Supplementary Materials:

Highly Porous Cyanometallic Spin-Crossover Frameworks Employing Pyridazino[4,5-d]pyridazine Bridge

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Contents of the Supplementary Materials:

1: [Fe(*pp*)Pd(CN)$_4$]·G

2: [Fe(*pp*)Pt(CN)$_4$]·G

where:

pp = pyridazino[4,5-d]pyridazine

G = guest solvent molecules (MeOH and H_2O)

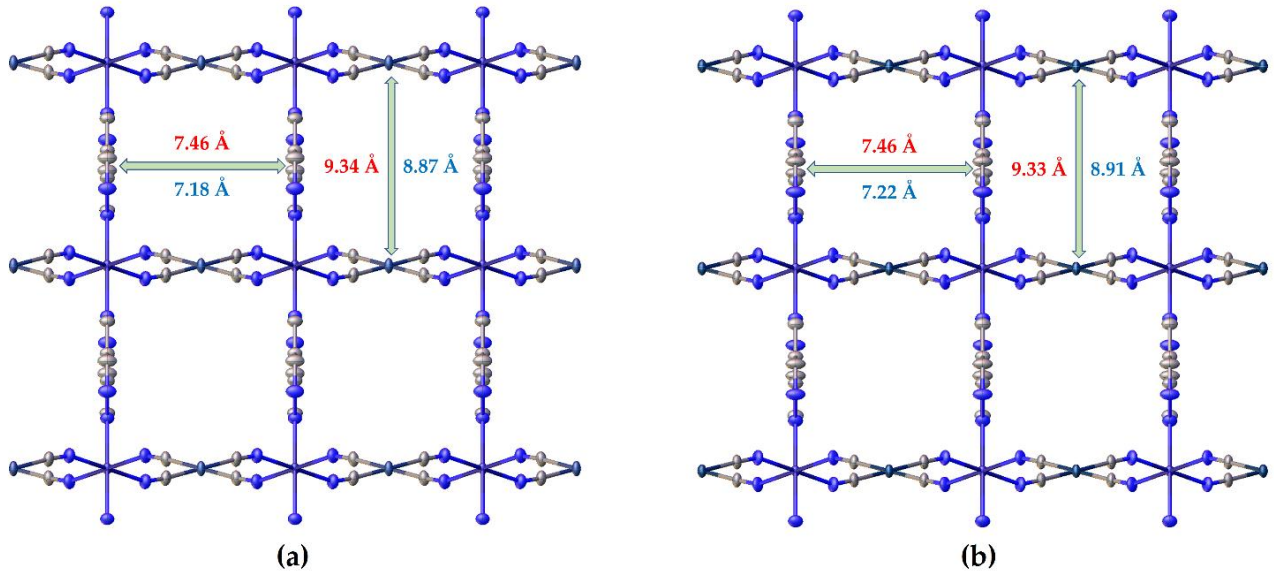

Figure S1. View of the 1D channel of **1** (**a**) and **2** (**b**) along the *a*-axis direction. The gate sizes of the pores of **1** and **2** in the LS (blue) and HS (red) states.

