

Supplementary information

Novel bis- and tris-cyclometalated iridium(III) complexes bearing a benzoyl group on each fluorinated 2-phenylpyridinate ligand aimed at development of blue phosphorescent materials for OLED

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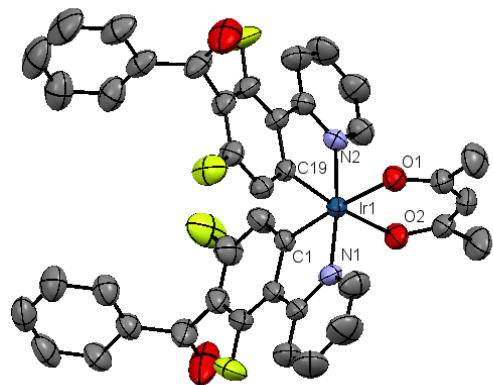
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- **Fig. S9** ¹H NMR spectra of **Ir-1c**, **Ir-2a–c**, and **Ir-3a–c**.

(a) **Ir-3a**



(b) **Ir-3c**

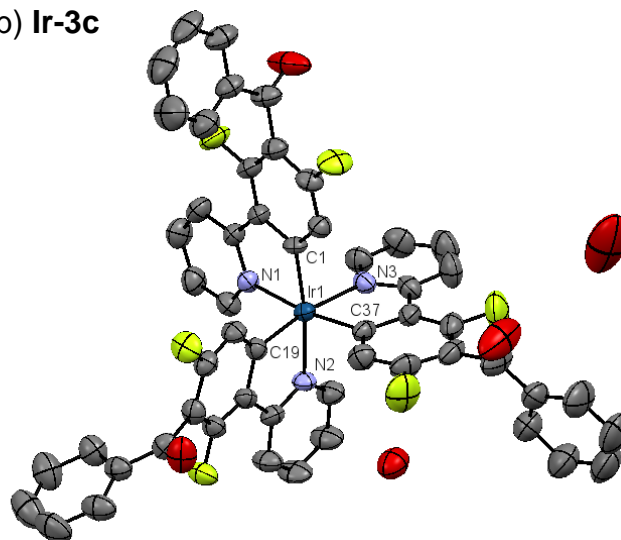


Fig. S1 ORTEP drawings of (a) **Ir-3a** and (b) **Ir-3c**·2H₂O with ellipsoids at the 50% probability level. Atom labels are added to the selected atoms around the metal center.

Table S1 Crystal data and structure refinement for **Ir-3a** and **Ir-3c**.

Parameter	Ir-3a	Ir-3c
Formula	C ₄₁ H ₂₇ F ₄ IrN ₂ O ₄	C ₅₄ H ₃₀ F ₆ IrN ₃ O ₃ ·2H ₂ O
Formula weight	879.89	1111.09
Crystal system	Monoclinic	Monoclinic
Space group	<i>C2/c</i> (#15)	<i>P2₁/a</i> (#14)
Lattice Parameters <i>a</i> /Å	41.393(9)	19.190 (3)
<i>b</i> /Å	8.1687(14) Å	10.3544 (16)
<i>c</i> /Å	23.774(5) Å	23.935 (4)
β /°	120.926(2)	101.5280 (19)
Volume / Å ³	6896(3)	4660.1 (13)
<i>Z</i>	8	4
Density ρ_{calc} /g cm ⁻³	1.695	1.584
μ /cm ⁻¹	39.508	29.496
<i>F</i> (000)	3456.00	2200.00
<i>T</i> /K	293	293
No. of reflections measured	28759	36255
No. of reflections used (<i>R</i> _{int})	9259 (0.0265)	12611 (0.040)
<i>R</i> ₁ , <i>wR</i> ₂	0.0390 (0.0459)	0.0509 (0.0567)
Goodness of fit on <i>F</i> ²	1.067	1.088
ρ_{fin} (max/min) /e Å ³	1.92 /-1.85	2.94 /-1.98

Table S2 Selected bond distance and angles for **Ir-3a**.

		Ir-3a
Distance /Å	Ir-O1	2.131(4)
	Ir-O2	2.133(3)
	Ir-C1	1.991(6)
	Ir-N1	2.043(5)
	Ir-C19	1.995(4)
	Ir-N2	2.036(5)
Angle /°	O1–Ir–O2	88.39(14)
	N1–Ir–C1	80.90(19)
	N2–Ir–C19	81.28(17)

Table S3 Selected bond distance and angles for **Ir-3c**.

		Ir-3c
Distance /Å	Ir-C1	2.017 (5)
	Ir-N1	2.129 (4)
	Ir-C19	2.016 (5)
	Ir-N2	2.119 (4)
	Ir-C37	2.031 (5)
	Ir-N3	2.129 (4)
Angle /°	N1–Ir–C1	79.56 (18)
	N2–Ir–C19	79.4 (2)
	N3–Ir–C37	78.2 (2)

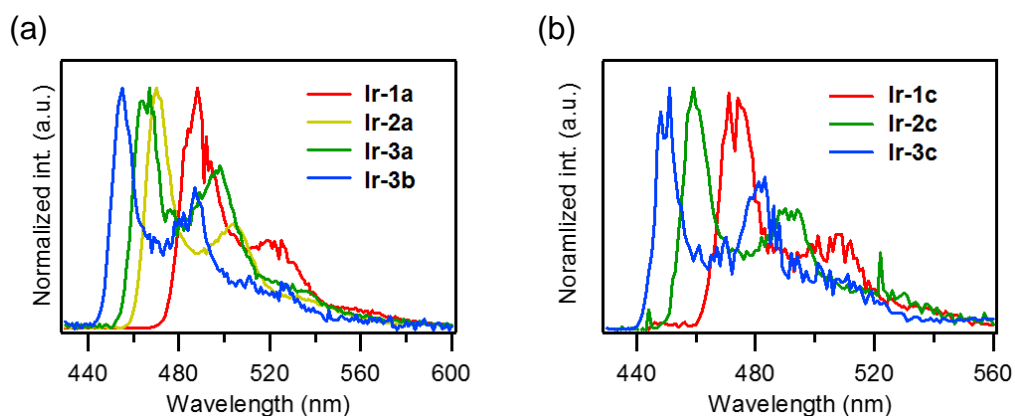


Fig. S2 Phosphorescence spectra of (a) bis-cyclometalated and (b) tris-cyclometalated complexes in 2-MeTHF glass matrix at 77 K.

