Supporting Information for

Actinide Tetracyanoplatinates: Synthesis and Structural Characterization Featuring Unique Fluorescent Properties from d-f Orbital Interactions

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Experimental Section

General Procedure: $UO_2(NO_3)_2.6H_2O$, $Th(NO_3)_4\cdot 6H_2O$ and $K_2[Pt(CN)_4]\cdot 3H_2O$ were purchased from Acros and used as received. The IR data were recorded as KBr pellets on SHIMADZU Inc. IR, Prestige-21 Fourier Transform Infrared Spectrophotometer in the range 400 – 4000 cm^{-1}. MALDI was performed on a Micromass QTOF mass spectrometer.

Synthesis: $Th(H_2O)_7[Pt(CN)_4]_2\cdot 10H_2O$ (**1**) was prepared by dissolving 0.0250 g (0.04 mmol) of $Th(NO_3)_4\cdot 6H_2O$ and 0.0235 g (0.06 mmol) of $K_2[Pt(CN)_4]\cdot xH_2O$ in 3 mL of H_2O in a test tube. The pH was brought to 2.5 with a small amount of 0.01 M KOH. The test tube was placed in a slow evaporation chamber, after 29 days green-yellow plates suitable for single crystal X-ray diffraction were observed.

$Th_2(H_2O)_{10}(OH)[Pt(CN)_4]\cdot 5H_2O$ (**2**) was prepared out by dissolving 0.0246 g (0.04 mmol) of $Th(NO_3)_4\cdot 6H_2O$ and 0.0237 g (.06 mmol) of $K_2[Pt(CN)_4]\cdot 3H_2O$ in 3 mL of H_2O in a test tube. The test tube was placed in a slow evaporation chamber, after 14 days green-yellow plates suitable for single crystal X-ray diffraction were observed.

$K_3[(UO_2)_2(OH)(Pt(CN)_4)_2]_2\cdot NO_3\cdot 1.5H_2O$ (**3**) was prepared dissolving 0.0248 g (0.05 mmol) of $UO_2(NO_3)_2\cdot 6H_2O$ and 0.0190 g (.05 mmol)of $K_2[Pt(CN)_4]\cdot xH_2O$ in 3 mL of H_2O. The test tube was placed in a slow evaporation chamber, after 20 days yellow plates suitable for single crystal X-ray diffraction were observed.

X-ray Crystallography: Crystals of compounds **2** and **3** were obtained in good yield from slow evaporation in water at room temperature. Crystals of **1** were obtained by slow evaporation of a water solution with a pH of 2.5. X-ray diffraction data for **1** were collected at -80 °C on a Bruker SMART APEX CCD X-ray diffractometer unit using Mo Kα radiation from crystals mounted in Paratone-N oil on glass fibers. SMART (v 5.624) was used for preliminary determination of cell constants and data collection control. Determination of integrated intensities and global cell refinement were performed with the Bruker SAINT Software package using a narrow-frame integration algorithm. X-ray data for **2** and **3** were collected using a Varian Oxford Xcalibur E single-crystal X-ray diffractometer. Intensity measurements were performed using Mo Kα radiation, from a sealed-tube Enhance X-ray source, and an Eos area detector. CrysAlis[R1] was used for preliminary determination of the cell constants, data collection strategy, and for data collection control. Following data collection, CrysAlis was also used to integrate the reflection intensities, apply an absorption correction to the data, and perform a global cell refinement. The program suite SHELXTL (v 5.1) was used for space group determination, structure solution, and refinement.[1] Refinement was performed against F^2 by weighted full-matrix least square, and empirical absorption correction (SADABS[3]) was applied. H atoms were found from the difference fourier maps.

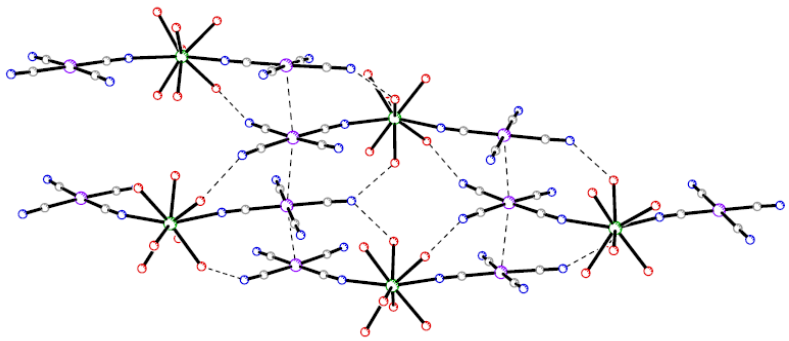


Fig. S1 Packing diagram of **1,** $Th(H_2O)_7[Pt(CN)_4]_2\cdot 10H_2O$. Pt-Pt interactions and hydrogen bonding shown with dotted lines.

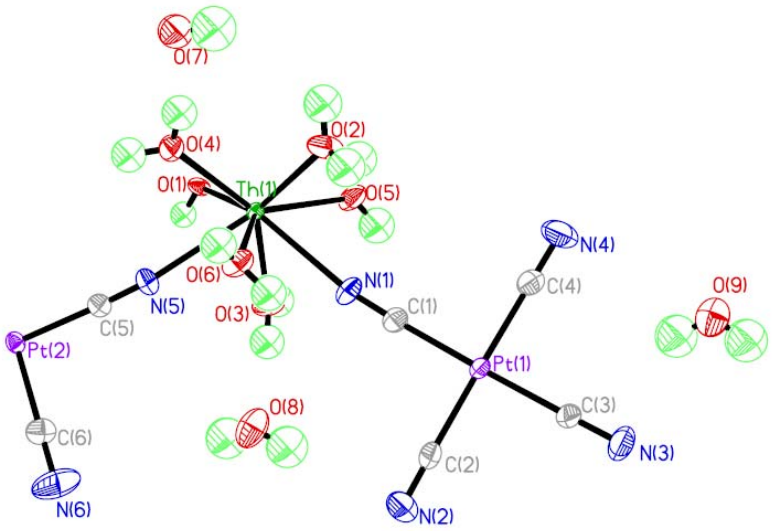


Fig. S2 Asymmetric unit of $Th_2(H_20)_{10}(OH)_2[Pt(CN)_4]_3 \cdot 5H_20$ **(2).**

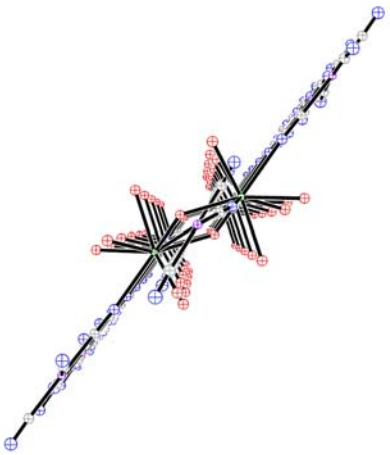


Fig. S3 Viewing down the C axis **2**. Two Th centers are bridged by a hydroxy group.

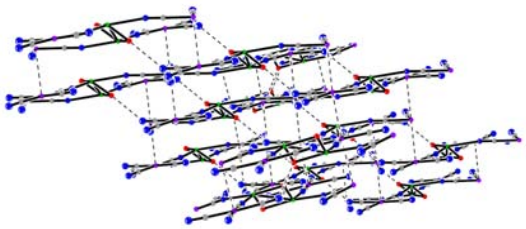


Fig. S4 Packing diagram of **2** Pt-Pt interactions and hydrogen bonding shown with dotted lines.

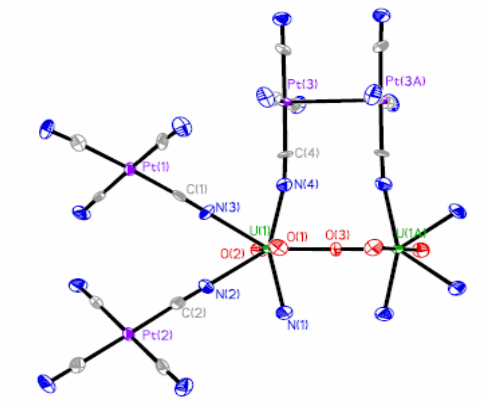


Fig. S5 Diagram showing dimeric Pt-Pt interactions (SHELX, 50% thermal ellipsoids) of $K_3[(UO_2)_2(OH)(Pt(CN)_4)_2]_2 \cdot NO_3 \cdot 1.5H_2O$ **(3)**.

