

Electronic Supplementary Informations for

Chemical Pressure-induced Pt(III)-I Mott-Hubbard Nanowire, $[\text{Pt}(\text{en})_2\text{I}](\text{Asp}-\text{C}_n)_2 \cdot \text{H}_2\text{O}$ ($13 \leq n$), Detected via Polarized Infrared Spectroscopy

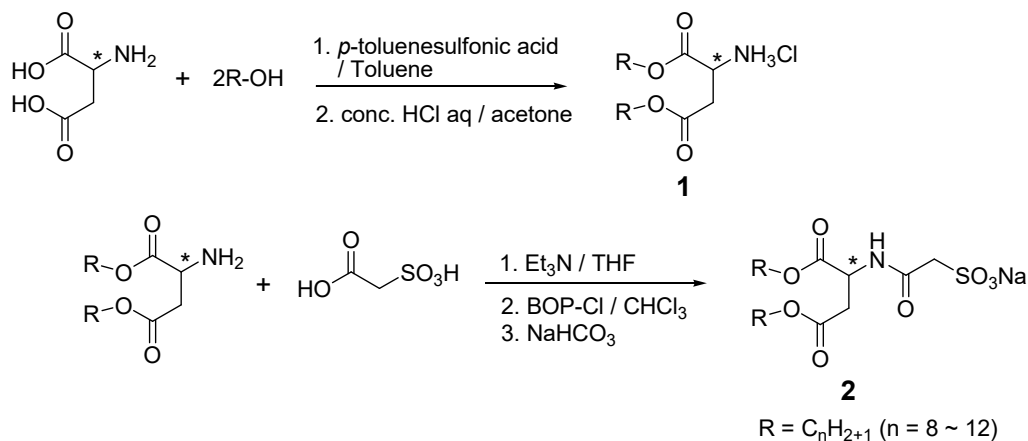
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Experimental details

Syntheses



Scheme S1 Synthetic route of Na(Asp-C_n).

Synthesis of Na(Asp-C₁₀)

4.00 g (30.1 mmol) of L-Aspartic acid, 11.43 g (72.2 mmol) of 1-Decanol and 5.95 g (31.3 mmol) of *p*-toluenesulfonic acid were dissolved in toluene, and water was removed as an azeotropic mixture with a Dean-Stark trap. The reaction was continued until the stoichiometric amount of water was recovered. After removing toluene under the reduced pressure, pale yellow solution was obtained. It was dissolved in 100 ml chloroform and washed with sodium carbonate solution and diluted water. Dry the organic layer with sodium sulfate. The filtrate was condensed and dissolved in acetone. White precipitation was obtained by adding hydrochloric acid solution and collected by suction filtration to give 11.86 g of white solid (Compound 1). The product was identified by NMR spectra.; Yield: 87.68 %, ¹H-NMR (500 MHz, chloroform-*d*). δ(ppm) 0.88 (6.0H*, t, CH₃-), 1.26-1.30 (28.2H, m, -(CH₂)₇-), 1.60 (4.0H, m, -(CH₂)₇-CH₂-CH₂-O), 3.16-3.34 (1.8H, dd, -C(=O)-CH₂-CH(-OCO)-), 4.08-4.24 (4.13H, m, -(CH₂)₈-CH₂-O-), 4.52 (1.0H, m, -CH₂-CH(-OCO)-NH₂-), 8.02 (2.0H, d, -C(=O)-CH-NH₂-).

3.80 g (8.45 mmol) of Compound 1 was dissolved in THF and add 3 ml of triethylamine, and filter white precipitation to obtain colorless solution. 1.24 g (8.58 mmol) of sulfoacetic acid, 2.28 g (8.96 mmol) of Bis(2-oxo-3-oxazolidinyl)phosphinic Chloride (BOP-Cl) and 3 ml of triethylamine were dissolved in 50 ml of chloroform and the mixture was cooled in ice bath, and was stirred for 18 h. After removing chloroform under the reduced pressure, colorless residue was obtained. It was dissolved in 50 ml of chloroform and washed with saturated sodium chloride solution, and then with 5% sodium bicarbonate solution. Dry the organic layer with sodium sulfate. After separating sodium sulfate by filtration, the filtrate was condensed (pale yellow oil) and added to ethyl acetate. Precipitate obtained was collected by suction filtration to give white solid. It was

recrystallized from methanol and then we obtained 0.66 g of Compound 2. The product was identified by NMR spectra; n = 10: Yield: 14.10 %, ¹H-NMR (500 MHz, chloroform-d). δ(ppm) 0.88 (6.0H*, t, CH₃-), 1.26-1.30 (28.4 H, m, -(CH₂)₇-), 1.60 (4.0H, m, -(CH₂)₇-CH₂-CH₂-O), 3.17-3.35 (1.8H, dd, -C(=O)-CH₂-CH(-OCO)-), 4.10-4.26 (4.0H, m, -(CH₂)₈-CH₂-O-), 4.42 (2.0H, m, -C(=O)-CH₂-SO₃-), 4.89 (1.0H, m, -CH₂-CH(-OCO)-NH-), 8.02 (0.9H, d, -CH-NH-C(=O)-).

Synthesis of Na(Asp-C₁₁)

4.00 g (30.1 mmol) of L-Aspartic acid, 12.44 g (72.2 mmol) of 1-Undecanol and 5.95 g (31.3 mmol) of p-toluenesulfonic acid were dissolved in toluene, and water was removed as an azeotropic mixture with a Dean-Stark trap. The reaction was continued until the stoichiometric amount of water was recovered. After removing toluene under the reduced pressure, pale yellow solution was obtained. It was dissolved in 100 ml chloroform and washed with sodium carbonate solution and diluted water. Dry the organic layer with sodium sulfate. The filtrate was condensed and dissolved in acetone. White precipitation was obtained by adding hydrochloric acid solution and collected by suction filtration to give 11.90 g of white solid (Compound 1). The product was identified by NMR spectra.; Yield: 82.84 %, ¹H-NMR (500 MHz, chloroform-d). δ(ppm) 0.88 (6.0H*, t, CH₃-), 1.26-1.30 (32.4 H, m, -(CH₂)₈-), 1.60 (4.0H, m, -(CH₂)₈-CH₂-CH₂-O), 3.16-3.34 (1.8H, dd, -C(=O)-CH₂-CH(-OCO)-), 4.08-4.24 (4.13H, m, -(CH₂)₉-CH₂-O-), 4.52 (1.0H, m, -CH₂-CH(-OCO)-NH₂-), 8.02 (2.0H, d, -C(=O)-CH-NH₂-).