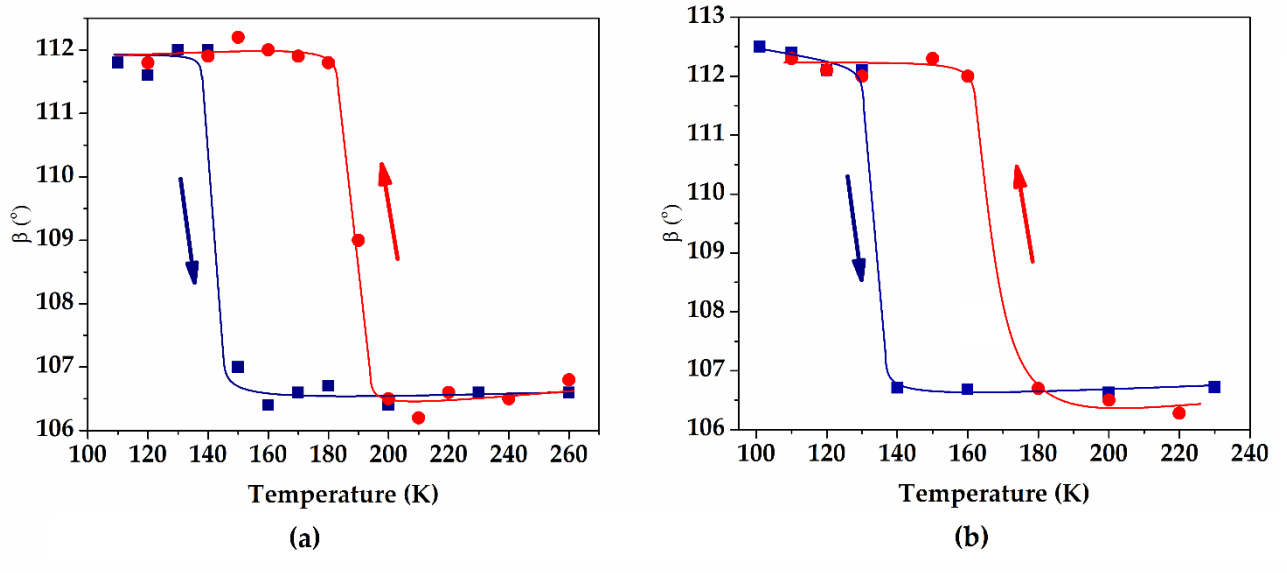

Figure S2. Temperature dependences of β angles of **1** (**a**) and **2** (**b**).

Table S1. Selected crystallographic data for **1** extracted from SCXRD pre-experiments at various temperatures.

Temperature (K)	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	V (Å³)
Cooling regime					
260	7.22(3)	7.398(18)	8.42(5)	106.6(5)	431(3)
230	7.20(2)	7.423(12)	8.39(2)	106.6(3)	430(2)
200	7.22(3)	7.400(17)	8.37(5)	106.4(5)	429(3)
180	7.20(3)	7.407(15)	8.40(4)	106.7(4)	429(3)
170	7.20(5)	7.375(15)	8.40(8)	106.6(9)	428(5)
160	7.18(3)	7.42(2)	8.40(6)	106.4(3)	429(7)
150	7.08(2)	7.40(2)	8.48(14)	107.0(9)	408(1)
140	7.08(2)	7.19(3)	8.72(4)	112.0(2)	409(2)
130	7.07(3)	7.125(14)	8.72(3)	112.0(4)	408(2)
120	7.05(4)	7.14(5)	8.73(2)	111.6(7)	406(5)
Heating regime					
120	7.12(4)	7.15(4)	8.61(5)	111.8(5)	407(4)
130	7.04(2)	7.138(8)	8.747(16)	111.4(5)	408(2)
140	7.08(5)	7.151(19)	8.68(4)	111.9(5)	408(4)
150	7.06(2)	7.14(2)	8.73(3)	112.2(3)	407(2)
160	7.08(5)	7.15(3)	8.72(4)	112.0(5)	409(4)
170	7.05(8)	7.129(18)	8.70(2)	111.9(2)	409(4)
180	7.08(5)	7.16(4)	8.65(5)	111.8(6)	408(5)
190	7.02(4)	7.33(11)	8.62(5)	109.0(4)	420(5)
200	7.20(9)	7.41(4)	8.40(6)	106.5(4)	429(6)
210	7.19(10)	7.47(8)	8.38(5)	106.2(5)	433(8)
220	7.18(3)	7.44(4)	8.39(4)	106.6(7)	430(4)
240	7.216(12)	7.47(3)	8.37(4)	106.5(1)	433(4)
260	7.19(6)	7.45(3)	8.39(2)	106.8(6)	430(3)

Table S2. Selected crystallographic data for **2** extracted from SCXRD pre-experiments at various temperatures.

Temperature (K)	*a* (Å)	*b* (Å)	*c* (Å)	β (°)	V (Å³)
Cooling regime					
230	7.181(4)	7.456(3)	8.386(7)	106.72(8)	430(1)
200	7.183(5)	7.447(3)	8.382(9)	106.63(9)	429.7(6)
160	7.187(6)	7.433(3)	8.372(9)	106.68(10)	428.5(6)
140	7.194(3)	7.433(2)	8.366(4)	106.71(5)	428.5(3)
130	7.01(4)	7.206(7)	8.760(4)	112.1(7)	410(3)
120	7.040(18)	7.186(6)	8.740(2)	112.1(4)	410(2)
110	7.06(3)	7.199(12)	8.750(3)	112.4(5)	411(3)
101	7.056(15)	7.179(6)	8.739(16)	112.5(3)	409(1)
Heating regime					
110	7.034(16)	7.184(14)	8.742(14)	112.3(2)	409(1)
120	7.038(9)	7.181(3)	8.721(17)	112.1(2)	408.4(1)
130	7.03(4)	7.214(11)	8.730(4)	112.0(7)	411(3)
140	7.04(3)	7.186(9)	8.720(2)	112.8(5)	407(2)
150	7.03(2)	7.188(14)	8.720(5)	112.3(6)	408(3)
160	7.03(6)	7.198(5)	8.73(14)	112(2)	409(7)
180	7.19(4)	7.411(15)	8.370(3)	106.7(8)	427(3)
200	7.189(12)	7.442(11)	8.34(3)	106.5(3)	428(2)
220	7.175(13)	7.451(7)	8.376(8)	106.28(14)	429.8(1)