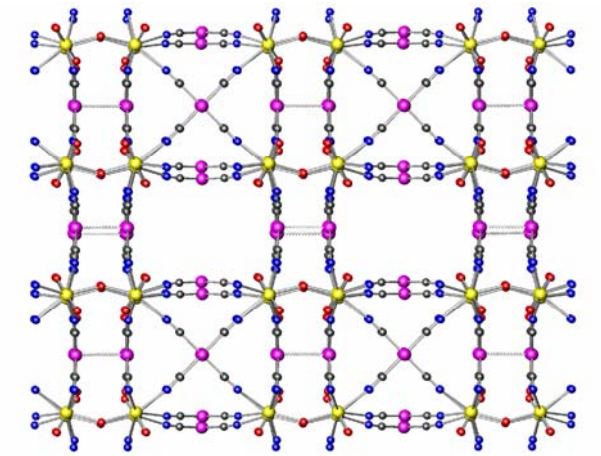
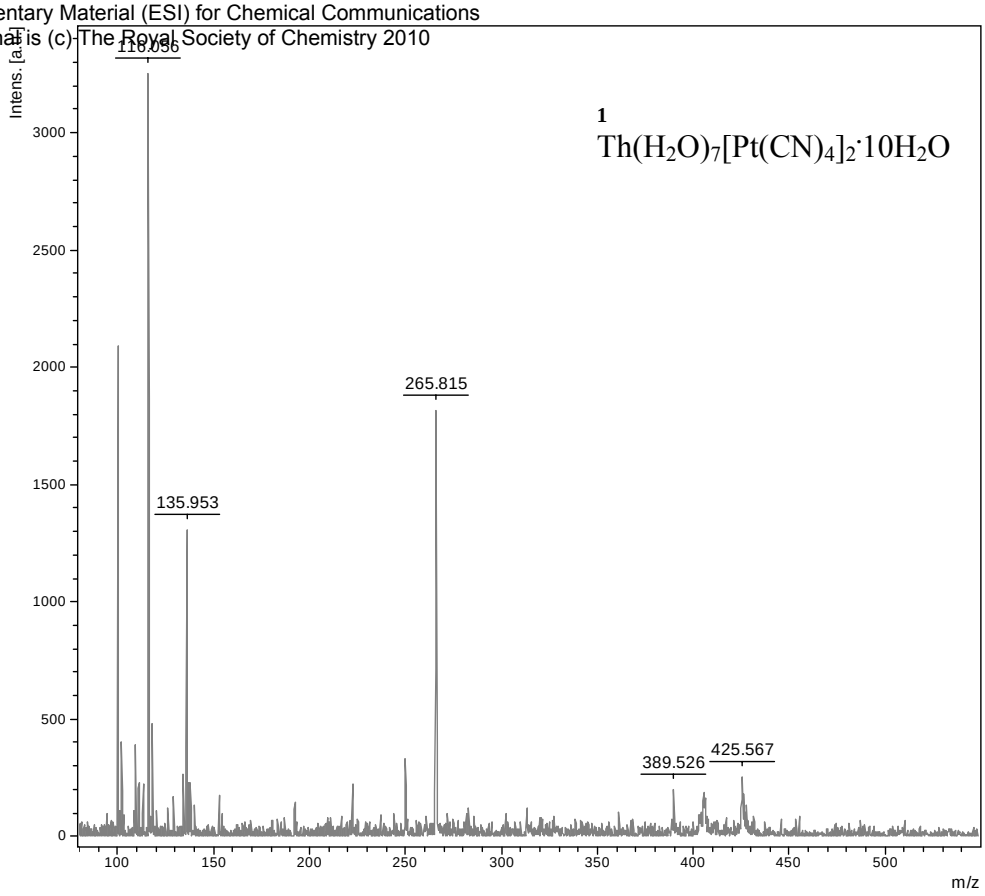
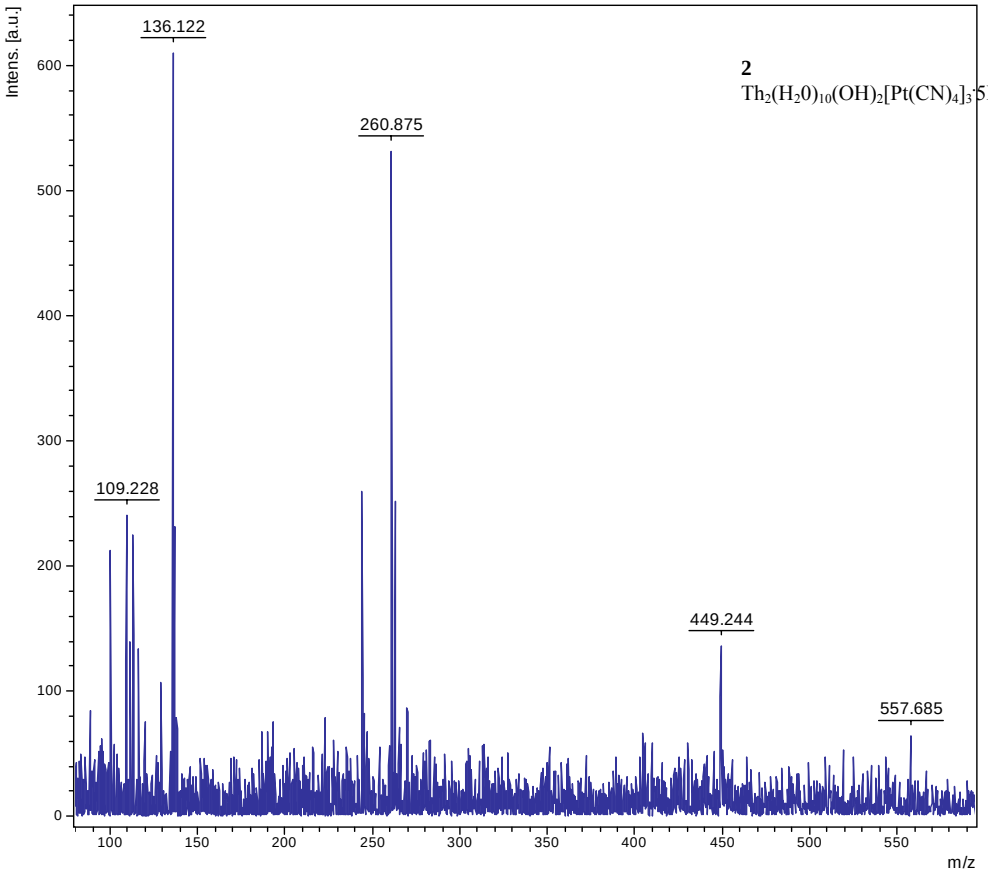


Fig. S6 Packing diagram of $K_3[(UO_2)_2(OH)(Pt(CN)_4)_2]_2 \cdot NO_3 \cdot 1.5H_2O$ **(3)** viewed perpendicular to the c axis.