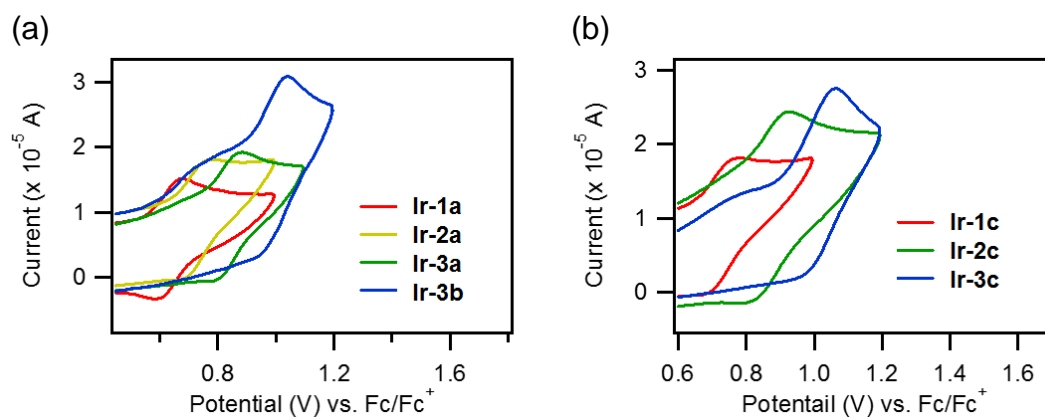


Fig. S3 Cyclic voltammograms of (a) bis-cyclometalated and (b) tris-cyclometalated complexes in anhydrous acetonitrile at a scan rate of 100 mV s⁻¹ at rt, where 0.1 M tetrabutylammonium perchlorate was used as a supporting electrolyte.

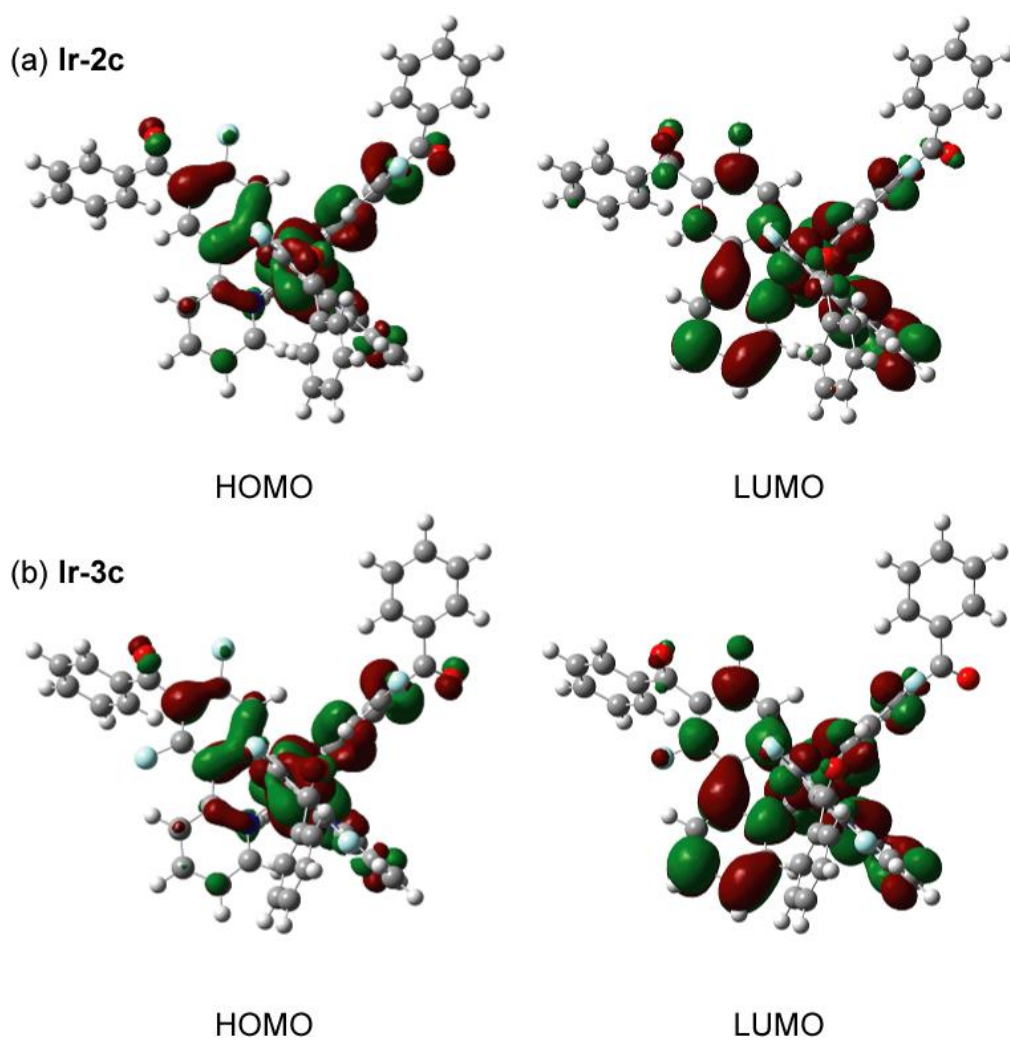


Fig. S4 Optimized geometry structures and electron configurations of HOMO and LUMO for (a) **Ir-2c** and (b) **Ir-3c**.