4.04 g (8.45 mmol) of Compound 1 was dissolved in THF and add 3 ml of triethylamine, and filter white precipitation to obtain colorless solution. Colorless solution, 1.24 g (8.58 mmol) of sulfoacetic acid, 2.28 g (8.96 mmol) of Bis(2-oxo-3-oxazolidinyl)phosphinic Chloride (BOP-Cl) and 3 ml of triethylamine were dissolved in 50 ml of chloroform and the mixture was cooled in ice bath, and was stirred for 18 h. After removing chloroform under the reduced pressure, colorless residue was obtained. It was dissolved in 50ml of chloroform and washed with saturated sodium chloride solution, and then with 5% sodium bicarbonate solution. Dry the organic layer with sodium sulfate. After separating sodium sulfate by filtration, the filtrate was condensed (pale yellow oil) and added to ethyl acetate. Precipitate obtained was collected by suction filtration to give white solid. It was recrystallized from methanol and then we obtained 0.82 g of Compound 2. The product was identified by NMR spectra.; Yield: 16.60 %, ¹H-NMR (500 MHz, chloroform-d). δ(ppm) 0.88 (6.0H*, t, CH₃-), 1.26-1.30 (32.4 H, m, -(CH₂)₈-), 1.60 (4.0H, m, -(CH₂)₈-CH₂-CH₂-O), 3.17-3.35 (1.8H, dd, -C(=O)-CH₂-CH(-OCO)-), 4.10-4.26 (4.0H, m, -(CH₂)₉-CH₂-O-), 4.42 (2.0H, m, -C(=O)-CH₂-SO₃-), 4.89 (1.0H, m, -CH₂-CH(-OCO)-NH-), 8.02 (0.9H, d, -CH-NH-C(=O)-).

Synthesis of Na(Asp-C₁₂)

4.00 g (30.1 mmol) of L-Aspartic acid, 13.45 g (72.2 mmol) of 1-Dodecanol and 5.95 g (31.3 mmol) of p-toluenesulfonic acid were dissolved in toluene, and water was removed as an azeotropic mixture with a Dean-Stark trap. The reaction was continued until the stoichiometric amount of water was recovered. After removing toluene under the reduced pressure, pale yellow solution was obtained. It was dissolved in 100 ml chloroform and washed with sodium carbonate solution and diluted water. Dry the organic layer with sodium sulfate. The

filtrate was condensed and dissolved in acetone. White precipitation was obtained by adding hydrochloric acid solution and collected by suction filtration to give 11.52 g of white solid (Compound 1). The product was identified by NMR spectra. ; Yield: 75.73 %, ¹H-NMR (500 MHz, chloroform-d). δ(ppm) 0.88 (6.0H*, t, CH₃-), 1.26-1.30 (36.6 H, m, -(CH₂)₉-) , 1.60 (4.0H, m, -(CH₂)₉-CH₂-CH₂-O), 3.16-3.34 (1.8H, dd, -C(=O)-CH₂-CH(-OCO)-), 4.08-4.24 (4.13H, m, -(CH₂)₁₀-CH₂-O-), 4.52 (1.0H, m, -CH₂-CH(-OCO)-NH₂-), 8.02 (2.0H, d, -C(=O)-CH-NH₂-).

4.28 g (8.45 mmol) of Compound 1 was dissolved in THF and add 3 ml of triethylamine, and filter white precipitation to obtain colorless solution. Colorless solution, 1.24 g (8.58 mmol) of sulfoacetic acid, 2.28 g (8.96 mmol) of Bis(2-oxo-3-oxazolidinyl)phosphinic Chloride (BOP-Cl) and 3 ml of triethylamine were dissolved in 50 ml of chloroform and the mixture was cooled in ice bath, and was stirred for 18 h. After removing chloroform under the reduced pressure, colorless residue was obtained. It was dissolved in 50ml of chloroform and washed with saturated sodium chloride solution, and then with 5% sodium bicarbonate solution. Dry the organic layer with sodium sulfate. After separating sodium sulfate by filtration, the filtrate was condensed (pale yellow oil) and added to ethyl acetate. Precipitate obtained was collected by suction filtration to give white solid. It was recrystallized from methanol and then we obtained 1.40 g of Compound 2. The product was identified by NMR spectra. ; Yield: 27.00 %, ¹H-NMR (500 MHz, chloroform-d). δ (ppm) 0.88 (6.0H*, t, CH₃-), 1.26-1.30 (36.8 H, m, -(CH₂)₉-) , 1.60 (4.0H, m, -(CH₂)₉-CH₂-CH₂-O), 3.17-3.35 (1.8H, dd, -C(=O)-CH₂-CH(-OCO)-), 4.10-4.26 (4.0H, m, -(CH₂)₁₀-CH₂-O-), 4.42 (2.0H, m, -C(=O)-CH₂-SO₃-), 4.89 (1.0H, m, -CH₂-CH(-OCO)-NH-), 8.02 (0.9H, d, -CH-NH-C(=O)-).

Synthesis of Na(Asp-C₁₃)

4.00 g (30.1 mmol) of L-Aspartic acid, 14.47 g (72.2 mmol) of 1-Tridecanol and 6.27 g (31.3 mmol) of p-toluenesulfonic acid were dissolved in toluene, and water was removed as an azeotropic mixture with a Dean-Stark trap. The reaction was continued until the stoichiometric amount of water was recovered. After removing toluene under the reduced pressure, pale yellow solution was obtained. It was dissolved in 100 ml chloroform and washed with sodium carbonate solution and diluted water. Dry the organic layer with sodium sulfate. The filtrate was condensed and dissolved in acetone. White precipitation was obtained by adding hydrochloric acid solution and collected by suction filtration to give 12.34 g of white solid (Compound 1). The product was identified by NMR spectra. ; Yield: 76.85 %, ¹H-NMR (500 MHz, chloroform-d). δ (ppm) 0.88 (6.0H*, t, CH₃-), 1.26-1.30 (39.0 H, m, -(CH₂)₁₀-), 1.60 (4.0H, m, -(CH₂)₁₀-CH₂-CH₂-O), 3.16-3.34 (1.8H, dd, -C(=O)-CH₂-CH(-OCO)-), 4.08-4.24 (4.13H, m, -(CH₂)₁₁-CH₂-O-), 4.52 (1.0H, m, -CH₂-CH(-OCO)-NH₂-), 8.02 (2.0H, d, -C(=O)-CH-NH₂-) .