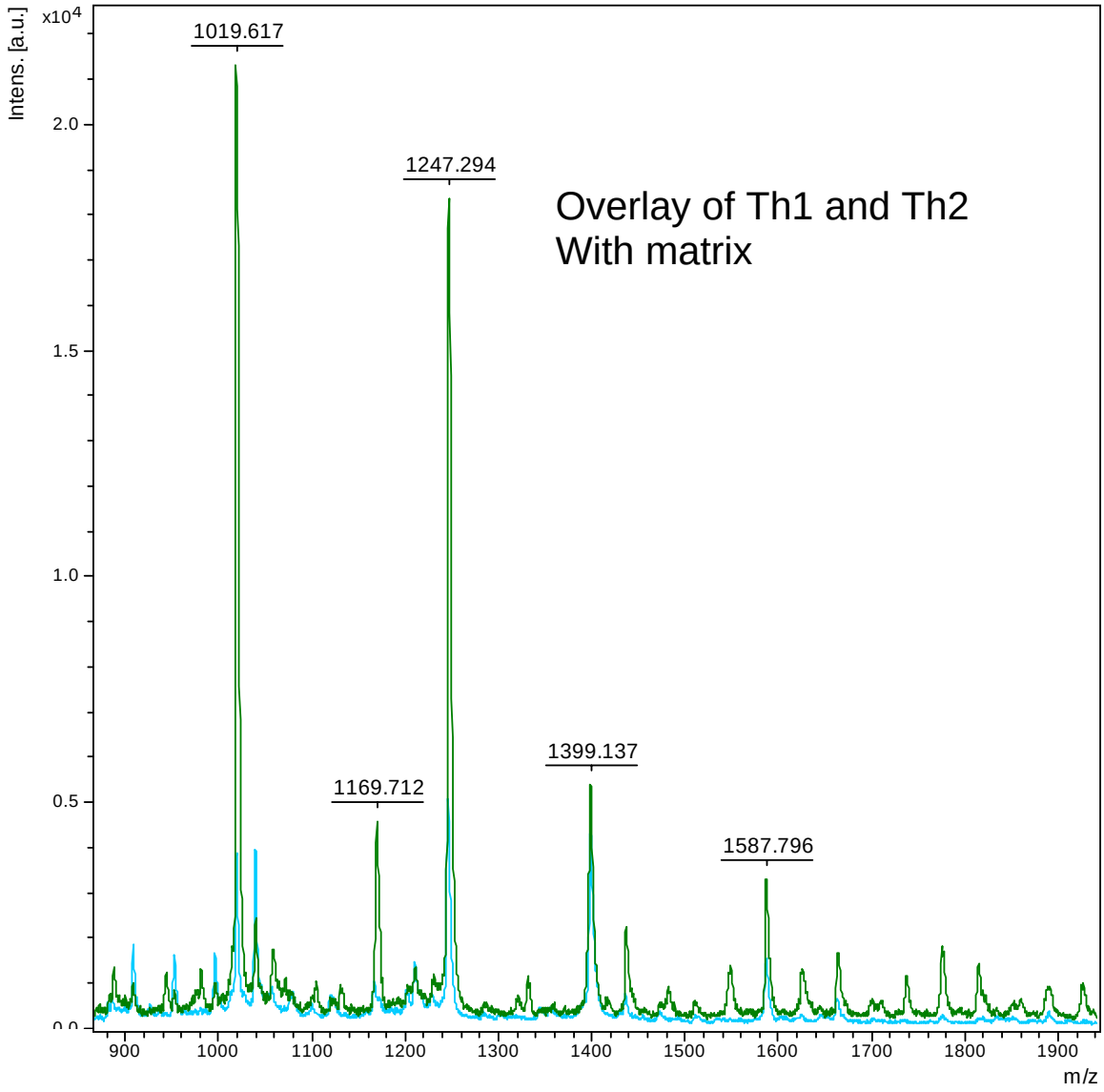
1

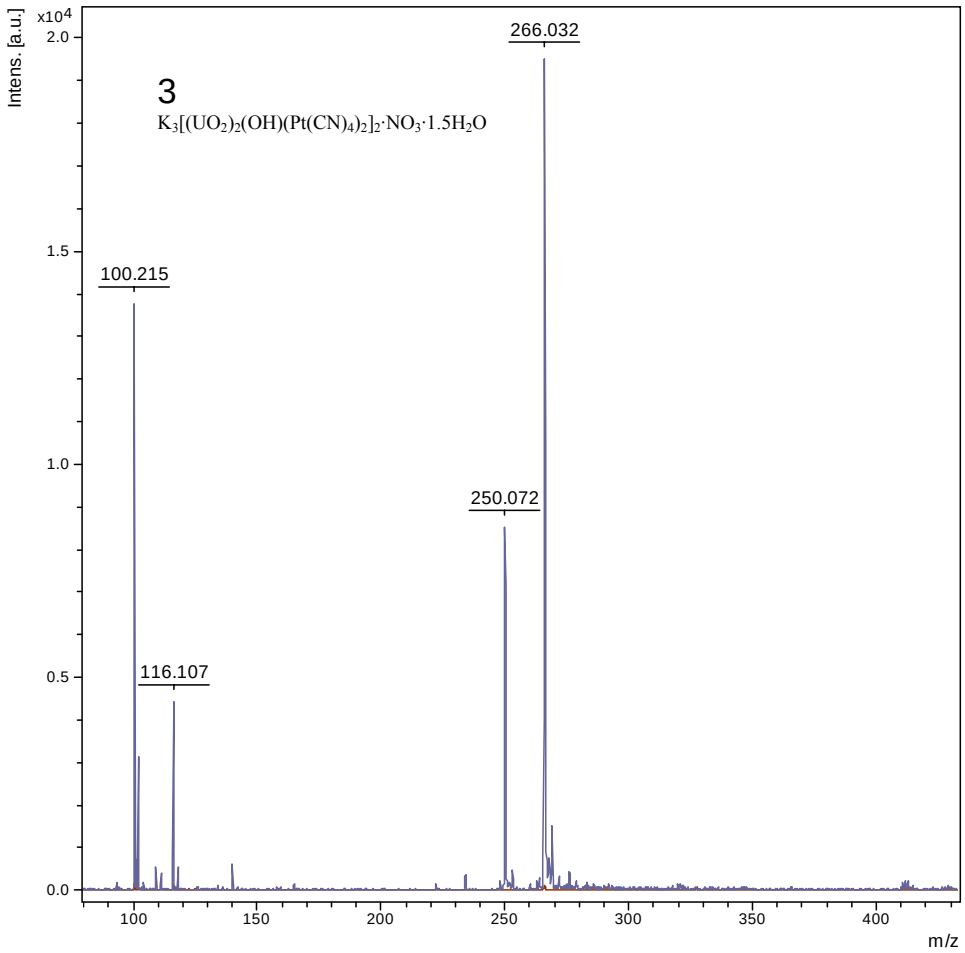
$Th(H_2O)_7[Pt(CN)_4]_2 \cdot 10H_2O$

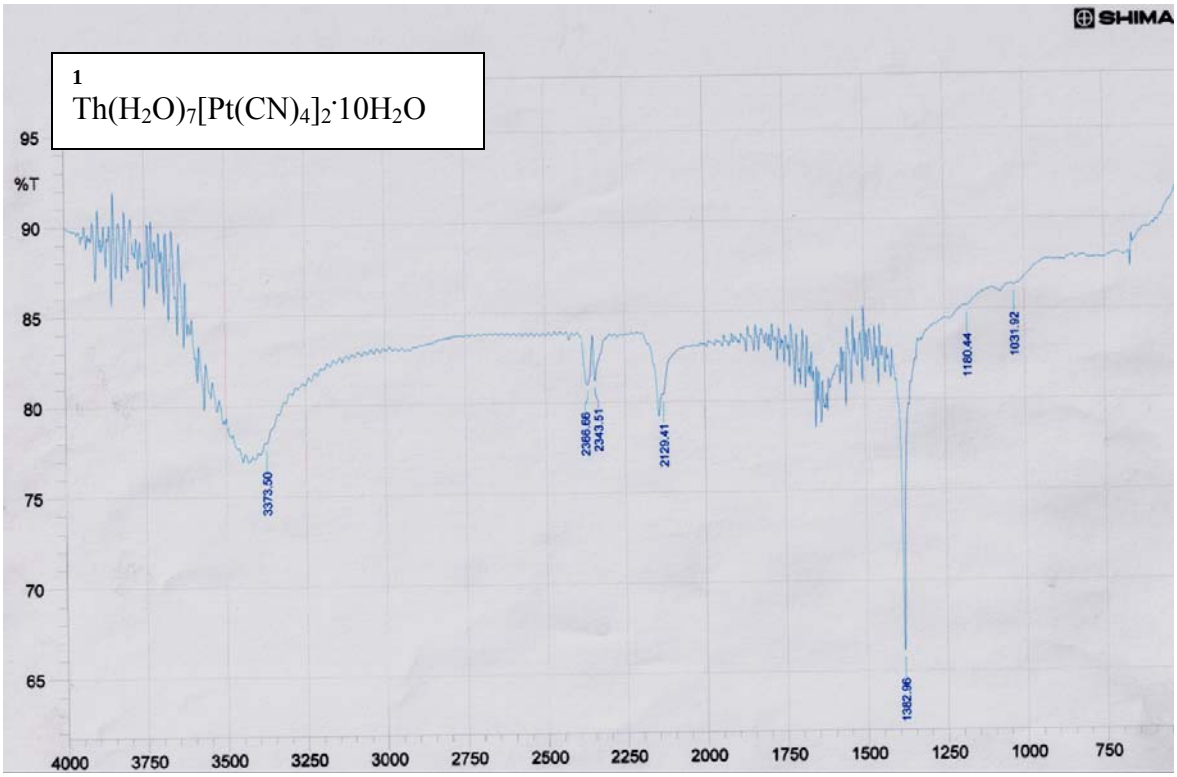


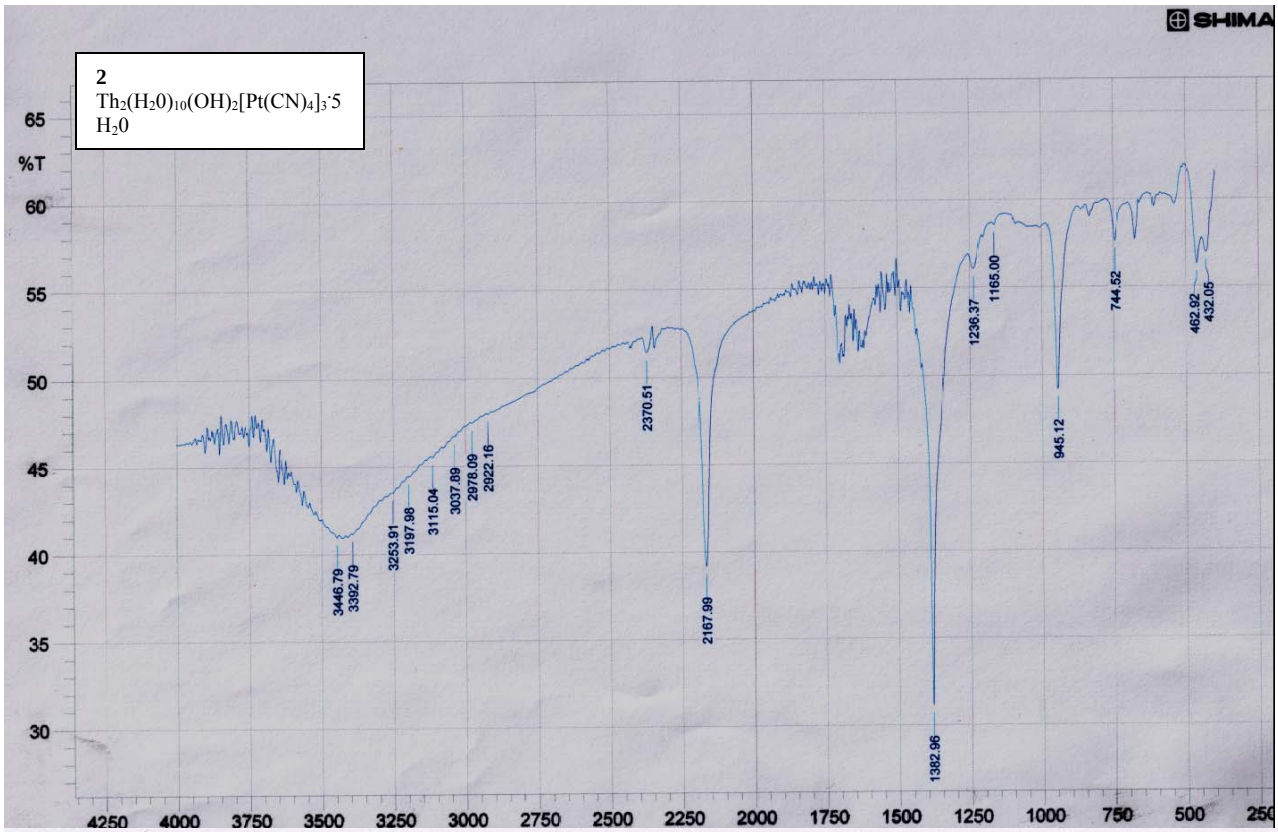
2

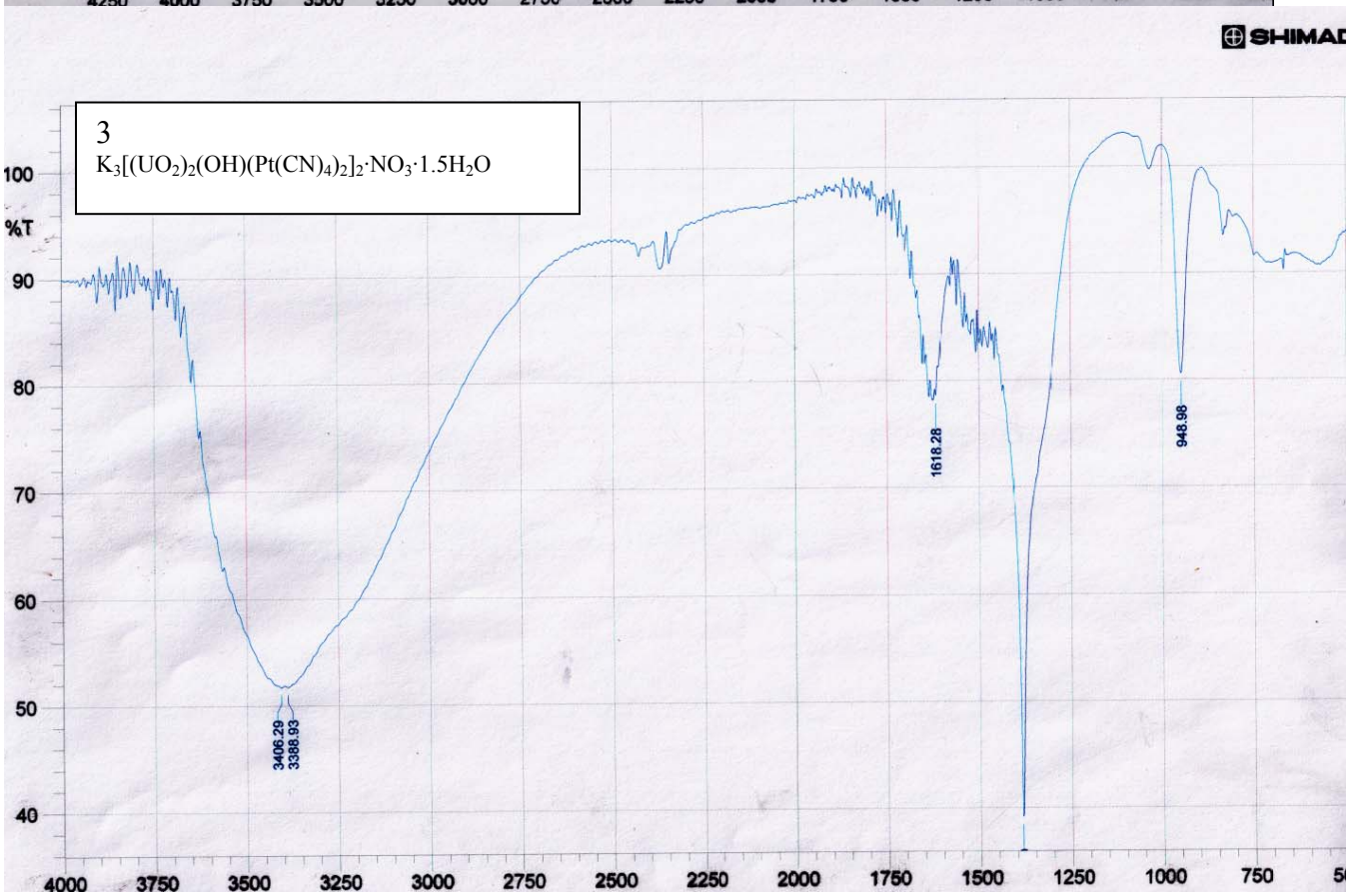
$Th_2(H_20)_{10}(OH)_2[Pt(CN)_4]_3 \cdot 5H_20$


Intens. [a.u.]
x10^4
2.0
1.5
1.0
0.5
0.0
1019.617
1247.294
1169.712
1399.137
1587.796
Overlay of Th1 and Th2
With matrix
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
1900
m/z


x10^4
Intens. [a.u.]
2.0
1.5
1.0
0.5
0.0
3
K3[(UO2)2(OH)(Pt(CN)4)2]2·NO3·1.5H2O
266.032
100.215
250.072
116.107
100
150
200
250
300
350
400
m/z


SHIMA
1
Th(H2O)7[Pt(CN)4]2·10H2O
95
%T
90
85
80
75
70
65
3373.50
2366.66
2343.51
2129.41
1382.96
1160.44
1031.92
4000
3750
3500
3250
3000
2750
2500
2250
2000
1750
1500
1250
1000
750


SHIMA
2
$Th_2(H_20)_{10}(OH)_2[Pt(CN)_4]_3{\cdot}5H_20$
%T
3446.79
3392.79
3253.91
3197.98
3115.04
3037.89
2978.09
2922.16
2370.51
2167.99
1382.96
1236.37
1165.00
945.12
744.52
462.92
432.05


SHIMAD
3
$K_3[(UO_2)_2(OH)(Pt(CN)_4)_2]_2{\cdot}NO_3{\cdot}1.5H_2O$
%T
3406.29
3388.93
1618.28