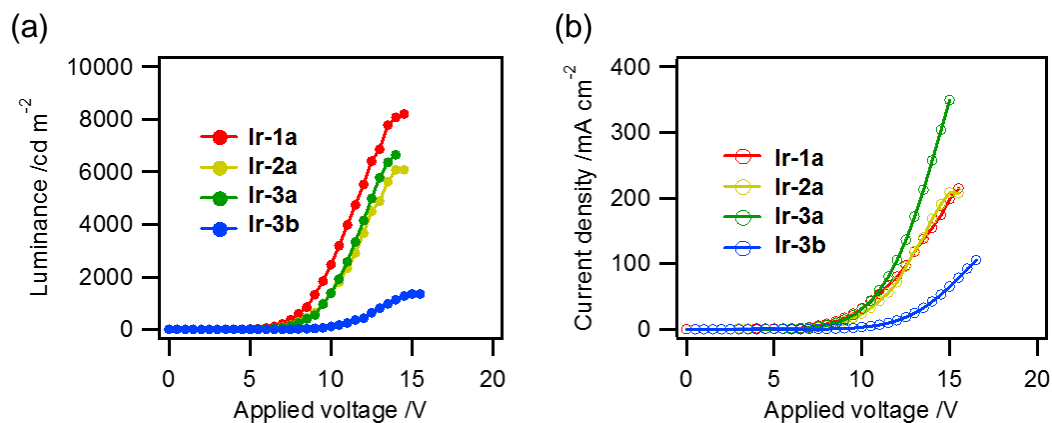


Fig. S5 (a) Voltage-luminance and (b) voltage-current density curves of the Device-1 employing bis-cyclometarated complexes.

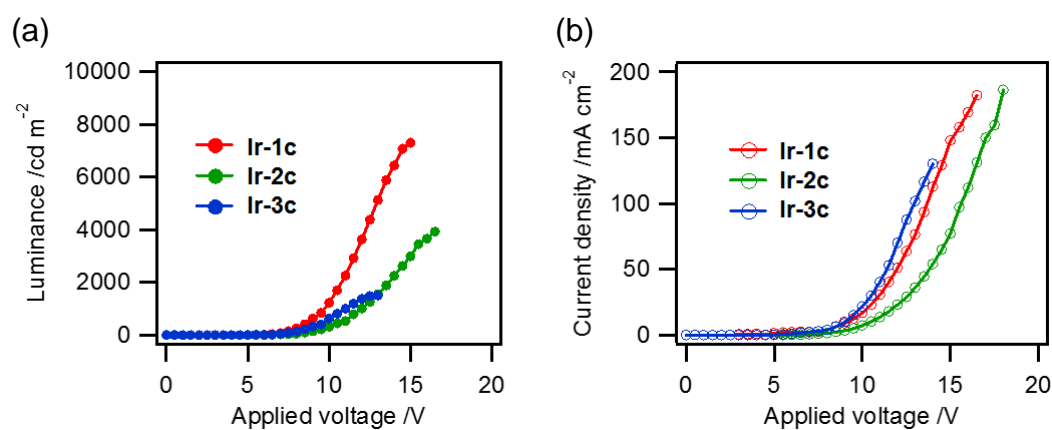


Fig. S6 (a) Voltage-luminance and (b) voltage-current density curves of the Device-1 employing tris-cyclometarated complexes.

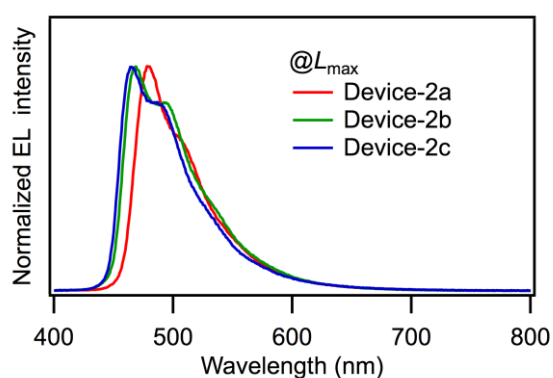


Fig. S7 EL spectra of **Device-2a–c**.

