

Luminescence color change of [3,4-difluoro-2,6-bis(5-methyl-2-pyridyl)phenyl- κ^3N,C^1,N']cyanidoplatinum(II) by aggregation

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Table S1. Color and luminescence color variations for Pt(L)CN upon exposure to solvent vapor.



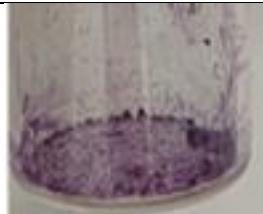

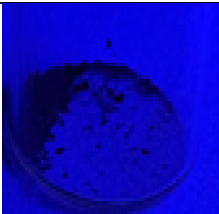

vapor	CHCl ₃	CH ₂ Cl ₂	No vapor
Color			
Luminescence color under UV light			

Table S2. Crystal data, bond lengths and bond angles for Pt(L)CN·2CHCl₃ crystal.

Space group	<i>P2₁/m</i>
Formulas	C ₂₁ H ₁₅ Cl _{6,12} F ₂ N ₃ Pt
Crystal system	Monoclinic
<i>a</i> /Å	13.7207(16)
<i>b</i> /Å	6.8784(6)
<i>c</i> /Å	28.022(2)
<i>α</i> /°	90
<i>β</i> /°	102.154
<i>γ</i> /°	90
<i>V</i> /Å ³	2585.34
<i>Z</i> , <i>Z</i> '	<i>Z</i> :4, <i>Z</i> ':1
<i>R</i> /%	7.97

	Bond length / Å		Bond angle /°
Pt1-N3	1.88	N3-Pt1-N5	163.1
Pt1-N5	2.07	N5-Pt1-C9	82.4
Pt1-C1	2.08	C9-Pt1-N3	81.0
Pt1-C9	1.98	N3-Pt1-C1	99.9
Pt2-N4	2.06	C1-Pt1-N5	97.0
Pt2-N6	2.07	C1-Pt1-C9	179.3
Pt2-C20	2.05	N4-Pt2-N6	162.9
Pt2-C28	1.91	N6-Pt2-C28	81.6
		C28-Pt2-N4	81.3
		N4-Pt2-C20	99.0
		C20-Pt2-N6	98.2
		C20-Pt2-C28	179.8

