Supporting Information

Structural Modifications to Platinum(II) Pincer Complexes Resulting in Changes in their Vapochromic and Solvatochromic Properties

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Synthesis of the Precursor Complexes

Chloro[acetyl 3,5-di(2-pyridyl)phenyl]platinum

The synthesis was adapted from a literature procedure.[1]

To a stirred solution of acetyl 3,5-di(2-pyridyl)benzene (100 mg, 0.34 mmol) in acetonitrile (15 ml), a solution of $K_2[PtCl]_4$ (144 mg, 0.34 mmol) in water (5 ml) was added, and the resulting orange mixture was refluxed at 100°C for 3 days.

This was then allowed to cool, resulting in a vivid yellow precipitate, which was retained in a filter and washed with water (20ml), ethanol (20 ml), acetonitrile (20ml), and Et_2O (10 ml). The bright yellow solid was then dried.

Yield: 85mg, 50%

1H NMR (400 MHz, CDCl$_3$) δ_H: 9.38 (d, $^3J_{H-H}$= 4.5 Hz, $^3J_{H-Pt}$= 38.7 Hz, 2H, *ortho-Py*), 8.06 (s, 2H, *pincer-Ph*), 8.02 (t, $^3J_{H-H}$= 7.0 Hz, *para-Py*), 7.82 (d, $^3J_{H-H}$= 6.9 Hz, 2H, *meta-Py*), 7.35 (t, obscured by CDCl$_3$ signal, *meta-Py*), 2.67 (s, 3H, CO*CH$_3$*) The NMR analysis consistent with literature.

Chloro[ethyl 3,5-di(2-pyridyl)benzoato]platinum

The synthesis was adapted from a literature procedure.[1]

To a stirred solution of ethyl 3,5-di(2-pyridyl)benzoate (100 mg, 0.34 mmol) in acetonitrile (15 ml), a solution of $K_2[PtCl]_4$ (144 mg, 0.34 mmol) in water (5 ml) was added, and the resulting orange mixture was refluxed at 100°C for 3 days.

This was then allowed to cool, resulting in a vivid yellow precipitate, which was retained in a filter and washed with water (20ml), ethanol (20 ml), acetonitrile (20ml), and Et_2O (10 ml). The bright yellow solid was then dried.

Yield: 150mg, 85.5%

IR (cm^{-1}): ν(C=O) 1708

1H NMR (500 MHz, CDCl$_3$) δ_H: 9.42 (d, $^3J_{H-H}$= 5.5 Hz, $^3J_{H-Pt}$= 42.4 Hz, 2H, *ortho-Py*), 8.20 (s, 2H, *pincer-Ph*), 8.04 (t, $^3J_{H-H}$= 7.6 Hz, 2H, *para-Py*), 7.86 (d, $^3J_{H-H}$= 8.1 Hz, 2H, *meta-Py*), 7.39 (t, $^3J_{H-H}$= 6.77 Hz, 2H, *meta-Py*), 4.46 (q, $^3J_{H-H}$ = 7.1 Hz, 2H, CO$_2$*CH$_2$*), 1.48 (t, $^3J_{H-H}$ = 7.1 Hz, 3H, CO$_2$CH$_2$*CH$_3$*)

Mass Spectrometry (positive loop injection): Chloride lost upon ionisation. Measured (MeOH) *m/z* – 498.0792, Calculated for [$C_{19}O_2N_2H_{15}Pt_1$]$^+$ – 498.078127. Correct isotope pattern.

Chloro[phenyl 3,5-di(2-pyridyl)benzoato]platinum

The synthesis was adapted from a literature procedure.[1]

To a stirred solution of phenyl 3,5-di(2-pyridyl)benzoate (100 mg, 0.34 mmol) in acetonitrile (15 ml), a solution of $K_2[PtCl]_4$ (144 mg, 0.34 mmol) in water (5 ml) was added, and the resulting orange mixture was refluxed at 100°C for 3 days.

This was then allowed to cool, resulting in a vivid yellow precipitate, which was retained in a filter and washed with water (20ml), ethanol (20 ml), acetonitrile (20ml), and Et_2O (10 ml). The bright yellow solid was then dried.

Yield: 150mg, 85.5%

IR (cm^{-1}): ν(C=O) 1708

1H NMR (500 MHz, CDCl$_3$) δ_H: 9.45 (d, $^3J_{H-H}$= 5.5 Hz, $^3J_{H-Pt}$= 41.9 Hz, 2H, *ortho-Py*), 8.34 (s, 2H, *pincer-Ph*), 8.06 (t, $^3J_{H-H}$= 7.6 Hz, 2H, *para-Py*), 7.89 (d, $^3J_{H-H}$= 8.1 Hz, 2H, *meta-Py*), 7.50 (m, 3H, *ortho+para-pendant Ph*), 7.42 (t, $^3J_{H-H}$= 7.2 Hz, 2H, *meta-Py*), 7.34 (t, $^3J_{H-H}$= 7.4 Hz, 2H, *meta-pendant Ph*)

Mass Spectrometry (positive loop injection): Chloride lost upon ionisation. Measured (MeOH) *m/z* – 546.0806, Calculated for [$C_{23}O_2N_2H_{15}Pt_1$]$^+$ – 546.078127. Correct isotope pattern.

Crystallographic Data

Data for 2a' (green)

Table S1 Crystal data and structure refinement for 2'_green.

Identification code	2_green
Empirical formula	$C_{19}H_{13}N_3O_8Pt$
Formula weight	606.41
Temperature/K	150.15
Crystal system	orthorhombic
Space group	Ibam
a/Å	35.828(2)
b/Å	18.4081(9)
c/Å	6.6356(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4376.4(4)
Z	8
ρ_{calc}g/cm^3	1.841
μ/mm^{-1}	11.789
F(000)	2320.0
Crystal size/mm^3	0.2 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.61 to 143.752
Index ranges	-37 ≤ h ≤ 43, -21 ≤ k ≤ 22, -8 ≤ l ≤ 4
Reflections collected	8374
Independent reflections	2305 [R_{int} = 0.0404, R_{sigma} = 0.0381]
Data/restraints/parameters	2305/0/168
Goodness-of-fit on F^2	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0813, wR_2 = 0.2449
Final R indexes [all data]	R_1 = 0.1065, wR_2 = 0.2750
Largest diff. peak/hole / e Å^{-3}	2.53/-2.13

Table S2 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for 2_green. U$_{eq}$ is defined as 1/3 of the trace of the orthogonalised U$_{IJ}$ tensor.

Atom	x	y	z	U(eq)
C1	4735(10)	2769(11)	5000	96(10)
C2	4724(8)	3581(11)	5000	71(7)
C3	4325(6)	3900(10)	5000	60(5)
C4	4301(6)	4651(9)	5000	48(4)
C5	3957(6)	5012(10)	5000	48(4)
C6	3649(7)	4561(10)	5000	59(5)
C7	3648(7)	3801(9)	5000	55(5)
C8	3994(6)	3495(9)	5000	51(5)
N1	3485(5)	5913(7)	5000	44(3)
C9	3871(5)	5771(11)	5000	48(4)
C10	4104(6)	6328(9)	5000	53(5)
C11	3993(5)	7047(10)	5000	53(5)
C12	3627(6)	7184(9)	5000	55(5)
C13	3368(7)	6587(10)	5000	56(5)
N2	2996(6)	3959(9)	5000	61(5)
C14	3294(7)	3485(11)	5000	57(5)
C15	3216(8)	2728(12)	5000	72(7)
C16	2853(9)	2485(13)	5000	84(8)
C17	2589(9)	2966(16)	5000	94(10)
C18	2651(7)	3747(14)	5000	73(6)
C19	2634(7)	5505(12)	5000	64(6)
N3	2336(7)	5733(11)	5000	87(6)
O1	4987(5)	3957(11)	5000	110(9)
Pt01	3155.5(2)	5021.9(4)	5000	50.0(5)
O2	1717(9)	5911(17)	8030(50)	256(17)
O3	4376(3)	941(6)	2372(15)	58(2)
O4	4365(3)	924(5)	3885(17)	62(2)
O5	4462(5)	925(9)	1060(30)	51(4)