4.51 g (8.45 mmol) of Compound 1 was dissolved in THF and add 3 ml of triethylamine, and filter white precipitation to obtain colorless solution. Colorless solution, 1.24 g (8.58 mmol) of sulfoacetic acid, 2.28 g (8.96 mmol) of Bis(2-oxo-3-oxazolidinyl)phosphinic Chloride (BOP-Cl) and 3 ml of triethylamine were dissolved in 50 ml of chloroform and the mixture was cooled in ice bath, and was stirred for 18 h. After removing chloroform under the reduced pressure, colorless residue was obtained. It was dissolved in 50ml of chloroform and washed

with saturated sodium chloride solution, and then with 5% sodium bicarbonate solution. Dry the organic layer with sodium sulfate. After separating sodium sulfate by filtration, the filtrate was condensed (pale yellow oil) and added to ethyl acetate. Precipitate obtained was collected by suction filtration to give white solid. It was recrystallized from methanol and then we obtained 1.36 g of Compound 2. The product was identified by NMR spectra.; Yield: 25.16 %, ¹H-NMR (500 MHz, chloroform-d). δ (ppm) 0.88 (6.0H*, t, CH₃-), 1.26-1.30 (39.5 H, m, -(CH₂)₁₀-), 1.60 (4.0H, m, -(CH₂)₁₀-CH₂-CH₂-O), 3.17-3.35 (1.8H, dd, -C(=O)-CH₂-CH(-OCO)-), 4.10-4.26 (4.0H, m, -(CH₂)₁₁-CH₂-O-), 4.42 (2.0H, m, -C(=O)-CH₂-SO₃-), 4.89 (1.0H, m, -CH₂-CH(-OCO)-NH-), 8.02 (0.9H, d, -CH-NH-C(=O)-).

Synthesis of Na(Asp-C₁₄)

4.00g (30.1 mmol) of L-Aspartic acid, 15.48 g (72.2 mmol) of 1-Tetradecanol and 6.71 g (31.3 mmol) of p-toluenesulfonic acid were dissolved in toluene, and water was removed as an azeotropic mixture with a Dean-Stark trap. The reaction was continued until the stoichiometric amount of water was recovered. After removing toluene under the reduced pressure, pale yellow solution was obtained. It was dissolved in 100 ml chloroform and washed with sodium carbonate solution and diluted water. Dry the organic layer with sodium sulfate. The filtrate was condensed and dissolved in acetone. White precipitation was obtained by adding hydrochloric acid solution and collected by suction filtration to give 13.53 g of white solid (Compound 1). The product was identified by NMR spectra.; Yield: 80.12 %, ¹H-NMR (500 MHz, chloroform-d). δ (ppm) 0.88 (6.0H*, t, CH₃-) · 1.26-1.30 (44.8 H, m, -(CH₂)₁₁-), 1.60 (4.0H, m, -(CH₂)₁₁-CH₂-CH₂-O), 3.16-3.34 (1.8H, dd, -C(=O)-CH₂-CH(-OCO)-), 4.08-4.24 (4.13H, m, -(CH₂)₁₂-CH₂-O-), 4.52 (1.0H, m, -CH₂-CH(-OCO)-NH₂-), 8.02 (2.0H, d, -C(=O)-CH-NH₂-).

4.75 g (8.45 mmol) of Compound 1 was dissolved in THF and add 3 ml of triethylamine, and filter white precipitation to obtain colorless solution. Colorless solution, 1.24 g (8.58 mmol) of sulfoacetic acid, 2.28 g (8.96 mmol) of Bis(2-oxo-3-oxazolidinyl)phosphinic Chloride (BOP-Cl) and 3 ml of triethylamine were dissolved in 50 ml of chloroform and the mixture was cooled in ice bath, and was stirred for 18 h. After removing chloroform under the reduced pressure, colorless residue was obtained. It was dissolved in 50ml of chloroform and washed with saturated sodium chloride solution, and then with 5% sodium bicarbonate solution. Dry the organic layer with sodium sulfate. After separating sodium sulfate by filtration, the filtrate was condensed (pale yellow oil) and added to ethyl acetate. Precipitate obtained was collected by suction filtration to give white solid. It was recrystallized from methanol and then we obtained 1.05 g of Compound 2. The product was identified by NMR spectra.; Yield: 18.50 %, ¹H-NMR (500 MHz, chloroform-d). δ (ppm) 0.88 (6.0H*, t, CH₃-), 1.26-1.30 (45.0 H, m, -(CH₂)₁₁-), 1.60 (4.0H, m, -(CH₂)₁₁-CH₂-CH₂-O), 3.17-3.35 (1.8H, dd, -C(=O)-CH₂-CH(-OCO)-), 4.10-4.26 (4.0H, m, -(CH₂)₁₂-CH₂-O-), 4.42 (2.0H, m, -C(=O)-CH₂-SO₃-), 4.89 (1.0H, m, -CH₂-CH(-OCO)-NH-), 8.02 (0.9H, d, -CH-NH-C(=O)-).

Syntheses of $[\text{Pt}^{\text{II}}(\text{en})_2]\text{I}_2$

0.45 g (1.0 mmol) of PtI_2 was dispersed in approximately 10 mL of water, followed by the addition of 0.9 g (15 mmol) of ethylenediamine (en). The mixture was stirred at 80°C for 1 hour. Any formed impurity, appearing as a black solid, was then removed by filtration. The solvent from the filtrate was largely evaporated using a rotary evaporator. Methanol (10 mL) and acetone (10 mL) were added to the remaining residue, resulting in the formation of a white precipitate. This white solid was collected through filtration, yielding 0.47 g of $[\text{Pt}^{\text{II}}(\text{en})_2]\text{I}_2$ (83% yield).

Syntheses of $[\text{Pt}^{\text{II}}(\text{en})_2][\text{Pt}^{\text{IV}}(\text{en})_2\text{I}_2](\text{ClO}_4)_4$

0.47 g (0.83 mmol) of $[\text{Pt}^{\text{II}}(\text{en})_2]\text{I}_2$ was dissolved in approximately 5 mL of water, and then 130 mg (1.0 mmol) of I_2 was added. Upon complete dissolution, approximately 0.5 mL of concentrated HClO_4 was added dropwise, resulting in the formation of a deep rust-green precipitate. The solid was collected by filtration and washed with methanol, yielding 413 mg (0.65 mmol, 78% yield) of $[\text{Pt}^{\text{II}}(\text{en})_2][\text{Pt}^{\text{IV}}(\text{en})_2\text{I}_2](\text{ClO}_4)_4$.