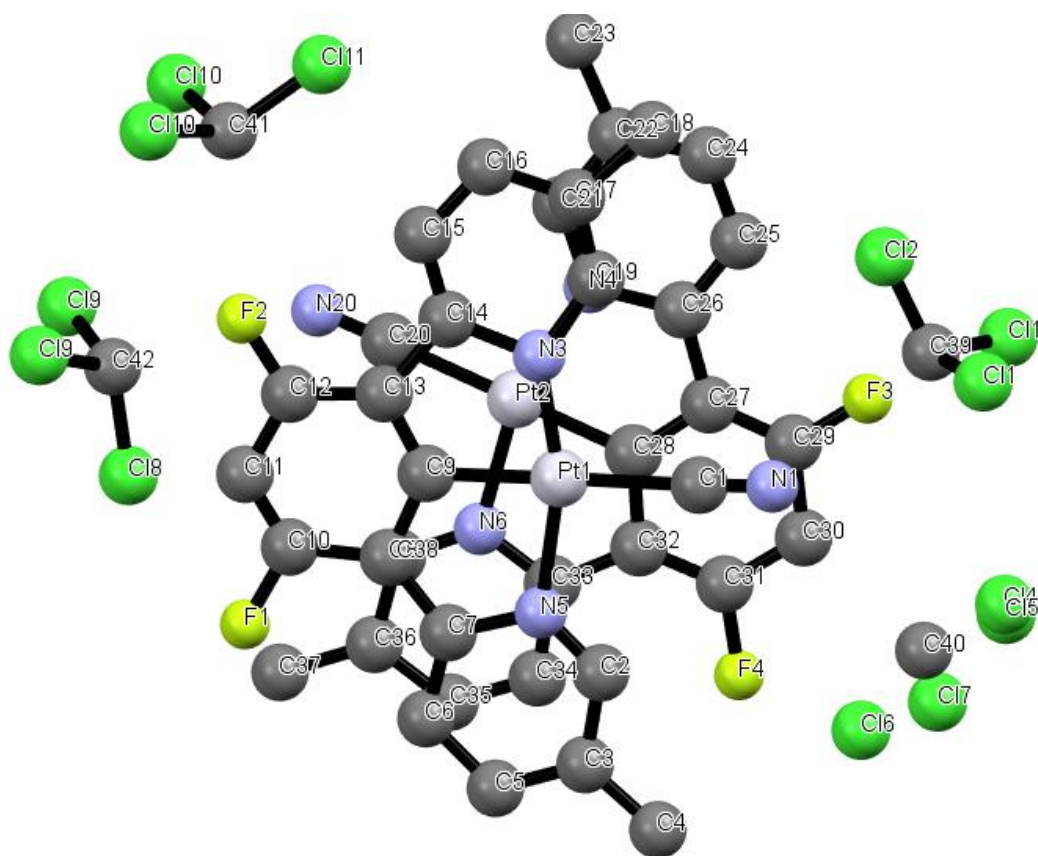


Figure S1. Structure of Pt(L)CN·2CHC

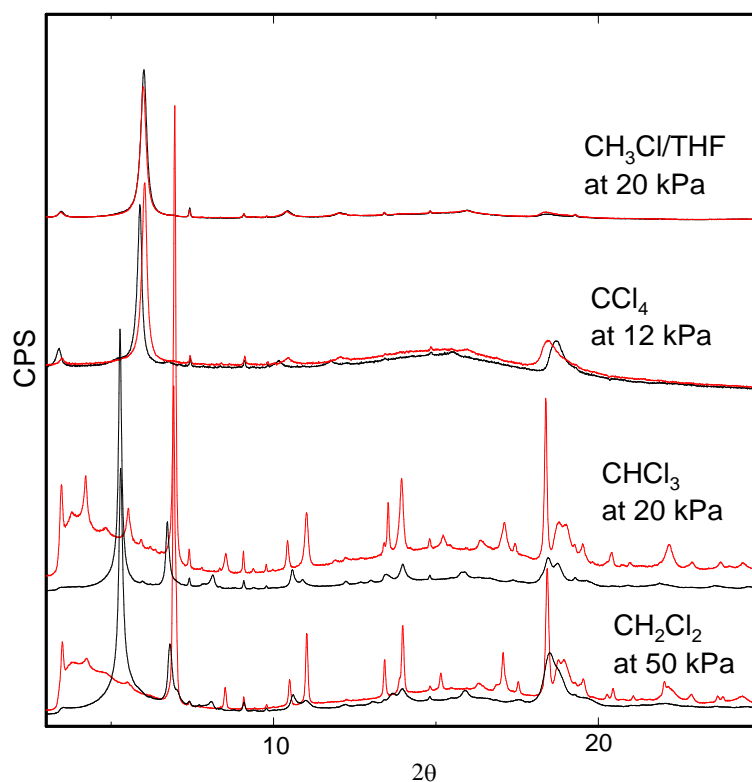


Figure S2. Red lines are PXRD patterns for Pt(L)CN crystal upon exposure to vapors. THF solution of CH₃Cl is employed for the exposure to CH₃Cl vapor. Black lines are respective PXRD patterns after evacuation.

For the CHCl₃ and CH₂Cl₂ adsorbed crystals, the PXRD patterns are very similar to each other. The peaks seem to be identical to each other within the experimental error. For the angles $2\theta = 18.38^\circ$ (CHCl₃) and 18.43° (CH₂Cl₂) providing distinct intense peak are transformed into 3.38 and 3.37 Å from the Bragg's law, respectively, which would correspond to the interplane separation between Pt(L)CN stacking pair. It seems that CH₃Cl in THF vapor doesn't contribute to the change in PXRD pattern. While the slight change in pattern can be seen upon exposure to CCl₄ vapor, the pattern is very different from those of CHCl₃ and CH₂Cl₂ adsorbed crystals.

Scheme S1. Synthesis of Pt(L)CN.

