

Supplementary Materials

Di- μ -(1-(3-(1*H*-imidazol-1-yl)propyl)-2-methyl-4-oxo-1,4-dihydropyridin-3-olate)-bis[(η^5 -pentamethylcyclopentadienyl)iridium(III)] chloride

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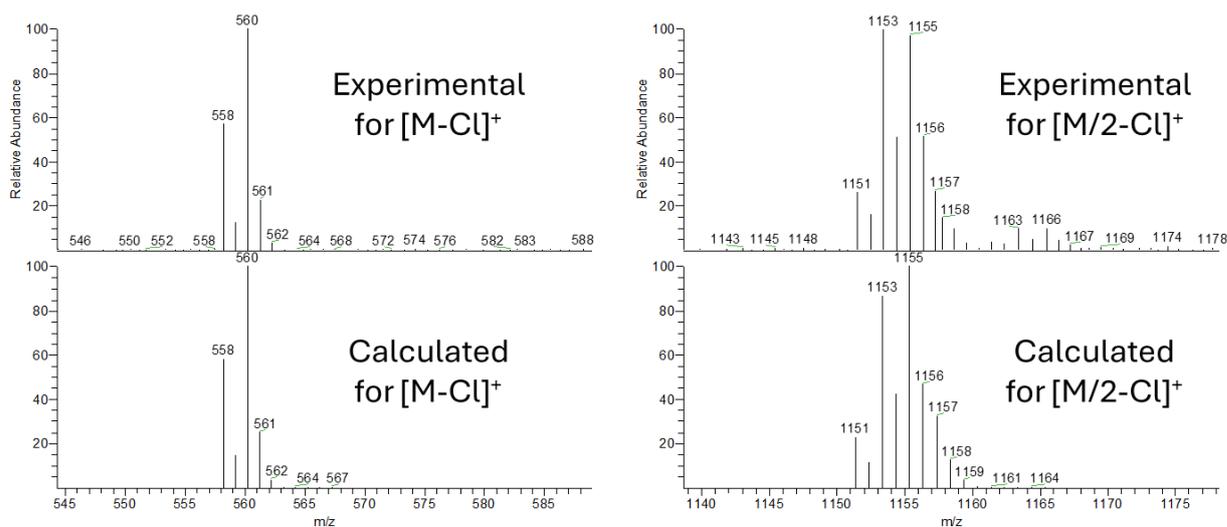


Figure S1. ESI mass-spectra of compound 2 in the mode of recording positively charged ions.