Syntheses of single crystals of $[\text{Pt}(\text{en})_2\text{I}](\text{Asp-C}_n)_2 \cdot \text{H}_2\text{O}$

In the pyrex glass tube (8 mm ϕ , 15 cm length), aqueous solution of $[\text{Pt}^{\text{II}}(\text{en})_2][\text{Pt}^{\text{IV}}(\text{en})_2\text{I}_2](\text{ClO}_4)_4$ (2 mL, 10 mM) was added to the bottom layer of the tube, followed by the H_2O /methanol 1:1 (v/v) mixture solution (2 mL) as the middle layer, and methanol solution of $\text{Na}(\text{Asp-C}_n)$ (2 mL, 40 mM) as the top layer were slowly added so as that the three layers of the solution was kept. After keeping a week, the thin single crystals (typically 1 \times 0.1 \times 0.01 mm) were obtained at the bottom of the glass tube. The schematic illustration is shown in Fig. S1. In some cases, colorless needle-like crystals (probably $[\text{Pt}^{\text{II}}(\text{en})_2](\text{Asp-C}_n)_2$) also form. They can be easily distinguished and separated by hand.

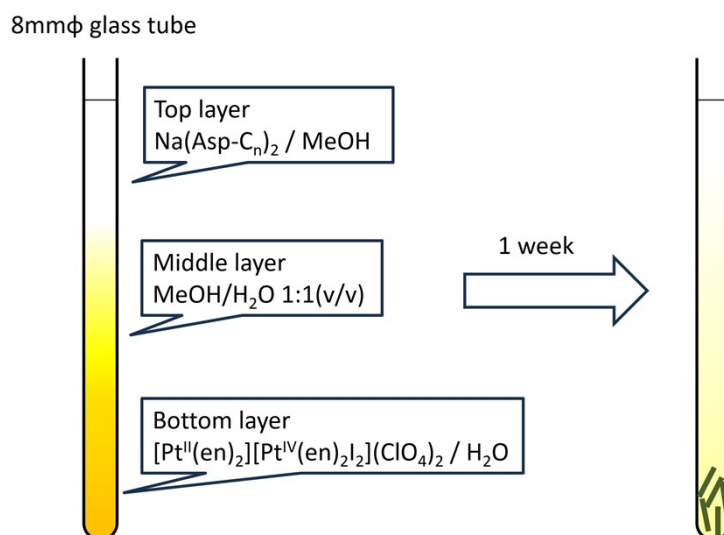


Fig. S1 Schematic illustration of the syntheses of $[\text{Pt}(\text{en})_2\text{I}](\text{Asp-C}_n)_2 \cdot \text{H}_2\text{O}$.

Experimental details for polarized FT-IR spectra

The polarized FT-IR spectra were measured using a Jasco IRT-5000 microscope equipped with a Jasco FT-IR 6200 spectrometer. Temperature control was achieved using a Janis ST-300MS cryostat and a Lakeshore 331 temperature controller. The photographs of the equipment are shown in Fig. S2(a) and (b). The schematic illustration of the measurement system is shown in Fig. S2(c). Two 0.1 mm diameter holes were made on the copper foil (0.03 mm thickness) using a precision drill. A thin single crystal (thickness less than 0.01 mm) of $[\text{Pt}(\text{en})_2\text{I}](\text{Asp}-\text{C}_n)_2 \cdot \text{H}_2\text{O}$ was mounted over one of the holes with a small amount of thermal conductive grease. The thickness direction of the single crystal is parallel to the a^* -axis (perpendicular to the bc -plane). The polarization of the incident light was set to be $E // c$ by rotating the polarizer of the incident light to maximize the magnitude of the transmitted light (a strong CT transition exists for $E // b$). The holes with and without crystal were used for the measurement of sample (S) and background (BG), respectively. The optical transmittance (T) of the sample was obtained by $T = S/BG$. The T was converted to absorbance (Abs) by using the equation of $Abs = -\log_{10}(T)$.

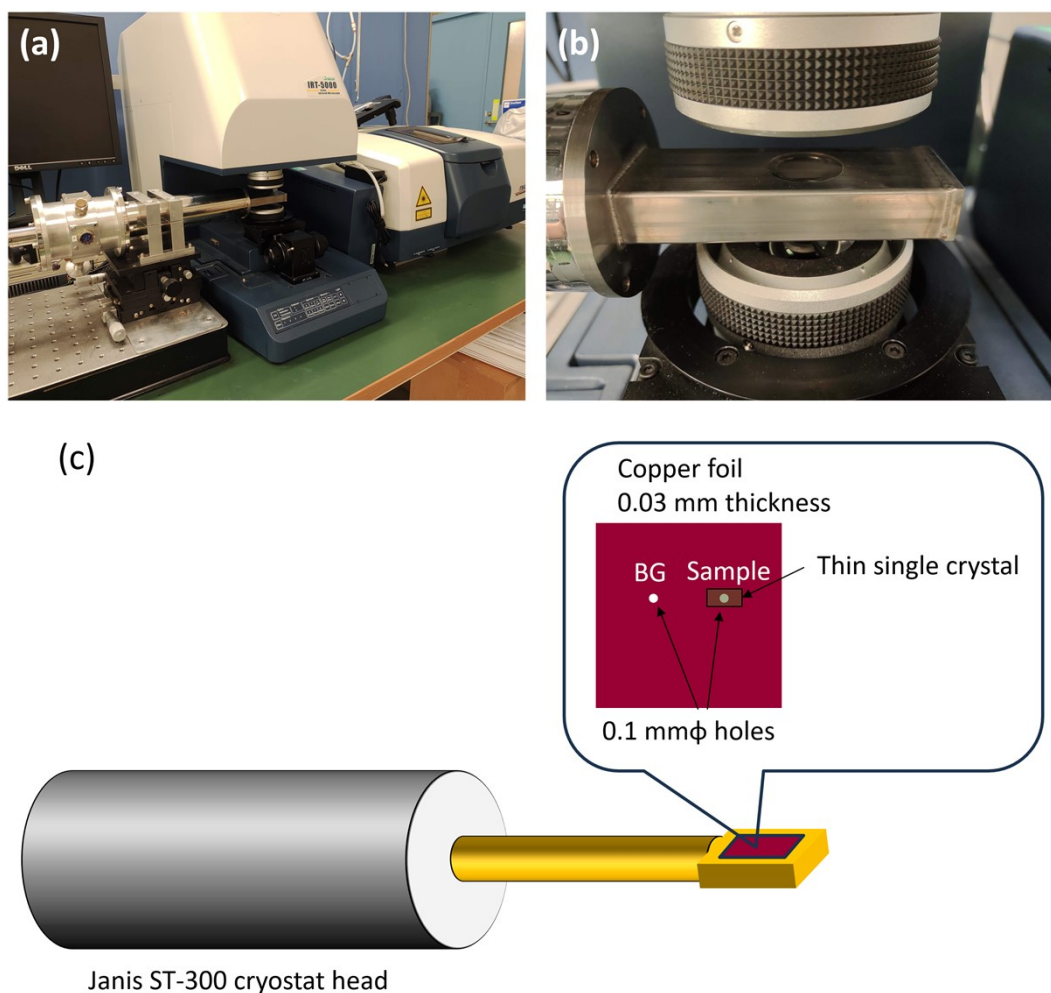


Fig. S2 Photograph (a) and (b), and schematic illustration of the experimental setup.

