



Copper(II) complexes with fluorinated 5-aryl-2,2'-bipyridine-6(6')-carboxylic acid tridentate ligands

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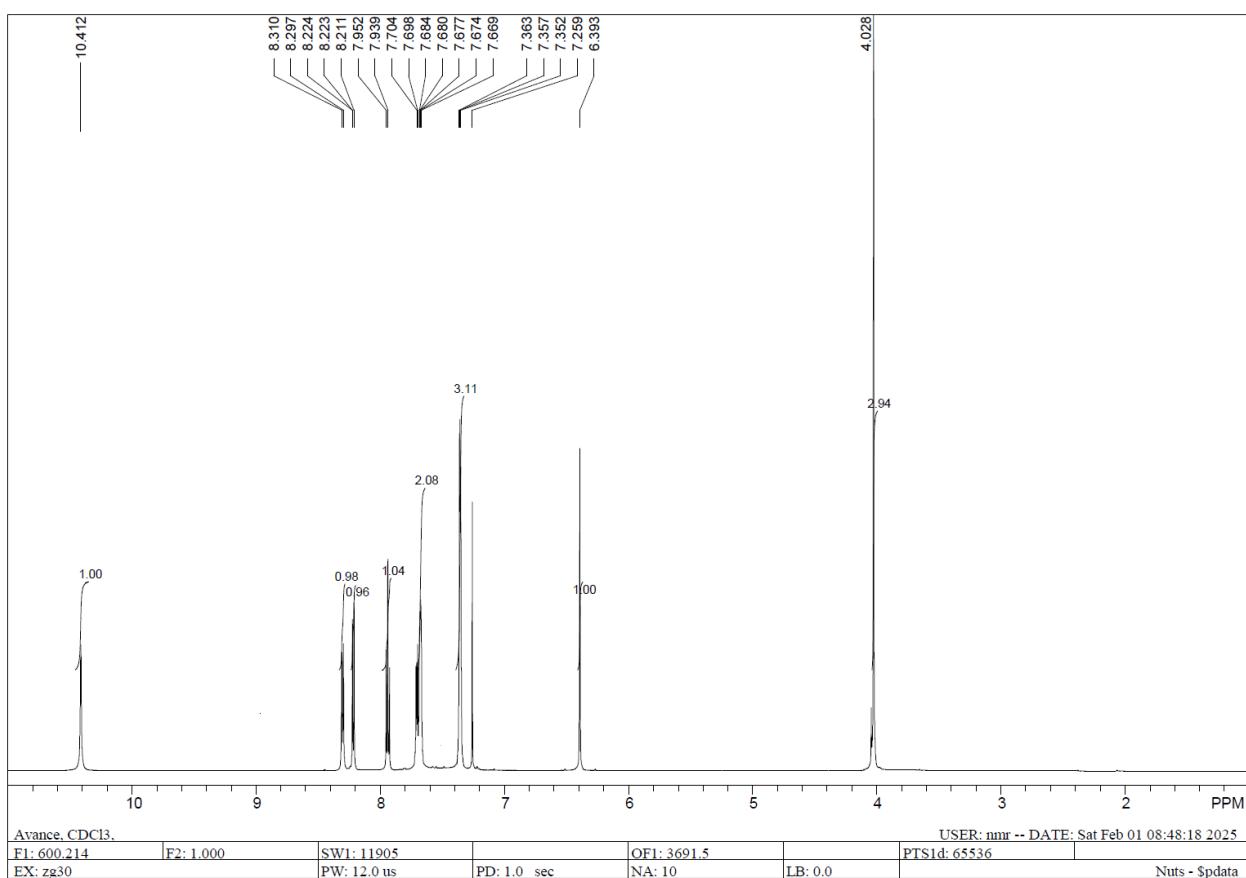


Figure S1 ¹H (600 MHz, CDCl₃, 295 K) NMR spectrum of **2**.