948.98

Crystallographic Information for **1**,**2** and **3**

Table 1. Crystal data and structure refinement for **1**, $Th(H_2O)_7[Pt(CN)_4]_2{\cdot}10H_2O$.

Identification code	Th1
Empirical formula	C8 H34 N8 O17 Pt2 Th
Formula weight	1136.65
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions	
	a = 13.2464(6) Å alpha = 90.0000(9) °
	b = 20.5599(10) Å beta = 90.0000(1) °
	c = 22.4536(11) Å gamma = 90.0000(9) °
Volume	6115.1(5) Å ^3
Z, Calculated density	8, 2.469 Mg/m^3
Absorption coefficient	14.053 mm^-1
F(000)	4160
Crystal size	0.80 x 0.80 x 0.09 mm
Theta range for data collection	1.81 to 28.27 °
Limiting indices	-17<=h<=17, -27<=k<=27, -29<=l<=29
Reflections collected / unique	59819 / 7574 [R(int) = 0.0737]
Completeness to theta = 28.27	99.9 %
Absorption correction	Analytical
Max. and min. transmission	0.3710 and 0.0314
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7574 / 0 / 313
Goodness-of-fit on F^2	0.999
Final R indices [I>2sigma(I)]	R1 = 0.0301, wR2 = 0.0766
R indices (all data)	R1 = 0.0373, wR2 = 0.0781
Largest diff. peak and hole	2.154 and -3.034 e. Å ^-3