Table S3. Crystal data and structure refinement for **1** at 293 K and 125 K.

Empirical formula	$C_{10}H_4FeN_8Pd$	$C_{10}H_4FeN_8Pd$
Formula weight	398.46	398.46
Temperature (K)	293	125
Crystal system	monoclinic	monoclinic
Space group	*P*2/*m*	*P*2/*m*
***a* (Å)**	7.1903(3)	7.0619(6)
***b* (Å)**	7.4599(2)	7.1811(5)
***c* (Å)**	8.4271(4)	8.6859(7)
α (°)	90	90
β (°)	107.071(5)	112.392(10)
γ (°)	90	90
Volume (Å^3)	432.11(3)	407.27(6)
Z	1	1
ϱ_{calc} (g cm^{-3})	1.531	1.625
μ (mm^{-1})	1.880	1.995
F(000)	192.0	192.0
Crystal size (mm^3)	0.25 × 0.25 × 0.05	0.25 × 0.15 × 0.04
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection (°)	5.056 to 65.124	5.072 to 64.724
Reflections collected	5312	2697
Independent reflections	1562 [R_{int} = 0.0398, R_{sigma} = 0.0393]	1438 [R_{int} = 0.0382, R_{sigma} = 0.0639]
Data/restraints/parameters	1562 / 0 / 57	1438 / 0 / 57
Goodness-of-fit on F^2	1.065	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0251, wR_2 = 0.0588	R_1 = 0.0425, wR_2 = 0.0886
Final R indexes [all data]	R_1 = 0.0309, wR_2 = 0.0606	R_1 = 0.0469, wR_2 = 0.0905
Largest diff. peak/hole (e Å^{-3})	0.63 / -0.39	1.47 / -1.41

Table S4. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **1** at 293 K (HS). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Pd1	5000	5000	5000	21.29(9)
Fe1	0	0	5000	16.19(11)
N2	2140(3)	0	7484(3)	24.3(4)
N1	1784(2)	2025(2)	4360(2)	28.9(4)
N3	1397(3)	0	8801(3)	32.6(5)
C3	5367(3)	0	9324(3)	24.3(5)
C1	2946(2)	3120(2)	4530(3)	25.6(4)
C2	4030(3)	0	7737(3)	26.1(5)
C4	2575(4)	0	10307(4)	33.4(6)

Table S5. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **1** at 293 K (HS). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd1	12.38(12)	12.93(12)	38.96(18)	0	8.17(11)	0
Fe1	9.00(19)	14.6(2)	23.0(3)	0	1.64(18)	0
N2	14.5(9)	33.2(11)	23.7(11)	0	3.2(8)	0
N1	23.1(7)	24.0(7)	38.2(10)	1.8(7)	6.9(7)	-4.9(6)
N3	13.2(9)	56.2(15)	27.7(12)	0	4.7(9)	0
C3	10.6(10)	37.9(13)	23.5(13)	0	3.6(10)	0
C1	17.9(8)	18.8(8)	39.5(11)	2.6(8)	7.5(8)	1.0(6)
C2	15.1(10)	41.2(14)	21.9(12)	0	5.2(10)	0
C4	13.1(11)	61.7(19)	25.6(14)	0	5.8(10)	0

Table S6. Bond Lengths for **1** at 293 K (HS).

