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SUPPLEMENTARY INFORMATION

9,10-dihydroanthracenyl structures: original ligands for the synthesis of polymetallic complexes through selective π-coordination

Ielyzaveta Bratko,[a] Sonia Mallet-Ladeira,[b] Nathalie Saffon,[b] Emmanuelle Teuma[a] and Montserrat Gómez[a]

[a] *Laboratoire Hétérochimie Fondamentale et Appliquée UMR CNRS 5069, Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse Cedex 9, France. E-mail: gomez@chimie.ups-tlse.fr. Fax: +33 561558204; Tel: +33 561557738.*

[b] *Université de Toulouse, UPS, Institut de Chimie de Toulouse FR2599, 118 route de Narbonne, 31062 Toulouse cedex 9, France.*

Figures

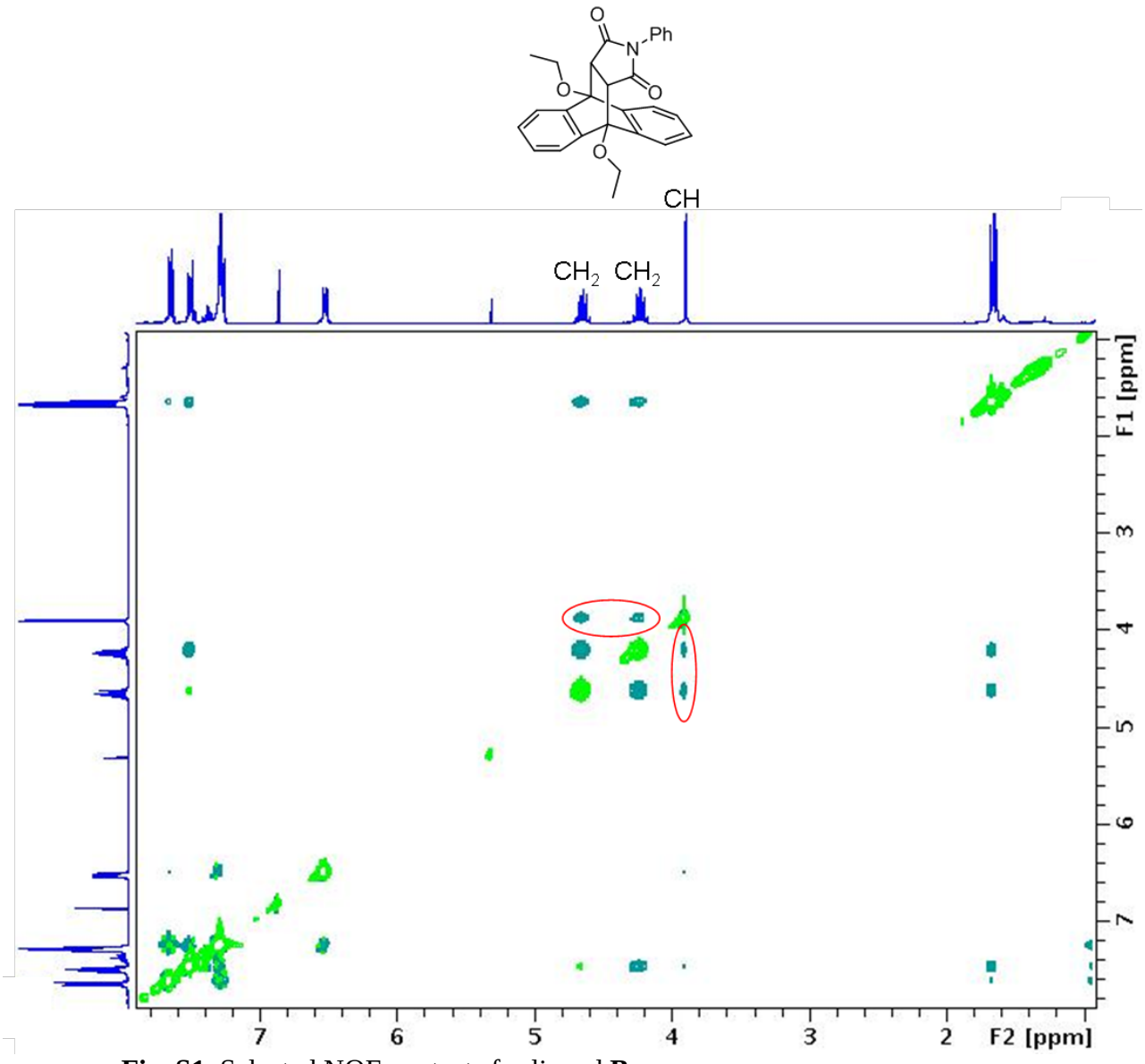

Fig. S1. Selected NOE contacts for ligand **B**.

