Anchoring of a Ruthenium Complex into Mesoporous Silica Via a Covalent Route

Imobilização de um Complexo de Rutênio em Sílica Mesoporosa Via Rota Covalente

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Nuclear magnetic spectra of *cis*-[RuCl(dppb)(ISN)(phen)](PF_6)

Figures S1 and S2 show the ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra of *cis*-[RuCl(dppb)(ISN)(phen)](PF_6).

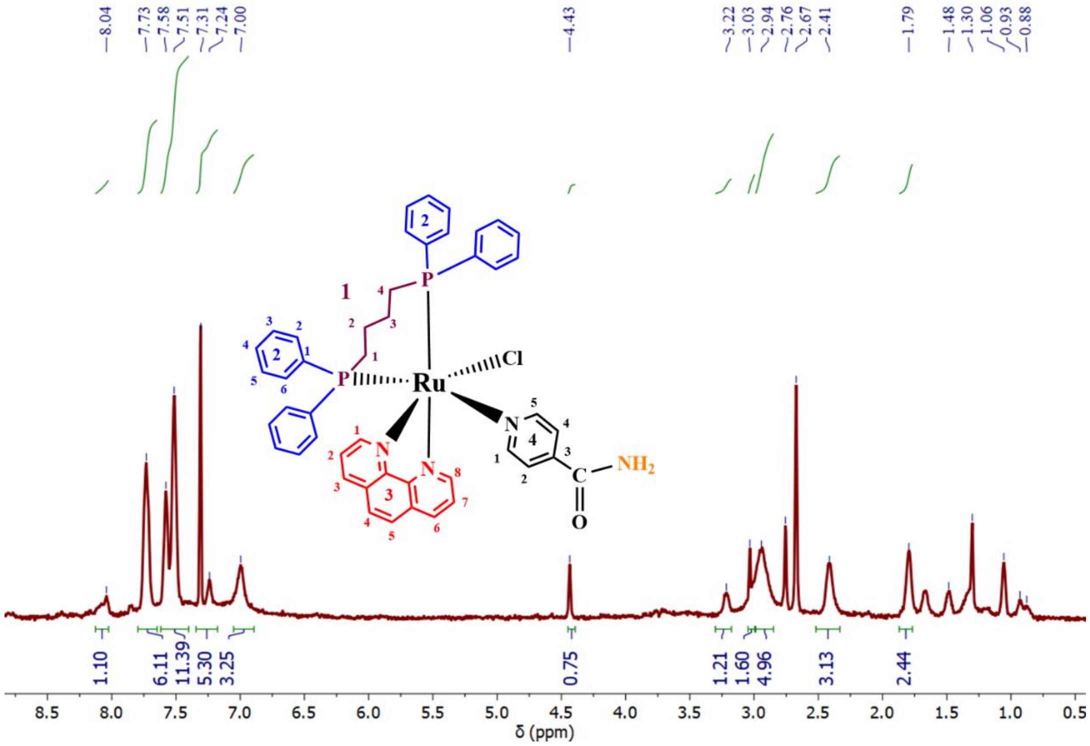

Figure S1. ^{1}H NMR spectrum of *cis*-[RuCl(dppb)(ISN)(phen)](PF_6) in $CDCl_3$ in a 500 MHz spectrometer. Inset: molecular structure with numbering scheme.

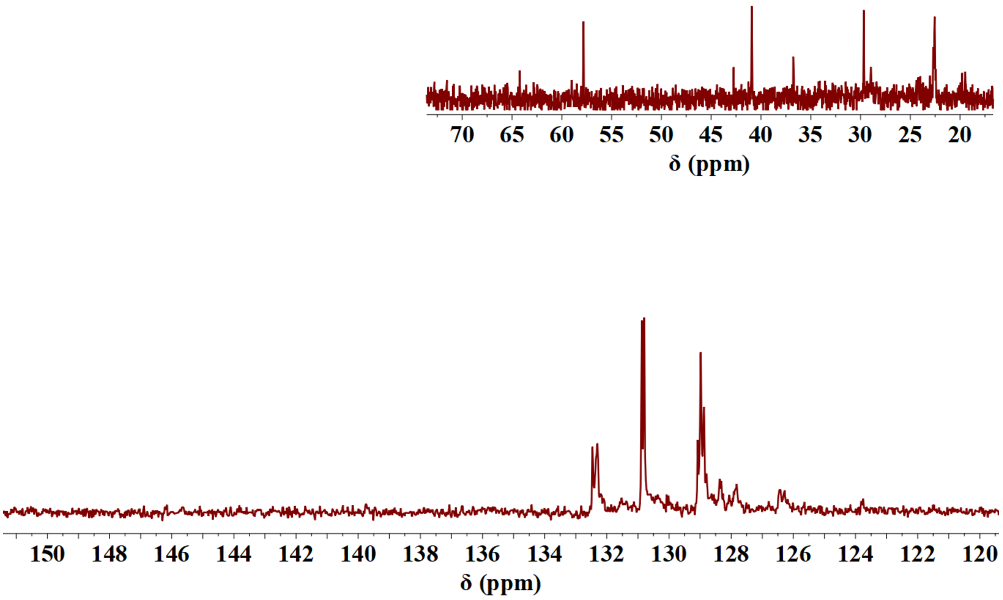

Figure S2. ^{13}C NMR spectrum of *cis*-[RuCl(dppb)(ISN)(phen)](PF_6) in $CDCl_3$ in a 500 MHz spectrometer.