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 2_green. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+...]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	170(30)	34(10)	82(19)	0	0	24(14)
C2	107(19)	37(10)	67(15)	0	0	28(11)
C3	69(13)	45(10)	65(13)	0	0	13(9)
C4	71(12)	30(8)	42(10)	0	0	15(8)
C5	58(10)	62(12)	23(9)	0	0	4(9)
C6	104(17)	38(9)	35(10)	0	0	3(10)
C7	88(15)	39(9)	38(10)	0	0	−5(9)
C8	81(14)	25(8)	46(11)	0	0	−3(8)
N1	67(9)	32(6)	33(8)	0	0	−1(6)
C9	56(11)	59(11)	30(9)	0	0	8(9)
C10	78(14)	37(9)	44(11)	0	0	−10(9)
C11	53(11)	50(10)	55(12)	0	0	−6(8)
C12	81(14)	29(8)	55(12)	0	0	8(8)
C13	73(14)	48(10)	46(11)	0	0	2(9)
N2	88(13)	53(9)	42(9)	0	0	−30(9)
C14	79(14)	58(11)	32(10)	0	0	−3(11)
C15	100(20)	57(12)	56(14)	0	0	−13(12)
C16	110(20)	46(12)	90(20)	0	0	−22(13)
C17	110(20)	100(20)	75(18)	0	0	−68(19)
C18	70(15)	86(16)	62(15)	0	0	−27(13)
C19	79(16)	52(11)	61(14)	0	0	2(11)
N3	88(15)	55(11)	117(19)	0	0	−1(11)
O1	79(12)	57(10)	190(30)	0	0	−1(9)
Pt01	65.1(7)	45.4(6)	39.6(7)	0	0	−2.9(4)
O2	164(19)	160(20)	450(50)	0(20)	70(20)	20(20)

Table S4 Bond Lengths for 2_green.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.49(3)	C10	C11	1.38(2)
C2	C3	1.55(3)	C11	C12	1.34(3)
C2	O1	1.17(3)	C12	C13	1.44(3)
C3	C4	1.38(2)	N2	C14	1.38(3)
C3	C8	1.40(3)	N2	C18	1.29(3)
C4	C5	1.40(3)	N2	Pt01	2.038(16)
C5	C6	1.38(3)	C14	C15	1.42(3)
C5	C9	1.43(2)	C15	C16	1.38(4)
C6	C7	1.40(2)	C16	C17	1.30(4)
C6	Pt01	1.96(2)	C17	C18	1.46(3)
C7	C8	1.36(3)	C19	N3	1.15(3)
C7	C14	1.40(3)	C19	Pt01	2.07(3)
N1	C9	1.41(2)	O3	O4	1.005(12)
N1	C13	1.31(2)	O3	O5	0.927(19)
N1	Pt01	2.022(14)	O4	O4^1	1.48(2)
C9	C10	1.32(3)	O5	O5^2	1.40(4)

[1]+X,+Y,1-Z; [2]+X,+Y,-Z

Table S5 Bond Angles for 2_green.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	C2	C3	114(2)	C12	C11	C10	117.6(19)
O1	C2	C1	125(3)	C11	C12	C13	119.4(18)
O1	C2	C3	121.4(19)	N1	C13	C12	121(2)
C4	C3	C2	116(2)	C14	N2	Pt01	113.0(14)
C4	C3	C8	118.6(19)	C18	N2	C14	123(2)
C8	C3	C2	125.5(18)	C18	N2	Pt01	123.8(18)
C3	C4	C5	122(2)	C7	C14	C15	126(2)
C4	C5	C9	130.9(18)	N2	C14	C7	116.0(18)
C6	C5	C4	114.6(17)	N2	C14	C15	118(2)
C6	C5	C9	114.5(18)	C16	C15	C14	120(2)
C5	C6	C7	127(2)	C17	C16	C15	118(2)
C5	C6	Pt01	117.4(13)	C16	C17	C18	124(3)
C7	C6	Pt01	115.4(19)	N2	C18	C17	116(3)
C8	C7	C6	114(2)	N3	C19	Pt01	176(2)
C8	C7	C14	130.9(17)	C6	Pt01	N1	79.9(7)
C14	C7	C6	115(2)	C6	Pt01	N2	80.6(8)
C7	C8	C3	123.4(16)	C6	Pt01	C19	179.8(8)
C9	N1	Pt01	115.0(12)	N1	Pt01	N2	160.5(7)
C13	N1	C9	119.6(17)	N1	Pt01	C19	100.3(7)
C13	N1	Pt01	125.5(15)	N2	Pt01	C19	99.1(8)
N1	C9	C5	113.3(17)	O5	O3	O4	162.2(19)
C10	C9	C5	128.3(19)	O3	O4	O4[1]	177.2(9)
C10	C9	N1	118.4(18)	O3	O5	O5[2]	160.4(13)
C9	C10	C11	124(2)				

[1]+X,+Y,1-Z; [2]+X,+Y,-Z

Table S6 Torsion Angles for 2_green.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	180.0	C9	N1	C13	C12	0.0
C1	C2	C3	C8	0.0	C9	C10	C11	C12	0.0
C2	C3	C4	C5	180.0	C10	C11	C12	C13	0.0
C2	C3	C8	C7	180.0	C11	C12	C13	N1	0.0
C3	C4	C5	C6	0.0	C13	N1	C9	C5	180.0
C3	C4	C5	C9	180.0	C13	N1	C9	C10	0.0
C4	C3	C8	C7	0.0	N2	C14	C15	C16	0.0
C4	C5	C6	C7	0.0	C14	C7	C8	C3	180.0
C4	C5	C6	Pt01	180.0	C14	N2	C18	C17	0.0
C4	C5	C9	N1	180.0	C14	C15	C16	C17	0.0
C4	C5	C9	C10	0.0	C15	C16	C17	C18	0.0
C5	C6	C7	C8	0.0	C16	C17	C18	N2	0.0
C5	C6	C7	C14	180.0	C18	N2	C14	C7	180.0
C5	C9	C10	C11	180.0	C18	N2	C14	C15	0.0
C6	C5	C9	N1	0.0	O1	C2	C3	C4	0.0
C6	C5	C9	C10	180.0	O1	C2	C3	C8	180.0
C6	C7	C8	C3	0.0	Pt01	C6	C7	C8	180.0
C6	C7	C14	N2	0.0	Pt01	C6	C7	C14	0.0
C6	C7	C14	C15	180.0	Pt01	N1	C9	C5	0.0
C7	C14	C15	C16	180.0	Pt01	N1	C9	C10	180.0
C8	C3	C4	C5	0.0	Pt01	N1	C13	C12	180.0
C8	C7	C14	N2	180.0	Pt01	N2	C14	C7	0.0
C8	C7	C14	C15	0.0	Pt01	N2	C14	C15	180.0
N1	C9	C10	C11	0.0	Pt01	N2	C18	C17	180.0
C9	C5	C6	C7	180.0	O4	O3	O5	O5[1]	174(3)
C9	C5	C6	Pt01	0.0					

[1] +X,+Y,-Z

Table S7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 2_green.

Atom	x	y	z	U(eq)
H1A	4499	2580	4465	145
H1B	4771	2594	6381	145
H1C	4942	2603	4154	145
H4	4524	4929	5000	57
H8	4012	2980	5000	61
H10	4364	6228	5000	64
H11	4170	7431	5000	63
H12	3538	7670	5000	66
H13	3107	6683	5000	67
H15	3415	2388	5000	86
H16	2797	1980	5000	100
H17	2338	2798	5000	113
H18	2450	4084	5000	87

Data for 2(yellow)

Table S8 Crystal data and structure refinement for 2_yellow.

