5)-Pt(1)	178.2(5)
N(6)-C(6)-Pt(1)	178.5(8)
N(7)-C(7)-C(8)	124.0(6)
N(7)-C(7)-H(7)	118.0
C(8)-C(7)-H(7)	118.0
C(9)-C(8)-C(7)	120.3(6)
C(9)-C(8)-H(8)	119.8
C(7)-C(8)-H(8)	119.8
C(8)-C(9)-C(10)	116.7(6)
C(8)-C(9)-H(9)	121.6
C(10)-C(9)-H(9)	121.6
C(9)-C(10)-C(11)	119.6(6)
C(9)-C(10)-C(12)	132.2(6)



C(11)-C(10)-C(12)	108.2(5)
N(7)-C(11)-C(10)	124.9(5)
N(7)-C(11)-C(13)	127.2(5)
C(10)-C(11)-C(13)	107.9(5)
O(10)-C(12)-C(14)	126.4(7)
O(10)-C(12)-C(10)	126.7(7)
C(14)-C(12)-C(10)	107.0(5)
N(8)-C(13)-C(14)	124.0(5)
N(8)-C(13)-C(11)	126.5(5)
C(14)-C(13)-C(11)	109.5(5)
C(15)-C(14)-C(13)	119.2(6)
C(15)-C(14)-C(12)	133.4(6)
C(13)-C(14)-C(12)	107.4(5)
C(14)-C(15)-C(16)	117.6(6)
C(14)-C(15)-H(15)	121.2
C(16)-C(15)-H(15)	121.2
C(17)-C(16)-C(15)	120.2(6)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
N(8)-C(17)-C(16)	123.7(6)
N(8)-C(17)-H(17)	118.1
C(16)-C(17)-H(17)	118.1
N(9)-C(18)-C(19)	124.1(5)
N(9)-C(18)-H(18)	118.0
C(19)-C(18)-H(18)	118.0
C(20)-C(19)-C(18)	120.5(6)
C(20)-C(19)-H(19)	119.7
C(18)-C(19)-H(19)	119.7
C(19)-C(20)-C(21)	116.4(5)
C(19)-C(20)-H(20)	121.8
C(21)-C(20)-H(20)	121.8
C(20)-C(21)-C(22)	119.9(5)
C(20)-C(21)-C(23)	131.2(5)
C(22)-C(21)-C(23)	108.9(4)
N(9)-C(22)-C(21)	124.4(5)
N(9)-C(22)-C(24)	126.5(4)

C(21)-C(22)-C(24)	109.1(4)
O(11)-C(23)-C(21)	128.1(5)
O(11)-C(23)-C(25)	127.2(5)
C(21)-C(23)-C(25)	104.7(4)
N(10)-C(24)-C(25)	124.3(5)
N(10)-C(24)-C(22)	127.5(5)
C(25)-C(24)-C(22)	108.2(4)
C(26)-C(25)-C(24)	120.1(5)
C(26)-C(25)-C(23)	130.7(5)
C(24)-C(25)-C(23)	109.2(4)
C(25)-C(26)-C(27)	116.1(5)
C(25)-C(26)-H(26)	122.0
C(27)-C(26)-H(26)	122.0
C(28)-C(27)-C(26)	120.4(5)
C(28)-C(27)-H(27)	119.8
C(26)-C(27)-H(27)	119.8
N(10)-C(28)-C(27)	123.9(5)
N(10)-C(28)-H(28)	118.0
C(27)-C(28)-H(28)	118.0
C(1)-N(1)-Eu(1)	177.7(4)
C(5)-N(5)-Eu(1)	173.8(5)
C(11)-N(7)-C(7)	114.4(5)
C(13)-N(8)-C(17)	115.3(5)
C(22)-N(9)-C(18)	114.6(5)
C(24)-N(10)-C(28)	115.1(5)
Eu(1)-O(1)-H(1A)	128.1
Eu(1)-O(1)-H(1B)	123.4
H(1A)-O(1)-H(1B)	108.6
Eu(1)-O(2)-H(2A)	123.5
Eu(1)-O(2)-H(2B)	121.1
H(2A)-O(2)-H(2B)	112.0
Eu(1)-O(3)-H(3A)	131.1
Eu(1)-O(3)-H(3B)	127.8
H(3A)-O(3)-H(3B)	101.1
Eu(1)-O(4)-H(4A)	120.9
Eu(1)-O(4)-H(4B)	122.2