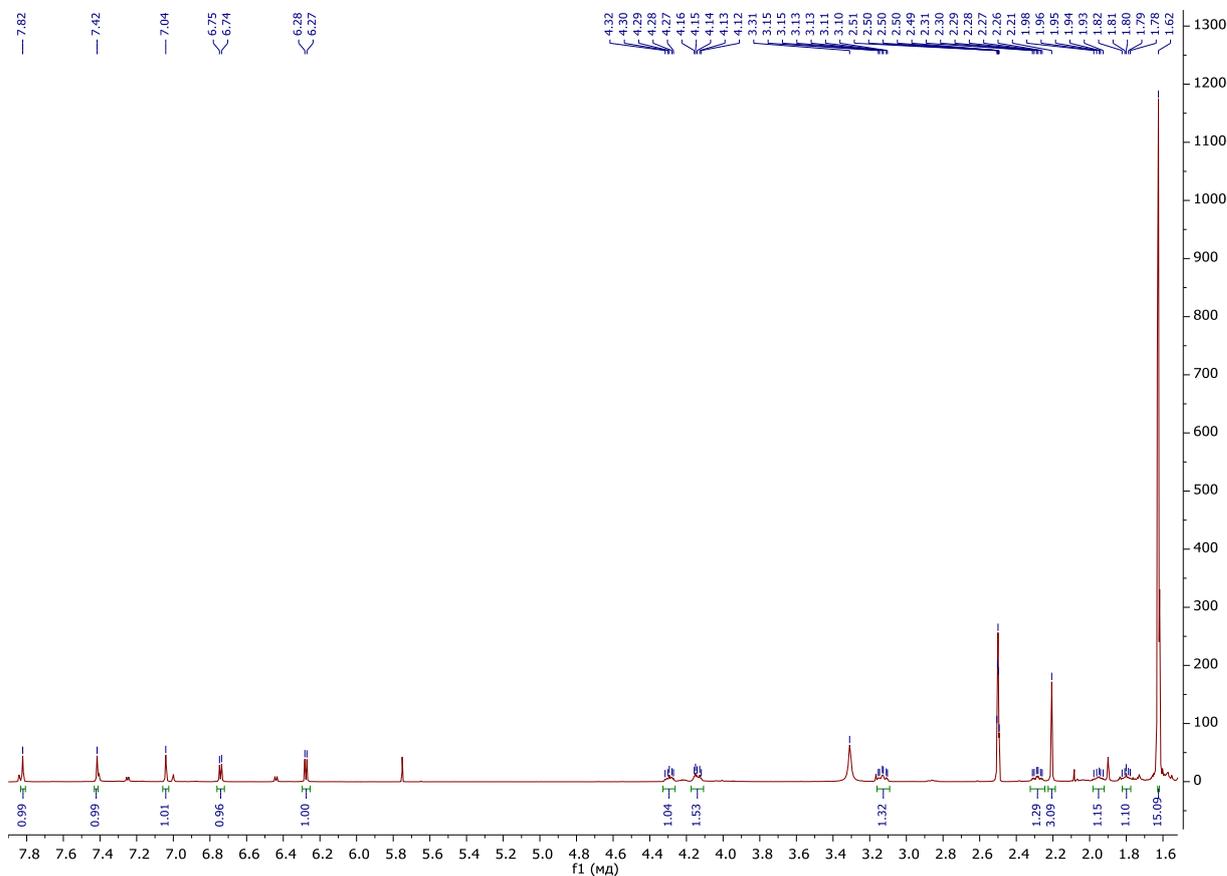


Figure S2. 1H NMR spectrum for metallacycle 2.