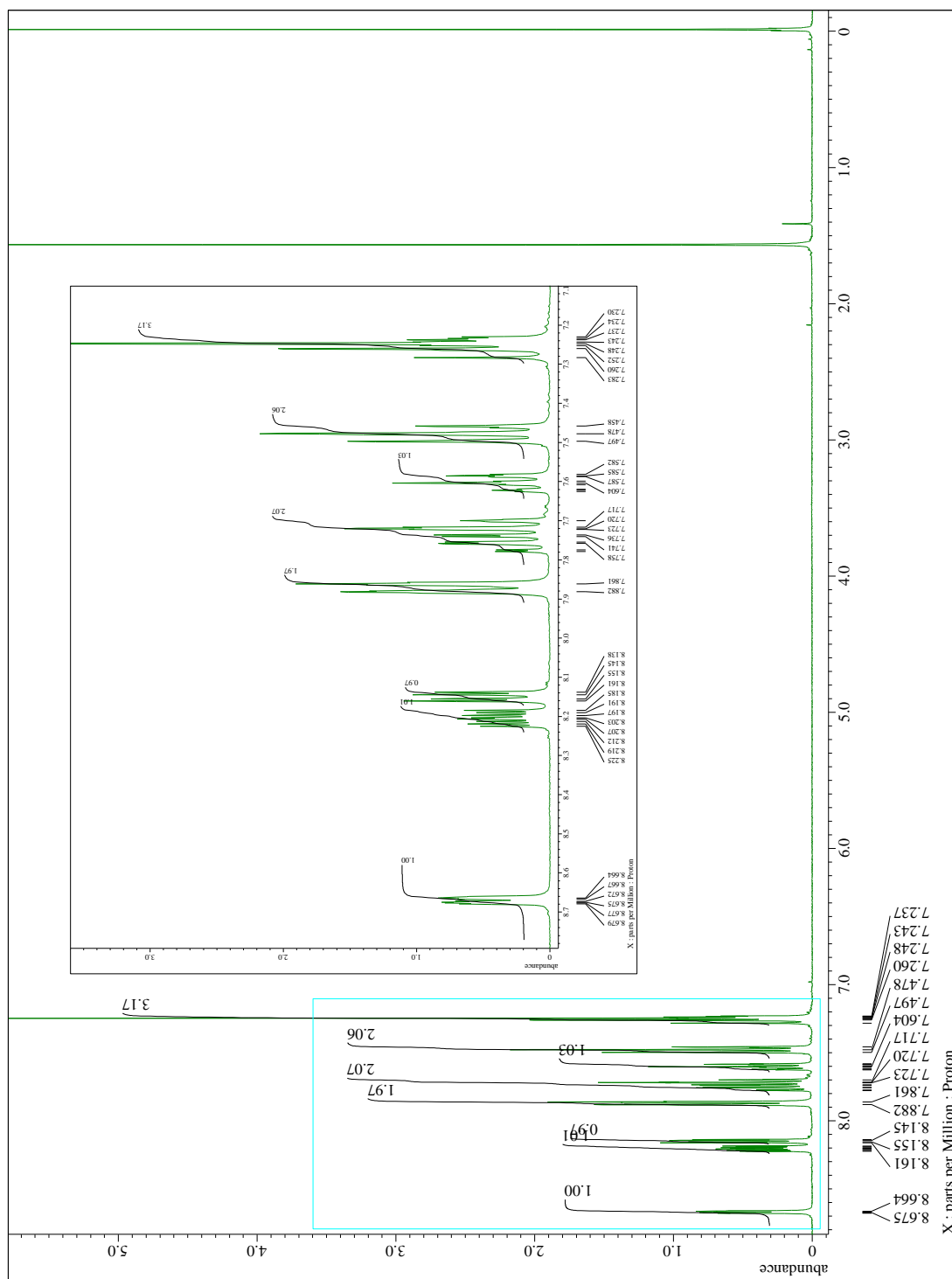


Fig. S8-1 ^1H NMR spectrum of $\text{HC}^{\text{N}}\text{-2}$ in CDCl_3 .

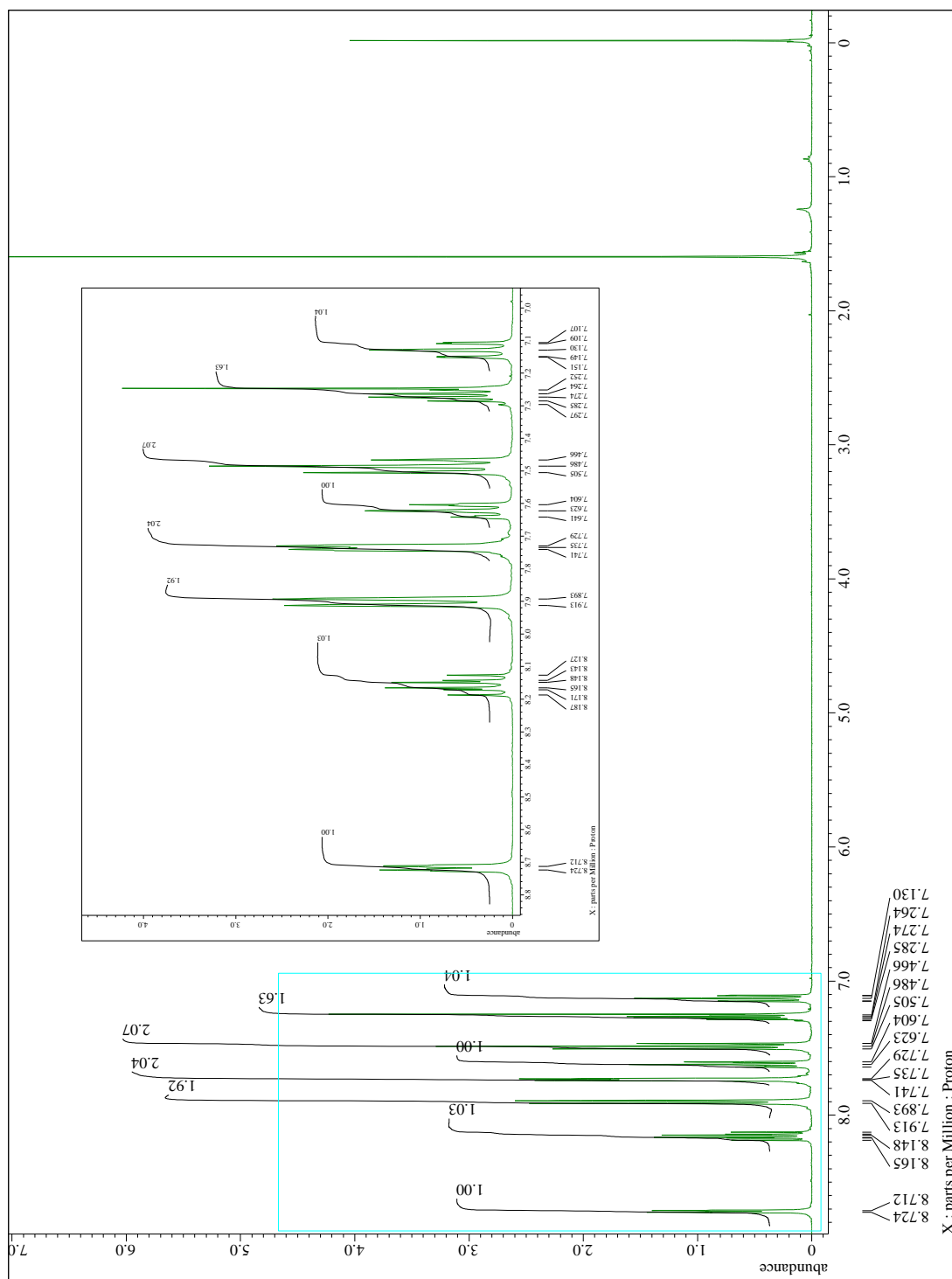


Fig. S8-2 ^1H NMR spectrum of $\text{HC}^{\text{N}}\text{-3}$ in CDCl_3 .