Atom	Atom	Length (Å)		Atom	Atom	Length (Å)
Pd1	C1	1.9907(17)		Fe1	N1[6]	2.1503(15)
Pd1	C1[1]	1.9907(17)		N2	N3	1.365(3)
Pd1	C1[2]	1.9907(17)		N2	C2	1.313(3)
Pd1	C1[3]	1.9907(17)		N1	C1	1.147(2)
Fe1	N2	2.204(2)		N3	C4	1.303(4)
Fe1	N2[4]	2.204(2)		C3	C3[7]	1.390(5)
Fe1	N1[5]	2.1503(15)		C3	C2	1.400(4)
Fe1	N1	2.1503(15)		C3	C4[7]	1.419(3)
Fe1	N1[4]	2.1503(15)				

[1]1-X,+Y,1-Z; [2]+X,1-Y,+Z; [3]1-X,1-Y,1-Z; [4]-X,-Y,1-Z; [5]-X,+Y,1-Z; [6]+X,-Y,+Z; [7]1-X,-Y,2-Z

Table S7. Bond Angles for **1** at 293 K (HS).

Atom	Atom	Atom	Angle (°)		Atom	Atom	Atom	Angle (°)
C1	Pd1	C1[1]	180.0		N1	Fe1	N1[5]	89.24(8)
C1[2]	Pd1	C1[3]	180.0		N1[4]	Fe1	N1[6]	89.24(8)
C1	Pd1	C1[2]	89.61(10)		N1	Fe1	N1[4]	180.0
C1[1]	Pd1	C1[3]	89.61(10)		N1	Fe1	N1[6]	90.76(8)
C1[1]	Pd1	C1[2]	90.39(10)		N1[5]	Fe1	N1[6]	180.00(9)
C1	Pd1	C1[3]	90.39(10)		N3	N2	Fe1	116.19(14)
N2	Fe1	N2[4]	180.0		C2	N2	Fe1	123.68(18)
N1[5]	Fe1	N2	86.38(6)		C2	N2	N3	120.1(2)
N1	Fe1	N2[4]	93.62(6)		C1	N1	Fe1	159.26(16)
N1	Fe1	N2	86.38(6)		C4	N3	N2	119.6(2)
N1[5]	Fe1	N2[4]	93.61(6)		C3[7]	C3	C2	117.6(3)
N1[4]	Fe1	N2	93.62(6)		C3[7]	C3	C4[7]	116.3(3)
N1[6]	Fe1	N2	93.62(6)		C2	C3	C4[7]	126.1(2)
N1[6]	Fe1	N2[4]	86.39(6)		N1	C1	Pd1	175.88(17)
N1[4]	Fe1	N2[4]	86.39(6)		N2	C2	C3	122.9(2)
N1[4]	Fe1	N1[5]	90.76(8)		N3	C4	C3[7]	123.5(2)

[1]1-X,1-Y,1-Z; [2]+X,1-Y,+Z; [3]1-X,+Y,1-Z; [4]-X,-Y,1-Z; [5]+X,-Y,+Z; [6]-X,+Y,1-Z; [7]1-X,-Y,2-Z

Table S8. Torsion Angles for **1** at 293 K (HS).

A	B	C	D	Angle (°)		A	B	C	D	Angle (°)
Fe1	N2	N3	C4	180.000(1)		C3[1]	C3	C2	N2	0.000(1)
Fe1	N2	C2	C3	180.000(1)		C2	N2	N3	C4	0.000(1)
N2	N3	C4	C3[1]	0.000(2)		C4[1]	C3	C2	N2	180.000(1)
N3	N2	C2	C3	0.000(1)						

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

Table S9. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for **1** at 293 K (HS).

Atom	*x*	*y*	*z*	U(eq)
H2	4501.41	0	6820.17	31
H4	2040.42	0	11186.33	40

Table S10. Solvent masks information for **1** at 293 K (HS).

X	Y	Z	Volume	Electron count Content
-0.619	0.500	0.000	159.1	35.0

Table S11. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **1** at 125 K (LS). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Pd1	5000	0	10000	8.02(12)
Fe1	10000	5000	10000	8.47(17)
N2	8026(5)	5000	7665(4)	10.6(7)
N3	8801(5)	5000	6438(4)	13.8(7)
N1	8330(4)	3082(4)	10436(3)	11.3(5)
C1	7147(4)	1952(4)	10379(3)	11.3(5)
C3	5386(6)	5000	4368(5)	10.9(8)
C4	6023(6)	5000	7278(5)	13.5(8)
C2	7547(6)	5000	4889(5)	15.0(8)

Table S12. Anisotropic Displacement Parameters (Å²×10³) for **1** at 125 K (LS). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd1	6.1(2)	4.00(19)	15.0(2)	0	5.15(16)	0
Fe1	7.0(4)	6.6(4)	11.9(4)	0	3.8(3)	0
N2	9.1(15)	11.7(16)	13.2(15)	0	6.6(13)	0
N3	11.7(16)	18.7(18)	13.5(16)	0	7.5(14)	0
N1	10.1(11)	10.5(11)	12.2(11)	-0.2(9)	3.0(9)	2.9(10)
C1	10.1(12)	9.9(12)	14.1(13)	-0.6(11)	4.8(11)	1.0(11)
C3	7.2(16)	13.6(19)	12.1(17)	0	3.9(15)	0
C4	11.9(18)	14.5(19)	15.5(18)	0	7.0(16)	0
C2	10.0(18)	22(2)	15.0(19)	0	6.4(16)	0

Table S13. Bond Lengths for **1** at 125 K (LS).