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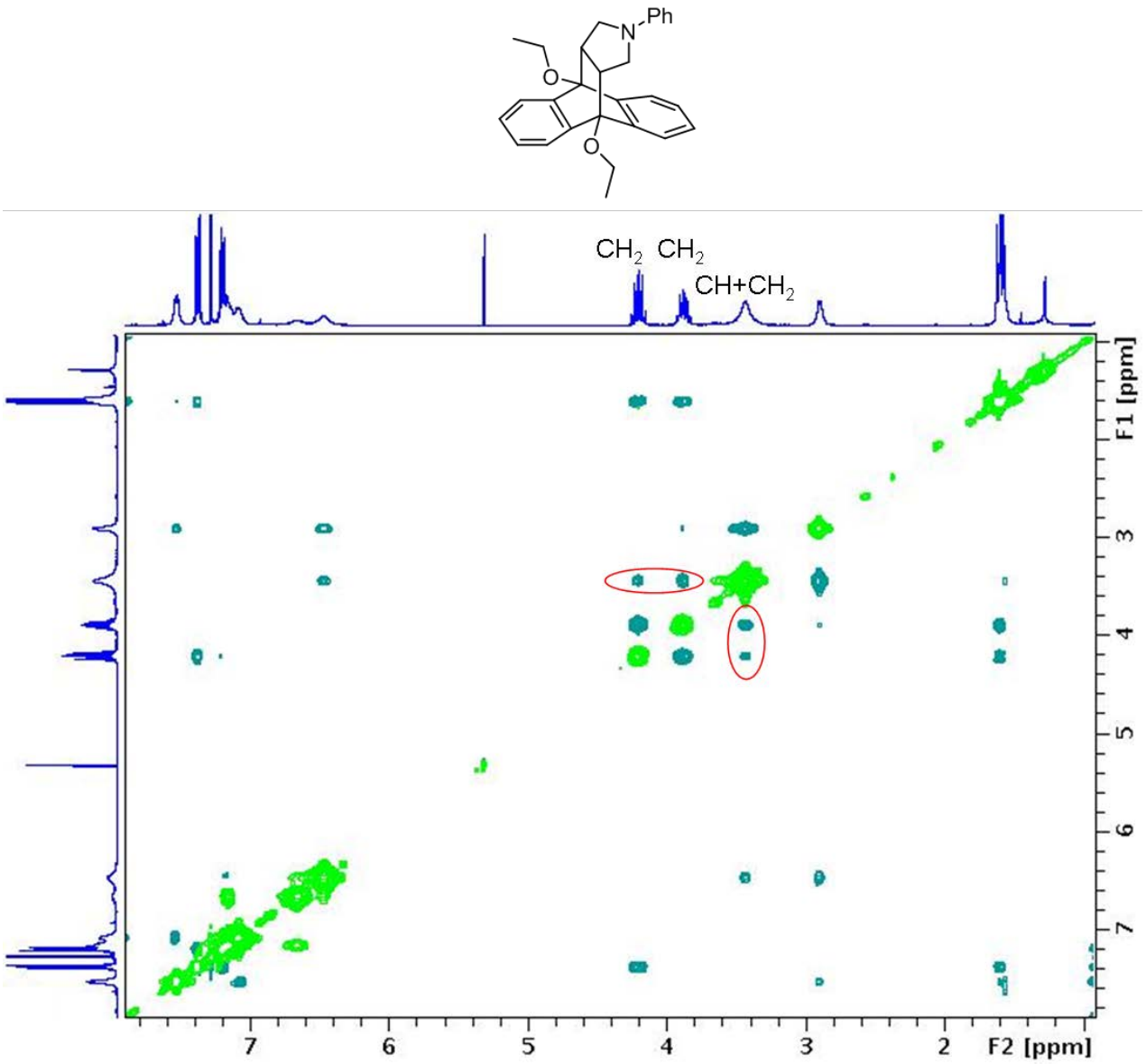

Fig. S2. Selected NOE contacts for ligand **D**.

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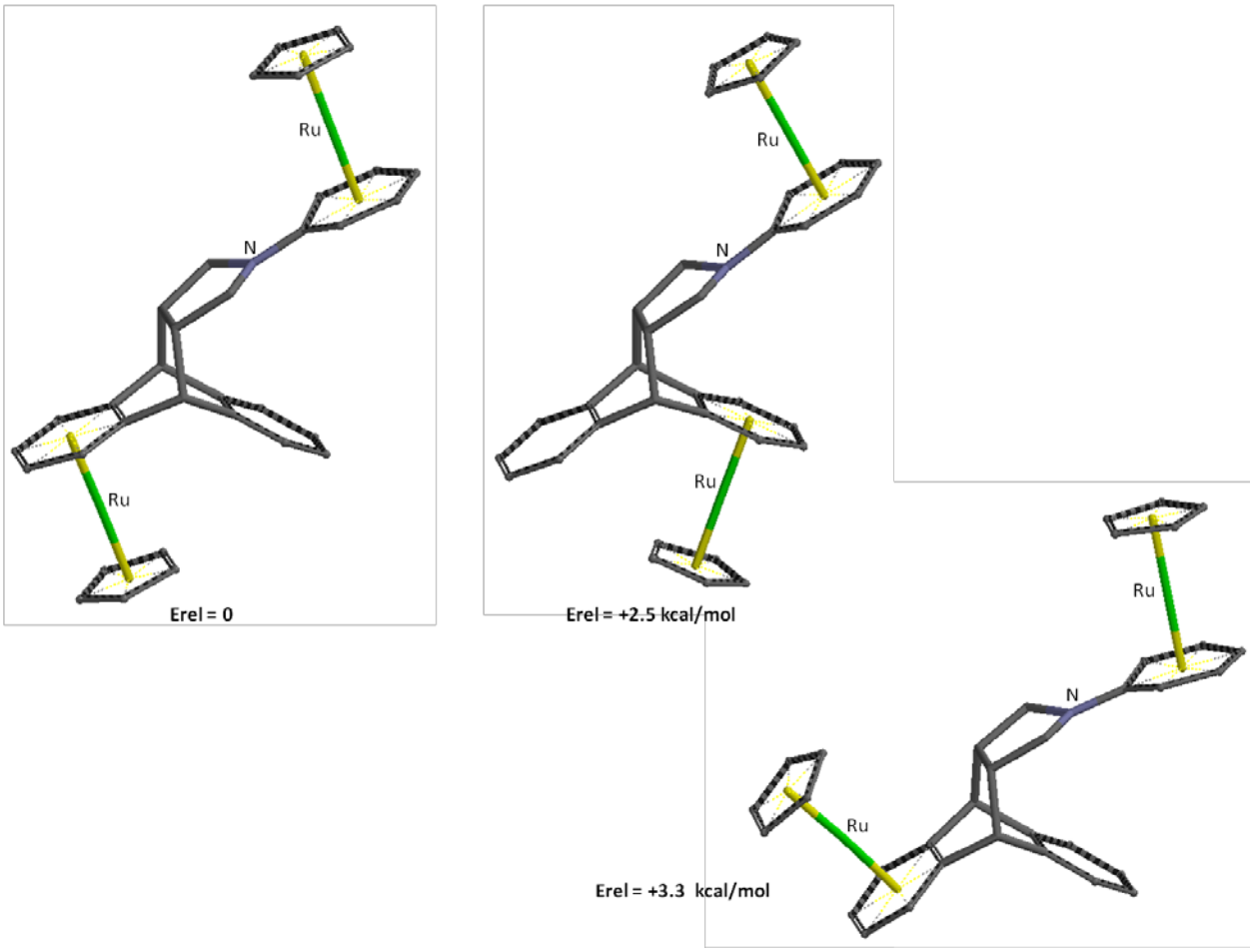