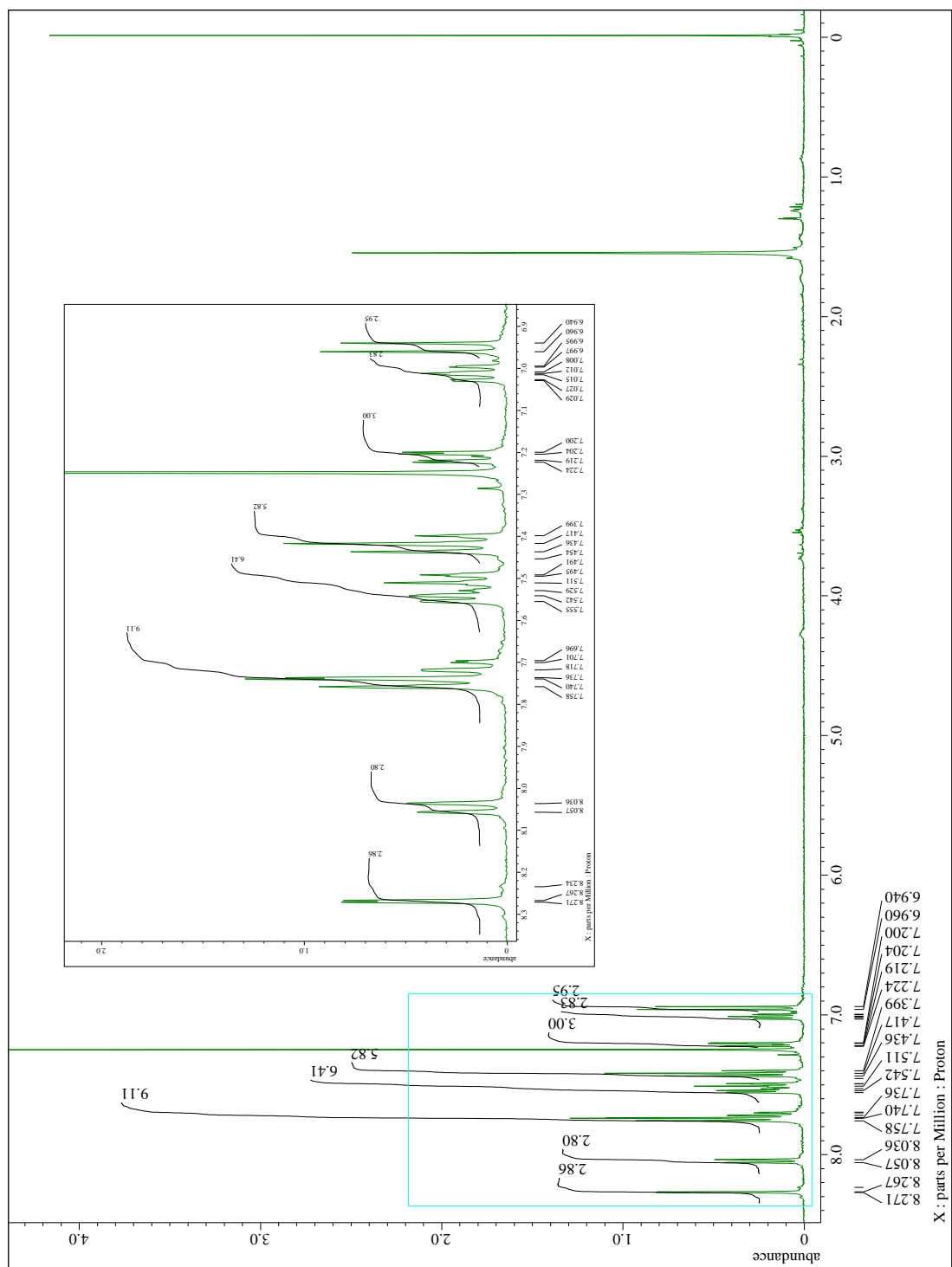


Fig. S9-1 ^1H NMR spectrum of **Ir-1c** in CDCl_3 .