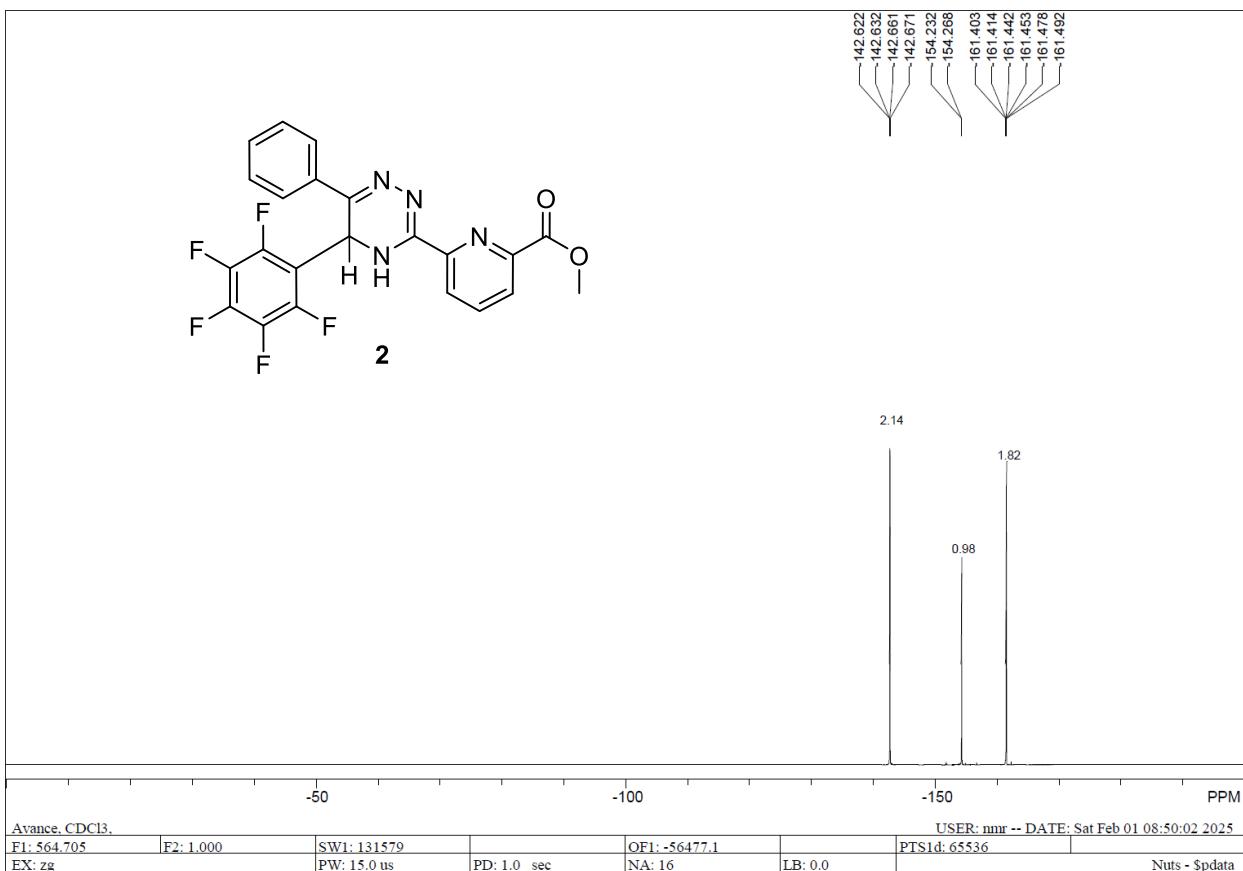


Figure S2 ¹⁹F (565 MHz, CDCl₃, 295 K) NMR spectrum of 2.

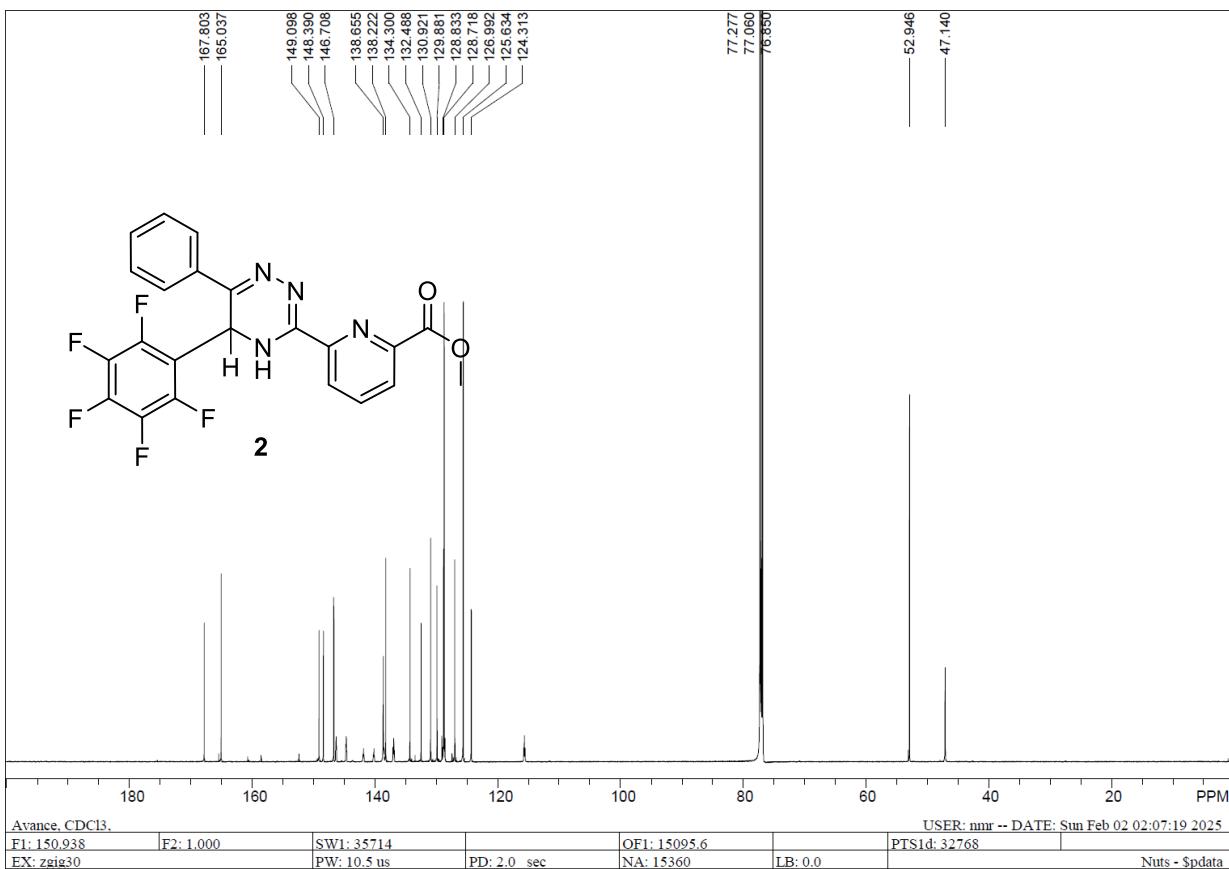


Figure S3 ¹³C (151 MHz, CDCl₃, 295 K) NMR spectrum of 2.