H(4A)-O(4)-H(4B)	114.7
Eu(1)-O(5)-H(5A)	124.0
Eu(1)-O(5)-H(5B)	127.4
H(5A)-O(5)-H(5B)	100.9
Eu(1)-O(6)-H(6A)	123.1
Eu(1)-O(6)-H(6B)	121.5
H(6A)-O(6)-H(6B)	110.4
H(7A)-O(7)-H(7B)	107.2
H(8A)-O(8)-H(8B)	107.8
H(9A)-O(9)-H(9B)	94.5

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Symmetry transformations used to generate equivalent atoms:

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

Table S4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $[(\text{Eu}(\text{H}_2\text{O})_6)_2(\text{Pt}(\text{CN})_4)_3] \cdot 4\text{C}_{11}\text{H}_6\text{N}_2\text{O} \cdot 4\text{H}_2\text{O}$ .  
The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Eu(1)	36(1)	21(1)	24(1)	1(1)	4(1)	5(1)
Pt(1)	78(1)	43(1)	59(1)	21(1)	39(1)	37(1)
Pt(2)	34(1)	46(1)	23(1)	3(1)	2(1)	-4(1)
C(1)	35(3)	34(3)	28(3)	0(2)	-3(2)	-3(2)
C(2)	39(3)	53(4)	35(3)	0(3)	-3(3)	1(3)
C(3)	41(3)	65(4)	27(3)	4(3)	0(3)	-23(3)
C(4)	38(3)	70(4)	30(3)	6(3)	2(3)	-2(3)
C(5)	68(4)	37(3)	55(4)	16(3)	25(3)	14(3)
C(6)	97(6)	47(5)	53(5)	6(3)	23(4)	22(4)
C(7)	69(4)	61(4)	51(4)	8(3)	-10(3)	-4(3)
C(8)	86(5)	79(5)	69(5)	27(4)	-35(4)	-16(4)
C(9)	96(6)	46(5)	106(6)	18(4)	-47(5)	-14(4)
C(10)	57(4)	45(4)	69(5)	5(3)	-27(3)	-1(3)
C(11)	29(3)	36(3)	60(4)	8(3)	-10(3)	-1(2)
C(12)	71(5)	36(4)	112(6)	-9(4)	-37(4)	8(3)
C(13)	25(3)	36(3)	51(3)	-8(3)	-2(2)	0(2)
C(14)	39(3)	40(4)	70(4)	-13(3)	-9(3)	7(3)
C(15)	65(4)	66(5)	80(5)	-39(4)	-6(4)	10(4)
C(16)	58(4)	78(5)	52(4)	-23(4)	-4(3)	7(4)
C(17)	47(3)	57(4)	50(4)	-5(3)	10(3)	-3(3)
C(18)	56(4)	72(5)	41(4)	-10(3)	7(3)	-5(3)
C(19)	64(4)	79(5)	44(4)	17(4)	1(3)	-9(4)
C(20)	58(4)	44(4)	65(4)	14(3)	-1(3)	-3(3)
C(21)	40(3)	33(3)	43(3)	2(2)	-1(3)	-3(2)
C(22)	30(3)	32(3)	40(3)	1(2)	0(2)	-7(2)
C(23)	37(3)	33(3)	62(4)	-5(3)	0(3)	-2(3)
C(24)	27(3)	35(3)	45(3)	3(3)	-4(2)	-4(2)
C(25)	36(3)	35(3)	43(3)	-7(3)	-6(3)	-3(2)
C(26)	52(4)	43(4)	57(4)	-17(3)	-2(3)	-5(3)
C(27)	58(4)	67(5)	37(3)	-3(3)	-8(3)	-6(3)
C(28)	49(4)	52(4)	52(4)	8(3)	-11(3)	-6(3)