Fig. S3. Calculated structures (DFT) for cations $[RuCp((\eta^6\text{-arene})_2\mathbf{C})]^{2+}$ showing the coordination through **Ar3** cycle (a), **Ar2** (b) and **Ar1** (c and d). Hydrogen atoms are omitted for clarity.

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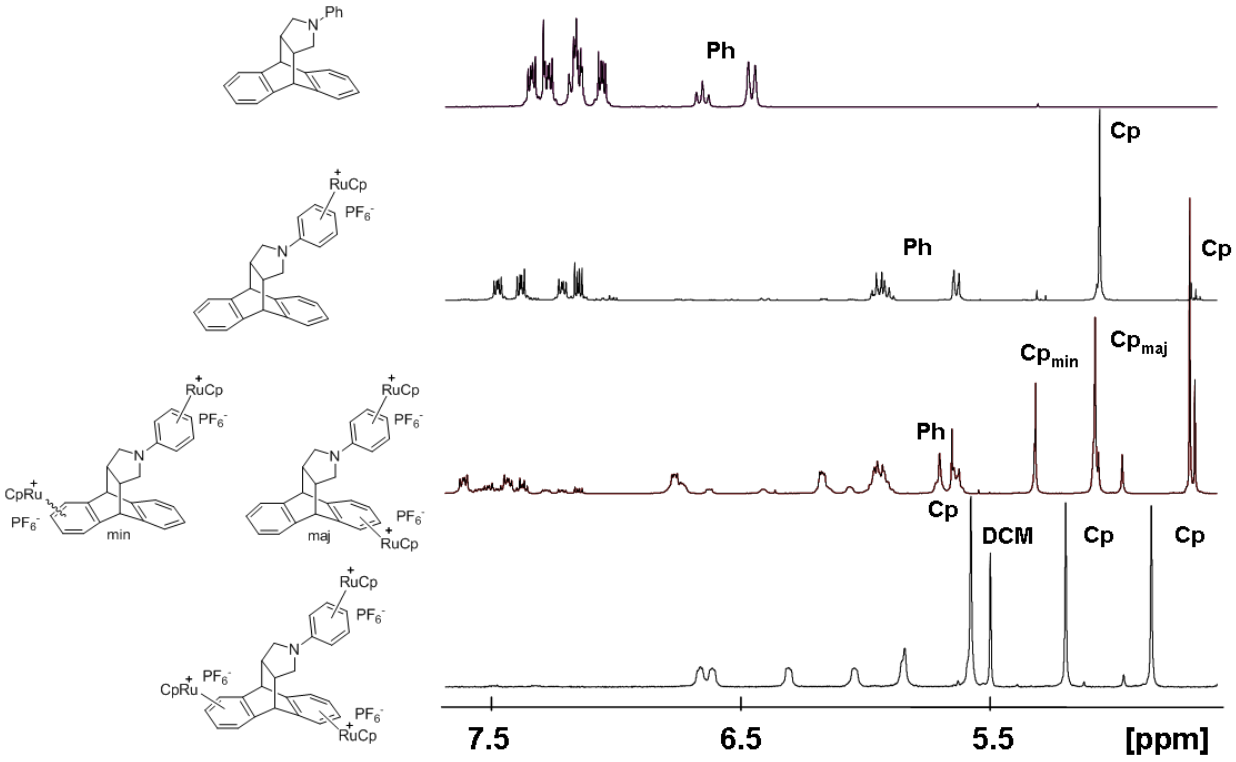