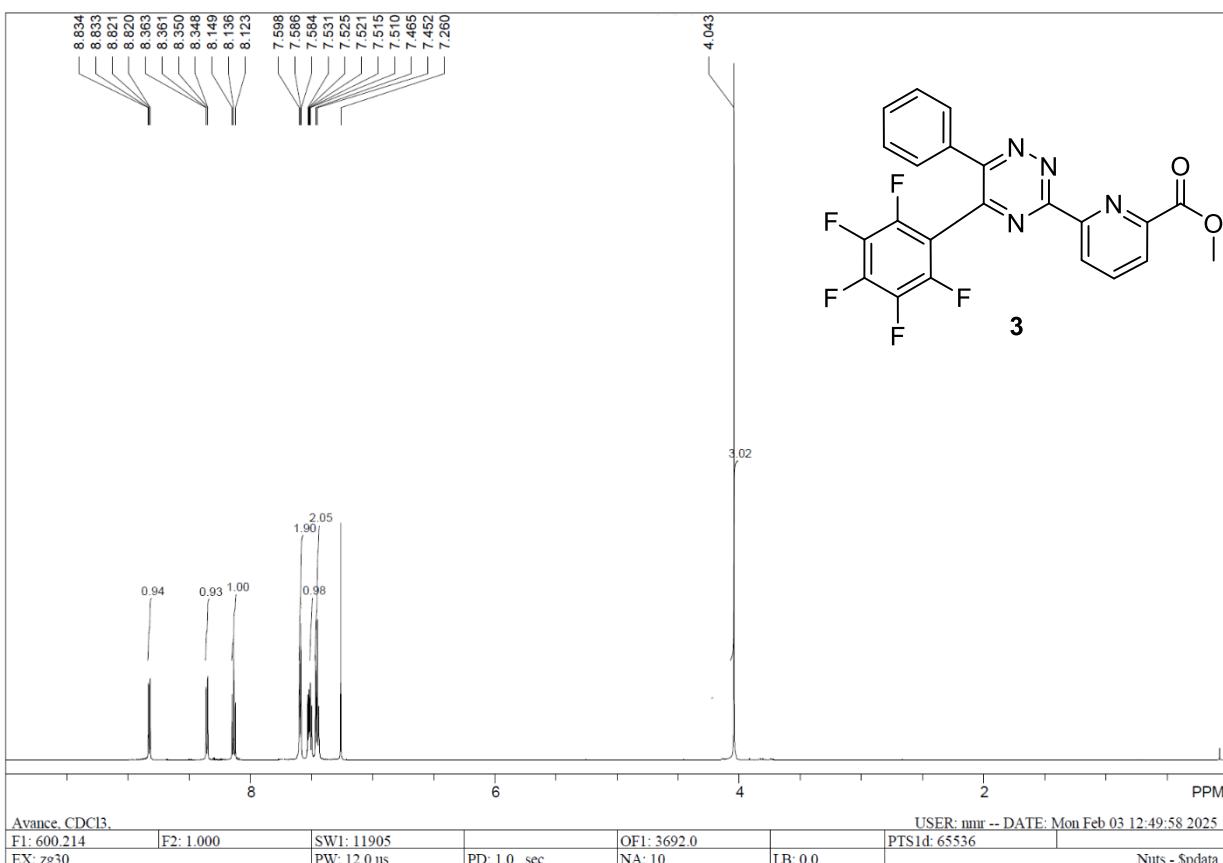


Figure S4 ¹H (600 MHz, CDCl₃, 295 K) NMR spectrum of 3.

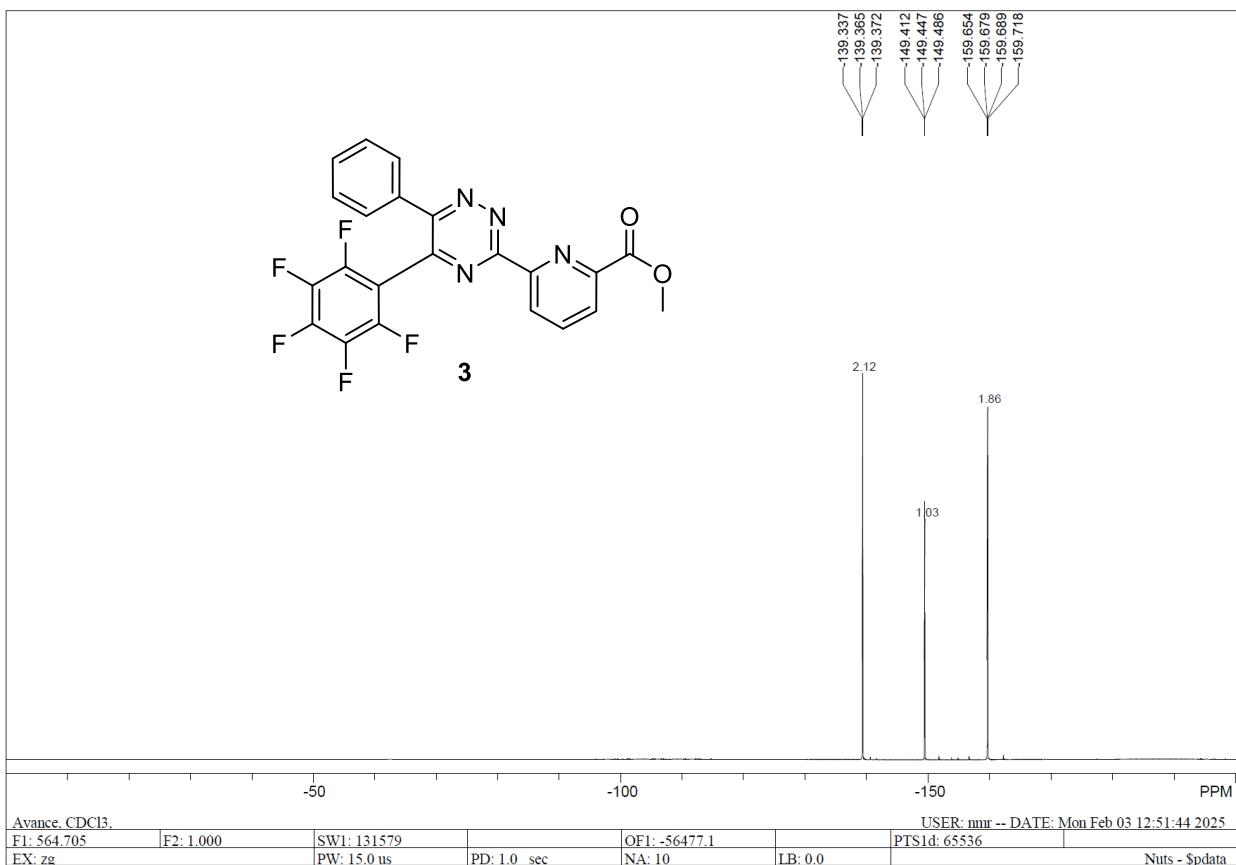


Figure S5 ¹⁹F (565 MHz, CDCl₃, 295 K) NMR spectrum of 3.