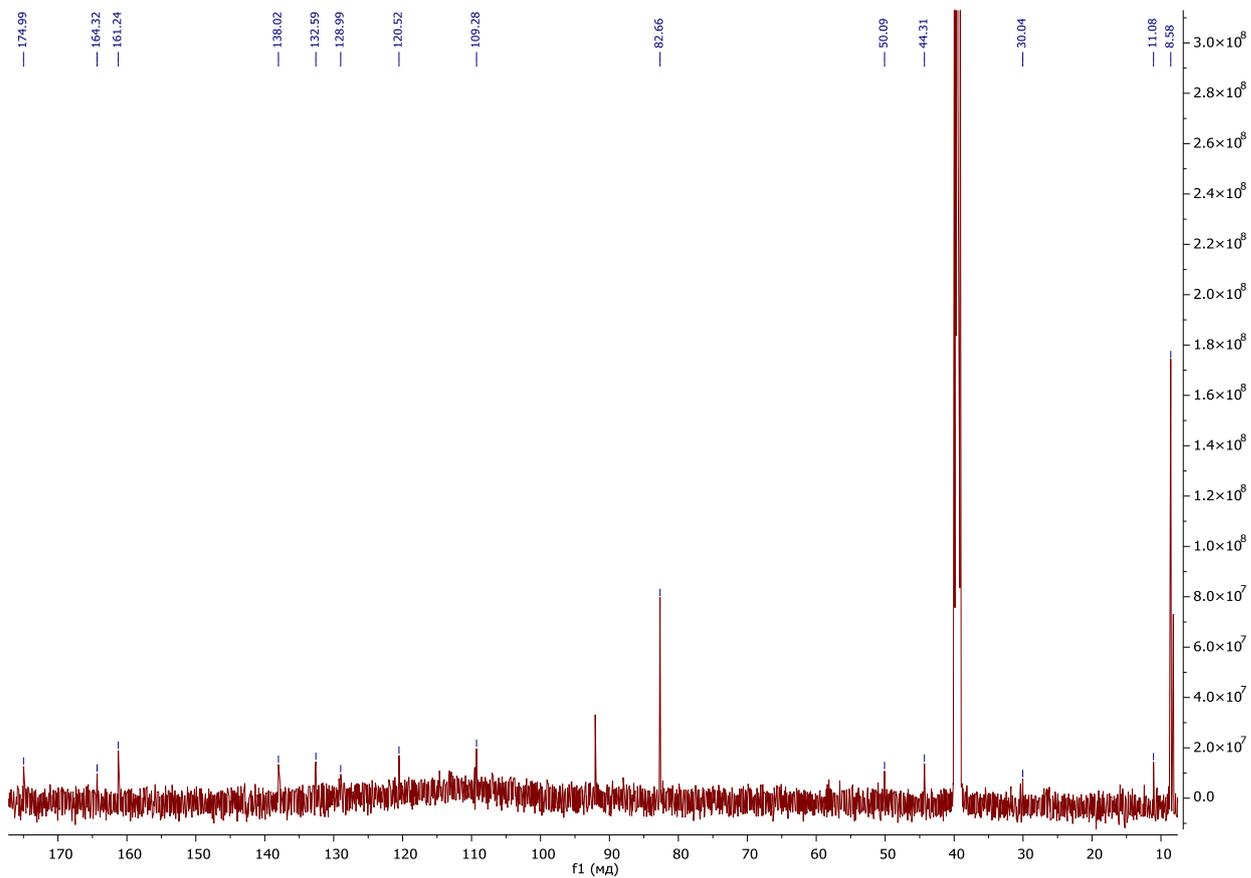


Figure S3. ^{13}C NMR spectrum for metallacycle **2**.