Fig. S4. ^{1}H NMR (300 MHz, $(CD_3)_2CO$, 298 K) monitoring of **C** by consecutive addition of $[RuCp(CH_3CN)_3]PF_6$

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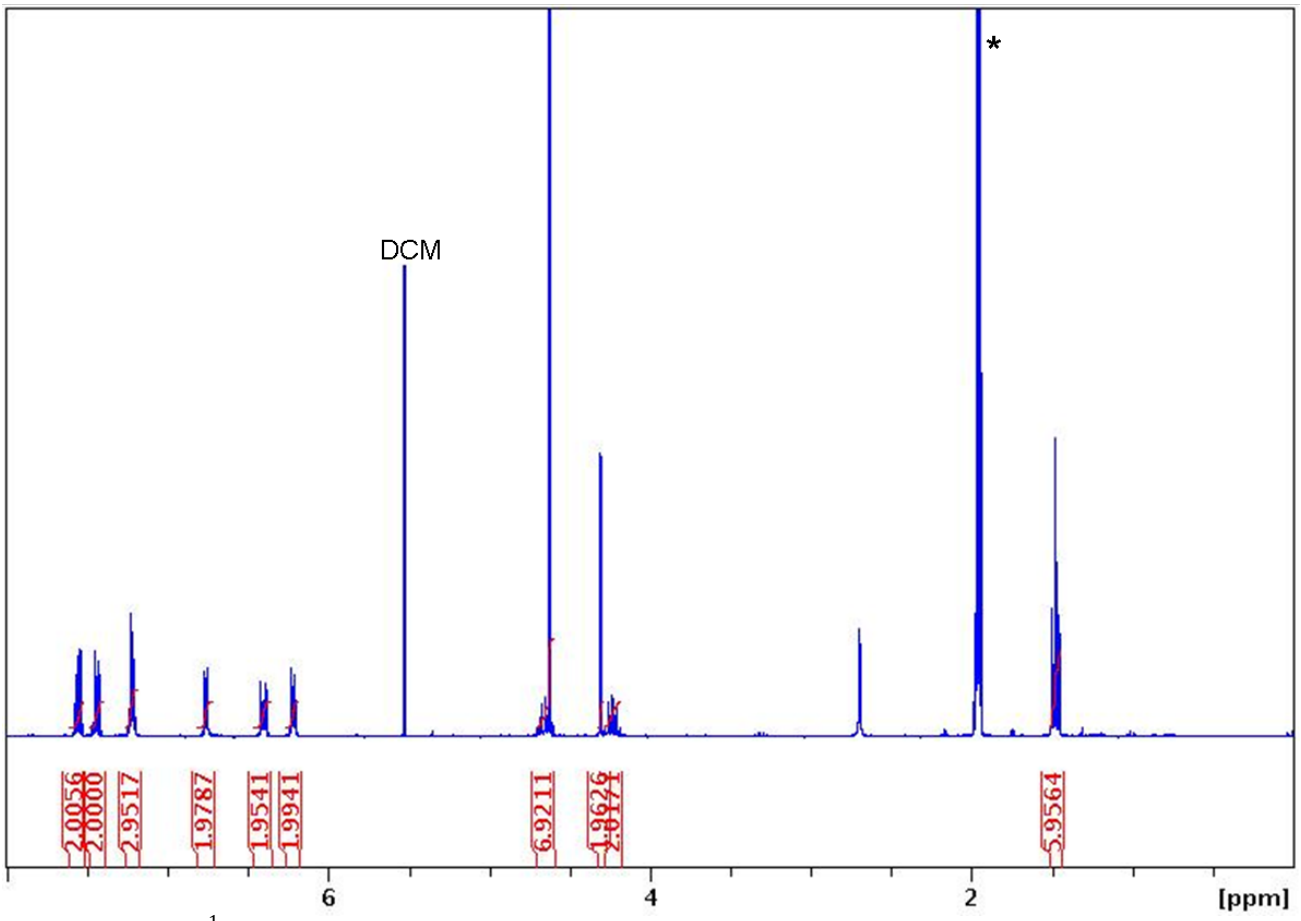

Fig. S5. ^{1}H NMR (300 MHz, $(CD_3)_2CO$, 298 K) spectrum for **BRu1.** * denotes partially protonated solvent.