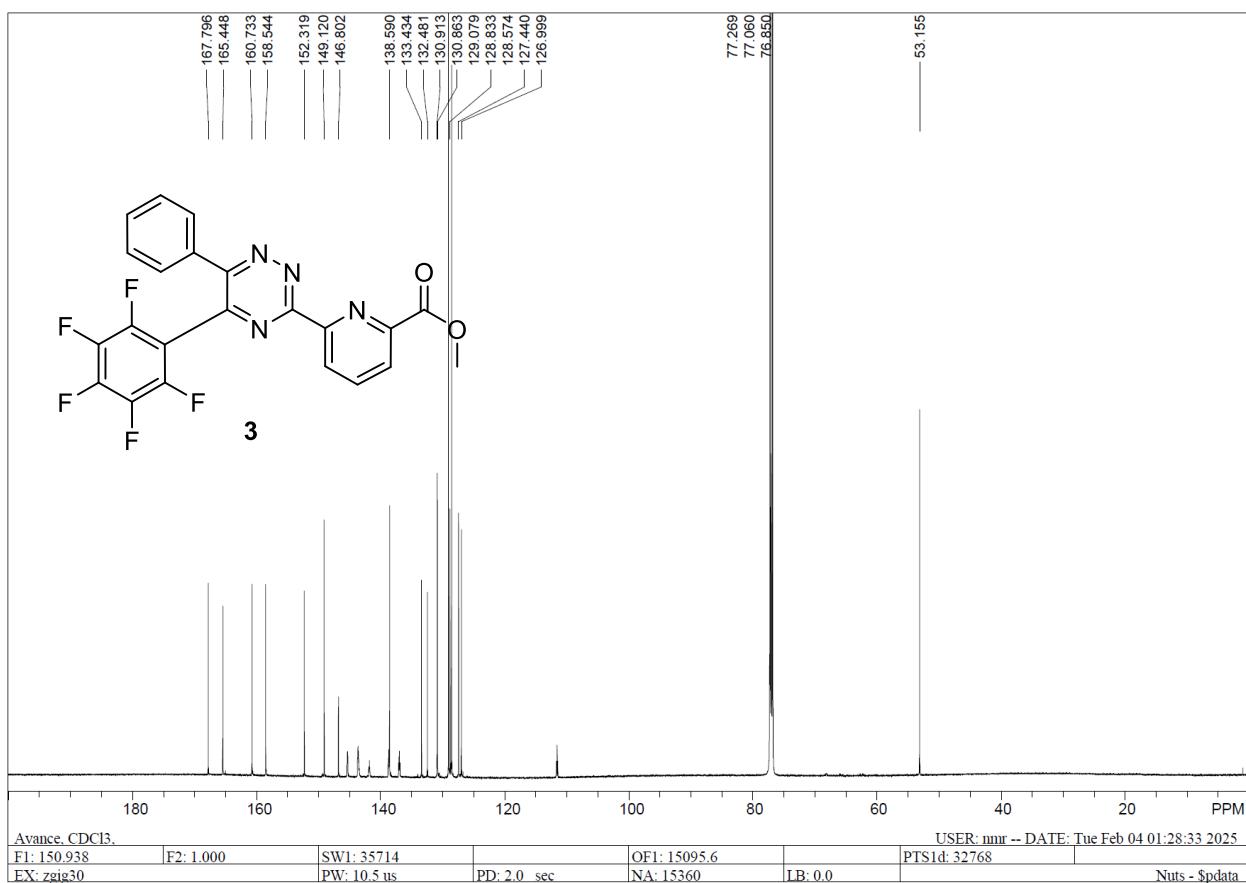


Figure S6 ¹³C (151 MHz, CDCl₃, 295 K) NMR spectrum of 3.