Identification code	2_yellow
Empirical formula	$C_{19}H_{13}N_3OPt$
Formula weight	494.41
Temperature/K	150.0(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.8945(2)
b/Å	15.5988(4)
c/Å	14.7127(5)
α/°	90
β/°	102.975(3)
γ/°	90
Volume/Å^3	1541.90(8)
Z	4
ρ_{calc}g/cm^3	2.130
μ/mm^{-1}	9.110
F(000)	936.0
Crystal size/mm^3	0.25 × 0.2 × 0.18
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.682 to 59.348
Index ranges	-9 ≤ h ≤ 9, -21 ≤ k ≤ 21, -20 ≤ l ≤ 19
Reflections collected	33906
Independent reflections	4100 [R_{int} = 0.0652, R_{sigma} = 0.0456]
Data/restraints/parameters	4100/0/218
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0290, wR_2 = 0.0402
Final R indexes [all data]	R_1 = 0.0501, wR_2 = 0.0448
Largest diff. peak/hole / e Å^{-3}	0.99/-0.71

Table S9 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for 2_yellow. U_eq is defined as 1/3 of the trace of the orthogonalised U_IJ tensor.

Atom	x	y	z	U(eq)
Pt1	3138.7(2)	975.1(2)	5744.5(2)	19.09(5)
N3	4449(6)	2950(2)	5861(2)	38.0(9)
C3	1714(5)	−1962(2)	5814(3)	23.8(8)
C2	1232(6)	−2889(2)	5870(3)	28.3(9)
C9	2970(5)	0(2)	7402(3)	22.2(8)
C18	2818(5)	1241(2)	3667(3)	24.0(8)
C1	960(7)	−3429(3)	5003(3)	39.1(11)
C10	3045(6)	−182(3)	8327(3)	27.0(9)
N1	3333(4)	816.2(18)	7134(2)	20.8(7)
O1	1082(5)	−3207.5(18)	6605(2)	43.4(8)
C6	2516(5)	−232(2)	5774(2)	19.2(8)
C19	3938(6)	2248(2)	5781(3)	24.3(8)
C8	1740(5)	−1570(2)	4965(3)	23.6(8)
N2	2699(4)	691.0(18)	4359(2)	21.1(7)
C12	3819(6)	1276(3)	8716(3)	32.8(10)
C15	1918(5)	−425(2)	3219(3)	24.0(8)
C4	2109(5)	−1489(2)	6650(3)	24.4(9)
C17	2533(6)	991(3)	2750(3)	27.6(9)
C13	3767(6)	1433(2)	7783(3)	28.6(9)
C7	2134(5)	−692(2)	4941(3)	20.9(8)
C14	2238(5)	−154(2)	4134(2)	19.9(8)
C11	3435(6)	463(3)	8987(3)	31.9(10)
C5	2506(5)	−616(2)	6625(3)	22.4(8)
C16	2073(5)	148(2)	2518(3)	26.7(9)

Table S10 Anisotropic Displacement Parameters (Å^2×10^3) for 2_yellow. The Anisotropic displacement factor exponent takes the form:

$-2\pi^2[h^2a*^2U_{11}+2hka*b*U_{12}+...]$.

Atom	U$_{11}$	U$_{22}$	U$_{33}$	U$_{23}$	U$_{13}$	U$_{12}$
Pt1	20.09(8)	19.53(7)	17.63(8)	−0.36(7)	4.18(5)	0.70(7)
N3	56(2)	33(2)	26(2)	−0.4(17)	10.9(17)	−5.5(19)
C3	21(2)	24.1(19)	27(2)	2.6(17)	6.6(16)	5.1(16)
C2	20(2)	25.3(19)	39(3)	2(2)	5.4(18)	1.0(17)
C9	17.6(19)	27(2)	20(2)	−1.0(17)	2.1(15)	3.7(16)
C18	24(2)	25.0(19)	23(2)	2.7(16)	4.1(16)	−0.5(16)
C1	47(3)	23(2)	47(3)	−2(2)	12(2)	−1.8(19)
C10	24(2)	31(2)	25(2)	5.2(18)	4.6(17)	6.1(17)
N1	20.1(16)	26.2(17)	15.5(16)	0.0(13)	3.1(13)	4.1(13)
O1	60(2)	30.5(16)	38.0(19)	8.3(14)	8.3(16)	−5.9(15)
C6	15.3(18)	18.8(17)	22(2)	1.4(15)	2.1(15)	1.8(14)
C19	33(2)	22(2)	18(2)	1.7(16)	6.2(17)	2.0(17)
C8	23(2)	22.1(19)	26(2)	−2.9(16)	5.2(17)	3.5(16)
N2	19.7(16)	22.2(15)	20.8(17)	0.1(13)	3.5(13)	2.4(13)
C12	40(3)	36(2)	20(2)	−5.8(18)	1.9(19)	10.2(19)
C15	19(2)	29(2)	24(2)	−0.5(17)	3.3(16)	2.2(16)
C4	20(2)	28(2)	26(2)	8.0(17)	6.6(16)	4.5(16)
C17	26(2)	37(2)	22(2)	6.8(19)	7.4(16)	−2.0(19)
C13	30(2)	28(2)	27(2)	−3.3(18)	3.6(18)	4.9(17)
C7	14.4(18)	27.0(19)	21(2)	−2.4(16)	3.6(15)	3.2(15)
C14	14.5(19)	24.8(18)	21(2)	0.1(16)	4.1(15)	0.6(15)
C11	35(2)	40(2)	21(2)	4.6(19)	4.3(18)	9.9(19)
C5	18(2)	26.9(19)	23(2)	2.7(17)	5.9(16)	7.2(16)
C16	21(2)	38(2)	21(2)	−2.5(18)	5.9(16)	2.3(18)

Table S11 Bond Lengths for 2_yellow.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pt1	N1	2.033(3)	C18	C17	1.376(5)
Pt1	C6	1.934(3)	C10	C11	1.383(5)
Pt1	C19	2.058(4)	N1	C13	1.342(5)
Pt1	N2	2.042(3)	C6	C7	1.393(5)
N3	C19	1.148(5)	C6	C5	1.390(5)
C3	C2	1.489(5)	C8	C7	1.398(5)
C3	C8	1.395(5)	N2	C14	1.379(4)
C3	C4	1.408(5)	C12	C13	1.387(5)
C2	C1	1.505(6)	C12	C11	1.373(6)
C2	O1	1.216(5)	C15	C14	1.381(5)
C9	C10	1.381(5)	C15	C16	1.387(5)
C9	N1	1.372(4)	C4	C5	1.391(5)
C9	C5	1.472(5)	C17	C16	1.378(5)
C18	N2	1.347(5)	C7	C14	1.468(5)

Table S12 Bond Angles for 2_yellow.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Pt1	C19	97.74(13)	C5	C6	C7	122.2(3)
N1	Pt1	N2	159.89(12)	N3	C19	Pt1	175.5(3)
C6	Pt1	N1	79.84(13)	C3	C8	C7	119.6(3)
C6	Pt1	C19	176.61(15)	C18	N2	Pt1	126.5(3)
C6	Pt1	N2	80.04(13)	C18	N2	C14	118.6(3)
N2	Pt1	C19	102.37(13)	C14	N2	Pt1	114.9(2)
C8	C3	C2	121.6(3)	C11	C12	C13	119.1(4)
C8	C3	C4	120.9(3)	C14	C15	C16	120.4(4)
C4	C3	C2	117.5(3)	C5	C4	C3	119.4(4)
C3	C2	C1	118.9(4)	C18	C17	C16	119.2(4)
O1	C2	C3	120.7(4)	N1	C13	C12	122.0(4)
O1	C2	C1	120.4(4)	C6	C7	C8	118.8(3)
C10	C9	C5	125.7(3)	C6	C7	C14	112.6(3)
N1	C9	C10	120.4(3)	C8	C7	C14	128.7(3)
N1	C9	C5	113.9(3)	N2	C14	C15	120.2(3)
N2	C18	C17	122.7(4)	N2	C14	C7	113.8(3)
C9	C10	C11	120.1(4)	C15	C14	C7	126.0(3)
C9	N1	Pt1	115.3(2)	C12	C11	C10	119.2(4)
C13	N1	Pt1	125.6(3)	C6	C5	C9	111.9(3)
C13	N1	C9	119.1(3)	C6	C5	C4	119.1(4)
C7	C6	Pt1	118.7(3)	C4	C5	C9	129.0(4)
C5	C6	Pt1	119.1(3)	C17	C16	C15	118.8(4)