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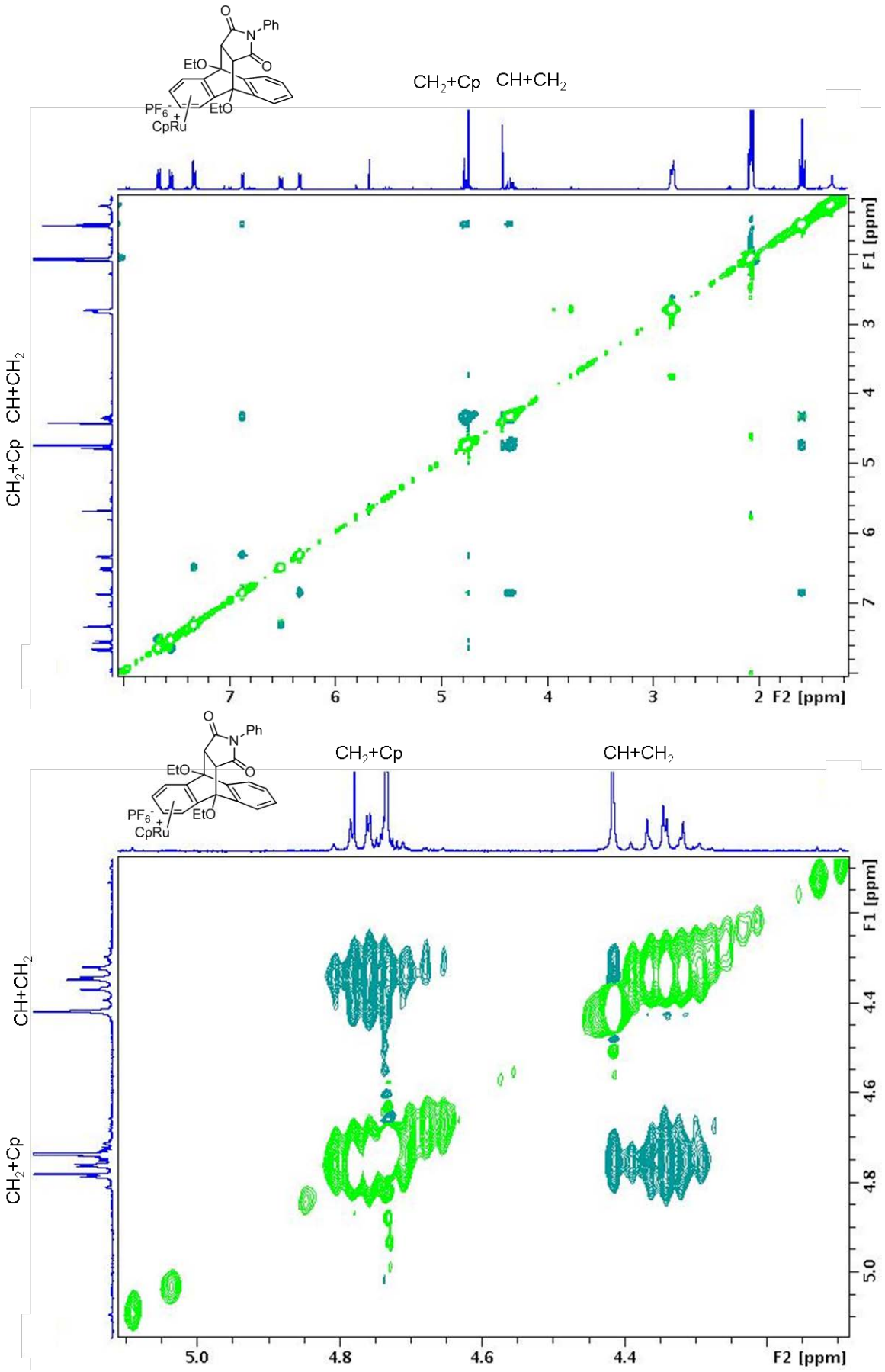

Fig. S6. NOESY NMR spectrum (300 MHz, $(CD_3)_2CO$, 298 K) and selected NOE contacts for **BRu1**.

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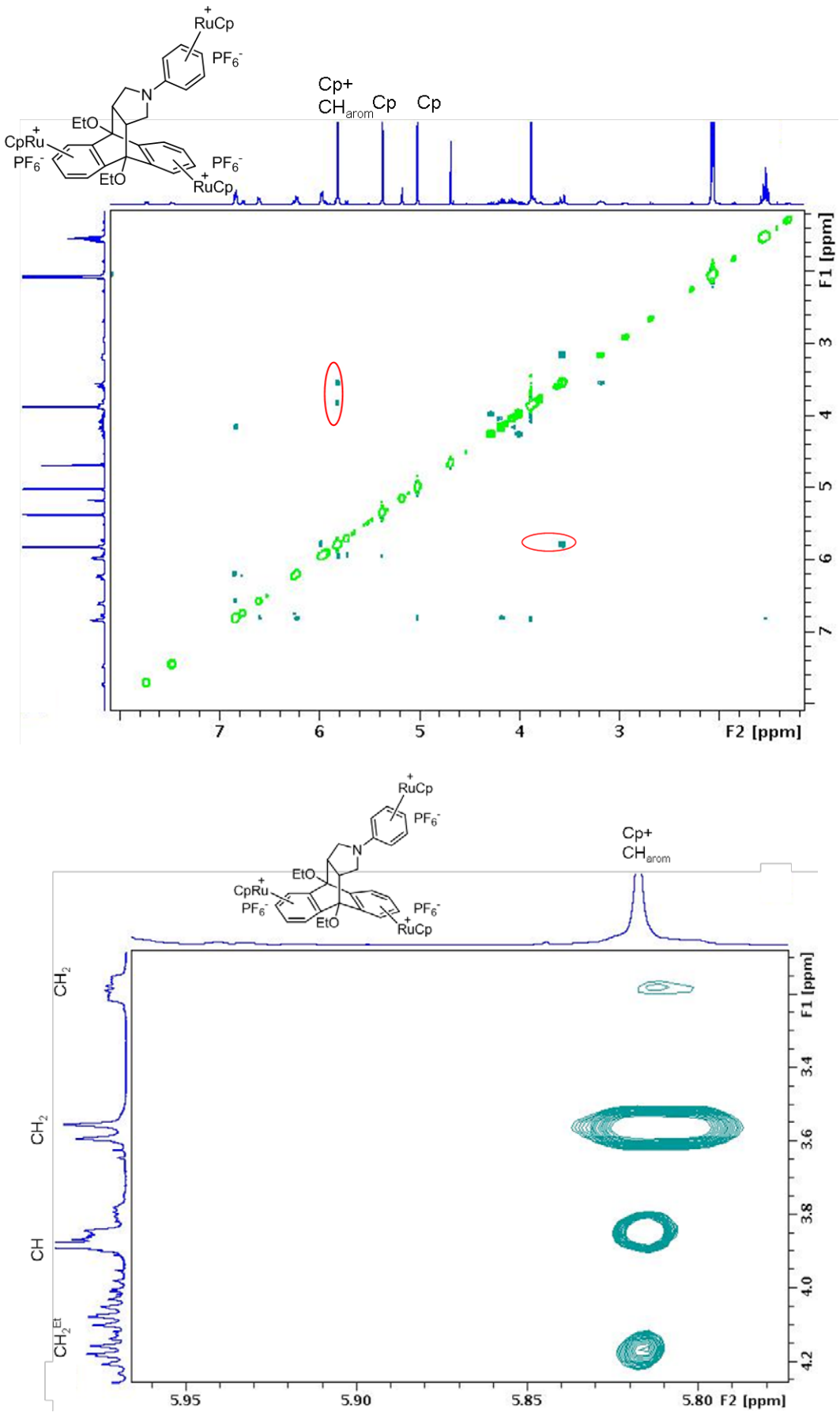