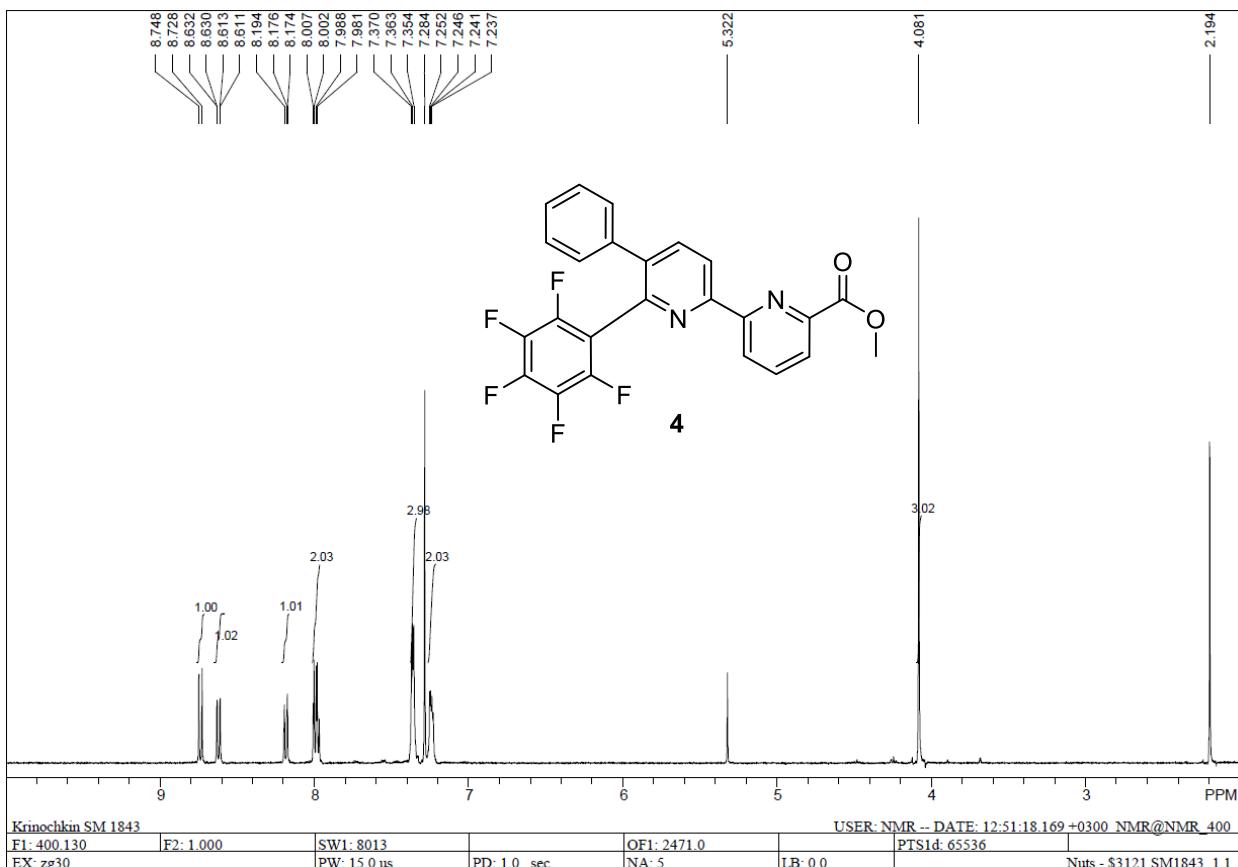


Figure S7 ^1H (400 MHz, CDCl_3 , 295 K) NMR spectrum of 4.

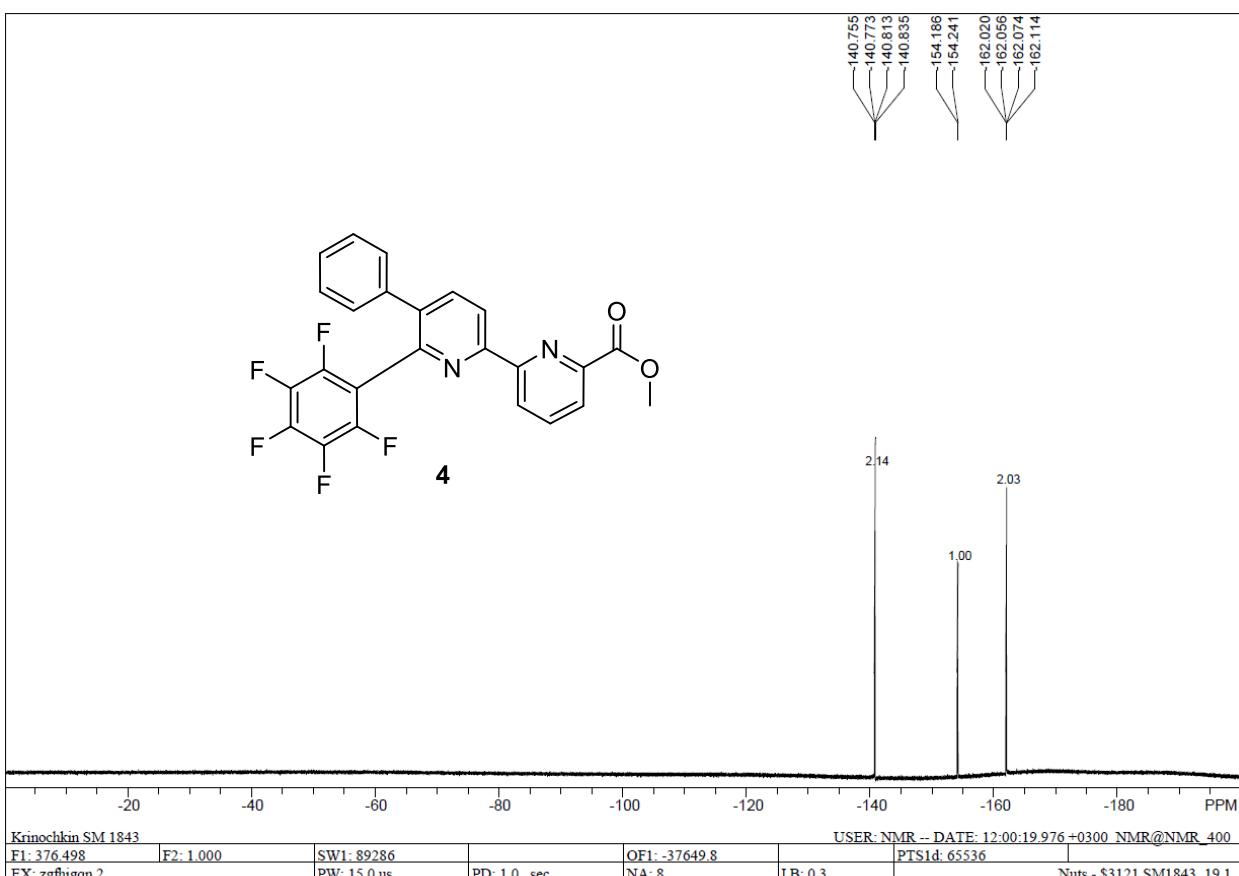


Figure S8 ^{19}F (376 MHz, CDCl_3 , 295 K) NMR spectrum of 4.