Powder X-ray diffraction patterns (PXRD) measurements

The unit cell parameters for $[\text{Pt}(\text{en})_2\text{I}](L\text{-Asp-C}_n)_2 \cdot \text{H}_2\text{O}$ ($n = 8, 9, 10, 11, 12, \text{ and } 14$) were determined by LeBail fitting with Rietica software of the powder X-ray diffraction (PXRD) patterns taken with the synchrotron generated X-ray source (beam line 8A) at photon-factory of High Energy Accelerator Research Organization. The polycrystalline samples were filled into the glass capillary ($0.5\text{mm}\phi$).

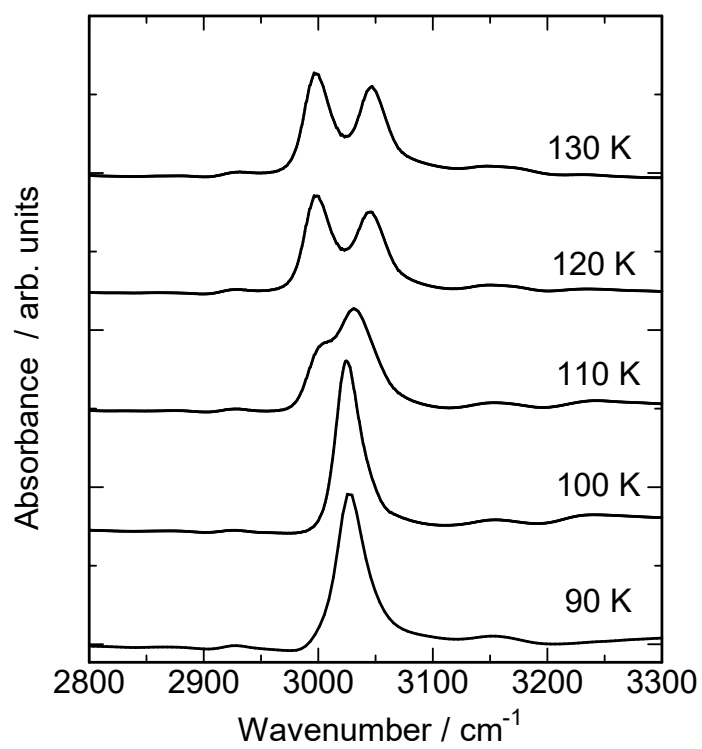


Fig. S3 Temperature dependence of FT-IR spectra in $[\text{Pd}(\text{cptn})_2\text{Br}]\text{Br}_2$.

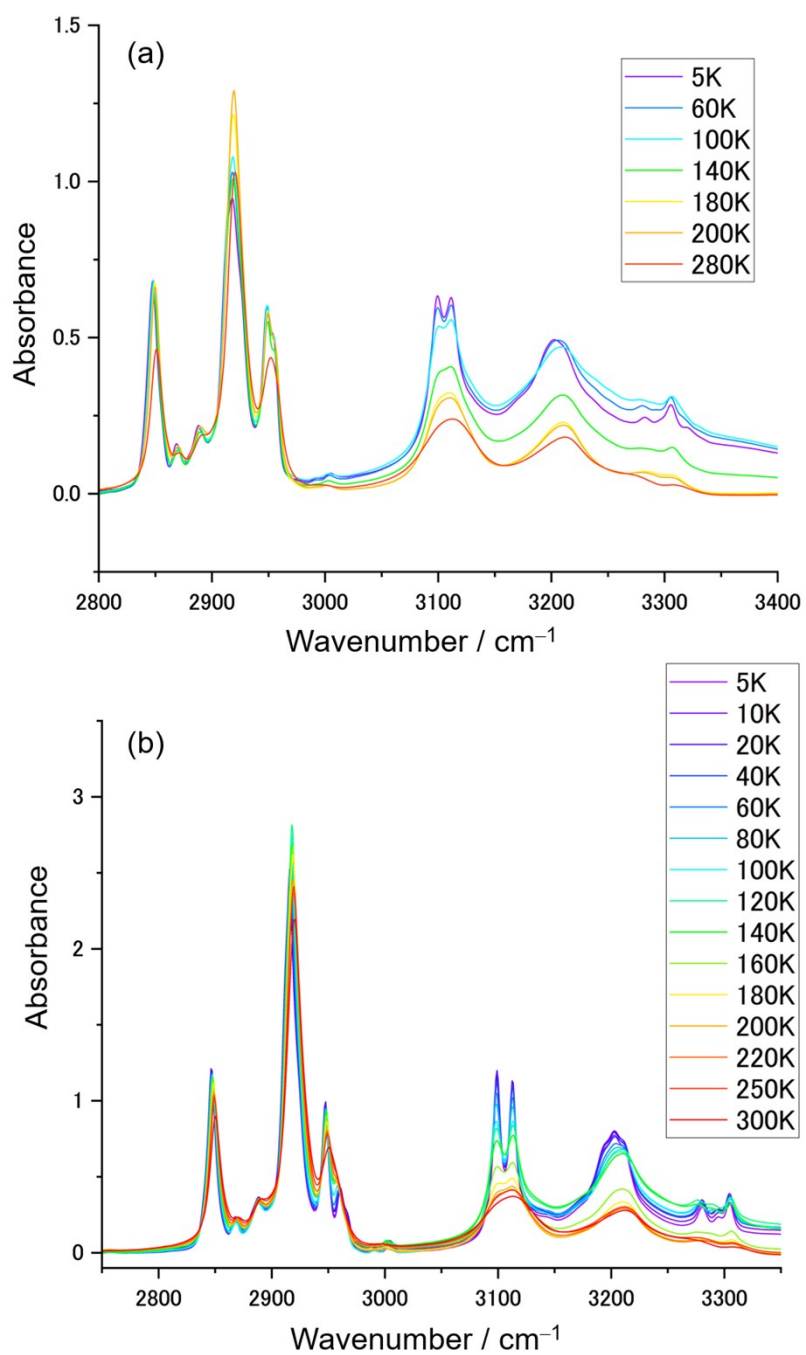


Fig. S4 Temperature dependence of FT-IR spectra in $[\text{Pt}(\text{en})_2\text{I}](\text{Asp-C}_n)_2 \cdot \text{H}_2\text{O}$. (a) $n = 11$ and (b) $n = 12$.