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

$Th(H_2O)_7[Pt(CN)_4]_2 \cdot 10H_2O$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Th(1)	3617(1)	3956(1)	8669(1)	14(1)
Pt(1)	3747(1)	6259(1)	7345(1)	16(1)
O(1)	2519(3)	3947(2)	7783(2)	28(1)
N(1)	3683(3)	5121(2)	8278(2)	22(1)
C(1)	3711(4)	5557(2)	7954(2)	18(1)
O(2)	4947(3)	3941(2)	7922(2)	25(1)
Pt(2)	3733(1)	1421(1)	7668(1)	15(1)
N(2)	1312(3)	2367(3)	8310(3)	33(1)
C(2)	3733(4)	6956(3)	7957(3)	21(1)
O(3)	2275(3)	3225(2)	9036(2)	23(1)
N(3)	6121(4)	2301(2)	8688(2)	31(1)
C(3)	3809(4)	6923(3)	6703(3)	24(1)
O(4)	2058(3)	4602(2)	8865(2)	25(1)
N(4)	3619(4)	5162(3)	6382(2)	35(1)
C(4)	3683(4)	5561(3)	6732(3)	26(1)
O(5)	5104(3)	4559(2)	9052(2)	25(1)
N(5)	3705(3)	2874(2)	8098(2)	18(1)
C(5)	3725(4)	2356(3)	7925(2)	18(1)
O(6)	4743(3)	3181(2)	9197(2)	24(1)
N(6)	3954(4)	1798(3)	6321(2)	33(1)
C(6)	3872(4)	1663(3)	6813(3)	22(1)
O(7)	3459(3)	4136(2)	9730(2)	27(1)
C(7)	3567(4)	1168(3)	8520(3)	20(1)
N(7)	3449(4)	1006(2)	9002(2)	31(1)
O(8)	127(3)	4252(2)	8998(2)	32(1)
N(8)	6239(3)	4929(3)	7635(2)	28(1)
C(8)	3755(4)	487(3)	7462(2)	21(1)
O(9)	4100(4)	2602(2)	10200(2)	36(1)
O(10)	4764(3)	3339(2)	6865(2)	30(1)
O(11)	4819(3)	1362(2)	9962(2)	38(1)
O(12)	6790(3)	3788(2)	177(2)	35(1)
O(13)	2101(3)	4223(2)	5978(2)	32(1)

O(14)	5082(3)	5813(2)	9419(2)	28(1)
O(15)	2691(3)	3258(2)	6760(2)	30(1)
O(16)	2020(4)	2537(2)	10071(2)	38(1)
O(17)	1751(4)	4061(3)	10301(3)	74(2)

Table 3. Bond lengths [Å] and angles [°] for $Th(H_2O)_7[Pt(CN)_4]_2 \cdot 10H_2O$.

Th(1)-O(7)	2.420(4)
Th(1)-O(2)	2.434(4)
Th(1)-O(1)	2.464(4)
Th(1)-O(3)	2.469(4)
Th(1)-O(5)	2.481(4)
Th(1)-O(6)	2.485(4)
Th(1)-O(4)	2.494(4)
Th(1)-N(1)	2.552(5)
Th(1)-N(5)	2.570(4)
Pt(1)-C(2)	1.985(6)
Pt(1)-C(3)	1.986(6)
Pt(1)-C(1)	1.990(6)
Pt(1)-C(4)	1.991(6)
N(1)-C(1)	1.155(7)
Pt(2)-C(8)	1.975(6)
Pt(2)-C(6)	1.991(6)
Pt(2)-C(7)	1.995(6)
Pt(2)-C(5)	2.007(6)
N(2)-C(2)#1	1.160(8)
C(2)-N(2)#2	1.160(8)
N(3)-C(3)#3	1.176(8)
C(3)-N(3)#4	1.176(8)
N(4)-C(4)	1.139(8)
N(5)-C(5)	1.135(7)
N(6)-C(6)	1.146(7)
C(7)-N(7)	1.142(8)
N(8)-C(8)#4	1.168(8)
C(8)-N(8)#3	1.168(8)

O(7)-Th(1)-O(2)	138.02(13)
O(7)-Th(1)-O(1)	138.15(13)
O(2)-Th(1)-O(1)	82.58(15)
O(7)-Th(1)-O(3)	72.68(13)
O(2)-Th(1)-O(3)	138.01(13)
O(1)-Th(1)-O(3)	80.77(13)
O(7)-Th(1)-O(5)	69.61(14)
O(2)-Th(1)-O(5)	70.74(14)
O(1)-Th(1)-O(5)	138.78(14)
O(3)-Th(1)-O(5)	139.48(14)
O(7)-Th(1)-O(6)	71.35(13)
O(2)-Th(1)-O(6)	83.43(13)
O(1)-Th(1)-O(6)	137.26(12)
O(3)-Th(1)-O(6)	83.24(13)
O(5)-Th(1)-O(6)	71.25(13)
O(7)-Th(1)-O(4)	70.93(13)
O(2)-Th(1)-O(4)	136.75(13)
O(1)-Th(1)-O(4)	70.01(13)
O(3)-Th(1)-O(4)	70.69(12)
O(5)-Th(1)-O(4)	109.29(13)
O(6)-Th(1)-O(4)	138.98(13)
O(7)-Th(1)-N(1)	101.46(15)
O(2)-Th(1)-N(1)	75.52(14)
O(1)-Th(1)-N(1)	75.52(14)
O(3)-Th(1)-N(1)	135.31(13)
O(5)-Th(1)-N(1)	67.86(14)
O(6)-Th(1)-N(1)	138.21(13)
O(4)-Th(1)-N(1)	65.79(13)
O(7)-Th(1)-N(5)	128.82(15)
O(2)-Th(1)-N(5)	67.17(13)
O(1)-Th(1)-N(5)	67.51(13)
O(3)-Th(1)-N(5)	70.85(13)
O(5)-Th(1)-N(5)	124.67(13)
O(6)-Th(1)-N(5)	69.82(13)
O(4)-Th(1)-N(5)	125.91(13)
N(1)-Th(1)-N(5)	129.71(15)

C(2)-Pt(1)-C(3)	90.4(2)
C(2)-Pt(1)-C(1)	92.6(2)
C(3)-Pt(1)-C(1)	176.8(2)
C(2)-Pt(1)-C(4)	177.0(2)
C(3)-Pt(1)-C(4)	89.8(2)
C(1)-Pt(1)-C(4)	87.2(2)
C(1)-N(1)-Th(1)	161.2(4)
N(1)-C(1)-Pt(1)	175.5(5)
C(8)-Pt(2)-C(6)	90.9(2)
C(8)-Pt(2)-C(7)	88.5(2)
C(6)-Pt(2)-C(7)	178.8(2)
C(8)-Pt(2)-C(5)	176.8(2)
C(6)-Pt(2)-C(5)	92.2(2)
C(7)-Pt(2)-C(5)	88.5(2)
N(2)#2-C(2)-Pt(1)	177.5(5)
N(3)#4-C(3)-Pt(1)	177.1(5)
N(4)-C(4)-Pt(1)	178.1(5)
C(5)-N(5)-Th(1)	170.1(4)
N(5)-C(5)-Pt(2)	176.4(5)
N(6)-C(6)-Pt(2)	179.5(6)
N(7)-C(7)-Pt(2)	177.6(5)
N(8)#3-C(8)-Pt(2)	177.1(5)

Symmetry transformations used to generate equivalent atoms:

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

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $Th(H_2O)_7[Pt(CN)_4]_2 \cdot 10H_2O$. 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}
Th(1)	18(1)	14(1)	10(1)	0(1)	0(1)	0(1)
Pt(1)	19(1)	16(1)	14(1)	2(1)	1(1)	0(1)
O(1)	38(2)	26(2)	19(2)	-3(2)	-8(2)	6(2)
N(1)	27(3)	18(2)	20(3)	2(2)	-2(2)	-1(2)
C(1)	24(3)	16(3)	14(3)	-4(2)	0(2)	0(2)
O(2)	36(2)	24(2)	16(2)	-2(2)	10(2)	-3(2)
Pt(2)	19(1)	15(1)	13(1)	-2(1)	1(1)	0(1)
N(2)	31(3)	30(3)	38(3)	-8(3)	3(2)	-1(2)
C(2)	21(3)	19(3)	23(3)	-1(2)	0(2)	-1(2)
O(3)	24(2)	24(2)	19(2)	-1(2)	3(2)	-6(2)
N(3)	35(3)	30(3)	29(3)	-9(2)	3(2)	0(2)
C(3)	25(3)	21(3)	25(3)	-1(2)	0(2)	0(2)
O(4)	23(2)	24(2)	27(2)	2(2)	5(2)	5(2)
N(4)	47(3)	36(3)	21(3)	-7(2)	-4(2)	0(2)
C(4)	35(3)	26(3)	16(3)	9(2)	0(2)	-1(2)
O(5)	26(2)	27(2)	23(2)	-3(2)	-6(2)	-3(2)
N(5)	26(2)	15(2)	13(2)	-2(2)	2(2)	-1(2)
C(5)	16(3)	25(3)	13(3)	4(2)	1(2)	0(2)
O(6)	31(2)	24(2)	16(2)	1(2)	-1(2)	6(2)
N(6)	40(3)	39(3)	21(3)	0(2)	3(3)	-4(2)
C(6)	24(3)	23(3)	18(3)	-6(2)	0(2)	0(2)
O(7)	26(2)	42(2)	12(2)	-3(2)	2(2)	-1(2)
C(7)	22(3)	18(3)	19(3)	-4(2)	1(2)	-3(2)
N(7)	43(3)	27(3)	24(3)	2(2)	3(2)	-6(2)
O(8)	31(2)	31(2)	35(3)	-2(2)	-1(2)	-1(2)
N(8)	32(3)	20(3)	32(3)	4(2)	5(2)	-1(2)
C(8)	28(3)	23(3)	11(3)	-3(2)	4(2)	0(2)
O(9)	56(3)	35(2)	16(2)	1(2)	4(2)	-1(2)
O(10)	37(2)	32(2)	21(2)	-2(2)	0(2)	1(2)
O(11)	45(3)	41(3)	28(3)	-1(2)	-6(2)	4(2)
O(12)	36(2)	40(3)	28(3)	1(2)	0(2)	4(2)