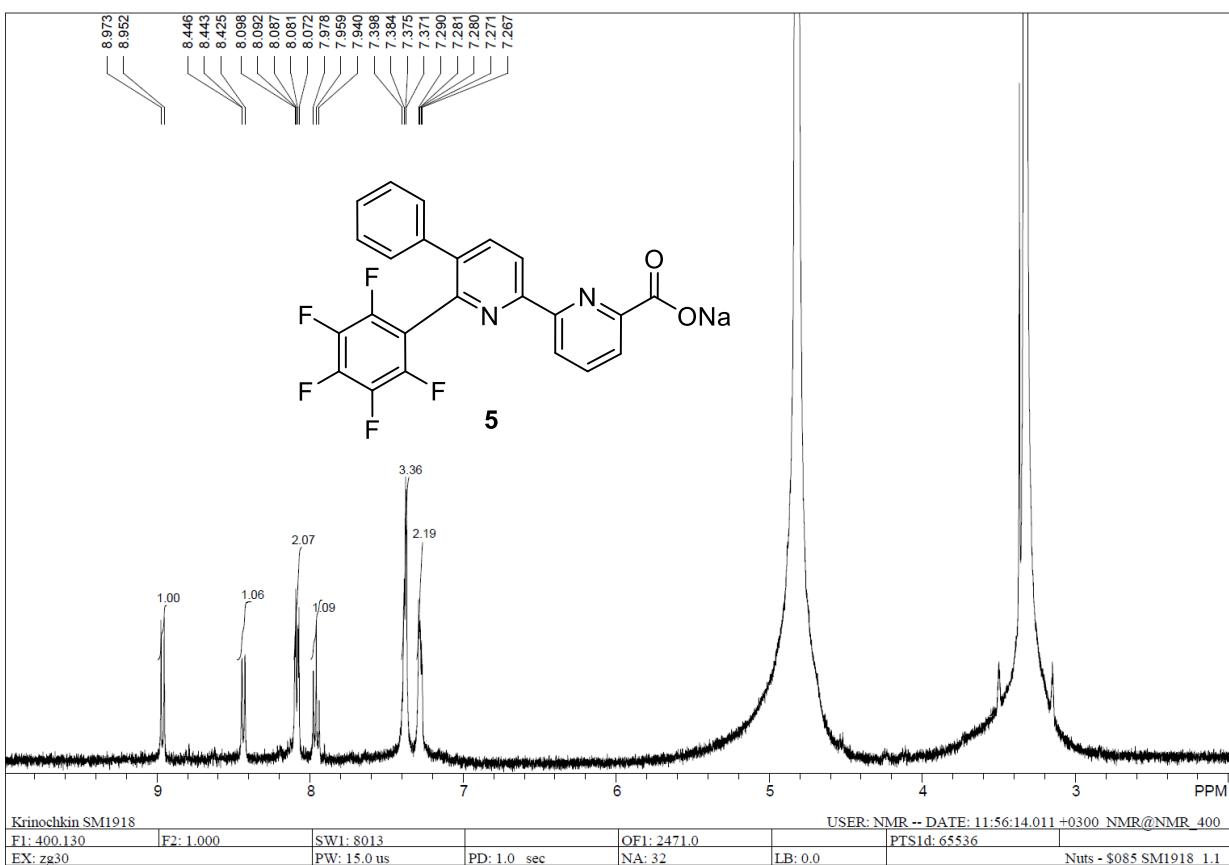


Figure S9 ^1H (400 MHz, CD_3OD , 295 K) NMR spectrum of **5**.

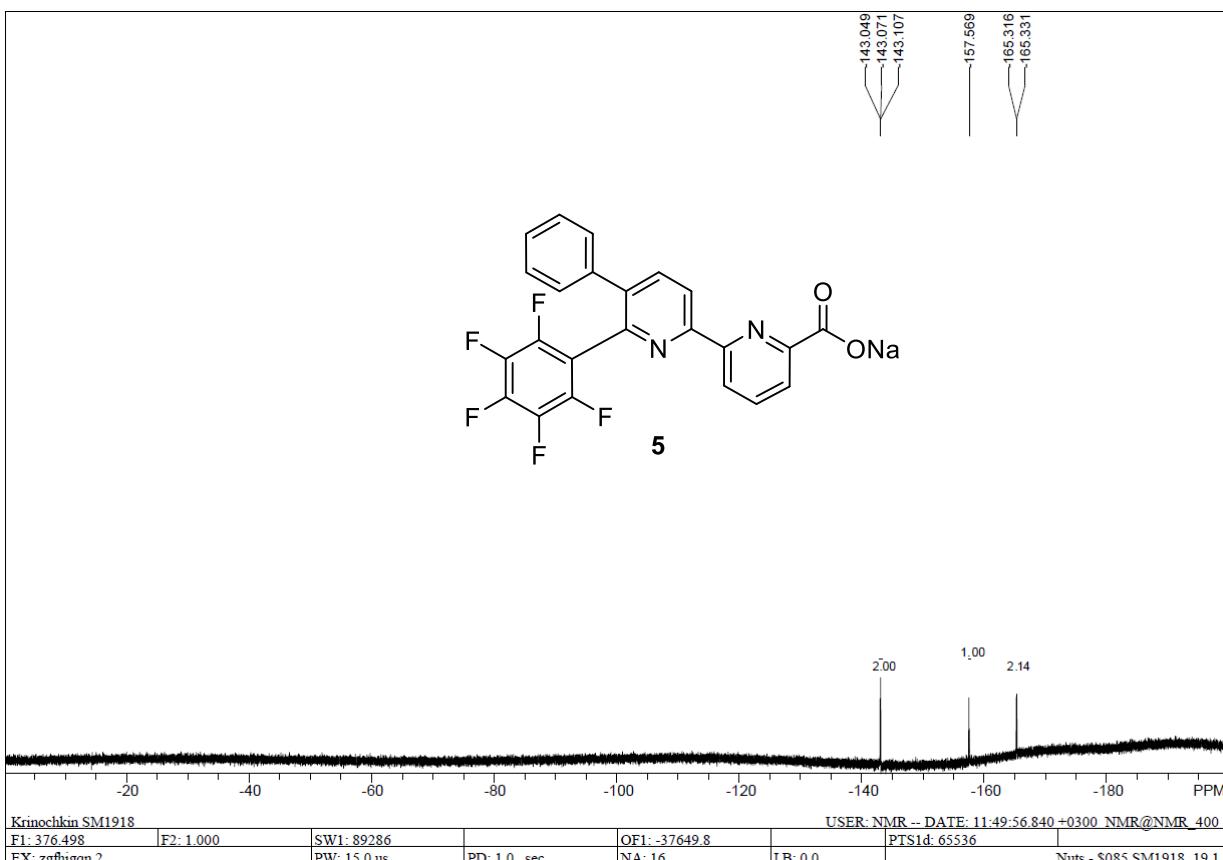


Figure S10 ¹⁹F (376 MHz, CD₃OD, 295 K) NMR spectrum of **5**.