Atom	Atom	Length (Å)		Atom	Atom	Length (Å)
Pd1	C1[1]	1.998(3)		Fe1	N1[6]	1.942(3)
Pd1	C1[2]	1.998(3)		N2	N3	1.371(5)
Pd1	C1[3]	1.998(3)		N2	C4	1.323(5)
Pd1	C1	1.998(3)		N3	C2	1.298(5)
Fe1	N2	1.976(3)		N1	C1	1.152(4)
Fe1	N2[4]	1.976(3)		C3	C3[7]	1.400(8)
Fe1	N1	1.942(3)		C3	C4[7]	1.396(6)
Fe1	N1[5]	1.942(3)		C3	C2	1.417(6)
Fe1	N1[4]	1.942(3)				

[1]1-X,-Y,2-Z; [2]1-X,+Y,2-Z; [3]+X,-Y,+Z; [4]2-X,1-Y,2-Z; [5]+X,1-Y,+Z; [6]2-X,+Y,2-Z; [7]1-X,1-Y,1-Z

Table S14. Bond Angles for **1** at 125 K (LS).

Atom	Atom	Atom	Angle (°)		Atom	Atom	Atom	Angle (°)
C1[1]	Pd1	C1[2]	90.87(16)		N1[4]	Fe1	N1[6]	89.64(14)
C1[2]	Pd1	C1	89.13(16)		N1[5]	Fe1	N1	89.64(14)
C1[1]	Pd1	C1	180.0		N1[4]	Fe1	N1	180.0
C1[1]	Pd1	C1[3]	89.13(16)		N1[6]	Fe1	N1	90.36(14)
C1[3]	Pd1	C1	90.87(16)		N1[4]	Fe1	N1[5]	90.36(14)
C1[2]	Pd1	C1[3]	180.0		N3	N2	Fe1	117.6(2)
N2[4]	Fe1	N2	180.00(19)		C4	N2	Fe1	121.9(3)
N1[5]	Fe1	N2[4]	87.52(10)		C4	N2	N3	120.5(4)
N1[5]	Fe1	N2	92.48(10)		C2	N3	N2	119.2(3)
N1[6]	Fe1	N2	87.52(10)		C1	N1	Fe1	167.3(2)
N1	Fe1	N2[4]	92.48(10)		N1	C1	Pd1	173.5(2)
N1	Fe1	N2	87.52(10)		C3[7]	C3	C2	116.3(5)
N14	Fe1	N2	92.48(10)		C4[7]	C3	C3[7]	117.7(4)
N1[6]	Fe1	N2[4]	92.48(10)		C4[7]	C3	C2	126.0(4)
N1[4]	Fe1	N2[4]	87.52(10)		N2	C4	C3[7]	122.4(4)
N1[6]	Fe1	N1[5]	180.0		N3	C2	C3	123.9(4)

[1]1-X,-Y,2-Z; [2]+X,-Y,+Z; [3]1-X,+Y,2-Z; [4]2-X,1-Y,2-Z; [5]2-X,+Y,2-Z; [6]+X,1-Y,+Z; [7]1-X,1-Y,1-Z

Table S15. Torsion Angles for **1** at 125 K (LS).

A	B	C	D	Angle (°)		A	B	C	D	Angle (°)
Fe1	N2	N3	C2	180.000(1)		C3[1]	C3	C2	N3	0.000(2)
Fe1	N2	C4	C3[1]	180.000(1)		C4	N2	N3	C2	0.000(2)
N2	N3	C2	C3	0.000(2)		C4[1]	C3	C2	N3	180.000(1)
N3	N2	C4	C3[1]	0.000(2)						

[1]1-X,1-Y,1-Z

Table S16. Hydrogen Atom Coordinates (Å×10[4]) and Isotropic Displacement Parameters (Å[2]×10[3]) for **1** at 125 K (LS).