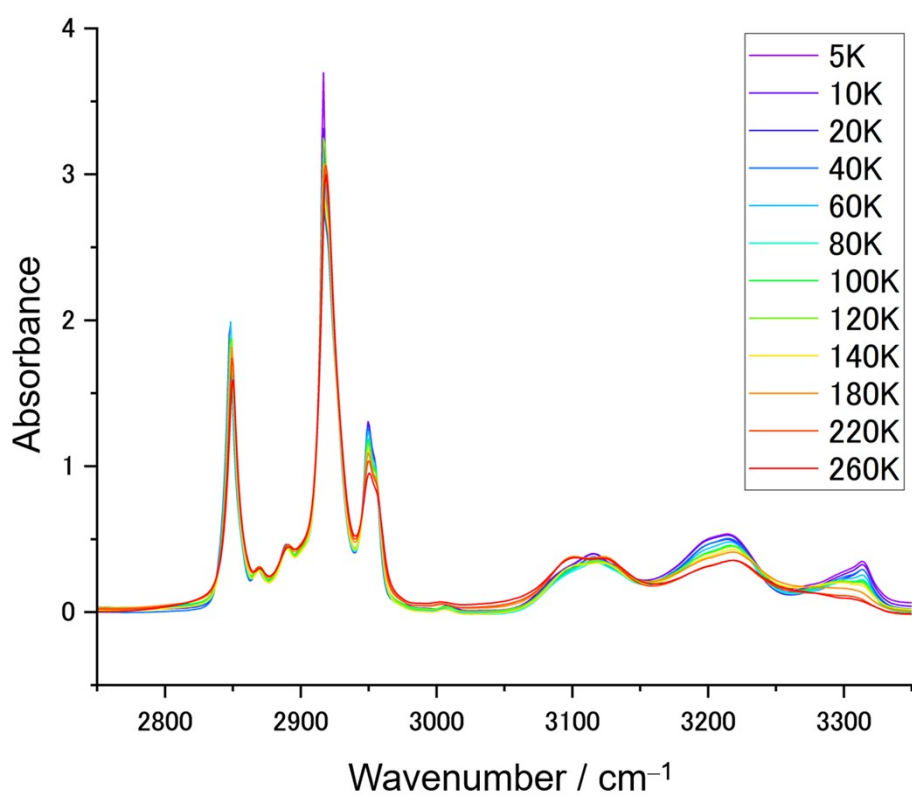


Fig. S5 Temperature dependence of FT-IR spectra in $[\text{Pt}(\text{en})_2\text{I}](\text{Asp-C}_n)_2 \cdot \text{H}_2\text{O}$ ($n = 13$).

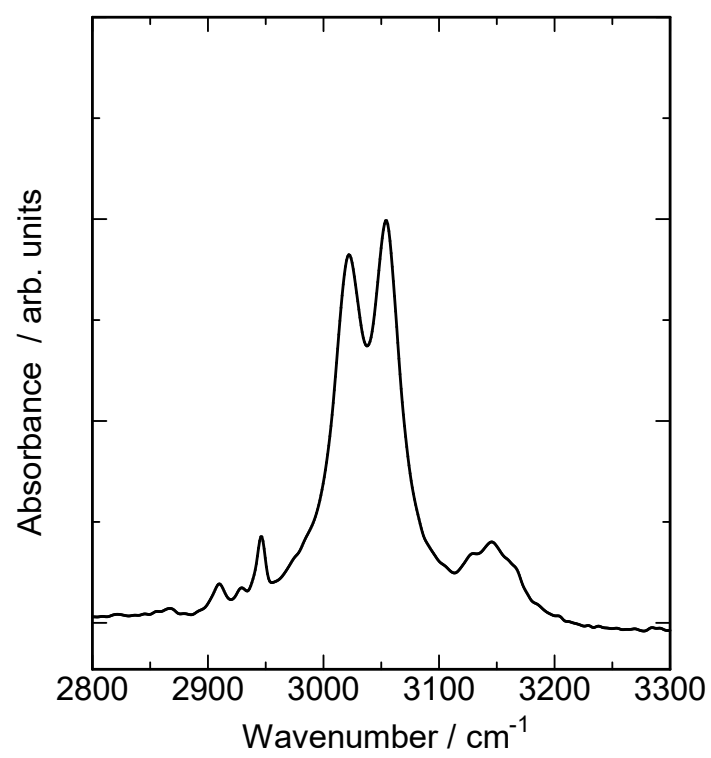


Fig. S6 FT-IR spectra in [Pt(chxn)₂I]₂ at room temperature.

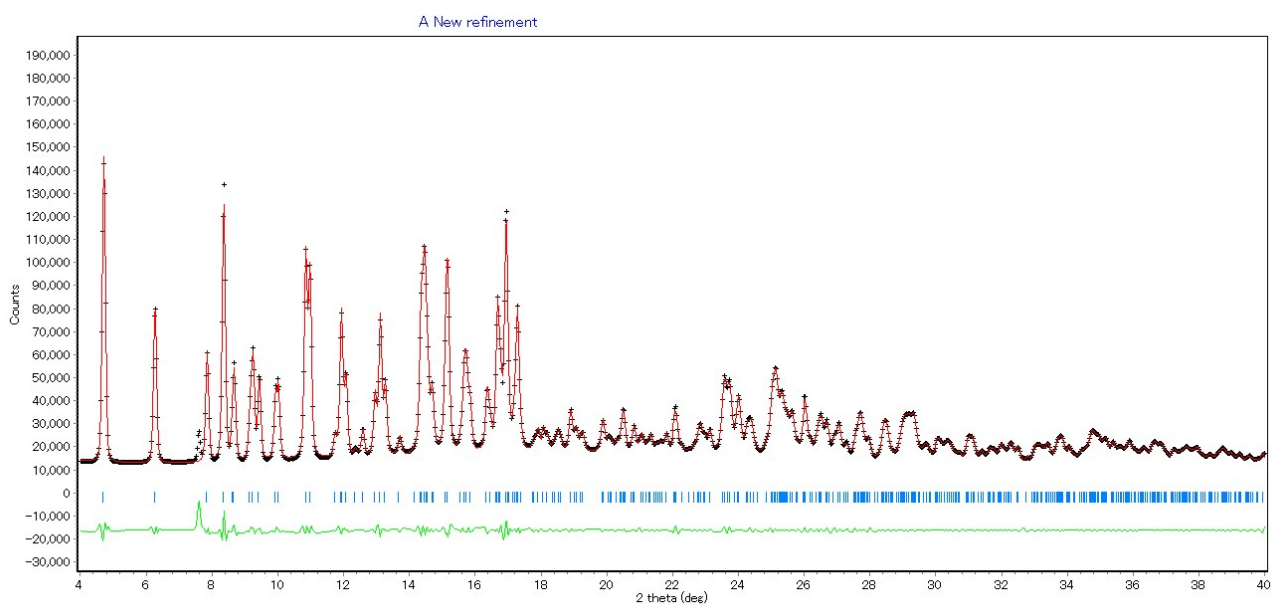


Fig. S7 PXRd pattern and LeBail fitting of $[\text{Pt}(\text{en})_2\text{I}](\text{L-Asp-C}_{10})_2 \cdot \text{H}_2\text{O}$ (300 K).