Table S13 Torsion Angles for 2_yellow.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Pt1	N1	C13	C12	178.3(3)	C6	C7	C14	N2	0.3(4)
Pt1	C6	C7	C8	178.2(3)	C6	C7	C14	C15	−179.6(3)
Pt1	C6	C7	C14	−1.0(4)	C8	C3	C2	C1	5.9(5)
Pt1	C6	C5	C9	0.9(4)	C8	C3	C2	O1	−174.9(4)
Pt1	C6	C5	C4	−178.3(3)	C8	C3	C4	C5	0.8(5)
Pt1	N2	C14	C15	−179.7(3)	C8	C7	C14	N2	−178.8(3)
Pt1	N2	C14	C7	0.5(4)	C8	C7	C14	C15	1.3(6)
C3	C8	C7	C6	0.8(5)	N2	C18	C17	C16	1.1(6)
C3	C8	C7	C14	179.8(3)	C4	C3	C2	C1	−175.3(3)
C3	C4	C5	C9	−179.5(3)	C4	C3	C2	O1	3.9(5)
C3	C4	C5	C6	−0.4(5)	C4	C3	C8	C7	−1.0(5)
C2	C3	C8	C7	177.8(3)	C17	C18	N2	Pt1	178.8(3)
C2	C3	C4	C5	−178.0(3)	C17	C18	N2	C14	−1.2(5)
C9	C10	C11	C12	−2.5(6)	C13	C12	C11	C10	1.3(6)
C9	N1	C13	C12	−1.4(6)	C7	C6	C5	C9	179.4(3)
C18	N2	C14	C15	0.4(5)	C7	C6	C5	C4	0.3(5)
C18	N2	C14	C7	−179.5(3)	C14	C15	C16	C17	−0.6(5)
C18	C17	C16	C15	−0.2(5)	C11	C12	C13	N1	0.7(6)
C10	C9	N1	Pt1	−179.5(3)	C5	C9	C10	C11	−177.8(4)
C10	C9	N1	C13	0.2(5)	C5	C9	N1	Pt1	0.1(4)
C10	C9	C5	C6	179.0(3)	C5	C9	N1	C13	179.8(3)
C10	C9	C5	C4	−1.9(6)	C5	C6	C7	C8	−0.4(5)
N1	C9	C10	C11	1.7(5)	C5	C6	C7	C14	−179.6(3)
N1	C9	C5	C6	−0.6(4)	C16	C15	C14	N2	0.5(5)
N1	C9	C5	C4	178.5(3)	C16	C15	C14	C7	−179.6(3)

Table S14 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 2_yellow.

Atom	x	y	z	U(eq)
H18	3112	1826	3819	29
H1A	797	−4031	5162	59
H1B	2131	−3371	4734	59
H1C	−226	−3237	4549	59
H10	2828	−752	8510	32
H8	1492	−1897	4406	28
H12	4117	1725	9162	39
H15	1590	−1007	3069	29
H4	2105	−1763	7226	29
H17	2652	1395	2282	33
H13	4048	1995	7598	34
H11	3436	345	9621	38
H16	1865	−38	1888	32

Table S15 Crystal data and structure refinement for 3_yellow.

Identification code	3_yellow
Empirical formula	$C_{41}H_{32}Cl_2N_6O_4Pt_2$
Formula weight	1133.80
Temperature/K	150.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	7.2730(2)
b/Å	11.5993(2)
c/Å	21.8397(4)
α/°	87.882(2)
β/°	85.973(2)
γ/°	83.861(2)
Volume/Å^3	1826.54(7)
Z	2
ρ_{calc}g/cm^3	2.062
μ/mm^{-1}	15.147
F(000)	1084.0
Crystal size/mm^3	0.18 × 0.12 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.786 to 143.84
Index ranges	-7 ≤ h ≤ 7, -14 ≤ k ≤ 14, -26 ≤ l ≤ 24
Reflections collected	21583
Independent reflections	5670 [R_{int} = 0.0594, R_{sigma} = 0.0444]
Data/restraints/parameters	5670/0/498
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0479, wR_2 = 0.1283
Final R indexes [all data]	R_1 = 0.0507, wR_2 = 0.1325
Largest diff. peak/hole / e Å^{-3}	2.18/-1.73

Table S16 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for 3_yellow. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
C1	−1229(16)	3825(8)	4801(4)	46(3)
C2	−1211(13)	3772(6)	4113(4)	26(2)
C3	−546(11)	4960(6)	3237(3)	21.9(19)
C4	14(11)	6102(6)	3015(3)	20.9(19)
C5	247(11)	6314(6)	2377(3)	20.1(19)
C6	719(11)	7371(6)	2150(3)	19.7(19)
C7	994(10)	8210(5)	2569(3)	17.4(18)
C8	799(11)	8026(6)	3195(3)	20.2(18)
C9	303(11)	6957(5)	3427(3)	20.8(19)
C10	1104(11)	7771(6)	1509(3)	20.9(19)
C11	1048(12)	7109(6)	996(3)	26(2)
C12	1458(13)	7578(6)	423(4)	34(2)
C13	1886(14)	8702(7)	352(4)	33(2)
C14	1982(12)	9335(6)	880(4)	26(2)
C15	1217(11)	9028(6)	3543(3)	19.8(19)
C16	1214(13)	9072(7)	4169(4)	29(2)
C17	1701(12)	10049(6)	4429(3)	26(2)
C18	2178(11)	10989(6)	4060(3)	25.2(19)
C19	2143(12)	10902(6)	3438(3)	25(2)
C20	2700(13)	11254(6)	1937(3)	29(2)
C21	6510(16)	6169(8)	−464(4)	51(3)
C22	6668(14)	7359(7)	−229(3)	35(2)
C23	6558(12)	8226(6)	737(3)	24(2)
C24	6253(11)	8065(6)	1421(3)	16.8(18)
C25	6548(11)	8974(6)	1782(3)	21.3(19)
C26	6355(11)	8855(6)	2424(3)	20.4(18)
C27	5818(11)	7811(6)	2675(3)	20.2(18)
C28	5503(11)	6889(6)	2313(3)	15.8(18)
C29	5699(12)	7013(6)	1686(3)	21.1(19)
C30	6606(11)	9683(6)	2882(3)	21.2(19)
C31	7064(12)	10795(6)	2775(4)	27(2)
C32	7280(11)	11498(6)	3248(4)	26(2)
C33	6962(11)	11082(6)	3846(3)	25.4(19)
C34	6532(12)	9968(6)	3944(3)	26(2)
C35	4979(11)	5875(5)	2691(3)	15.6(18)
C36	4531(11)	4843(5)	2473(3)	19.8(18)
C37	4039(12)	3964(6)	2875(3)	27(2)
C38	4030(11)	4125(6)	3502(3)	24(2)
C39	4502(11)	5145(6)	3701(3)	24(2)
C40	5702(13)	7345(6)	4507(3)	29(2)
C41	8630(20)	3134(8)	1569(5)	72(4)
Cl1	8326(4)	4399.7(19)	1099.5(12)	54.7(7)
Cl2	8403(4)	1888.1(19)	1181.5(10)	52.5(7)
N1	1594(9)	8875(4)	1455(2)	20.0(15)
N2	1727(9)	9955(5)	3174(3)	22.8(16)
N3	3223(13)	12107(6)	1803(3)	45(2)
N4	6347(9)	9268(5)	3480(3)	18.6(15)