Atom	*x*	*y*	*z*	U(eq)
H4	5536.48	5000	8133.55	16
H2	8099.87	5000	4073.98	18

Table S17. Solvent masks information for **1** at 125 K (LS).

X	Y	Z	Volume	Electron count Content
0.026	0.000	0.500	146.5	33.7

Table S18. Crystal data and structure refinement for **2** at 293 K and 123 K.

Empirical formula	$C_{10}H_4FeN_8Pt$	$C_{10}H_4FeN_8Pt$
Formula weight	487.15	487.15
Temperature (K)	293	123
Crystal system	monoclinic	monoclinic
Space group	*P*2/*m*	*P*2/*m*
***a* (Å)**	7.1806(5)	7.0971(6)
***b* (Å)**	7.4575(5)	7.2163(4)
***c* (Å)**	8.4389(8)	8.7642(8)
α (°)	90	90
β (°)	107.185(9)	112.610(10)
γ (°)	90	90
Volume (Å^3)	431.72(6)	414.36(6)
Z	1	1
ϱ_{calc} (g cm^{-3})	1.874	1.952
μ (mm^{-1})	8.933	9.307
F(000)	224.0	224.0
Crystal size (mm^3)	0.2 × 0.15 × 0.05	0.2 × 0.1 × 0.04
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection (°)	5.462 to 58.996	5.034 to 65.188
Reflections collected	2512	2392
Independent reflections	1299 [R_{int} = 0.0711, R_{sigma} = 0.0925]	1462 [R_{int} = 0.0402, R_{sigma} = 0.0743]
Data/restraints/parameters	1299 / 0 / 57	1462 / 0 / 57
Goodness-of-fit on F^2	0.891	1.019
Final R indexes [I>=2σ (I)]	R_1 = 0.0373, wR_2 = 0.0585	R_1 = 0.0359, wR_2 = 0.0737
Final R indexes [all data]	R_1 = 0.0383, wR_2 = 0.0593	R_1 = 0.0367, wR_2 = 0.0744
Largest diff. peak/hole (e Å^{-3})	1.82 / -1.93	4.21 / -3.61

Table S19. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **2** at 293 K (HS). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Pt1	0	0	5000	18.44(11)
Fe1	5000	5000	5000	15.7(3)
C2	7574(10)	5000	10292(8)	35(2)
N1	3233(6)	2982(6)	5660(5)	27.6(10)
C4	9023(9)	5000	7737(8)	26.8(17)
N2	7132(8)	5000	7481(7)	26.3(14)
C3	9613(9)	5000	10667(8)	24.8(17)
C1	2057(7)	1870(7)	5447(6)	23.7(11)
N3	6392(8)	5000	8788(7)	34.8(18)

Table S20. Anisotropic Displacement Parameters (Å²×10³) for **2** at 293 K (HS). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt1	12.07(17)	13.54(19)	30.2(2)	0	6.94(14)	0
Fe1	8.6(6)	16.0(7)	20.4(6)	0	1.3(5)	0
C2	16(3)	68(7)	20(4)	0	4(3)	0
N1	24(2)	20(2)	40(3)	2(2)	11(2)	-8(2)
C4	13(3)	44(5)	25(4)	0	6(3)	0
N2	14(3)	38(4)	25(3)	0	1(2)	0
C3	14(3)	39(5)	22(4)	0	6(3)	0
C1	20(2)	15(3)	36(3)	-1(2)	7(2)	1(2)
N3	16(3)	66(6)	22(3)	0	5(2)	0

Table S21. Bond Lengths for **2** at 293 K (HS).

Atom	Atom	Length (Å)		Atom	Atom	Length (Å)
Pt1	C1[1]	1.985(5)		Fe1	N2[6]	2.199(5)
Pt1	C1	1.985(5)		C2	C3	1.404(9)
Pt1	C1[2]	1.985(5)		C2	N3	1.302(8)
Pt1	C1[3]	1.985(5)		N1	C1	1.159(6)
Fe1	N1[4]	2.145(4)		C4	N2	1.310(8)
Fe1	N1	2.145(4)		C4	C3[7]	1.412(9)
Fe1	N1[5]	2.145(4)		N2	N3	1.358(7)
Fe1	N1[6]	2.145(4)		C3	C3[7]	1.395(11)
Fe1	N2	2.199(5)				

[1]-X,-Y,1-Z; [2]+X,-Y,+Z; [3]-X,+Y,1-Z; [4]1-X,+Y,1-Z; [5]+X,1-Y,+Z; [6]1-X,1-Y,1-Z; [7]2-X,1-Y,2-Z

Table S22. Bond Angles for **2** at 293 K (HS).