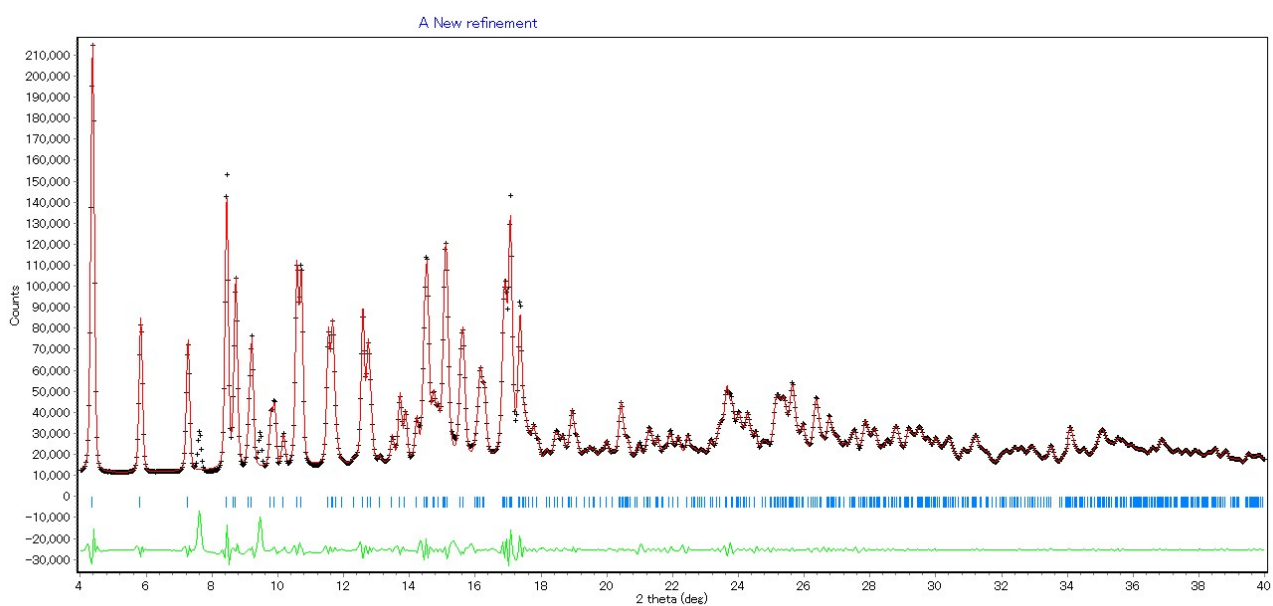


Fig. S8 PXRd pattern and LeBail fitting of $[\text{Pt}(\text{en})_2\text{I}](\text{L-Asp-C}_{11})_2 \cdot \text{H}_2\text{O}$ (300 K).

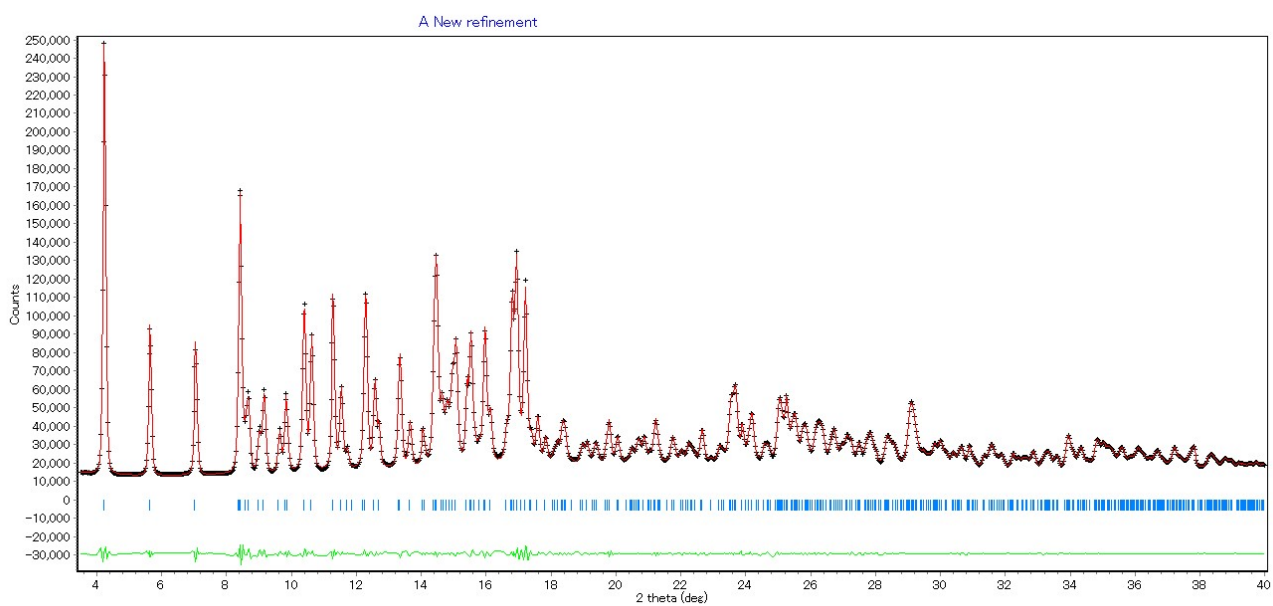


Fig. S9 PXR D pattern and LeBail fitting of $[\text{Pt}(\text{en})_2\text{I}](\text{L-Asp-C}_{12})_2 \cdot \text{H}_2\text{O}$ (300 K).