Atom	*x*	*y*	*z*	U(eq)
N5	4983(9)	6013(5)	3312(3)	20.6(16)
N6	5751(13)	7240(6)	5022(3)	45(2)
O1	-892(8)	4207(4)	2913(2)	29.9(14)
O2	-613(8)	4865(4)	3856(2)	23.5(13)
O3	6897(9)	9130(4)	487(3)	39.5(17)
O4	6392(8)	7247(4)	431(2)	30.5(14)
Pt1	1759.2(5)	9684.2(2)	2251.0(2)	19.36(15)
Pt2	5667.0(4)	7595.3(2)	3560.8(2)	17.12(15)

Table S17 Anisotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for 3_yellow. The Anisotropic displacement factor exponent takes the form:

$-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+...].$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	65(8)	40(5)	40(5)	20(4)	−17(5)	−37(5)
C2	35(6)	14(3)	33(4)	7(3)	−13(4)	−15(3)
C3	19(5)	20(3)	27(4)	1(3)	−3(3)	−2(3)
C4	14(5)	21(3)	30(4)	6(3)	−6(4)	−10(3)
C5	19(5)	15(3)	27(4)	0(3)	−6(3)	−1(3)
C6	15(5)	25(3)	17(3)	5(3)	2(3)	2(3)
C7	10(4)	20(3)	21(3)	3(2)	0(3)	1(3)
C8	17(5)	19(3)	25(4)	−1(3)	−4(3)	0(3)
C9	26(5)	21(3)	13(3)	6(2)	1(3)	0(3)
C10	16(5)	26(3)	20(4)	9(3)	−2(3)	−3(3)
C11	23(5)	27(4)	28(4)	−1(3)	−2(4)	−10(3)
C12	43(6)	29(4)	31(4)	−2(3)	−5(4)	−9(4)
C13	47(7)	33(4)	22(4)	6(3)	−6(4)	−17(4)
C14	20(5)	25(4)	33(4)	6(3)	−5(4)	−7(3)
C15	15(5)	19(3)	25(4)	2(3)	−8(3)	1(3)
C16	33(6)	26(4)	27(4)	4(3)	−3(4)	0(4)
C17	30(6)	27(4)	22(4)	0(3)	−12(4)	−9(4)
C18	23(5)	29(4)	26(4)	−5(3)	−9(4)	−9(3)
C19	32(6)	16(3)	30(4)	0(3)	−5(4)	−13(3)
C20	38(6)	26(4)	24(4)	2(3)	−4(4)	−8(4)
C21	76(9)	54(5)	26(4)	3(4)	1(5)	−23(6)
C22	44(6)	45(4)	20(4)	5(3)	−5(4)	−17(4)
C23	26(5)	30(4)	18(3)	1(3)	−7(3)	−3(4)
C24	14(5)	20(3)	16(3)	3(2)	−4(3)	0(3)
C25	15(5)	17(3)	32(4)	7(3)	−3(3)	−6(3)
C26	18(5)	17(3)	28(4)	1(3)	−9(3)	−8(3)
C27	12(5)	17(3)	32(4)	1(3)	−3(3)	−5(3)
C28	10(5)	17(3)	20(3)	5(3)	−5(3)	−3(3)
C29	22(5)	19(3)	24(4)	−3(3)	−7(3)	−8(3)
C30	17(5)	21(3)	27(4)	−1(3)	−9(3)	0(3)
C31	30(6)	15(3)	37(4)	3(3)	−4(4)	−5(3)
C32	23(5)	18(3)	37(4)	3(3)	−6(4)	−2(3)
C33	24(5)	23(3)	32(4)	−9(3)	−13(4)	−5(3)
C34	32(6)	23(3)	27(4)	−1(3)	−6(4)	−7(3)
C35	14(5)	11(3)	21(3)	3(2)	−6(3)	1(3)
C36	17(5)	18(3)	24(4)	4(3)	−4(3)	−4(3)
C37	33(6)	18(3)	31(4)	6(3)	−4(4)	−9(3)
C38	26(5)	19(3)	28(4)	9(3)	−4(4)	−6(3)
C39	25(5)	19(3)	26(4)	7(3)	4(4)	−1(3)
C40	43(6)	20(3)	27(4)	1(3)	−2(4)	−9(4)
C41	125(12)	42(5)	41(5)	0(4)	−19(6)	35(6)
Cl1	71(2)	36.7(11)	57.1(14)	−4.5(9)	−14.8(14)	0.2(12)
Cl2	84(2)	40.4(11)	34.4(11)	8.7(8)	−1.9(12)	−19.3(12)
N1	25(4)	17(3)	19(3)	0(2)	−1(3)	−4(3)
N2	19(4)	19(3)	31(3)	1(2)	−7(3)	0(3)
N3	75(7)	27(3)	37(4)	7(3)	−7(4)	−20(4)
N4	16(4)	16(3)	26(3)	−2(2)	−6(3)	−10(3)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N5	20(4)	22(3)	21(3)	5(2)	−3(3)	−7(3)
N6	73(7)	38(4)	25(4)	6(3)	−10(4)	−11(4)
O1	44(4)	21(2)	28(3)	−2(2)	−3(3)	−12(3)
O2	33(4)	15(2)	25(3)	5.2(19)	−7(3)	−11(2)
O3	61(5)	25(3)	34(3)	10(2)	1(3)	−19(3)
O4	42(4)	33(3)	19(3)	0(2)	−4(3)	−16(3)
Pt1	22.6(3)	15.01(17)	20.72(19)	3.64(12)	−2.91(16)	−3.72(15)
Pt2	18.7(3)	15.86(17)	17.50(18)	1.60(11)	−3.63(15)	−4.14(14)

Table S18 Bond Lengths for 3_yellow.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.505(12)	C23	O3	1.205(8)
C2	O2	1.464(8)	C23	O4	1.359(9)
C3	C4	1.482(9)	C24	C25	1.384(10)
C3	O1	1.201(9)	C24	C29	1.417(9)
C3	O2	1.350(8)	C25	C26	1.402(10)
C4	C5	1.407(10)	C26	C27	1.394(9)
C4	C9	1.404(11)	C26	C30	1.447(10)
C5	C6	1.374(10)	C27	C28	1.401(10)
C6	C7	1.399(10)	C27	Pt2	1.939(7)
C6	C10	1.477(8)	C28	C29	1.370(9)
C7	C8	1.375(9)	C28	C35	1.481(8)
C7	Pt1	1.944(6)	C30	C31	1.374(10)
C8	C9	1.396(9)	C30	N4	1.382(9)
C8	C15	1.482(10)	C31	C32	1.367(11)
C10	C11	1.386(11)	C32	C33	1.387(10)
C10	N1	1.364(9)	C33	C34	1.367(10)
C11	C12	1.372(10)	C34	N4	1.346(9)
C12	C13	1.373(11)	C35	C36	1.382(10)
C13	C14	1.399(13)	C35	N5	1.370(9)
C14	N1	1.370(9)	C36	C37	1.381(9)
C15	C16	1.369(10)	C37	C38	1.387(10)
C15	N2	1.386(8)	C38	C39	1.362(11)
C16	C17	1.377(12)	C39	N5	1.353(8)
C17	C18	1.392(9)	C40	N6	1.129(10)
C18	C19	1.368(10)	C40	Pt2	2.078(8)
C19	N2	1.332(10)	C41	Cl1	1.763(9)
C20	N3	1.119(10)	C41	Cl2	1.729(11)
C20	Pt1	2.089(7)	N1	Pt1	2.022(6)
C21	C22	1.508(12)	N2	Pt1	2.051(6)
C22	O4	1.446(8)	N4	Pt2	2.051(6)
C23	C24	1.501(9)	N5	Pt2	2.054(6)

