## **Supplementary Information**

## (Pyridyl)benzoazoleRuthenium(II) and Ruthenium(III) Complexes: Role of

Heteroatom and Ancillary Phosphine Ligand in the Transfer Hydrogenation of

## Ketones

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Fig. S1: HR-MS mass spectrum of complex 1



Fig. S2: ESI-MS mass spectrum of complex 2



Fig. S3: ESI-MS mass spectrum of complex 3



Fig. S4: ESI-MS mass spectrum of complex 4



**Figure S5**: ES-MS spectrum of complex **6** showing m/z signal at 892.90 (50%) corresponding to the molecular ion,  $M^+$  of **6**. The base peak at m/z peak at 923.31 could result form internal reactions in the column.



**(a)** 

so\_so35\_31p.20130312.nmr5 1 1 C:\Bruker\TOPSPIN Aloice



**(b)** 

**Fig. S6**:  ${}^{31}P$  { ${}^{1}H$ } NMR spectra of complexes [Ru(L1)PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>] **4** (a) and [Ru(L2)PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>] **5** (b) in DMSO. The free PPh<sub>3</sub> signals at -6.72 ppm indicate the displacement of one coordinated PPh<sub>3</sub>.



**Fig. S7**: ORTEP view of **6** showing the atom labeling and 50% probability ellipsoids (the structure could not be satisfactorily refined due to desolvation and the data obtained are not suitable for publication and discussion of bond parameters).



Fig. S8: <sup>1</sup>H NMR spectrum of ligand 1-propyl-2-(pyridin-2-yl)-1H-benzo[d]imidazole (L4)



Fig. S9: Mass spectrum of complex of [Ru(L4)Cl<sub>3</sub>] (7) indicating the formation of a dimer.



**Fig. S10**: <sup>31</sup>P{<sup>1</sup>H} NMR spectra showing evidence of displacement of PPh<sub>3</sub> in iPrOH/KOH solution to form metal-alkoxide **6-I** from complex **6**. The signal at -5.29 ppm reveals the generation of a free PPh<sub>3</sub> (inset; <sup>31</sup>P NMR spectrum of **6** in CDCl<sub>3</sub>, the signal at 29.83 ppm indicates that the two *trans*-PPh<sub>3</sub> ligands are chemically equivalent).



**Fig. S11**: Typical <sup>1</sup>H NMR spectrum of the 2-phenylethanol product obtained from the transfer hydrogenation of acetophenone confirming the identity and purity of the product.