Atom	Atom	Atom	Angle (°)		Atom	Atom	Atom	Angle (°)
C1[1]	Pt1	C1	180.0		N1[5]	Fe1	N2	87.06(15)
C1	Pt1	C1[2]	89.2(3)		N1[5]	Fe1	N2[4]	92.94(15)
C1[1]	Pt1	C1[2]	90.8(3)		N1[4]	Fe1	N2	87.06(15)
C1	Pt1	C1[3]	90.8(3)		N1[6]	Fe1	N2	92.94(15)
C1[1]	Pt1	C1[3]	89.2(3)		N2	Fe1	N2[4]	180.0
C1[2]	Pt1	C1[3]	180.0		N3	C2	C3	123.8(6)
N1	Fe1	N1[4]	180.0		C1	N1	Fe1	157.1(4)
N1	Fe1	N1[5]	90.9(2)		N2	C4	C3[7]	123.3(6)
N1[4]	Fe1	N1[6]	90.9(2)		C4	N2	Fe1	123.5(5)
N1[6]	Fe1	N1[5]	180.0(2)		C4	N2	N3	120.1(6)
N1[4]	Fe1	N1[5]	89.1(2)		N3	N2	Fe1	116.4(4)
N1	Fe1	N1[6]	89.1(2)		C2	C3	C4[7]	126.7(6)
N1	Fe1	N2	92.94(15)		C3[7]	C3	C2	117.1(8)
N1[6]	Fe1	N2[4]	87.06(15)		C3[7]	C3	C4[7]	116.2(8)
N1[4]	Fe1	N2[4]	92.94(15)		N1	C1	Pt1	177.9(5)
N1	Fe1	N2[4]	87.06(15)		C2	N3	N2	119.5(6)

[1]-X,-Y,1-Z; [2]+X,-Y,+Z; [3]-X,+Y,1-Z; [4]1-X,1-Y,1-Z; [5]1-X,+Y,1-Z; [6]+X,1-Y,+Z; [7]2-X,1-Y,2-Z

Table S23. Torsion Angles for **2** at 293 K (HS).

A	B	C	D	Angle (°)		A	B	C	D	Angle (°)
Fe1	N2	N3	C2	180.000(3)		C3[1]	C4	N2	N3	0.000(3)
C4	N2	N3	C2	0.000(4)		N3	C2	C3	C4[1]	180.000(4)
C3	C2	N3	N2	0.000(4)		N3	C2	C3	C3[1]	0.000(6)
C3[1]	C4	N2	Fe1	180.000(2)						

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

Table S24. Hydrogen Atom Coordinates (Å×10[4]) and Isotropic Displacement Parameters (Å[2]×10[3]) for **2** at 293 K (HS).

Atom	*x*	*y*	*z*	U(eq)
H2	7036.86	5000	11168.57	42
H4	9490.29	5000	6819.77	32

Table S25. Solvent masks information for **2** at 293 K (HS).

X	Y	Z	Volume	Electron count Content
0.471	0.000	-0.013	160.1	35.3

Table S26. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **2** at 123 K (LS). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Pt1	10000	10000	10000	8.72(10)
Fe1	5000	5000	10000	7.5(2)
N2	3023(8)	5000	7675(7)	9.5(10)
C4	2548(10)	5000	4895(8)	13.8(12)
C2	1034(9)	5000	7285(8)	11.6(12)
N3	3818(8)	5000	6455(7)	13.7(11)
N1	6672(5)	6922(5)	9578(5)	11.8(7)
C1	7873(7)	8053(6)	9648(6)	12.1(8)
C3	-378(10)	5000	5614(8)	13.4(12)

Table S27. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **2** at 123 K (LS). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt1	8.40(15)	7.14(15)	11.38(16)	0	4.66(12)	0
Fe1	8.5(5)	6.2(5)	8.2(5)	0	3.6(4)	0
N2	9(2)	9(2)	10(2)	0	4.0(19)	0
C4	15(3)	18(3)	10(3)	0	6(2)	0
C2	16(3)	8(3)	10(3)	0	5(2)	0
N3	10(2)	18(3)	13(3)	0	4(2)	0
N1	11.6(17)	11.4(17)	12.5(17)	3.4(15)	4.6(14)	0.6(13)
C1	14(2)	8.3(18)	15(2)	1.4(17)	6.4(17)	4.7(15)
C3	14(3)	15(3)	11(3)	0	4(2)	0

Table S28. Bond Lengths for **2** at 123 K (LS).