N(1)	51(3)	42(3)	29(3)	0(2)	2(2)	-3(2)
N(2)	56(3)	52(3)	60(3)	1(3)	2(3)	-4(3)
N(3)	125(5)	105(5)	25(3)	7(3)	3(3)	-34(4)
N(4)	75(4)	57(4)	75(4)	-6(3)	-1(3)	-19(3)
N(5)	59(3)	30(3)	65(3)	4(2)	24(3)	20(2)
N(6)	122(6)	65(5)	91(5)	-1(4)	17(4)	24(4)
N(7)	49(3)	41(3)	44(3)	4(2)	-1(2)	0(2)
N(8)	33(2)	37(3)	48(3)	-1(2)	2(2)	3(2)
N(9)	49(3)	34(3)	43(3)	-7(2)	0(2)	0(2)
N(10)	45(3)	37(3)	40(3)	-1(2)	-5(2)	0(2)
O(1)	88(3)	38(2)	22(2)	-2(2)	2(2)	-12(2)
O(2)	67(2)	34(2)	42(2)	14(2)	14(2)	21(2)
O(3)	41(2)	31(2)	66(2)	-2(2)	5(2)	-2(2)
O(4)	55(2)	31(2)	93(3)	6(2)	40(2)	7(2)
O(5)	73(3)	40(2)	44(2)	-7(2)	10(2)	-23(2)
O(6)	57(2)	34(2)	29(2)	-3(2)	-1(2)	15(2)
O(7)	83(3)	59(3)	52(2)	0(2)	7(2)	-14(2)
O(8)	50(3)	128(5)	197(6)	94(4)	-11(3)	-7(3)
O(9)	174(5)	84(4)	85(3)	-25(3)	70(4)	-44(4)
O(10)	140(5)	43(3)	151(5)	-8(3)	-37(4)	26(3)
O(11)	75(3)	31(2)	87(3)	-6(2)	-2(2)	0(2)

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Table S5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for  $[(\text{Eu}(\text{H}_2\text{O})_6)_2(\text{Pt}(\text{CN})_4)_3] \cdot 4\text{C}_{11}\text{H}_6\text{N}_2\text{O} \cdot 4\text{H}_2\text{O}$ .

	x	y	z	U(eq)
H(7)	-160	3031	-1842	72
H(8)	-676	3867	-2367	94
H(9)	-1025	4532	-1209	100
H(15)	-944	4377	3073	85
H(16)	-466	3646	4055	75
H(17)	-17	2860	3335	62
H(18)	2862	2945	-868	67
H(19)	2551	3803	-1351	75
H(20)	2397	4469	-164	67
H(26)	2756	4282	4093	61
H(27)	3004	3508	5049	65
H(28)	3056	2701	4289	61
H(1A)	1356	1897	3143	74
H(1B)	2090	2226	2591	74
H(2A)	1956	484	2310	71
H(2B)	1049	749	2849	71
H(3A)	3150	2305	764	69
H(3B)	3823	1875	860	69
H(4A)	-1057	1652	2020	88
H(4B)	-1053	1085	1915	88
H(5A)	74	412	680	78
H(5B)	431	540	-219	78
H(6A)	304	2377	164	60
H(6B)	221	2464	1194	60
H(7A)	-409	-253	1861	97
H(7B)	-1312	109	1652	97
H(8A)	862	3059	6069	188
H(8B)	933	3595	5878	188
H(9A)	27	240	3821	170
H(9B)	233	518	4586	170

Figure S1.