O(13)	30(2)	36(2)	29(3)	-3(2)	-4(2)	-2(2)
O(14)	37(2)	29(2)	18(2)	-6(2)	-4(2)	-3(2)
O(15)	39(2)	30(2)	21(2)	-2(2)	-3(2)	-1(2)
O(16)	58(3)	36(2)	20(2)	7(2)	6(2)	-1(2)
O(17)	44(3)	139(6)	40(3)	-45(4)	17(3)	-24(3)

Table 5. Crystal data and structure refinement for (2), $Th_2(H_20)_{10}(OH)_2[Pt(CN)_4]_3{\cdot}5H_20$.

Identification code	Th2	
Empirical formula	$C_{12}H_{32}N_{12}O_{17}Pt_3Th_2$	
Formula weight	1665.85	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	a = 16.4915(4) Å	α= 90°.
	b = 12.1941(4) Å	β= 114.016(4)°.
	c = 19.5380(5) Å	γ = 90°.
Volume	3588.9(2) $Å^3$	
Z	4	
Density (calculated)	3.083 Mg/m^3	
Absorption coefficient	19.989 mm^{-1}	
F(000)	2952	
Crystal size	0.29 x 0.03 x 0.03 mm^3	
Theta range for data collection	3.34 to 30.61°.	
Index ranges	-22<=h<=23, -16<=k<=17, -27<=l<=27	
Reflections collected	32269	
Independent reflections	5166 [R(int) = 0.0281]	
Completeness to theta = 29.00°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0 and 0.30	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5166 / 0 / 211	
Goodness-of-fit on F^2	0.918	

Final R indices [I>2sigma(I)]	R1 = 0.0141, wR2 = 0.0239
R indices (all data)	R1 = 0.0211, wR2 = 0.0244
Extinction coefficient	0.000167(4)
Largest diff. peak and hole	0.652 and -0.703 e.Å^{-3}

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for $Th_2(H_20)_{10}(OH)_2[Pt(CN)_4]_3{\cdot}5H_20$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Th(1)	1439(1)	1950(1)	149(1)	15(1)
Pt(1)	-838(1)	2711(1)	1667(1)	19(1)
Pt(2)	2500	-2500	0	19(1)
O(1)	2912(1)	1674(1)	321(1)	21(1)
O(2)	327(1)	3347(2)	-470(1)	39(1)
O(3)	2138(1)	1128(2)	1407(1)	36(1)
O(4)	978(1)	1541(2)	-1193(1)	32(1)
O(5)	1993(2)	3462(2)	1087(1)	41(1)
O(6)	-40(1)	1005(2)	-412(1)	31(1)
O(7)	0	2667(3)	-2500	48(1)
O(8)	1252(2)	-571(2)	1772(1)	52(1)
O(9)	-1371(2)	6087(2)	2690(1)	51(1)
C(1)	-39(2)	2306(2)	1173(2)	25(1)
C(2)	-1040(2)	1152(2)	1838(2)	30(1)
C(3)	-1609(2)	3159(2)	2176(2)	28(1)
C(4)	-705(2)	4284(2)	1463(2)	30(1)
C(5)	1985(2)	-1034(2)	46(1)	22(1)
C(6)	1855(2)	-3191(2)	550(2)	32(1)
N(1)	429(2)	2110(2)	888(1)	30(1)
N(2)	-1182(2)	261(2)	1927(2)	53(1)
N(3)	-2028(2)	3433(2)	2486(2)	47(1)
N(4)	-661(2)	5176(2)	1329(2)	49(1)
N(5)	1694(2)	-181(2)	51(1)	27(1)
N(6)	1490(2)	-3589(3)	873(2)	63(1)

Table 7. Bond lengths [Å] and angles [°] for $Th_2(H_20)_{10}(OH)_2[Pt(CN)_4]_3 \cdot 5H_20$.

Th(1)-O(1)	2.3369(17)
Th(1)-O(1)#1	2.3675(17)
Th(1)-O(2)	2.4342(18)
Th(1)-O(3)	2.4631(18)
Th(1)-O(4)	2.4650(18)
Th(1)-O(5)	2.4962(19)
Th(1)-O(6)	2.5113(18)
Th(1)-N(1)	2.619(2)
Th(1)-N(5)	2.651(2)
Th(1)-Th(1)#1	4.0045(2)
Pt(1)-C(2)	1.982(3)
Pt(1)-C(3)	1.982(3)
Pt(1)-C(1)	1.987(3)
Pt(1)-C(4)	1.988(3)
Pt(2)-C(6)#2	1.982(3)
Pt(2)-C(6)	1.982(3)
Pt(2)-C(5)#2	1.997(3)
Pt(2)-C(5)	1.997(3)
O(1)-Th(1)#1	2.3675(17)
O(1)-H(1A)	0.8501
O(2)-H(2A)	0.8500
O(2)-H(2B)	0.8499
O(3)-H(3A)	0.8500
O(3)-H(3B)	0.8501
O(4)-H(4A)	0.8500
O(4)-H(4B)	0.8500
O(5)-H(5A)	0.8500
O(5)-H(5B)	0.8500
O(6)-H(6A)	0.8500
O(6)-H(6B)	0.8501
O(7)-H(7)	0.8501
O(8)-H(8A)	0.8499
O(8)-H(8B)	0.8500

O(9)-H(9A)	0.8500
O(9)-H(9B)	0.8500
C(1)-N(1)	1.145(3)
C(2)-N(2)	1.140(4)
C(3)-N(3)	1.139(4)
C(4)-N(4)	1.129(4)
C(5)-N(5)	1.147(3)
C(6)-N(6)	1.141(4)
O(1)-Th(1)-O(1)#1	63.31(7)
O(1)-Th(1)-O(2)	134.55(6)
O(1)#1-Th(1)-O(2)	71.29(6)
O(1)-Th(1)-O(3)	76.19(6)
O(1)#1-Th(1)-O(3)	125.04(6)
O(2)-Th(1)-O(3)	137.08(7)
O(1)-Th(1)-O(4)	88.66(7)
O(1)#1-Th(1)-O(4)	73.94(6)
O(2)-Th(1)-O(4)	76.67(7)
O(3)-Th(1)-O(4)	142.68(7)
O(1)-Th(1)-O(5)	87.31(7)
O(1)#1-Th(1)-O(5)	70.95(6)
O(2)-Th(1)-O(5)	79.88(8)
O(3)-Th(1)-O(5)	71.65(7)
O(4)-Th(1)-O(5)	142.45(6)
O(1)-Th(1)-O(6)	139.91(6)
O(1)#1-Th(1)-O(6)	131.91(6)
O(2)-Th(1)-O(6)	72.66(7)
O(3)-Th(1)-O(6)	103.04(6)
O(4)-Th(1)-O(6)	67.57(6)
O(5)-Th(1)-O(6)	131.24(7)
O(1)-Th(1)-N(1)	142.06(7)
O(1)#1-Th(1)-N(1)	130.56(7)
O(2)-Th(1)-N(1)	72.63(7)
O(3)-Th(1)-N(1)	67.93(7)
O(4)-Th(1)-N(1)	127.69(7)
O(5)-Th(1)-N(1)	70.37(7)
O(6)-Th(1)-N(1)	63.37(7)

