

Supporting Information

Enantiomerically Pure Cyclopentadienyl- and Indenyl-Functionalized N-Heterocyclic Carbene Complexes of Iridium and Rhodium

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1 – ESI-MS of (*R*)-**3** in acetonitrile.

2 – ESI-MS of (*R*)-**4** in acetonitrile

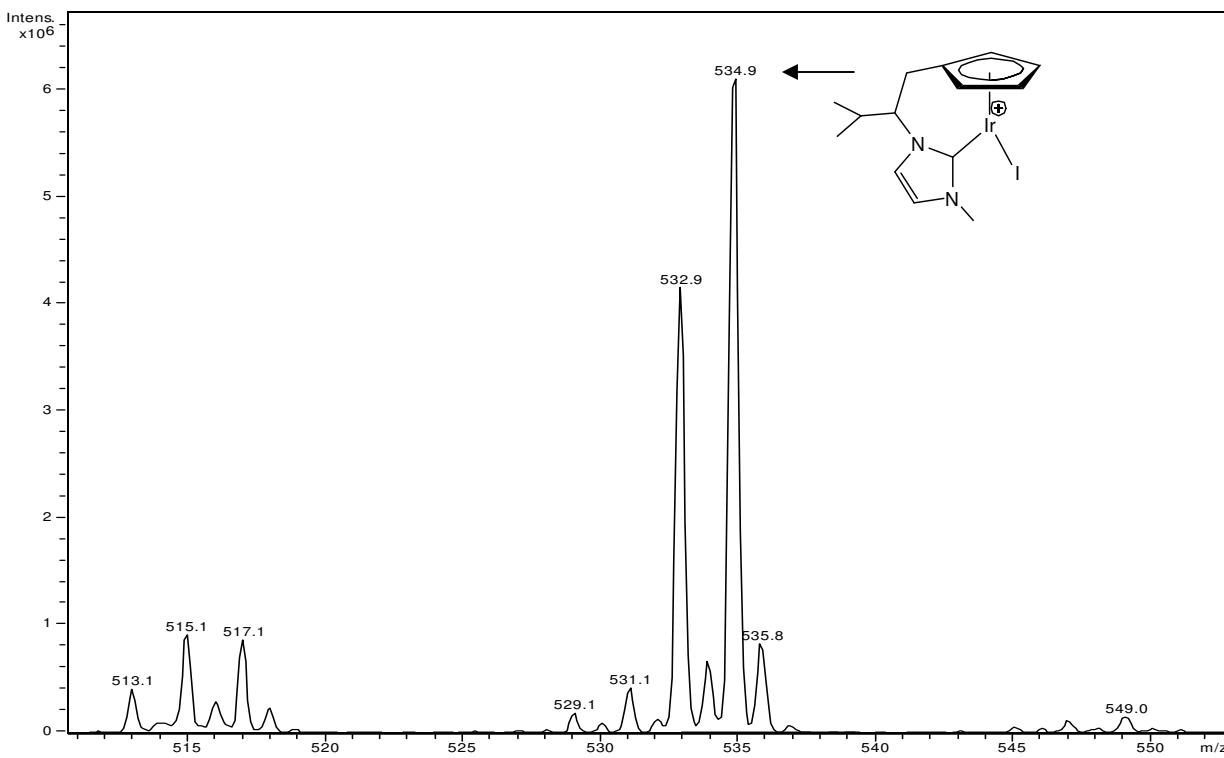
3 – ESI-MS of **5** in acetonitrile

4 – ESI-MS of **7** in acetonitrile.

5- Table 1. Details of the data collection, cell dimensions and structure refinement of (*R*)-**3**

