
Stereochemistry assignment of triskelion-shaped trishelvicenic Iridium complexes

Elsa Caytan^{*1}, Etienne Gauthier¹, Nora Hellou¹, Samuel Del Fré², Vincent Dorcet¹, Nicolas Vanthuyne³, Ludovic Favereau¹, Monika Srebro-Hooper², Gareth Williams⁴, and Jeanne Crassous¹

¹Institut des Sciences Chimiques de Rennes (ISCR) – Centre National de la Recherche Scientifique : UMR6226, Université de Rennes 1 – Campus de Beaulieu - Bât. 10 Avenue du Général Leclerc 35042 Rennes Cedex, France

²Department of Theoretical Chemistry, Faculty of Chemistry, Jagiellonian University – R. Ingardena 3, 30-060 Krakow, Pologne

³Institut des Sciences Moléculaires de Marseille (ISM2) – Aix Marseille Université : UMR7313, Ecole Centrale de Marseille : UMR7313, Centre National de la Recherche Scientifique : UMR7313 – Campus Saint Jérôme Av. escadrille Normandie Niemen BP 531 13397 MARSEILLE CEDEX 20, France

⁴Department of Chemistry [Durham, UK] – Stockton Road, Durham DH1 3LE, Royaume-Uni

Résumé

Enantiopure tris-helicenic chiral-at-iridium complexes have been prepared, constituting the first examples of organometallic metal-tris-helicenes. Thanks to their Ir(III)-based multi-helicenic architecture, the complexes display strong electronic circular dichroism and optical rotation along with long-lived yellow phosphorescence.

When synthesis is performed with an enantiopure helicenic precursor (either (*P*) or (*M*)), the octahedral complex can be statistically obtained in 4 different configurations, due to the chirality-at-iridium (*D*Ir/*L*Ir) and the two coordination geometries (meridional = *mer* / facial = *fac*).

Only 3 configurations were found experimentally. They were separated using HPLC, and the complete NMR studies (¹H, ¹³C, 2D homonuclear and heteronuclear NMR, performed on 500 MHz or 900 MHz spectrometers) of the optically pure stereoisomers were conducted in CD₂Cl₂. The analysis of the resulting NMR signals with reference to the calculated geometries of such molecular configurations enabled their stereochemistries to be definitively assigned.

*Intervenant