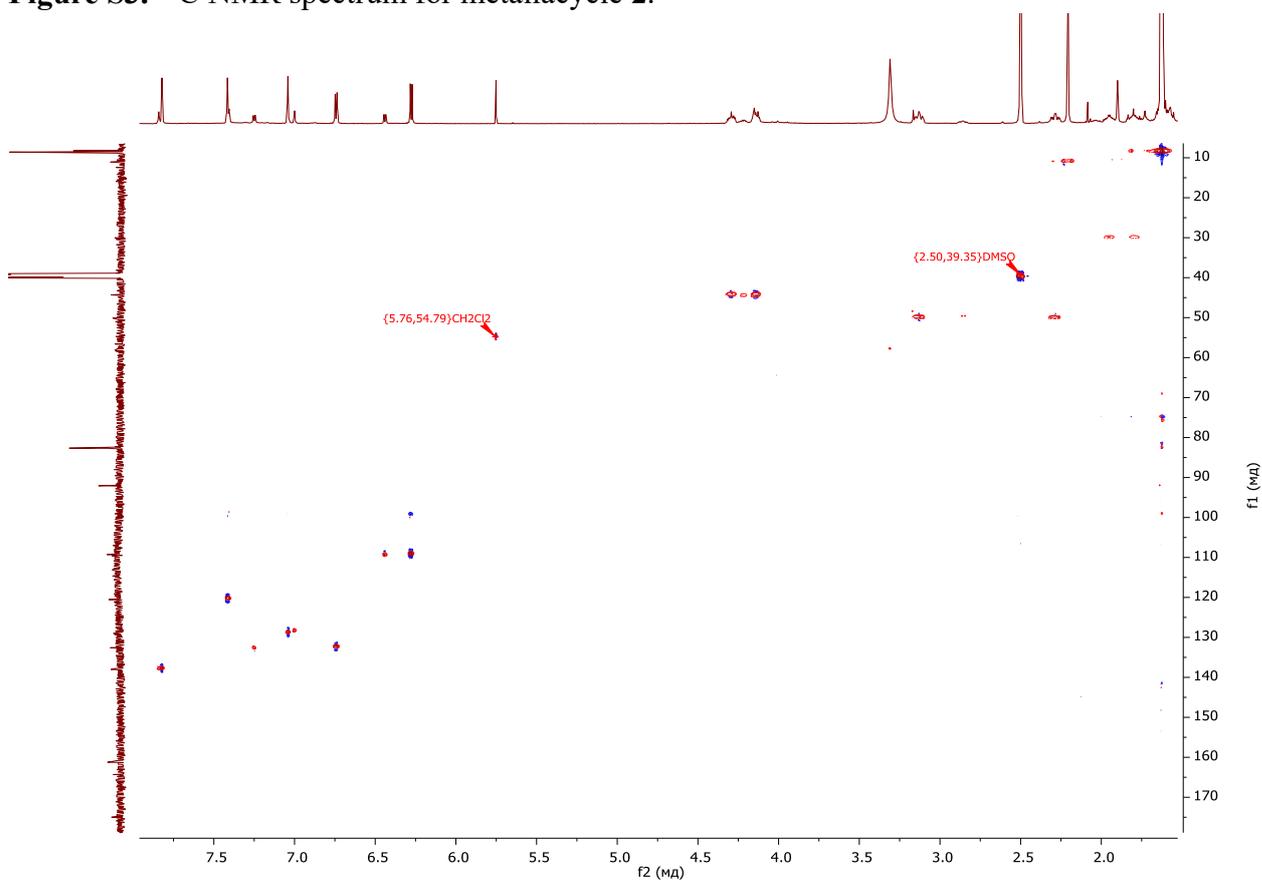


Figure S4. HSQC NMR spectrum for metallacycle **2**.