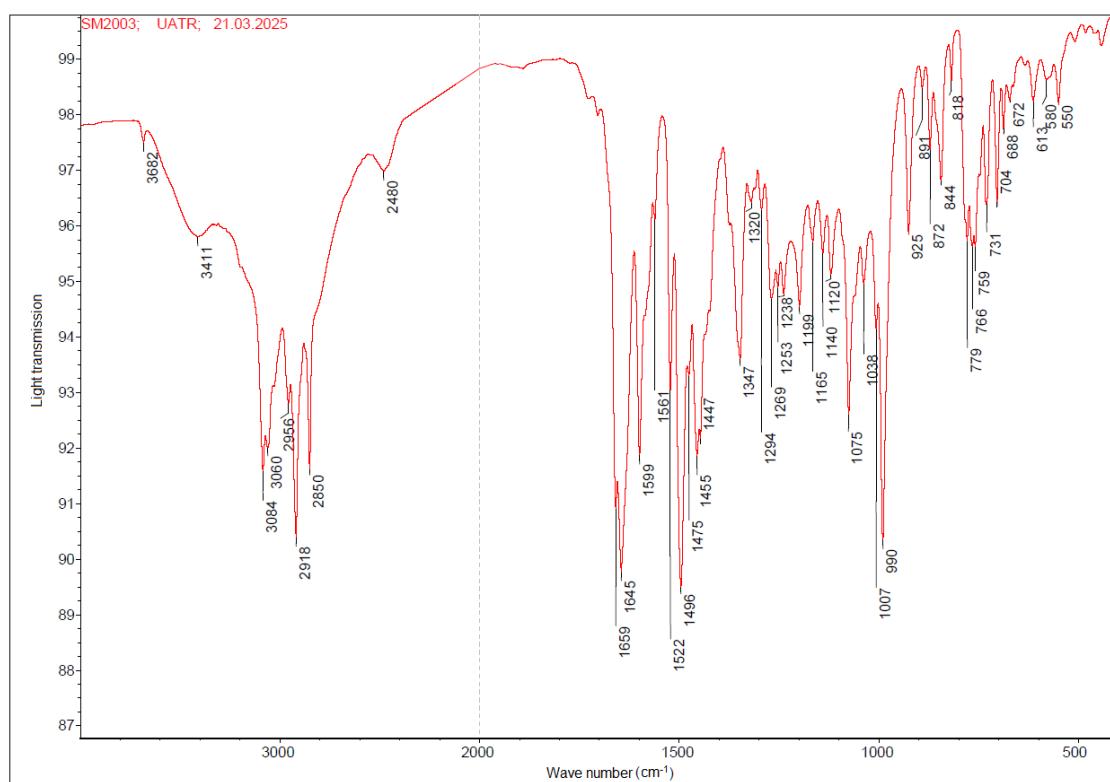


Figure S11 IR spectrum of complex Cu•5 at room temperature.

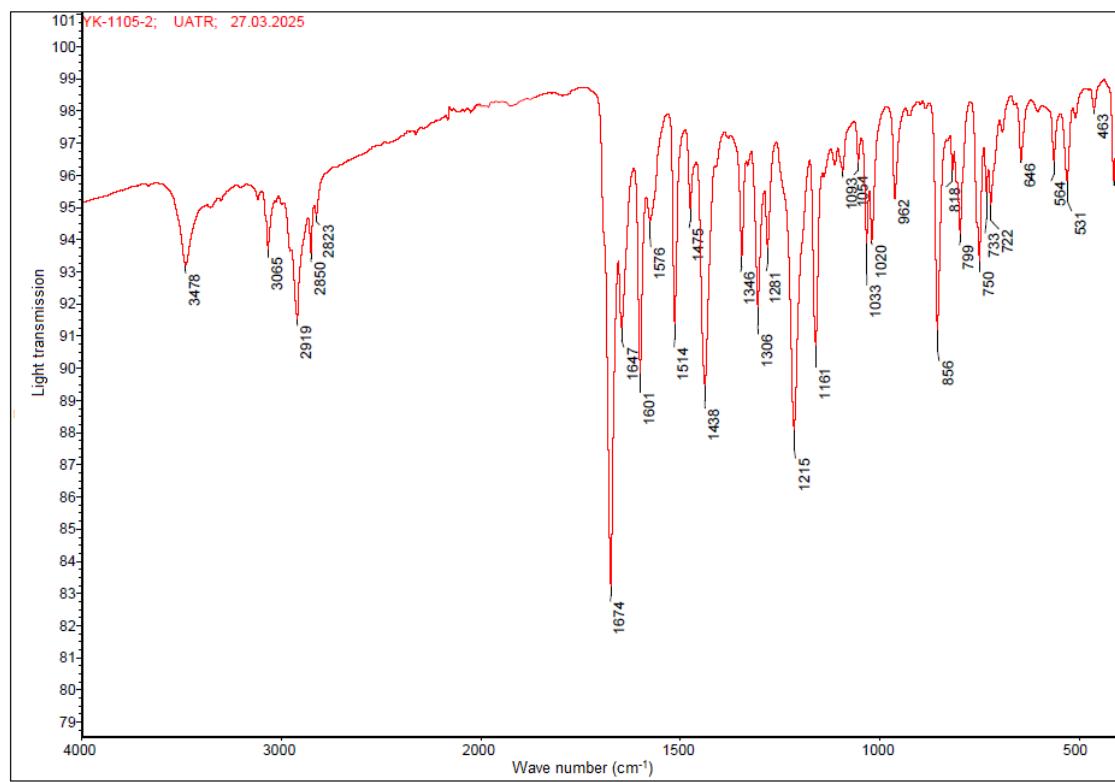


Figure S12 IR spectrum of complex Cu•6 at room temperature.

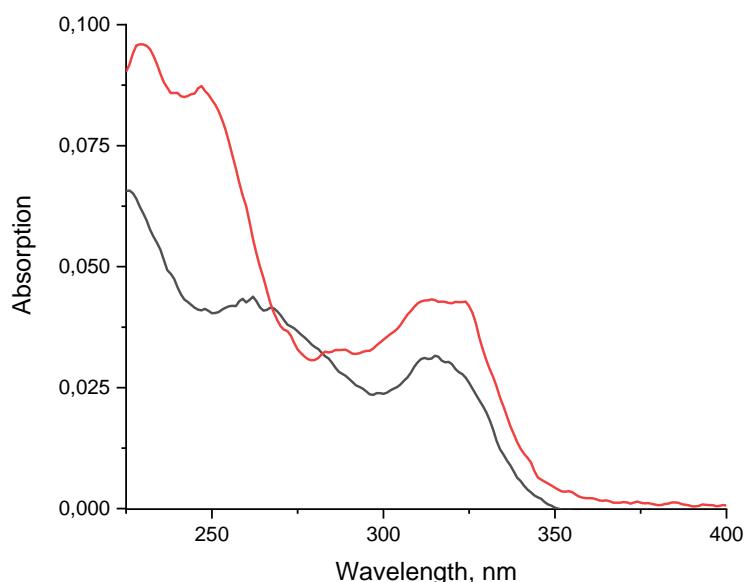


Figure S13 Absorption spectra of complexes Cu•5 (black line) and Cu•6 (red line) in acetonitrile at room temperature.