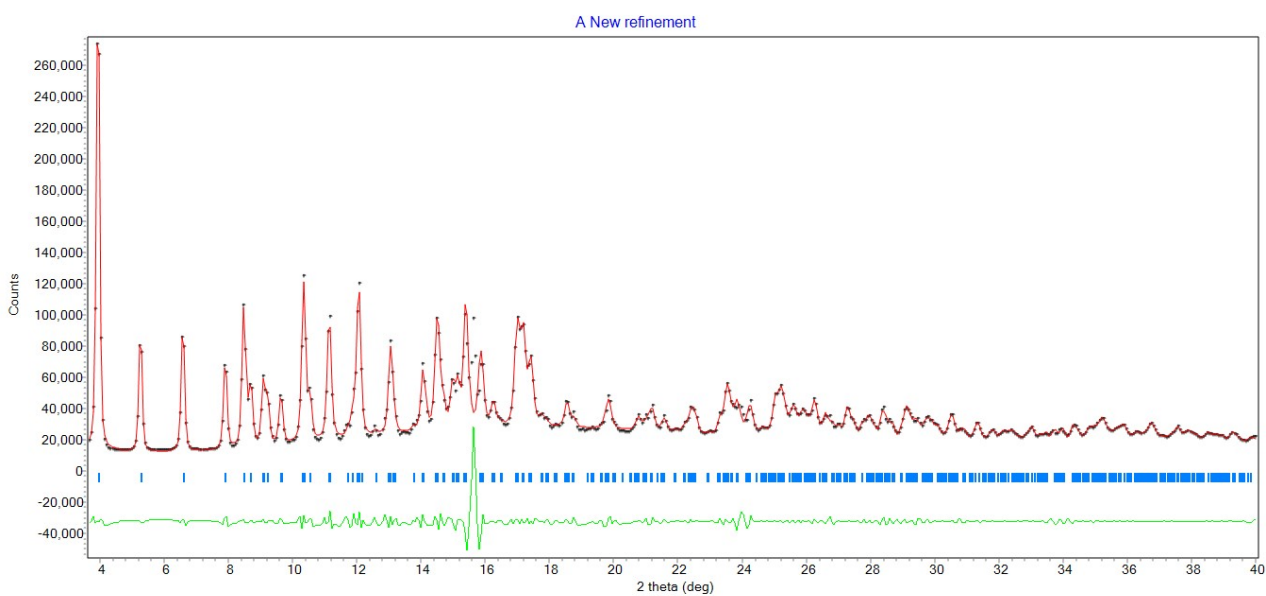


Fig. S10 PXR D pattern and LeBail fitting of $[\text{Pt}(\text{en})_2\text{I}](\text{L-Asp-C}_{13})_2 \cdot \text{H}_2\text{O}$ (300 K).

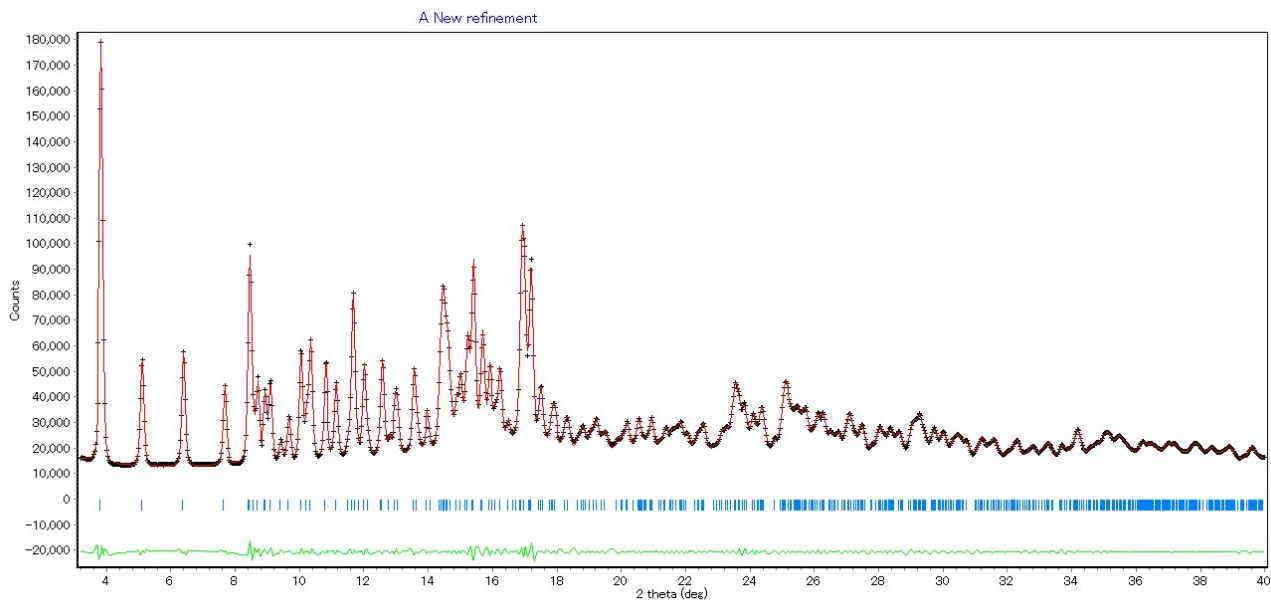


Fig. S11 PXR D pattern and LeBail fitting of $[\text{Pt}(\text{en})_2\text{I}](\text{L-Asp-C}_{14})_2 \cdot \text{H}_2\text{O}$ (300 K)

Table S1 Crystallographic parameters of [Pt(en)₂I](L-Asp-C_n)₂·H₂O (n = 10, 11, 12, 13 and 14)

n	10	11	12	13	14
Empirical formula	C ₅₀ H ₁₁₄ IN ₆ O ₁₇ PtS ₂	C ₆₀ H ₁₂₂ IN ₆ O ₁₇ PtS ₂	C ₆₄ H ₁₃₀ IN ₆ O ₁₇ PtS ₂	C ₆₈ H ₁₃₈ IN ₆ O ₁₇ PtS ₂	C ₇₂ H ₁₄₆ IN ₆ O ₁₇ PtS ₂
Formula weight	1529.65	1585.75	1641.86	1697.99	1754.07
Temperature / K	300(2)	300(2)	300(2)	300(2)	300(2)
λ / Å	1.1267	1.1267	1.1267	1.1267	1.1267
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	C2	C2	C2	C2	C2
<i>a</i> / Å	82.658(6)	89.388(9)	91.942(3)	98.63(2)	101.270(6)
<i>b</i> / Å	5.5260(3)	5.5118(5)	5.5312(2)	5.5359(13)	5.5274(3)
<i>c</i> / Å	7.7794(5)	7.7106(8)	7.7291(3)	7.6558(12)	7.6803(5)
β	94.721(2)	94.226(3)	93.546	94.249(19)	92.574(2)
Rp, Rwp	0.0172, 0.0322	0.0236, 0.0510	0.0130, 0.0198	0.0372, 0.0479	0.0138, 0.0198