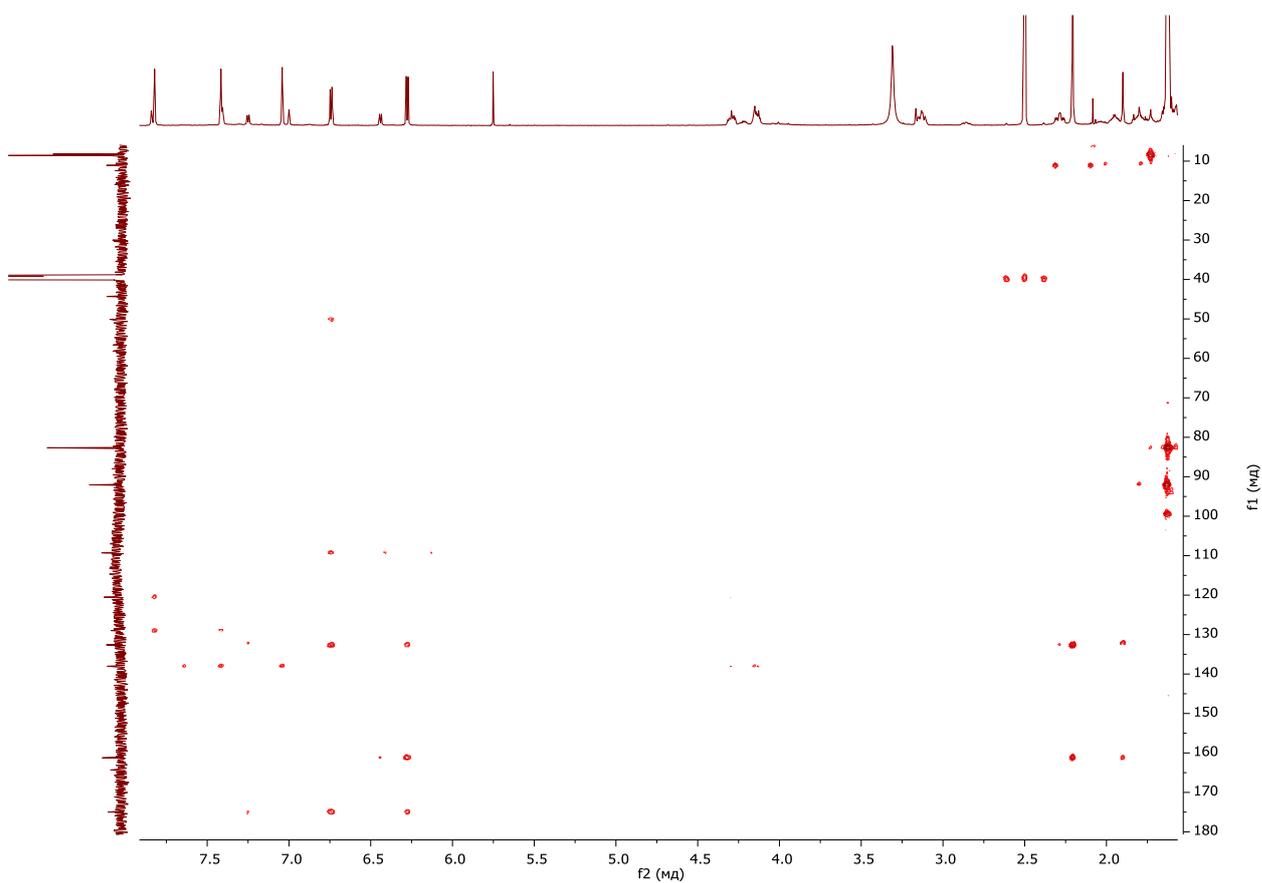


Figure S5. HMBC NMR spectrum for metallacycle **2**.

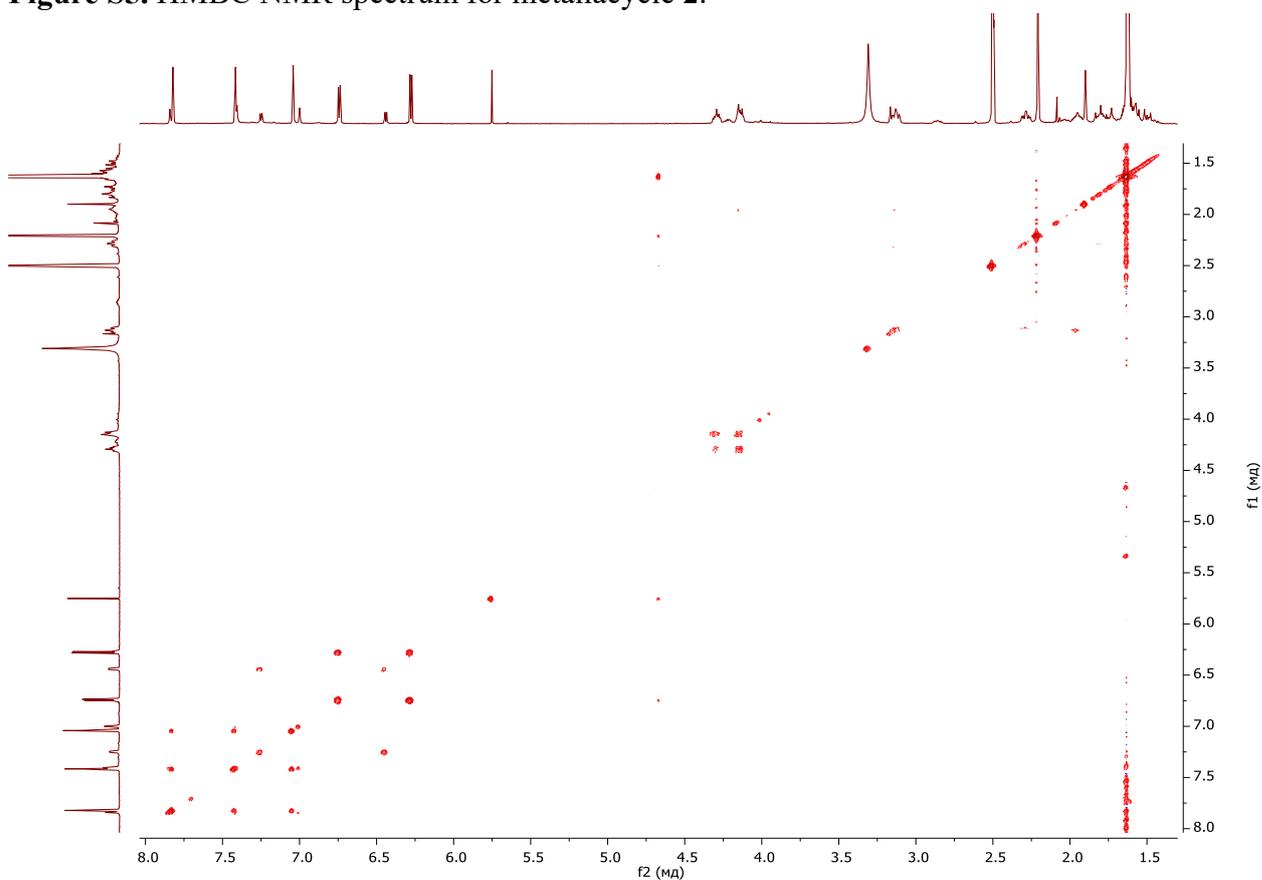


Figure S6. COSY NMR spectrum for metallacycle **2**.