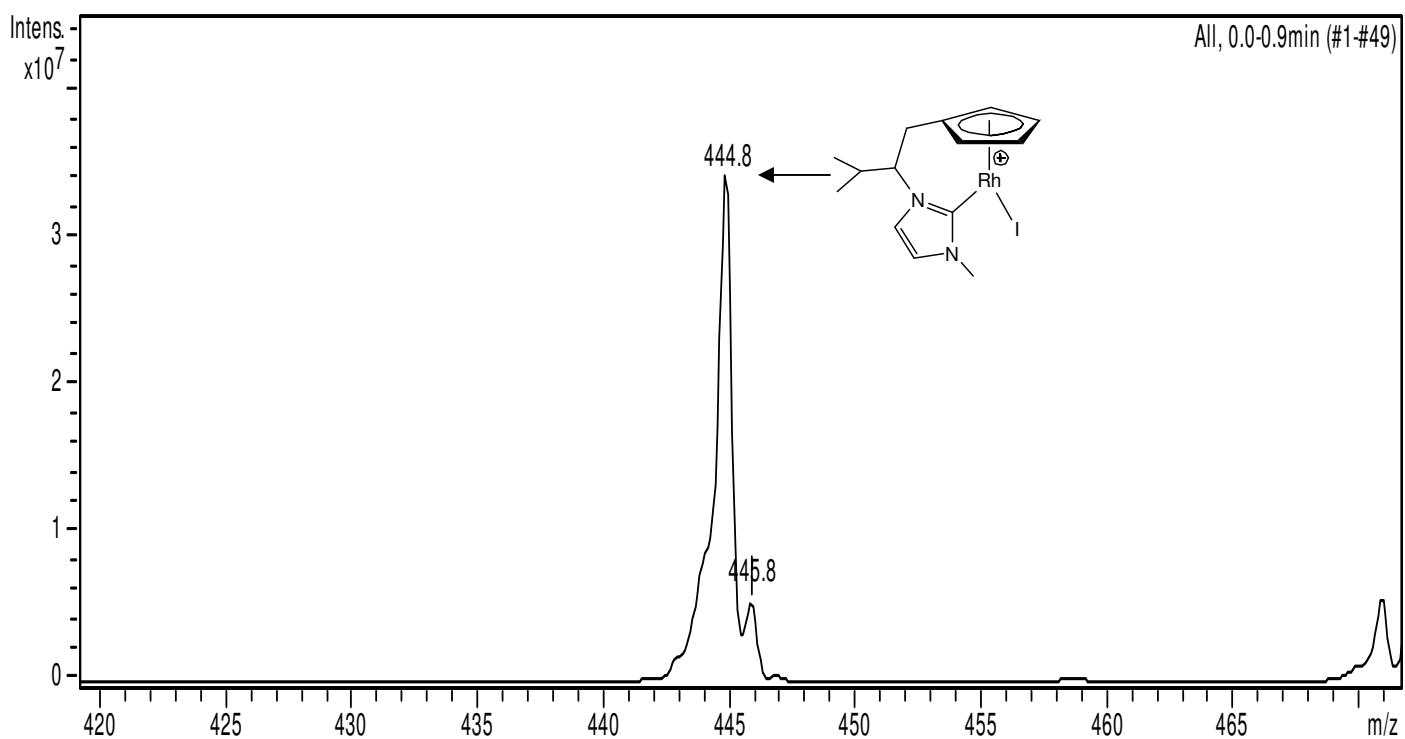
6- Figure 1. Molecular diagram of the iridium complex **5**