Table S19 Bond Angles for 3_yellow.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	C2	C1	107.3(6)	C27	C28	C35	111.9(6)
O1	C3	C4	125.0(7)	C29	C28	C27	119.4(6)
O1	C3	O2	123.8(6)	C29	C28	C35	128.8(7)
O2	C3	C4	111.2(6)	C28	C29	C24	119.0(7)
C5	C4	C3	118.2(7)	C31	C30	C26	126.6(7)
C9	C4	C3	121.3(6)	C31	C30	N4	119.4(7)
C9	C4	C5	120.5(6)	N4	C30	C26	114.0(6)
C6	C5	C4	120.3(7)	C32	C31	C30	121.3(7)
C5	C6	C7	118.2(6)	C31	C32	C33	118.7(7)
C5	C6	C10	129.8(7)	C34	C33	C32	119.2(7)
C7	C6	C10	111.9(6)	N4	C34	C33	122.3(7)
C6	C7	Pt1	118.4(5)	C36	C35	C28	126.1(6)
C8	C7	C6	122.9(6)	N5	C35	C28	114.3(6)
C8	C7	Pt1	118.6(6)	N5	C35	C36	119.7(6)
C7	C8	C9	119.0(7)	C37	C36	C35	120.6(7)
C7	C8	C15	113.0(6)	C36	C37	C38	118.9(7)
C9	C8	C15	128.0(6)	C39	C38	C37	119.1(6)
C8	C9	C4	119.1(6)	N5	C39	C38	122.5(7)
C11	C10	C6	125.1(7)	N6	C40	Pt2	177.7(8)
N1	C10	C6	113.7(7)	Cl2	C41	Cl1	112.7(6)
N1	C10	C11	121.2(6)	C10	N1	C14	118.6(6)
C12	C11	C10	119.5(7)	C10	N1	Pt1	116.1(4)
C13	C12	C11	120.7(8)	C14	N1	Pt1	125.3(5)
C12	C13	C14	118.3(7)	C15	N2	Pt1	114.1(5)
N1	C14	C13	121.6(8)	C19	N2	C15	119.1(6)
C16	C15	C8	125.8(7)	C19	N2	Pt1	126.8(5)
C16	C15	N2	120.3(7)	C30	N4	Pt2	114.6(5)
N2	C15	C8	113.8(6)	C34	N4	C30	119.1(6)
C15	C16	C17	119.5(7)	C34	N4	Pt2	126.3(5)
C16	C17	C18	120.3(7)	C35	N5	Pt2	114.9(4)
C19	C18	C17	117.8(7)	C39	N5	C35	119.2(6)
N2	C19	C18	123.0(6)	C39	N5	Pt2	125.8(5)
N3	C20	Pt1	176.0(8)	C3	O2	C2	114.6(6)
O4	C22	C21	105.5(6)	C23	O4	C22	114.9(6)
O3	C23	C24	123.5(7)	C7	Pt1	C20	177.0(3)
O3	C23	O4	123.7(7)	C7	Pt1	N1	79.9(3)
O4	C23	C24	112.8(6)	C7	Pt1	N2	80.4(3)
C25	C24	C23	117.7(6)	N1	Pt1	C20	101.8(3)
C25	C24	C29	121.3(6)	N1	Pt1	N2	160.2(2)
C29	C24	C23	121.0(7)	N2	Pt1	C20	97.8(3)
C24	C25	C26	120.2(6)	C27	Pt2	C40	176.1(3)
C25	C26	C30	129.1(6)	C27	Pt2	N4	79.7(3)
C27	C26	C25	117.6(7)	C27	Pt2	N5	80.0(3)
C27	C26	C30	113.3(6)	N4	Pt2	C40	99.5(3)
C26	C27	C28	122.6(7)	N4	Pt2	N5	159.7(2)
C26	C27	Pt2	118.3(6)	N5	Pt2	C40	100.8(3)
C28	C27	Pt2	118.9(5)				

Table S20 Hydrogen Bonds for 3_yellow.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
C13	H13	Cl2[1]	0.95	2.81	3.469(9)	127.6
C13	H13	O3[2]	0.95	2.46	3.221(9)	137.5
C18	H18	N6[3]	0.95	2.57	3.449(12)	153.8
C31	H31	Cl2[4]	0.95	2.82	3.759(8)	170.0
C41	H41A	N3[5]	0.99	2.59	3.493(16)	152.5

[1]1-X,1-Y,-Z; [2]1-X,2-Y,-Z; [3]1-X,2-Y,1-Z; [4]+X,1+Y,+Z; [5]1+X,-1+Y,+Z

Table S21 Torsion Angles for 3_yellow.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	O2	C3	−179.2(7)	C25	C26	C30	C31	1.4(14)
C3	C4	C5	C6	178.3(7)	C25	C26	C30	N4	−178.4(8)
C3	C4	C9	C8	−178.9(7)	C26	C27	C28	C29	−1.0(12)
C4	C3	O2	C2	178.3(6)	C26	C27	C28	C35	179.0(7)
C4	C5	C6	C7	1.3(11)	C26	C30	C31	C32	−179.5(8)
C4	C5	C6	C10	177.4(8)	C26	C30	N4	C34	−179.5(7)
C5	C4	C9	C8	0.9(12)	C26	C30	N4	Pt2	−0.2(8)
C5	C6	C7	C8	−0.5(11)	C27	C26	C30	C31	−177.5(8)
C5	C6	C7	Pt1	177.6(6)	C27	C26	C30	N4	2.7(10)
C5	C6	C10	C11	0.2(13)	C27	C28	C29	C24	1.3(11)
C5	C6	C10	N1	−178.0(8)	C27	C28	C35	C36	178.1(7)
C6	C7	C8	C9	−0.1(11)	C27	C28	C35	N5	−2.7(9)
C6	C7	C8	C15	178.2(7)	C28	C35	C36	C37	−179.1(7)
C6	C10	C11	C12	−179.2(8)	C28	C35	N5	C39	179.1(6)
C6	C10	N1	C14	−180.0(7)	C28	C35	N5	Pt2	1.0(8)
C6	C10	N1	Pt1	1.8(8)	C29	C24	C25	C26	2.0(12)
C7	C6	C10	C11	176.4(8)	C29	C28	C35	C36	−1.8(13)
C7	C6	C10	N1	−1.7(9)	C29	C28	C35	N5	177.4(7)
C7	C8	C9	C4	−0.1(11)	C30	C26	C27	C28	−179.8(7)
C7	C8	C15	C16	−177.1(8)	C30	C26	C27	Pt2	−4.1(9)
C7	C8	C15	N2	−0.1(9)	C30	C31	C32	C33	−2.2(13)
C8	C15	C16	C17	177.5(7)	C31	C30	N4	C34	0.7(11)
C8	C15	N2	C19	−179.7(7)	C31	C30	N4	Pt2	179.9(6)
C8	C15	N2	Pt1	0.1(8)	C31	C32	C33	C34	3.1(12)
C9	C4	C5	C6	−1.5(12)	C32	C33	C34	N4	−2.1(13)
C9	C8	C15	C16	1.0(13)	C33	C34	N4	C30	0.2(12)
C9	C8	C15	N2	178.0(7)	C33	C34	N4	Pt2	−178.9(6)
C10	C6	C7	C8	−177.2(7)	C35	C28	C29	C24	−178.7(7)
C10	C6	C7	Pt1	0.8(8)	C35	C36	C37	C38	−1.0(12)
C10	C11	C12	C13	−1.3(14)	C36	C35	N5	C39	−1.6(10)
C11	C10	N1	C14	1.8(11)	C36	C35	N5	Pt2	−179.7(5)
C11	C10	N1	Pt1	−176.4(6)	C36	C37	C38	C39	0.1(12)
C11	C12	C13	C14	3.1(15)	C37	C38	C39	N5	0.0(12)
C12	C13	C14	N1	−2.5(15)	C38	C39	N5	C35	0.8(11)
C13	C14	N1	C10	0.1(13)	C38	C39	N5	Pt2	178.7(6)
C13	C14	N1	Pt1	178.1(7)	N1	C10	C11	C12	−1.2(12)
C15	C8	C9	C4	−178.2(7)	N2	C15	C16	C17	0.7(12)
C15	C16	C17	C18	0.6(13)	N4	C30	C31	C32	0.4(12)
C16	C15	N2	C19	−2.5(11)	N5	C35	C36	C37	1.8(11)
C16	C15	N2	Pt1	177.2(6)	O1	C3	C4	C5	−3.1(12)
C16	C17	C18	C19	0.0(12)	O1	C3	C4	C9	176.7(8)
C17	C18	C19	N2	−1.9(12)	O1	C3	O2	C2	−2.0(11)
C18	C19	N2	C15	3.2(12)	O2	C3	C4	C5	176.6(7)
C18	C19	N2	Pt1	−176.5(6)	O2	C3	C4	C9	−3.5(10)
C21	C22	O4	C23	177.4(8)	O3	C23	C24	C25	−6.2(12)
C23	C24	C25	C26	−177.5(7)	O3	C23	C24	C29	174.4(8)
C23	C24	C29	C28	177.6(7)	O3	C23	O4	C22	0.4(12)
C24	C23	O4	C22	179.8(7)	O4	C23	C24	C25	174.5(7)
C24	C25	C26	C27	−1.6(11)	O4	C23	C24	C29	−5.0(11)
C24	C25	C26	C30	179.6(8)	Pt1	C7	C8	C9	−178.1(5)