Atom	Atom	Length (Å)		Atom	Atom	Length (Å)
Pt1	C1	1.997(5)		Fe1	$N1^6$	1.951(4)
Pt1	$C1^1$	1.997(4)		N2	C2	1.318(8)
Pt1	$C1^2$	1.997(4)		N2	N3	1.387(8)
Pt1	$C1^3$	1.997(5)		C4	N3	1.317(8)
Fe1	$N2^4$	1.980(5)		C4	$C3^7$	1.429(9)
Fe1	N2	1.980(5)		C2	C3	1.421(9)
Fe1	$N1^5$	1.951(4)		N1	C1	1.165(6)
Fe1	N1	1.951(4)		C3	$C3^7$	1.375(13)
Fe1	$N1^4$	1.951(4)				

^{1}2-X,+Y,2-Z; ^{2}+X,2-Y,+Z; ^{3}2-X,2-Y,2-Z; ^{4}1-X,1-Y,2-Z; ^{5}1-X,+Y,2-Z; ^{6}+X,1-Y,+Z; ^{7}-X,1-Y,1-Z

Table S29. Bond Angles for **2** at 123 K (LS).

Atom	Atom	Atom	Angle (°)		Atom	Atom	Atom	Angle (°)
C1	Pt1	C1[1]	180.00(19)		N1[6]	Fe1	N1[5]	180.0
C1[2]	Pt1	C1[3]	180.0		N1	Fe1	N1[5]	89.4(2)
C1	Pt1	C1[2]	89.4(2)		N1	Fe1	N1[6]	90.6(2)
C1[1]	Pt1	C1[3]	89.4(2)		N1	Fe1	N1[4]	180.0
C1[1]	Pt1	C1[2]	90.6(2)		N1[4]	Fe1	N1[5]	90.6(2)
C1	Pt1	C1[3]	90.6(2)		C2	N2	Fe1	122.1(5)
N2[4]	Fe1	N2	180.0		C2	N2	N3	120.8(5)
N1[5]	Fe1	N2	87.31(15)		N3	N2	Fe1	117.1(4)
N1[6]	Fe1	N2[4]	87.31(15)		N3	C4	C3[7]	123.4(6)
N1[4]	Fe1	N2[4]	92.69(15)		N2	C2	C3	121.9(6)
N1	Fe1	N2	92.69(15)		C4	N3	N2	118.7(5)
N1[5]	Fe1	N2[4]	92.69(15)		C1	N1	Fe1	167.0(4)
N1	Fe1	N2[4]	87.31(16)		N1	C1	Pt1	174.6(4)
N1[4]	Fe1	N2	87.31(16)		C2	C3	C4[7]	124.8(6)
N1[6]	Fe1	N2	92.69(15)		C3[7]	C3	C4[7]	117.0(7)
N1[4]	Fe1	N1[6]	89.4(2)		C3[7]	C3	C2	118.2(7)

[1]2-X,2-Y,2-Z; [2]+X,2-Y,+Z; [3]2-X,+Y,2-Z; [4]1-X,1-Y,2-Z; [5]1-X,+Y,2-Z; [6]+X,1-Y,+Z; [7]-X,1-Y,1-Z

Table S30. Torsion Angles for **2** at 123 K (LS).

A	B	C	D	Angle (°)		A	B	C	D	Angle (°)
Fe1	N2	C2	C3	180.000(2)		C2	N2	N3	C4	0.000(3)
Fe1	N2	N3	C4	180.000(2)		N3	N2	C2	C3	0.000(3)
N2	C2	C3	C4[1]	180.000(3)		C3[1]	C4	N3	N2	0.000(3)
N2	C2	C3	C3[1]	0.000(4)						

[1]-X,1-Y,1-Z

Table S31. Hydrogen Atom Coordinates (Å×10[4]) and Isotropic Displacement Parameters (Å[2]×10[3]) for **2** at 123 K (LS).

Atom	*x*	*y*	*z*	U(eq)
H4	3102.14	5000	4066.49	17
H2	530.95	5000	8144.57	14

Table S32. Solvent masks information for **2** at 123 K (LS).

X	Y	Z	Volume	Electron count Content
-0.205	0.000	0.500	149.3	13.4