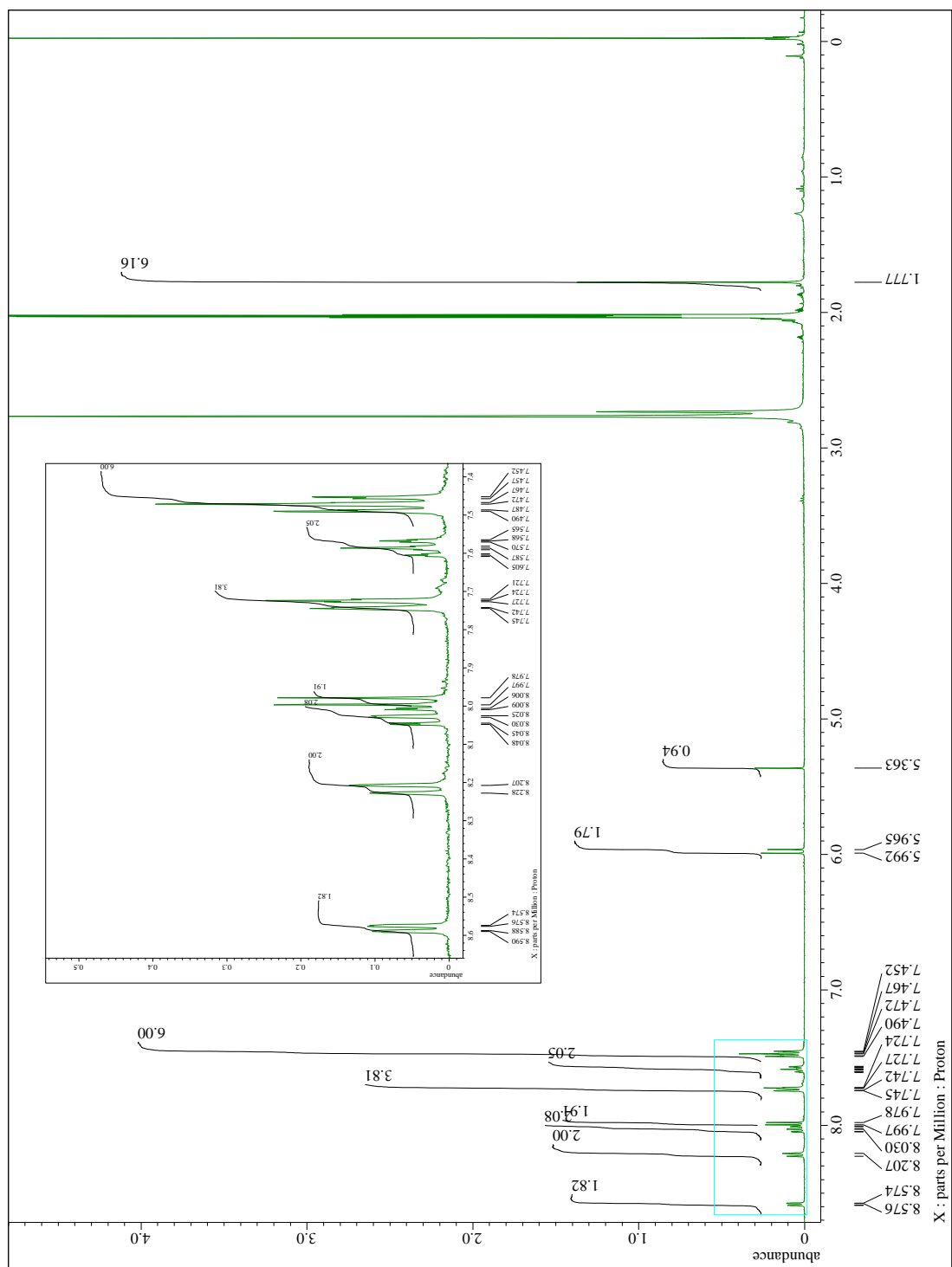


Fig. S9-2 ^1H NMR spectrum of **Ir-2a** in acetone-d_6 .

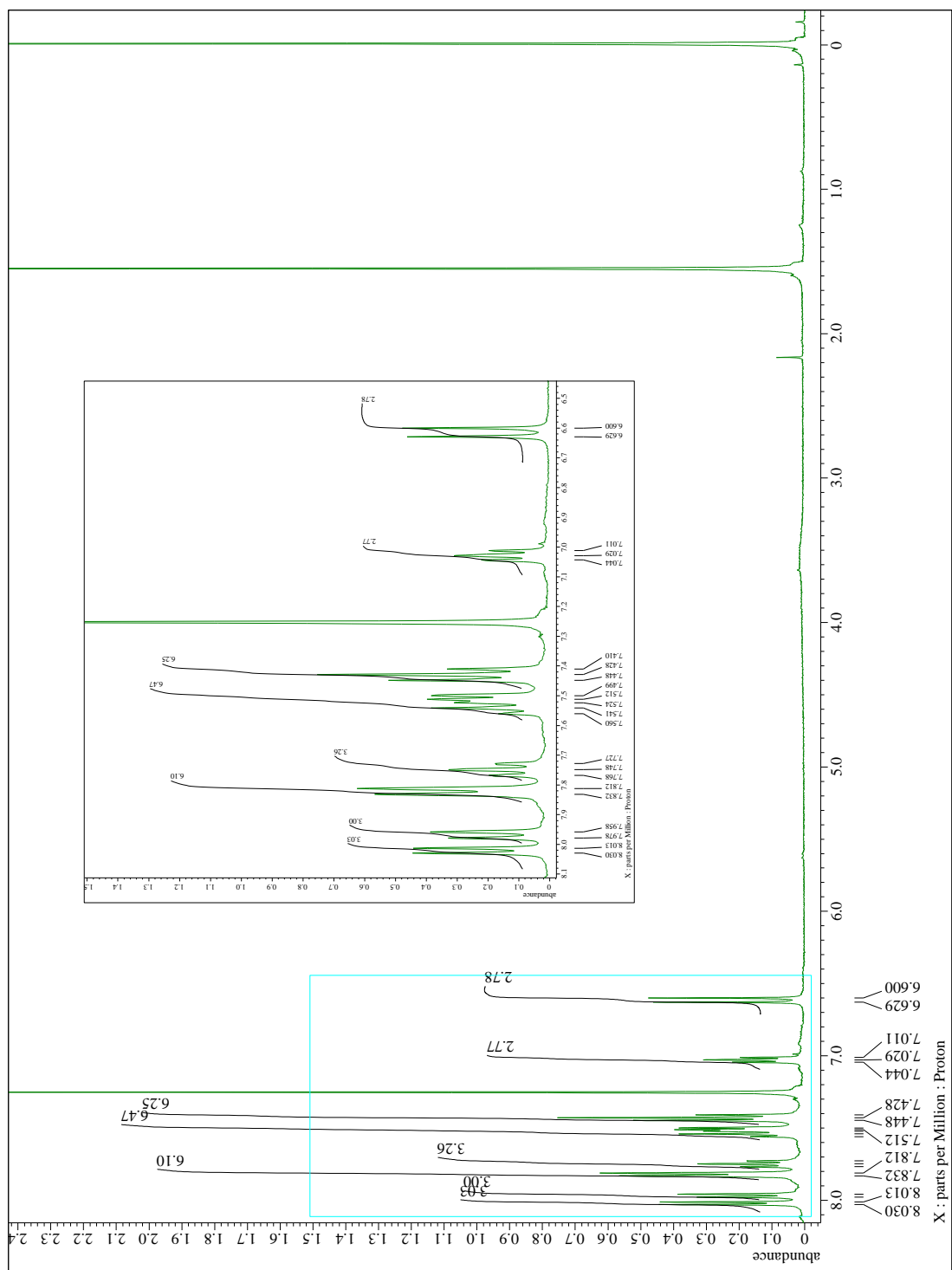


Fig. S9-3 ^1H NMR spectrum of **Ir-2c** in CDCl_3 .