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C25	C24	C29	C28	−1.9(12)	Pt1	C7	C8	C15	0.2(9)
C25	C26	C27	C28	1.1(11)	Pt2	C27	C28	C29	−176.7(6)
C25	C26	C27	Pt2	176.8(6)	Pt2	C27	C28	C35	3.3(9)

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C25	C24	C29	C28	−1.9(12)	Pt1	C7	C8	C15	0.2(9)
C25	C26	C27	C28	1.1(11)	Pt2	C27	C28	C29	−176.7(6)
C25	C26	C27	Pt2	176.8(6)	Pt2	C27	C28	C35	3.3(9)

Table S22 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3_yellow.

Atom	x	y	z	U(eq)
H1A	47	3778	4924	69
H1B	−1836	3173	4990	69
H1C	−1908	4557	4935	69
H2A	−344	3109	3963	31
H2B	−2465	3672	3987	31
H5	78	5724	2103	24
H9	162	6809	3857	25
H11	728	6336	1041	31
H12	1446	7121	72	41
H13	2110	9041	−45	40
H14	2326	10103	838	31
H16	877	8433	4421	35
H17	1712	10082	4863	31
H18	2517	11669	4234	30
H19	2429	11548	3182	30
H21A	7530	5625	−323	77
H21B	6572	6203	−914	77
H21C	5324	5906	−307	77
H22A	7906	7608	−350	42
H22B	5712	7934	−396	42
H25	6881	9682	1595	26
H29	5466	6402	1433	25
H31	7235	11081	2364	33
H32	7639	12256	3169	31
H33	7043	11565	4183	30
H34	6357	9679	4355	32
H36	4562	4739	2043	24
H37	3711	3260	2725	32
H38	3699	3532	3787	29
H39	4494	5251	4131	29
H41A	9870	3073	1732	86
H41B	7695	3197	1923	86

Figures

Figure S1. Solid-State IR spectroscopy for **2** in both green form-I and yellow form-II.
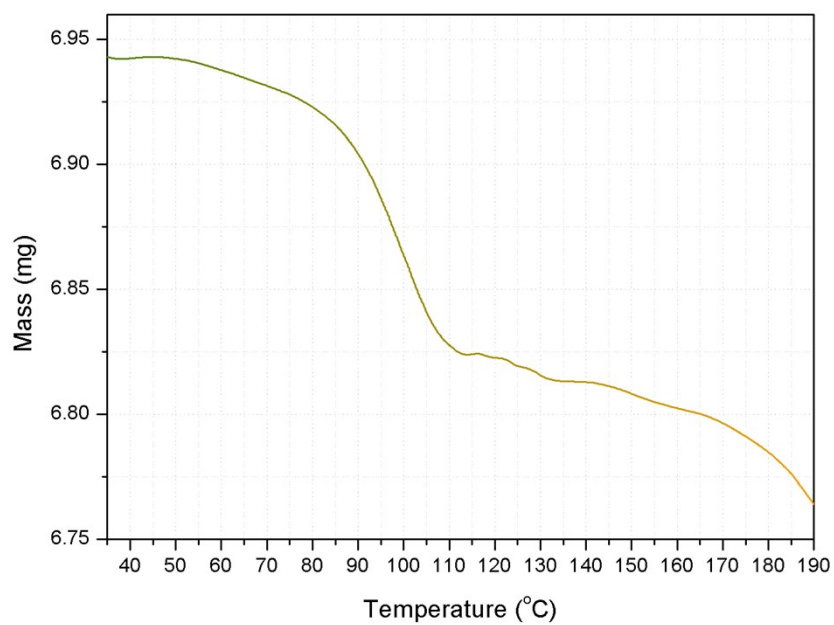

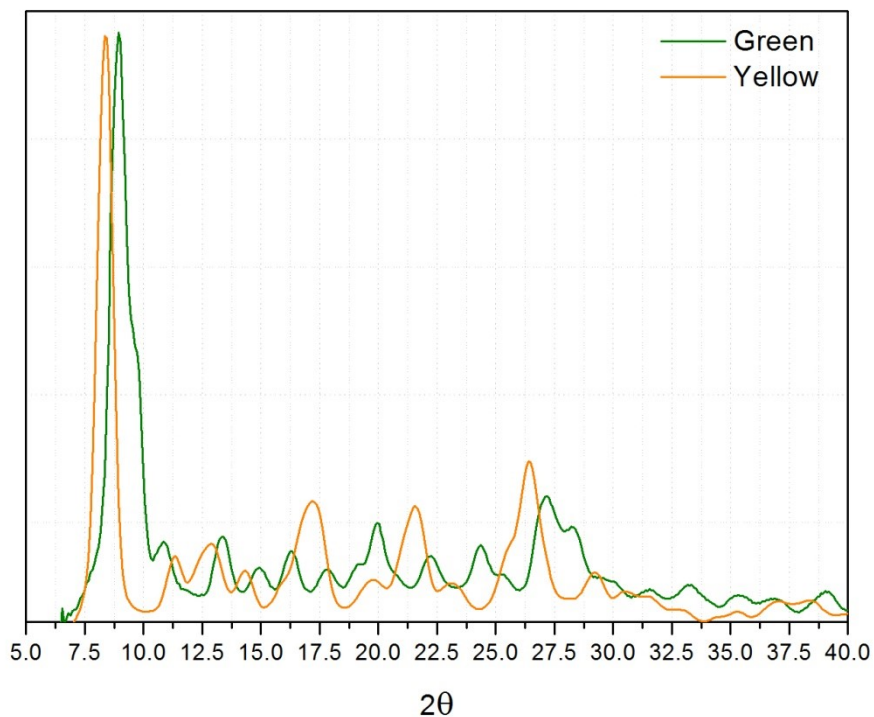Figure S2. Thermogravimetric analysis of **2** showing a two-step loss of 3.45% mass.