Fig. S7. NOESY NMR spectrum (300 MHz, $(CD_3)_2CO$, 298 K) and selected NOE contacts for **DRu3**.

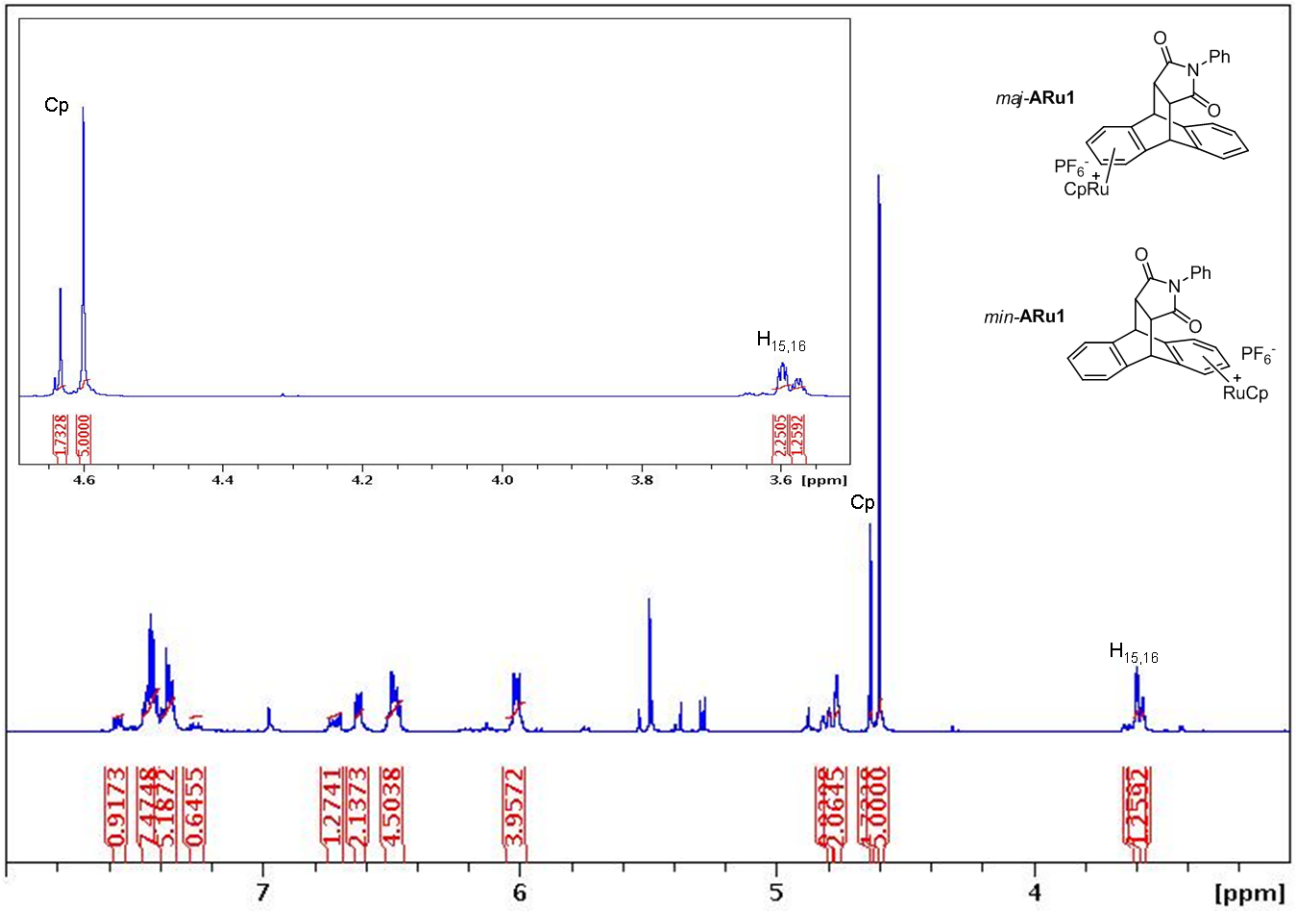

Fig. S8. ^{1}H NMR (300 MHz, CD_3CN, 298 K) spectrum for **ARu1**.