The peaks seen at δ 2.76, 2.67, and 1.03 ppm and at δ 58 ppm, respectively, in the ^{1}H and ^{13}C NMR spectra of *cis*-[RuCl(dppb)(ISN)(phen)](PF_6) are assigned to ethanol, which was the solvent used in the synthetic procedure. The ^{1}H NMR spectrum also shows peaks at δ 1.67 and 1.48 ppm ascribed to residual water of $CDCl_3$ (c.a. 0.01%) while the peak of $CDCl_3$ solvent is observed in the range δ 7.13-7.26 ppm. [1, 2]

Thermogravimetric data of silica-based samples

Figure S3 shows the thermogravimetric (TG) and differential thermal analysis (DTA) curves obtained for the material produced at each modification step

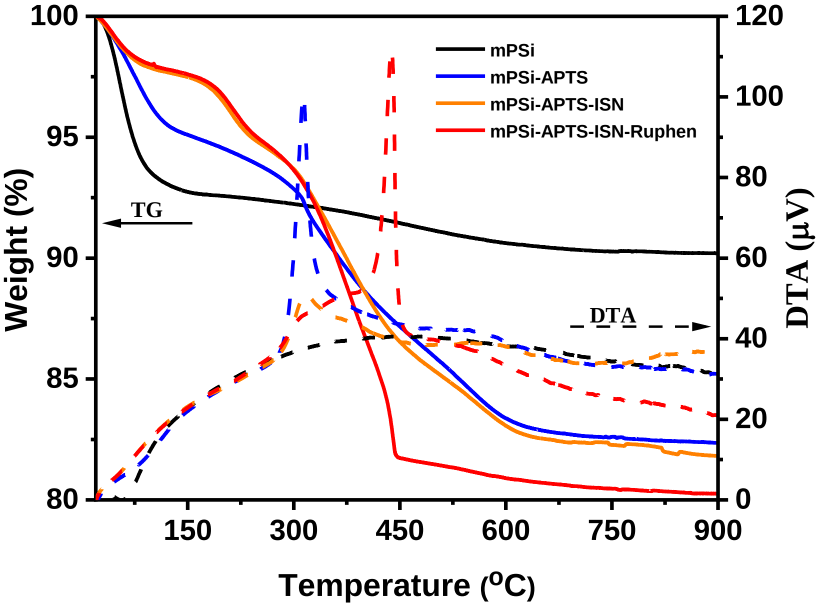

Figure S3. TG (solid lines) and DTA (dashed lines) curves obtained in air (heating hamp of 10 °C min^{-1}) for the mPSi (black), mPSi-APTS (blue), mPSi-APTS-ISN (orange), and mPSI-APTS-ISN-Ruphen (red) samples.

Leaching monitoring

Figure S4 shows the UV-Vis spectrum obtained after 24 h of stirring of mPSI-APTS-ISN-Ruphen in a 0.02 mol L^{-1} solution of KOH in isopropyl alcohol at 100 °C and 2 atm H_2 pressure.

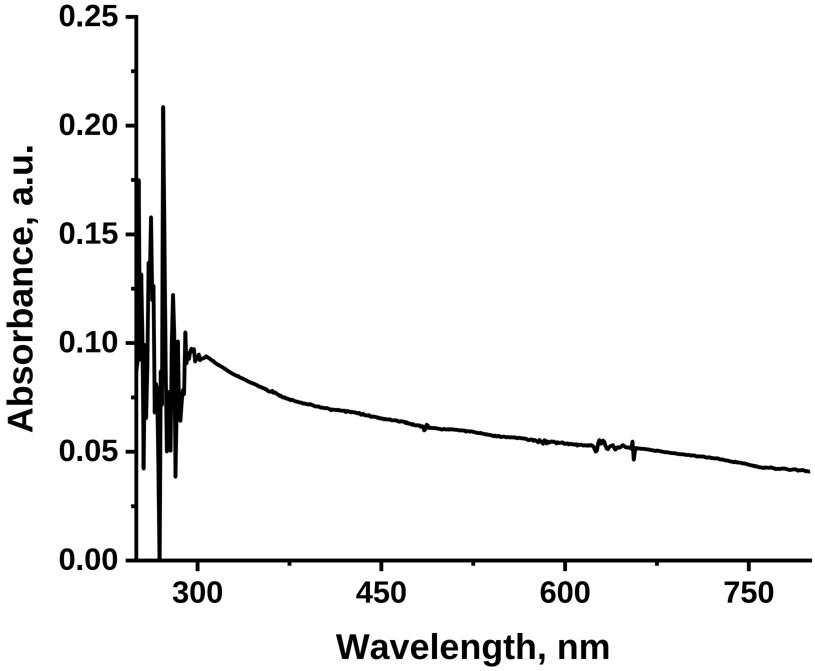

Figure S4. UV-Vis spectrum of a 0.02 mol L^{-1} solution of KOH in isopropyl alcohol after 24 h of stirring of the mPSI-APTS-ISN-Ruphen material at 100 °C and 2 atm H_2 pressure.

References

1. Fulmer, G. R.; Miller, A. J. M.; Sherden, N. H.; Gottlieb, H. E.; Nudelman, A.; Stoltz, B. M.; Bercaw, J. E.; Goldberg, K. I. NMR Chemical shifts of trace impurities: common laboratory solvents, organics, and gases in deuterated solvents relevant to the organometallic chemist. *Organometallics* **2010**, *29* (9), 2176-2179. https//doi.org/10.1021/om100106e.
2. Gottlieb, H. E.; Kotlyar, V.; Nudelman, A. NMR chemical shifts of common laboratory solvents as trace impurities. *The Journal of Organic Chemistry* **1997**, *62* (21), 7512-7515. https//doi.org/10.1021/jo971176v.