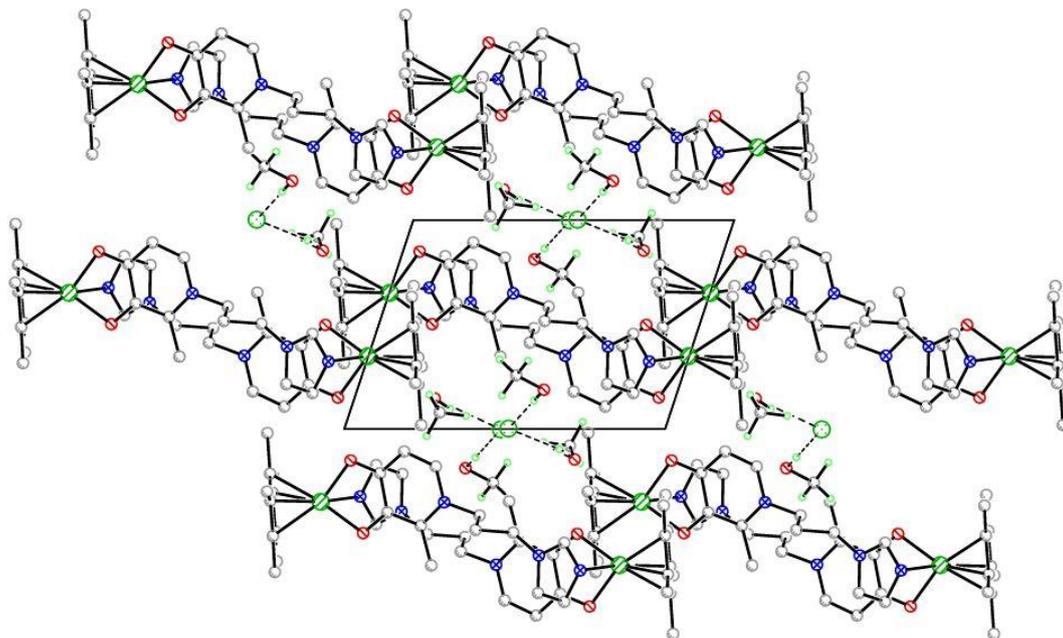


Figure S7. Molecular packing of 2

Table S1. Selected crystallographic data and refinement parameters for **2** from single crystal X-ray diffraction.

Chemical formula	C ₄₈ H ₇₄ Cl ₂ Ir ₂ N ₆ O ₈
Formula mass, g mol ⁻¹	1318.43
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> , Å	7.9907(12)
<i>b</i> , Å	12.7188(18)
<i>c</i> , Å	14.746(2)
α	114.437(4)
β	92.482(5)
γ	105.428(5)
<i>V</i> , Å ³	1295.0(3)
<i>Z</i> (<i>Z'</i>)	1(0.5)
<i>T</i> , K	110(2)
<i>d</i> _{calcd.} , g cm ³	1.691
μ , mm ⁻¹	52.92
θ range, °	3.846 < θ < 26.987
Collected reflections	21037
Independent reflections	7562
<i>R</i> _σ / <i>R</i> _{int}	0.0596/0.0679
Reflections with <i>I</i> > 2σ(<i>I</i>)	6505
Refined parameters	338
Largest difference peak/hole, e Å ⁻³	2.965/-2.892
<i>R</i> ₁ [<i>I</i> > 2σ(<i>I</i>)] / <i>R</i> ₁ [all data]	0.0379/0.0478
<i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)] / <i>wR</i> ₂ [all data]	0.0789/0.0823
<i>GoF</i>	1.025