Figure S3. X-ray powder diffraction experiment of **2** before heating (form-I) and after heating (form-II).
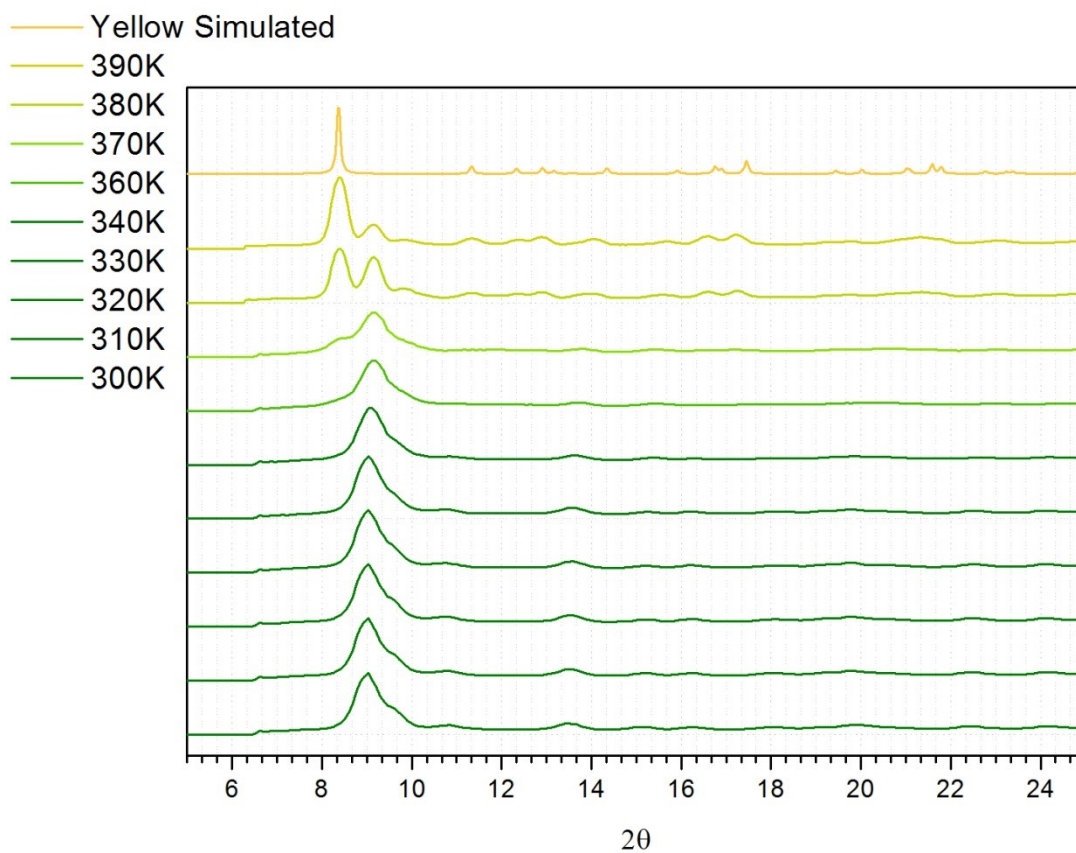

Figure S4. Powder diffraction patterns for **2** run at increasing cryostat temperature intervals, indicating a crystalline transition between the yellow and green forms at high temperatures.
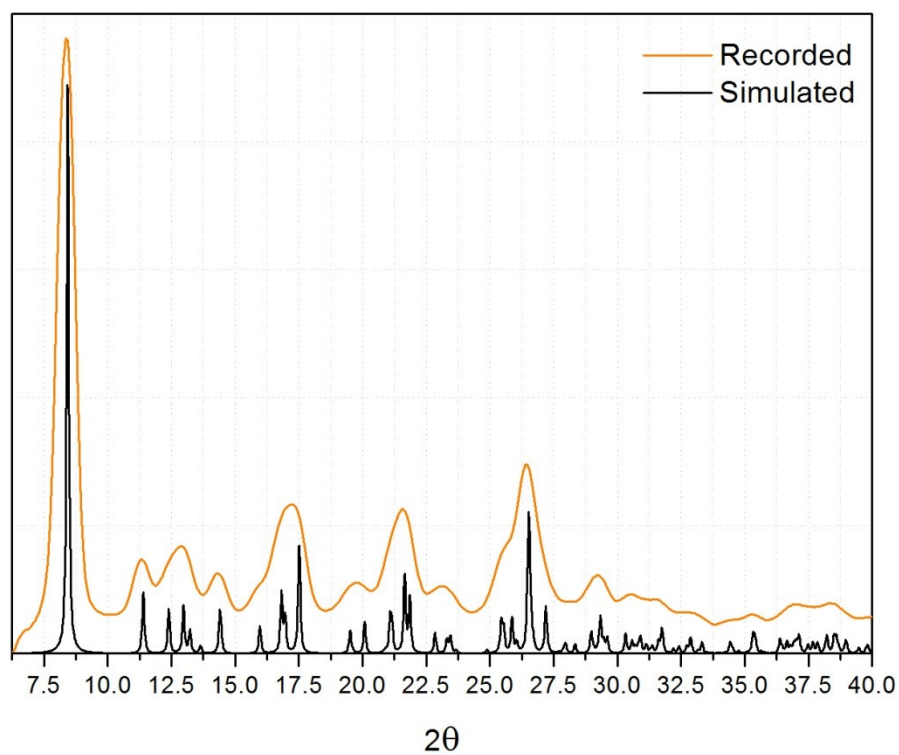
Figure S5. Comparison of the recorded powder pattern for **2** after heating (form-II) and the simulated powder pattern from the yellow crystals grown.
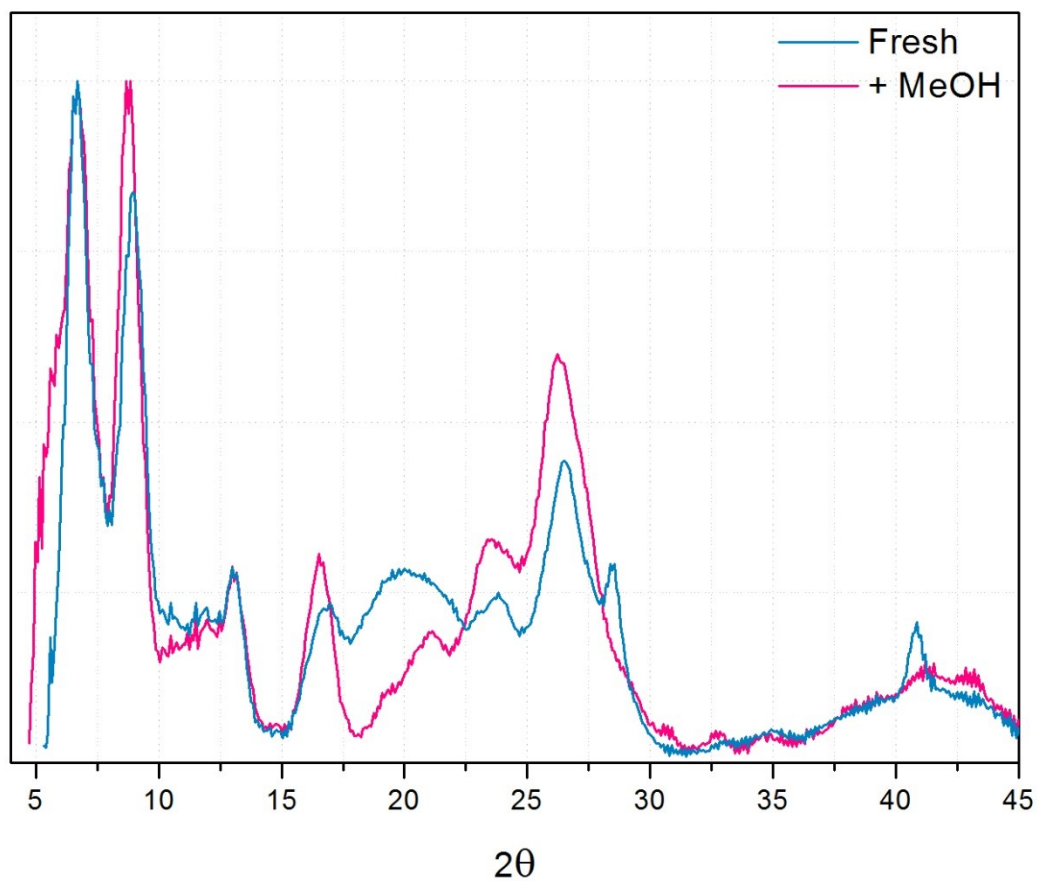
Figure S6. Powder diffraction of **4** before and after methanol exposure.

References

1.   J. A. G. Williams, A. Beeby, E. S. Davies, J. A. Weinstein and C. Wilson, *Inorg, Chem.*, 2003, **42**, 8609