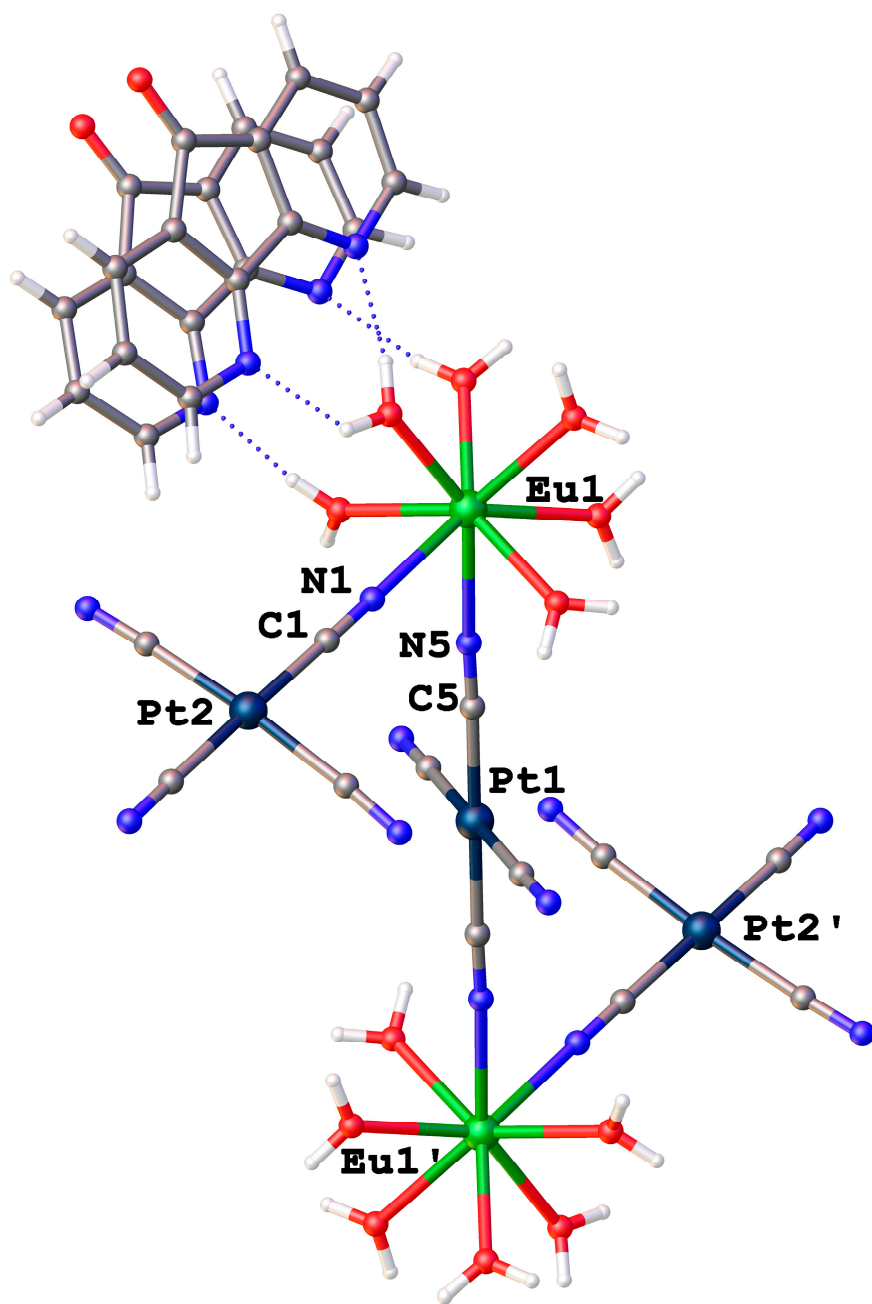


Figure S2.