O(1)-Th(1)-N(5)	71.54(6)
O(1)#1-Th(1)-N(5)	123.85(7)
O(2)-Th(1)-N(5)	139.42(7)
O(3)-Th(1)-N(5)	69.49(7)
O(4)-Th(1)-N(5)	73.40(6)
O(5)-Th(1)-N(5)	139.08(7)
O(6)-Th(1)-N(5)	70.93(7)
N(1)-Th(1)-N(5)	105.55(7)
O(1)-Th(1)-Th(1)#1	31.89(4)
O(1)#1-Th(1)-Th(1)#1	31.43(4)
O(2)-Th(1)-Th(1)#1	102.69(5)
O(3)-Th(1)-Th(1)#1	101.54(5)
O(4)-Th(1)-Th(1)#1	79.79(5)
O(5)-Th(1)-Th(1)#1	77.27(5)
O(6)-Th(1)-Th(1)#1	147.28(4)
N(1)-Th(1)-Th(1)#1	147.64(5)
N(5)-Th(1)-Th(1)#1	98.31(5)
C(2)-Pt(1)-C(3)	89.65(11)
C(2)-Pt(1)-C(1)	91.90(11)
C(3)-Pt(1)-C(1)	178.04(11)
C(2)-Pt(1)-C(4)	176.96(12)
C(3)-Pt(1)-C(4)	88.88(12)
C(1)-Pt(1)-C(4)	89.63(11)
C(6)#2-Pt(2)-C(6)	180.00(19)
C(6)#2-Pt(2)-C(5)#2	91.37(11)
C(6)-Pt(2)-C(5)#2	88.63(11)
C(6)#2-Pt(2)-C(5)	88.63(11)
C(6)-Pt(2)-C(5)	91.37(11)
C(5)#2-Pt(2)-C(5)	180.00(15)
Th(1)-O(1)-Th(1)#1	116.69(7)
Th(1)-O(1)-H(1A)	121.4
Th(1)#1-O(1)-H(1A)	121.1
Th(1)-O(2)-H(2A)	118.3
Th(1)-O(2)-H(2B)	119.7
H(2A)-O(2)-H(2B)	120.5
Th(1)-O(3)-H(3A)	123.6

Th(1)-O(3)-H(3B)	120.5
H(3A)-O(3)-H(3B)	115.6
Th(1)-O(4)-H(4A)	124.4
Th(1)-O(4)-H(4B)	124.7
H(4A)-O(4)-H(4B)	110.7
Th(1)-O(5)-H(5A)	109.8
Th(1)-O(5)-H(5B)	128.6
H(5A)-O(5)-H(5B)	121.4
Th(1)-O(6)-H(6A)	129.4
Th(1)-O(6)-H(6B)	112.5
H(6A)-O(6)-H(6B)	112.0
H(8A)-O(8)-H(8B)	104.9
H(9A)-O(9)-H(9B)	108.9
N(1)-C(1)-Pt(1)	177.6(3)
N(2)-C(2)-Pt(1)	177.9(3)
N(3)-C(3)-Pt(1)	177.7(3)
N(4)-C(4)-Pt(1)	177.5(3)
N(5)-C(5)-Pt(2)	177.6(3)
N(6)-C(6)-Pt(2)	179.4(3)
C(1)-N(1)-Th(1)	171.5(2)
C(5)-N(5)-Th(1)	165.5(2)

Symmetry transformations used to generate equivalent atoms:

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

Table 8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Th_2(H_20)_{10}(OH)_2[Pt(CN)_4]_3 \cdot 5H_20$. 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}
Th(1)	15(1)	15(1)	18(1)	1(1)	10(1)	1(1)
Pt(1)	21(1)	21(1)	19(1)	1(1)	12(1)	2(1)
Pt(2)	16(1)	16(1)	24(1)	0(1)	9(1)	2(1)
O(1)	19(1)	17(1)	33(1)	9(1)	15(1)	5(1)
O(2)	24(1)	38(1)	61(1)	26(1)	24(1)	11(1)

O(3)	32(1)	48(1)	25(1)	10(1)	8(1)	-2(1)
O(4)	44(1)	29(1)	23(1)	0(1)	13(1)	5(1)
O(5)	61(2)	39(1)	34(1)	-15(1)	32(1)	-23(1)
O(6)	23(1)	43(1)	29(1)	-3(1)	13(1)	-9(1)
O(7)	61(2)	42(2)	39(2)	0	18(2)	0
O(8)	41(1)	80(2)	32(1)	-5(1)	12(1)	9(1)
O(9)	45(2)	66(2)	36(1)	-4(1)	11(1)	6(1)
C(1)	23(1)	28(2)	23(1)	-1(1)	10(1)	-2(1)
C(2)	39(2)	30(2)	27(2)	-3(1)	20(1)	4(1)
C(3)	33(2)	27(2)	27(1)	6(1)	17(1)	6(1)
C(4)	29(2)	34(2)	28(2)	3(1)	15(1)	1(1)
C(5)	17(1)	23(1)	25(1)	-1(1)	7(1)	-2(1)
C(6)	22(1)	36(2)	37(2)	7(1)	13(1)	4(1)
N(1)	27(1)	41(2)	29(1)	-3(1)	18(1)	-1(1)
N(2)	90(2)	28(2)	55(2)	-1(1)	42(2)	-2(2)
N(3)	57(2)	55(2)	45(2)	11(1)	36(2)	23(2)
N(4)	57(2)	31(2)	60(2)	14(1)	25(2)	0(1)
N(5)	26(1)	20(1)	33(1)	-2(1)	11(1)	2(1)
N(6)	35(2)	97(3)	64(2)	31(2)	28(2)	6(2)

Table 9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $Th_2(H_20)_{10}(OH)_2[Pt(CN)_4]_3 \cdot 5H_20$.

	x	y	z	U(eq)
H(1A)	3224	1161	599	32
H(2A)	-179	3287	-455	58
H(2B)	404	3789	-774	58
H(3A)	2634	1337	1739	54
H(3B)	1864	649	1548	54
H(4A)	1123	964	-1361	48
H(4B)	686	1975	-1548	48
H(5A)	2123	4017	890	61

H(5B)	2032	3478	1535	61
H(6A)	-392	931	-870	47
H(6B)	-316	1026	-127	47
H(7)	-404	3069	-2467	72
H(8A)	1693	-1006	1930	78
H(8B)	1195	-358	2164	78
H(9A)	-1049	5514	2794	76
H(9B)	-1483	6254	3064	76

Table 10 Crystal data and structure refinement for U**3,** $K_3[(UO_2)_2(OH)(Pt(CN)_4)_2]_2 \cdot NO_3 \cdot 1.5H_2O$.

Identification code	U3
Empirical formula	C16 H5 K3 N17 O14.50 Pt4 U4
Formula weight	2517.15
Temperature	290(2) K
Wavelength	0.71073 Å
Crystal system, space group	Tetragonal, P 4/m b m
Unit cell dimensions	a = 22.1073(2) Å alpha = 90 º.
	b = 22.1073(2) Å beta = 90 º.
	c = 12.6202(2) Å gamma = 90 º.
Volume	6167.90(13) Å ^3
Z, Calculated density	4, 2.711 Mg/m^3
Absorption coefficient	19.750 mm^-1
F(000)	4292
Crystal size	0.344 x 0.174 x 0.096 mm
Theta range for data collection	2.91 to 26.37 º.
Limiting indices	-27<=h<=27, -25<=k<=26, -15<=l<=15
Reflections collected / unique	6733 / 3423 [R(int) = 0.0564]
Completeness to theta = 26.37	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00 and 0.31193
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	3423 / 55 / 146
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0522, wR2 = 0.1500
R indices (all data)	R1 = 0.0687, wR2 = 0.1562
Largest diff. peak and hole	4.241 and -9.542 e. Å ^-3

Table 11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for final. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

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	x	y	z	U(eq)
K(1)	607(3)	5607(3)	0	51(2)
K(2)	3617(7)	3695(7)	-5000	152
U(1)	2379(1)	5072(1)	-1713(1)	19(1)
Pt(1)	1464(1)	6464(1)	-5000	22(1)
Pt(2)	1234(1)	3766(1)	-5000	22(1)
Pt(3)	2432(1)	2568(1)	-1276(1)	15(1)
C(1)	1902(7)	6004(6)	-3904(11)	22(3)
C(2)	1676(8)	4216(7)	-3896(12)	26(3)
C(3)	2423(7)	3463(7)	-1306(12)	24(3)
C(4)	3325(6)	2575(7)	-1294(11)	20(3)
N(1)	2118(7)	5718(6)	-3255(11)	39(3)
N(2)	1937(7)	4471(7)	-3235(11)	39(3)
N(3)	2409(7)	3985(6)	-1344(11)	39(3)
N(4)	2579(7)	6157(6)	-1344(11)	38(3)
N(5)	0	5000	-2660(20)	74(11)
O(1)	1634(5)	5159(5)	-1214(9)	36(2)
O(2)	3103(5)	5001(5)	-2198(9)	33(2)
O(3)	2746(8)	5044(7)	0	29(3)
O(4)	0	5000	-1682(19)	55(5)
O(5)	326(12)	5326(12)	-3270(30)	210(20)
O(6)	728(10)	4272(10)	0	63(6)

O(7)	0	0	5000	56(12)

Table 12. Bond lengths [Å] and angles [º] for final.