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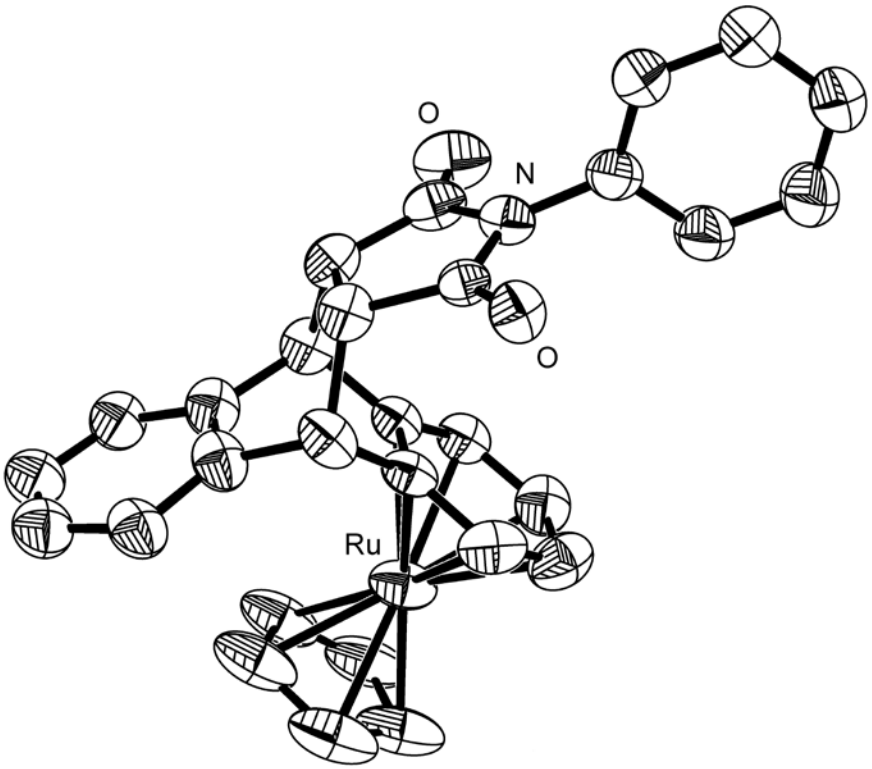

Fig. S9. Molecular view of the cation corresponding to complex **ARu1** (ellipsoids representing 50% probability). Hydrogen atoms and the hexafluorophosphate anion are omitted for clarity.

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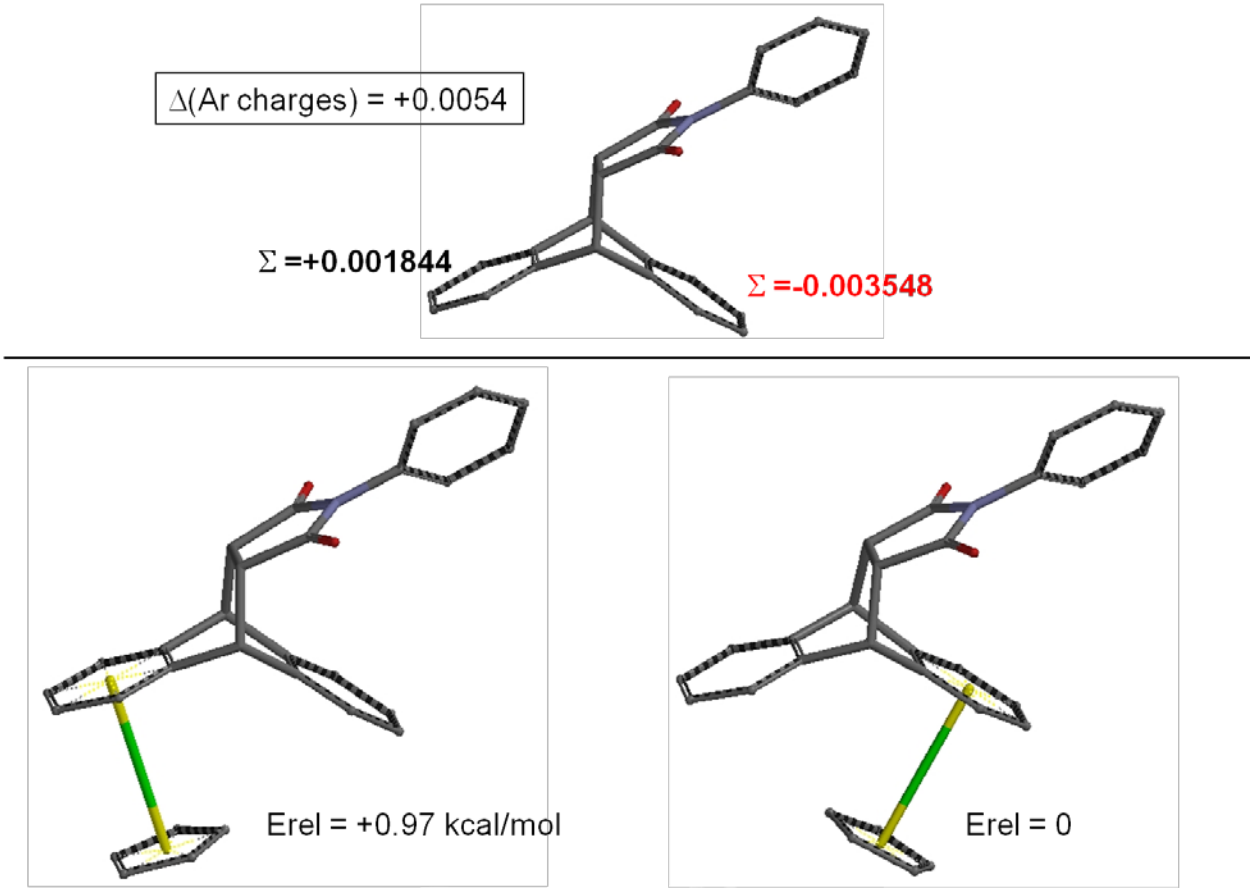