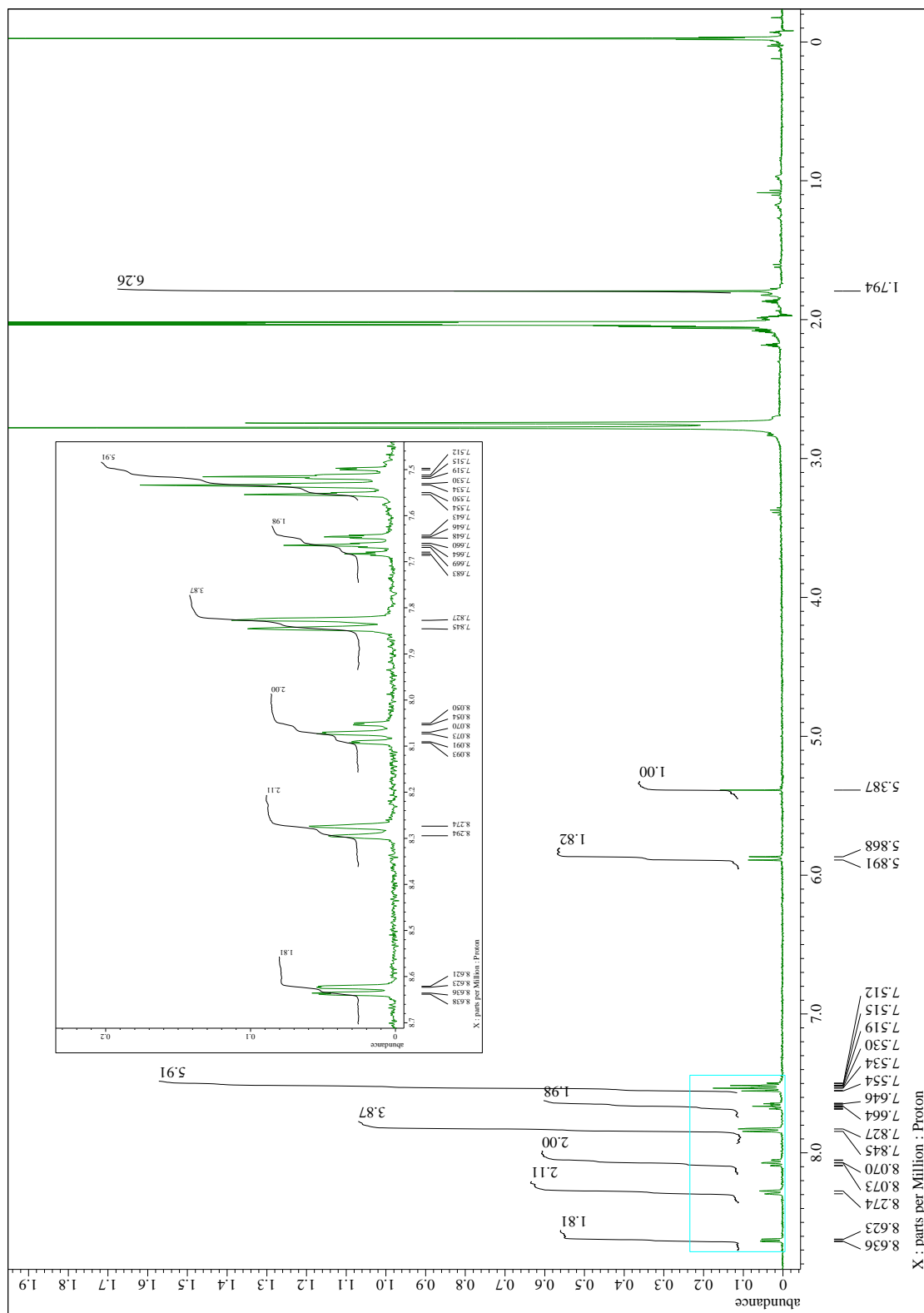


Fig. S9-4 ^1H NMR spectrum of **Ir-3a** in $\text{acetone-}d_6$.