1.– MS (ESI-MS) in acetonitrile of **3**

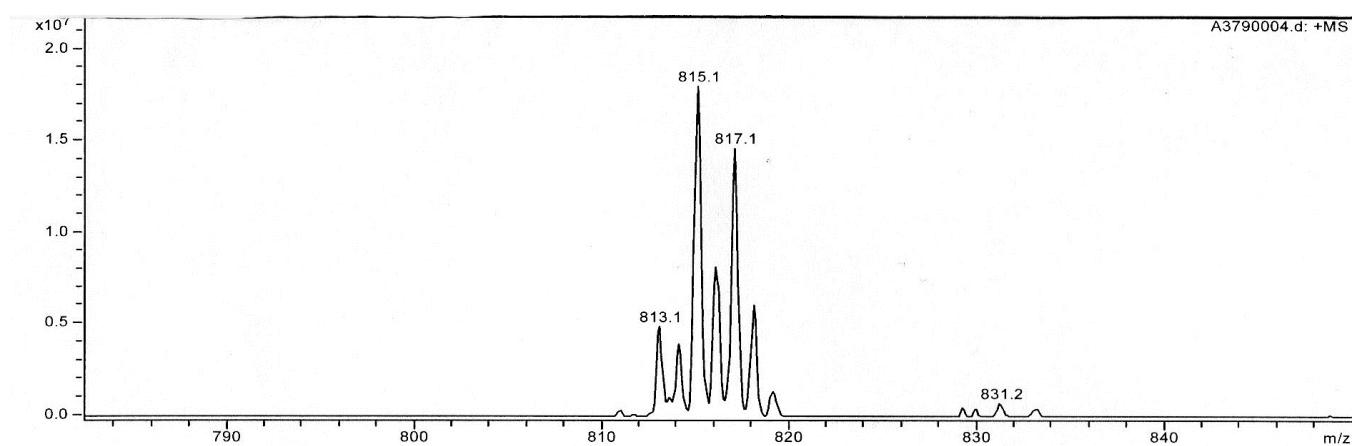


Peak (m/z)	Theoretical mass
534.9	535.02

2.– MS (ESI-MS) in acetonitrile of 4

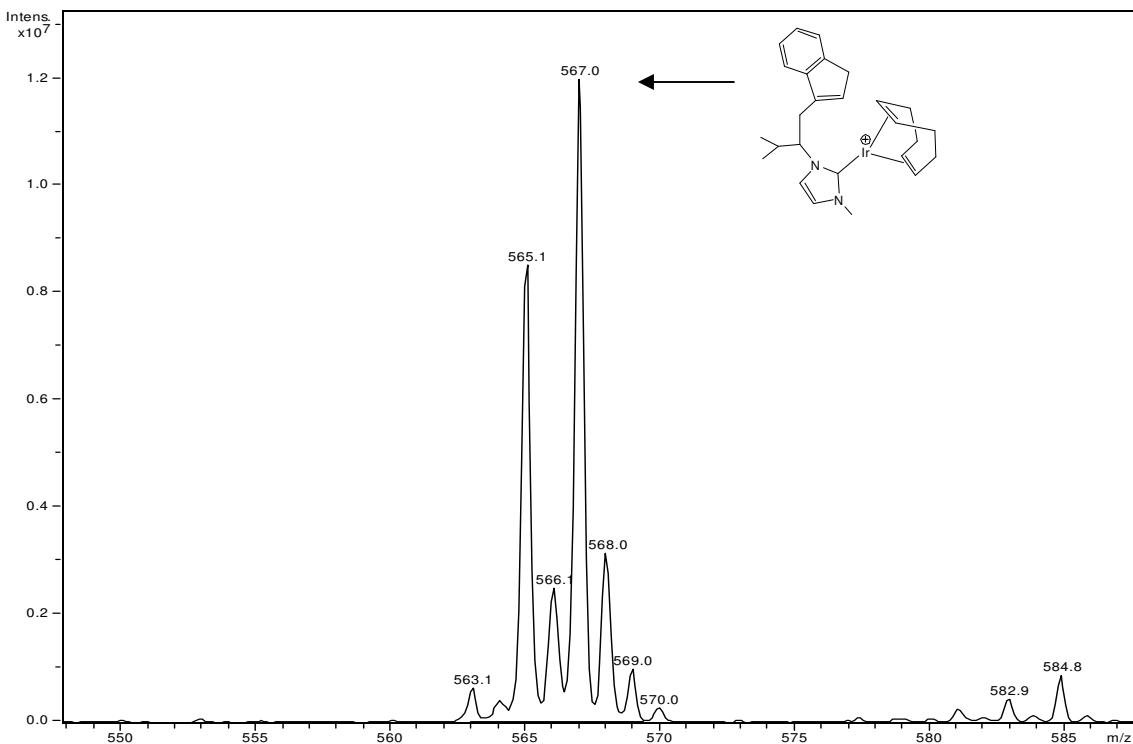


3.– MS (ESI-MS) in acetonitrile of 5



Peak (m/z)	Theoretical mass
815.3	815.1

4.- MS (ESI) of **7 in acetonitrile**



5- Table 1. Details of the data collection, cell dimensions and structure refinement of complex **3**

Table 1. Crystallographic data for complex **3**.

3	
empirical formula	C ₁₄ H ₁₉ I ₂ IrN ₂
mol wt	661.12
radiation	Mo K α (monochr)
T (K)	293(2)
cryst syst	Orthorhombic
space group	P 21 21 21
<i>a</i> (\AA)	9.0445(6)
<i>b</i> (\AA)	12.7406(9)
<i>c</i> (\AA)	17.8947(12)
α (deg)	90.00
β (deg)	90.00
γ (deg)	90.00
<i>V</i> (\AA^3)	2062.0(2)
<i>Z</i>	4
<i>D</i> _{calcd} (Mg m^{-3})	2.130
crystal size (mm^3)	0.31x0.22x0.1
<i>F</i> (000)	1200
θ range for data collection (deg)	1.96-27.5
μ (Mo K α) (mm^{-1})	1.83
reflns collected	13068
<i>R</i> _{int}	0.047
Independent reflections	5002
<i>R</i> [$F^2 > 2\sigma(F^2)$]	0.0328
w <i>R</i> (F^2)	0.0912
Flack	0.076(9)
<i>S</i>	1.113

6- Figure 1. Molecular diagram of the iridium complex **5**

