Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2021

Supporting Information

NHC Ligand-Based Half-Sandwich Iridium Complexes: Synthesis, Structure and Catalytic Activity in Acceptorless Dehydrogenation and Transfer Hydrogenation

Rong-Jian Li,^{a,c} Yang Wang,^a Yan Jin,^{a,c} Wei Deng,^{*a} Zhen-Jiang Liu,^{*a} Zi-Jian Yao,^{*ab}

^a School of Chemical and Environmental Engineering, Shanghai Institute of Technology, Shanghai,

201418, China.

^b Anhui Laboratory of Molecular-Based Materials, College of Chemistry and Materials Science, Anhui Normal University, Wuhu, 241002, China.

^c State Key Laboratory of Transducer Technology, Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai, 200050, China

Corresponding author: Email: zjyao@sit.edu.cn; Tel: +86-21-60877231, Fax: +86-21-60873335.







Figure S2. ¹H NMR spectra of A2







Figure S4. ¹H NMR spectra of A4







Figure S6. ¹H NMR spectra of L2



Figure S8. ¹H NMR spectra of L4



Figure S10. ¹³C NMR spectra of **1**



Figure S12. ¹³C NMR spectra of 2



Figure S14. ¹³C NMR spectra of **3**



Figure S16. ¹³C NMR spectra of 4