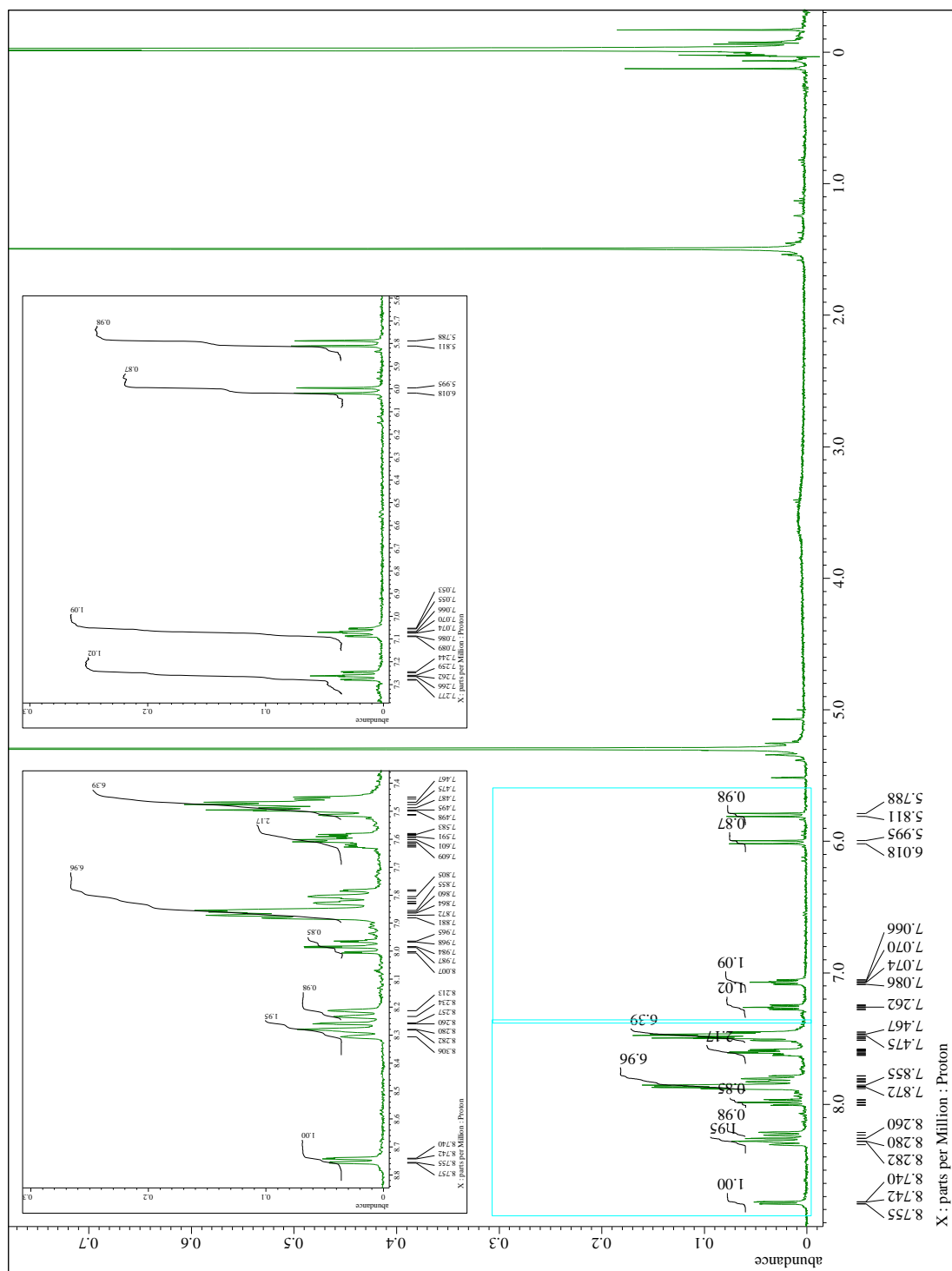


Fig. S9-5 ¹H NMR spectrum of Ir-3b in CD₂Cl₂.

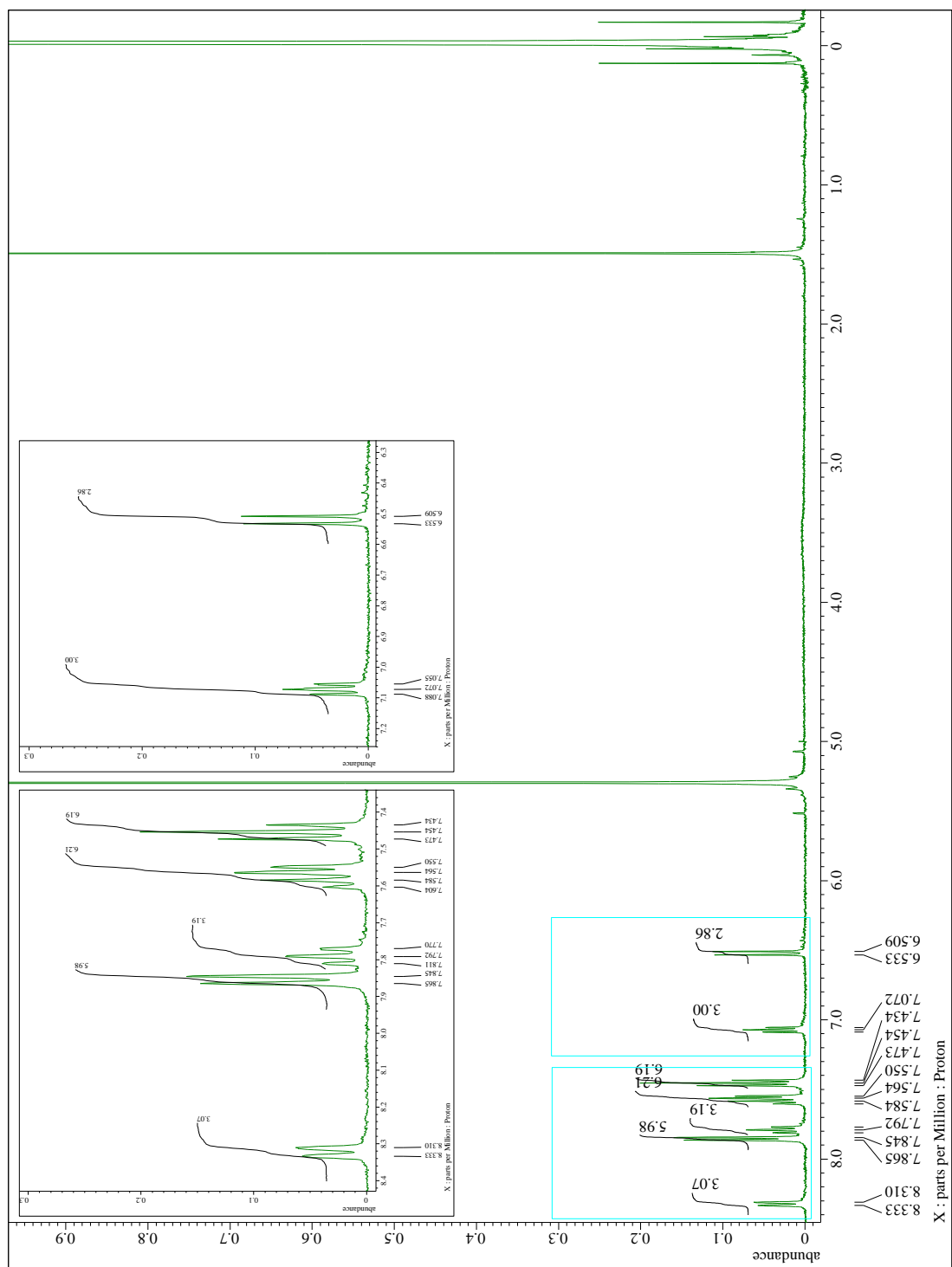


Fig. S9-6 ^1H NMR spectrum of **Ir-3c** in CD_2Cl_2 .