Table S1 Absorption maxima of complexes.

	Absorption maxima, nm
Cu•5:	262, 315
Cu•6:	247, 314

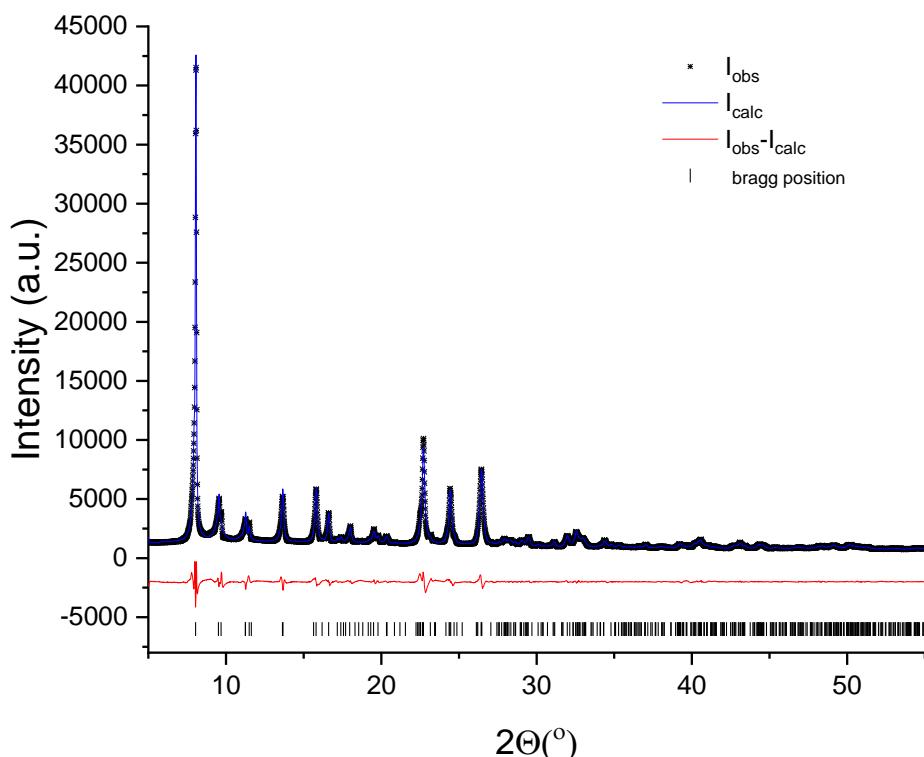


Figure S14 Powder X-ray data for complex **Cu•6**.


Table S2 Crystal data and structure refinement for **Cu•5**, **Cu•6** and **Cu•6A**.

Parameters	Compound Cu•5	Compound Cu•6	Compound Cu•6A
Empirical formula	C ₄₆ H ₂₀ CuF ₁₀ N ₄ O ₄	C ₄₂ H ₃₆ Cl ₂ Cu ₂ F ₂ N ₄ O ₆	C ₄₀ H ₃₀ Cl ₂ Cu ₂ F ₂ N ₄ O ₅
Formula weight	946.20	928.73	882.66
Temperature/K	295(2)	293(2)	295(2)
Crystal system	triclinic	triclinic	orthorhombic
Space group	P-1	P-1	Iba2
a/Å	11.7831(3)	9.8605(3)	8.7606(5)
b/Å	13.0797(2)	10.0445(3)	19.0270(12)
c/Å	15.2403(3)	11.4638(3)	21.3162(13)
α/°	113.603(2)	74.800(2)	90
β/°	98.476(2)	75.626(3)	90
γ/°	94.389(2)	68.759(3)	90
Volume/Å ³	2104.88(8)	1006.33(6)	3553.2(4)
Z	2	1	4
ρ _{calcd} /g/cm ³	1.493	1.532	1.650
μ/mm ⁻¹	0.612	1.252	1.412
F(000)	950.0	474.0	1792.0
Crystal size/mm ³	0.49 × 0.15 × 0.09	0.263 × 0.09 × 0.04	0.47 × 0.23 × 0.09
Radiation	MoKα (λ = 0.71073)	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	5.488 to 59.086 -16 ≤ h ≤ 16; -17 ≤ k ≤ 17; -20 ≤ l ≤ 20	5.224 to 59.116 -13 ≤ h ≤ 13; -13 ≤ k ≤ 13; -15 ≤ l ≤ 15	7.648 to 54.206 -11 ≤ h ≤ 11; -24 ≤ k ≤ 24; -27 ≤ l ≤ 27
Reflections collected	69764	33993	11565
Independent reflections	10578 [R _{int} = 0.0668, R _{sigma} = 0.0536]	5048 [R _{int} = 0.0624, R _{sigma} = 0.0434]	3757 [R _{int} = 0.0486, R _{sigma} = 0.0521]
Data/restraints/parameters	10578/0/586	5048/0/264	3757/19/261
Goodness-of-fit on F ²	1.014	1.035	0.984
Final R indexes [I>=2σ (I)]	R ₁ = 0.0515; wR ₂ = 0.1308	R ₁ = 0.0441; wR ₂ = 0.1115	R ₁ = 0.0437; wR ₂ = 0.1143
Final R indexes [all data]	R ₁ = 0.0949, wR ₂ = 0.1530	R ₁ = 0.0656; wR ₂ = 0.1228	R ₁ = 0.0625, wR ₂ = 0.1368
Largest diff. peak/hole / e Å ⁻³	0.72/-0.28	0.52/-0.42	0.61/-0.43