Fig. S10. Calculated structures (DFT) for cations $[RuCp((\eta^6\text{-arene})\mathbf{A})]^+$ showing the coordination through **Ar1** (bottom, left) and **Ar2** (bottom, right). Hydrogen atoms are omitted for clarity. NAP charges calculated for ligand **A** for both aromatic cycles, **Ar1** and **Ar2**. Energy values relative to the most stable isomer.

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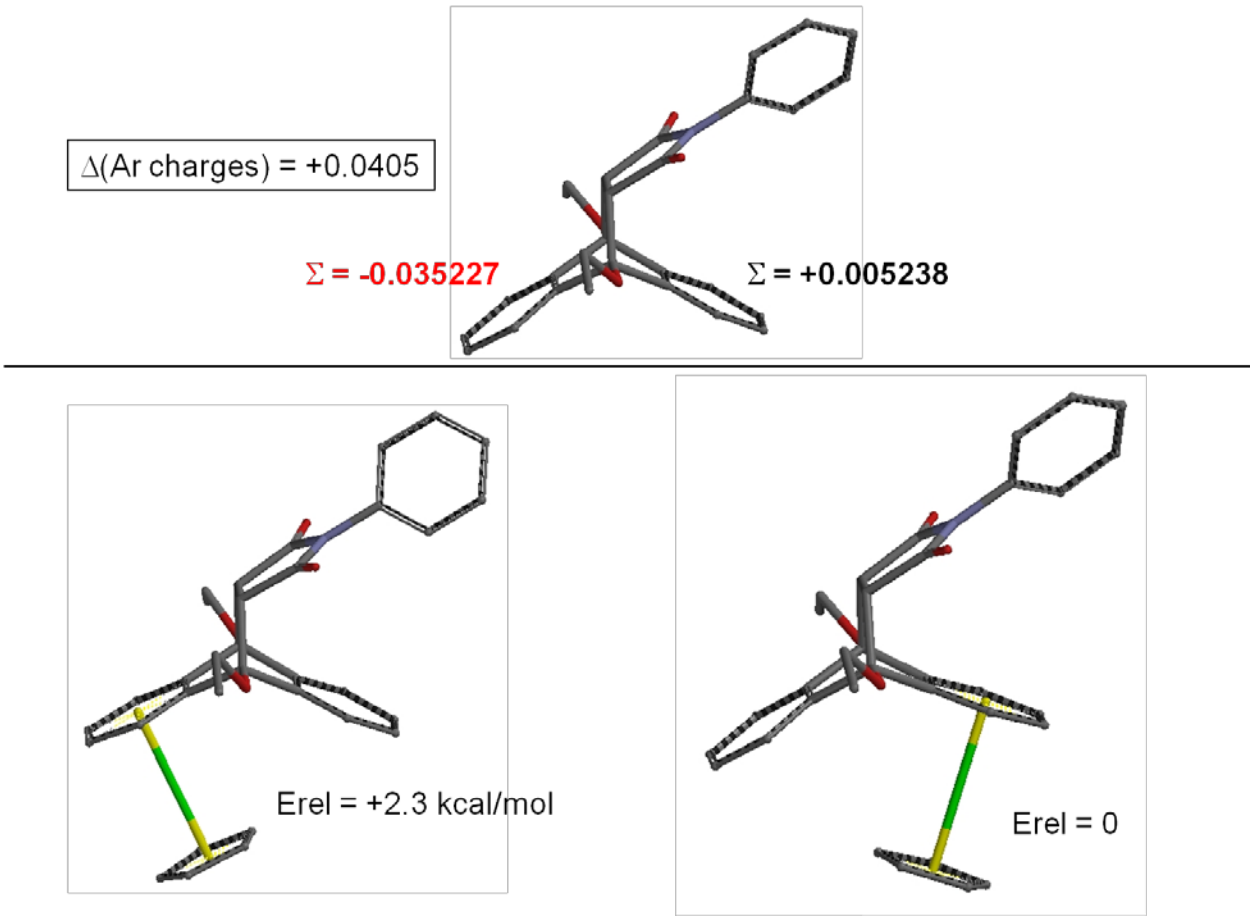

Fig. S11. Calculated structures (DFT) for cations [RuCp((η^6-arene)**B**)]$^+$ showing the coordination through **Ar1** (bottom, left) and **Ar2** (bottom, right). Hydrogen atoms are omitted for clarity. NAP charges calculated for ligand **B** for both aromatic cycles, **Ar1** and **Ar2**. Energy values relative to the most stable isomer.