K(1)-O(4)	2.848(19)
K(1)-O(4)#1	2.848(19)
K(1)-O(1)#2	2.912(12)
K(1)-O(1)#3	2.912(12)
K(1)-O(1)	2.912(12)
K(1)-O(1)#4	2.912(12)
K(1)-O(6)#1	2.96(3)
K(1)-O(6)	2.96(3)
K(1)-K(1)#1	3.80(2)
U(1)-O(2)	1.720(12)
U(1)-O(1)	1.774(12)
U(1)-O(3)	2.310(6)
U(1)-N(3)	2.449(14)
U(1)-N(1)	2.482(13)
U(1)-N(4)	2.483(14)
U(1)-N(2)	2.531(14)
Pt(1)-C(1)#5	1.971(15)
Pt(1)-C(1)#4	1.971(15)
Pt(1)-C(1)	1.971(15)
Pt(1)-C(1)#6	1.971(15)
Pt(2)-C(2)#7	1.971(15)
Pt(2)-C(2)	1.971(15)
Pt(2)-C(2)#8	1.971(15)
Pt(2)-C(2)#6	1.971(15)
Pt(3)-C(4)	1.975(14)
Pt(3)-C(4)#8	1.975(14)
Pt(3)-C(3)	1.978(15)
Pt(3)-C(3)#8	1.978(15)
Pt(3)-Pt(3)#2	3.2214(15)
C(1)-N(1)	1.139(19)
C(2)-N(2)	1.16(2)
C(3)-N(3)	1.16(2)

C(4)-N(4)#9	1.15(2)
N(4)-C(4)#10	1.15(2)
N(5)-O(4)	1.238(18)
N(5)-O(5)#11	1.279(18)
N(5)-O(5)	1.279(18)
O(3)-U(1)#2	2.310(6)
O(4)-K(1)#1	2.848(19)
O(6)-K(1)#1	2.96(3)
O(4)-K(1)-O(4)#1	96.4(7)
O(4)-K(1)-O(1)#2	126.8(3)
O(4)#1-K(1)-O(1)#2	79.3(3)
O(4)-K(1)-O(1)#3	126.8(3)
O(4)#1-K(1)-O(1)#3	79.3(3)
O(1)#2-K(1)-O(1)#3	104.7(5)
O(4)-K(1)-O(1)	79.3(3)
O(4)#1-K(1)-O(1)	126.8(3)
O(1)#2-K(1)-O(1)	63.5(5)
O(1)#3-K(1)-O(1)	143.8(6)
O(4)-K(1)-O(1)#4	79.3(3)
O(4)#1-K(1)-O(1)#4	126.8(3)
O(1)#2-K(1)-O(1)#4	143.8(6)
O(1)#3-K(1)-O(1)#4	63.5(5)
O(1)-K(1)-O(1)#4	104.7(5)
O(4)-K(1)-O(6)#1	64.7(3)
O(4)#1-K(1)-O(6)#1	64.7(3)
O(1)#2-K(1)-O(6)#1	143.8(3)
O(1)#3-K(1)-O(6)#1	65.9(4)
O(1)-K(1)-O(6)#1	143.8(3)
O(1)#4-K(1)-O(6)#1	65.9(4)
O(4)-K(1)-O(6)	64.7(3)
O(4)#1-K(1)-O(6)	64.7(3)
O(1)#2-K(1)-O(6)	65.9(4)
O(1)#3-K(1)-O(6)	143.8(3)
O(1)-K(1)-O(6)	65.9(4)
O(1)#4-K(1)-O(6)	143.8(3)
O(6)#1-K(1)-O(6)	100.3(9)

O(4)-K(1)-K(1)#1	48.2(4)
O(4)#1-K(1)-K(1)#1	48.2(4)
O(1)#2-K(1)-K(1)#1	108.1(3)
O(1)#3-K(1)-K(1)#1	108.1(3)
O(1)-K(1)-K(1)#1	108.1(3)
O(1)#4-K(1)-K(1)#1	108.1(3)
O(6)#1-K(1)-K(1)#1	50.1(4)
O(6)-K(1)-K(1)#1	50.1(4)
O(2)-U(1)-O(1)	179.1(5)
O(2)-U(1)-O(3)	90.2(5)
O(1)-U(1)-O(3)	89.8(5)
O(2)-U(1)-N(3)	87.3(5)
O(1)-U(1)-N(3)	93.7(5)
O(3)-U(1)-N(3)	77.6(5)
O(2)-U(1)-N(1)	89.4(5)
O(1)-U(1)-N(1)	90.0(5)
O(3)-U(1)-N(1)	146.2(5)
N(3)-U(1)-N(1)	136.1(5)
O(2)-U(1)-N(4)	89.4(5)
O(1)-U(1)-N(4)	89.7(5)
O(3)-U(1)-N(4)	77.8(5)
N(3)-U(1)-N(4)	155.1(5)
N(1)-U(1)-N(4)	68.5(5)
O(2)-U(1)-N(2)	92.3(5)
O(1)-U(1)-N(2)	88.2(5)
O(3)-U(1)-N(2)	146.2(5)
N(3)-U(1)-N(2)	68.9(5)
N(1)-U(1)-N(2)	67.5(5)
N(4)-U(1)-N(2)	135.9(5)
C(1)#5-Pt(1)-C(1)#4	89.1(8)
C(1)#5-Pt(1)-C(1)	178.0(9)
C(1)#4-Pt(1)-C(1)	90.8(8)
C(1)#5-Pt(1)-C(1)#6	90.8(8)
C(1)#4-Pt(1)-C(1)#6	178.0(9)
C(1)-Pt(1)-C(1)#6	89.1(8)
C(2)#7-Pt(2)-C(2)	179.3(10)

C(2)#7-Pt(2)-C(2)#8	90.0(8)
C(2)-Pt(2)-C(2)#8	90.0(8)
C(2)#7-Pt(2)-C(2)#6	90.0(8)
C(2)-Pt(2)-C(2)#6	90.0(8)
C(2)#8-Pt(2)-C(2)#6	179.3(10)
C(4)-Pt(3)-C(4)#8	90.8(9)
C(4)-Pt(3)-C(3)	90.1(6)
C(4)#8-Pt(3)-C(3)	178.0(6)
C(4)-Pt(3)-C(3)#8	178.0(6)
C(4)#8-Pt(3)-C(3)#8	90.1(6)
C(3)-Pt(3)-C(3)#8	88.9(9)
C(4)-Pt(3)-Pt(3)#2	90.6(4)
C(4)#8-Pt(3)-Pt(3)#2	90.6(4)
C(3)-Pt(3)-Pt(3)#2	91.1(4)
C(3)#8-Pt(3)-Pt(3)#2	91.1(4)
N(1)-C(1)-Pt(1)	175.3(15)
N(2)-C(2)-Pt(2)	178.8(15)
N(3)-C(3)-Pt(3)	178.3(15)
N(4)#9-C(4)-Pt(3)	177.5(13)
C(1)-N(1)-U(1)	168.5(15)
C(2)-N(2)-U(1)	172.8(15)
C(3)-N(3)-U(1)	171.4(13)
C(4)#10-N(4)-U(1)	166.7(13)
O(4)-N(5)-O(5)#11	127(2)
O(4)-N(5)-O(5)	127(2)
O(5)#11-N(5)-O(5)	106(5)
U(1)-O(1)-K(1)	161.3(6)
U(1)-O(3)-U(1)#2	138.7(8)
N(5)-O(4)-K(1)	138.2(4)
N(5)-O(4)-K(1)#1	138.2(4)
K(1)-O(4)-K(1)#1	83.6(7)
K(1)-O(6)-K(1)#1	79.7(9)

Symmetry transformations used to generate equivalent atoms:

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

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

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

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

#11 -x,-y+1,z

Table 13. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for final. 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}
K(1)	50(3)	50(3)	53(5)	0	0	5(4)
U(1)	27(1)	11(1)	18(1)	0(1)	-2(1)	-1(1)
Pt(1)	25(1)	25(1)	14(1)	0	0	5(1)
Pt(2)	25(1)	25(1)	15(1)	0	0	-8(1)
Pt(3)	11(1)	11(1)	23(1)	0(1)	0(1)	0(1)
C(1)	36(9)	13(7)	17(6)	-5(5)	0(6)	-1(6)
C(2)	36(9)	22(8)	21(7)	4(6)	2(6)	-12(7)
C(3)	24(8)	16(5)	33(8)	-8(6)	1(7)	2(6)
C(4)	9(6)	27(8)	24(7)	4(6)	-5(5)	-1(5)
N(1)	55(10)	29(7)	33(6)	9(5)	-12(6)	0(7)
N(2)	53(9)	32(7)	30(6)	-2(5)	-11(6)	-13(7)
N(3)	58(10)	20(4)	39(7)	2(5)	-10(7)	2(5)
N(4)	55(10)	22(5)	36(7)	2(5)	-8(7)	-8(6)
N(5)	86(17)	86(17)	48(10)	0	0	20(20)
O(1)	31(5)	37(6)	41(6)	-4(5)	1(4)	0(4)
O(2)	34(5)	31(6)	35(5)	1(5)	1(4)	0(4)
O(3)	36(8)	29(8)	22(5)	0	0	-3(7)
O(4)	61(8)	61(8)	45(10)	0	0	-8(12)
O(5)	240(30)	240(30)	140(30)	100(20)	100(20)	20(40)
O(6)	54(8)	54(8)	83(18)	0	0	-16(10)
O(7)	72(19)	72(19)	22(17)	0	0	0

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