

# Controlling Chiral Self-Sorting in Truxene-Based Self-Assembled Cages

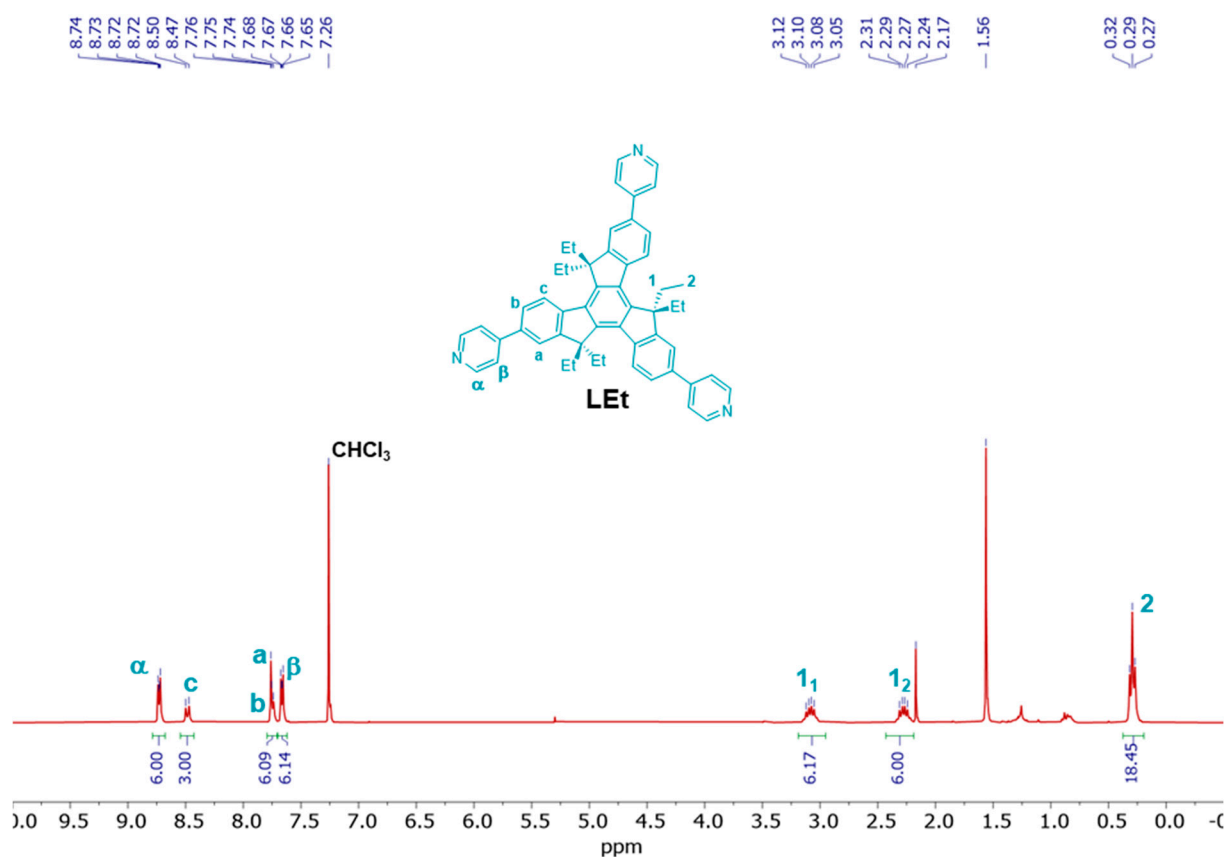
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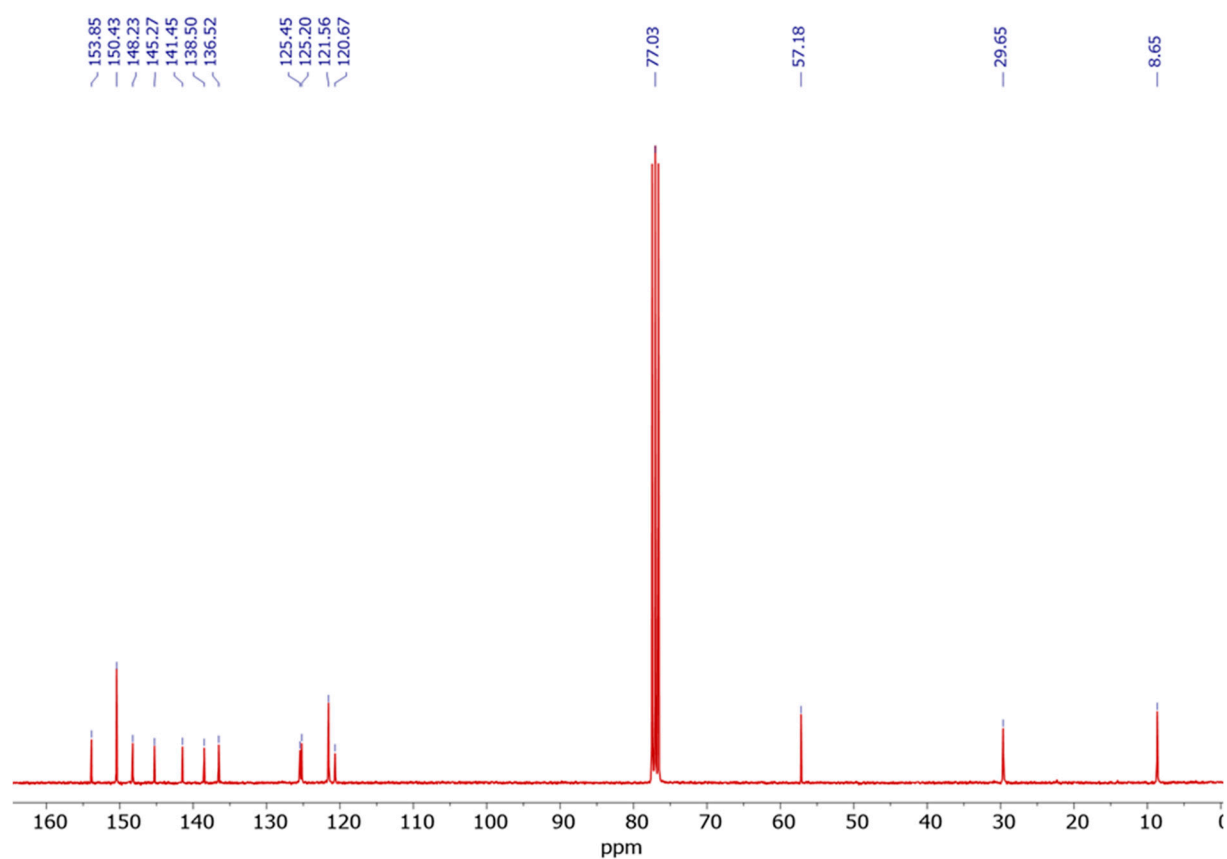
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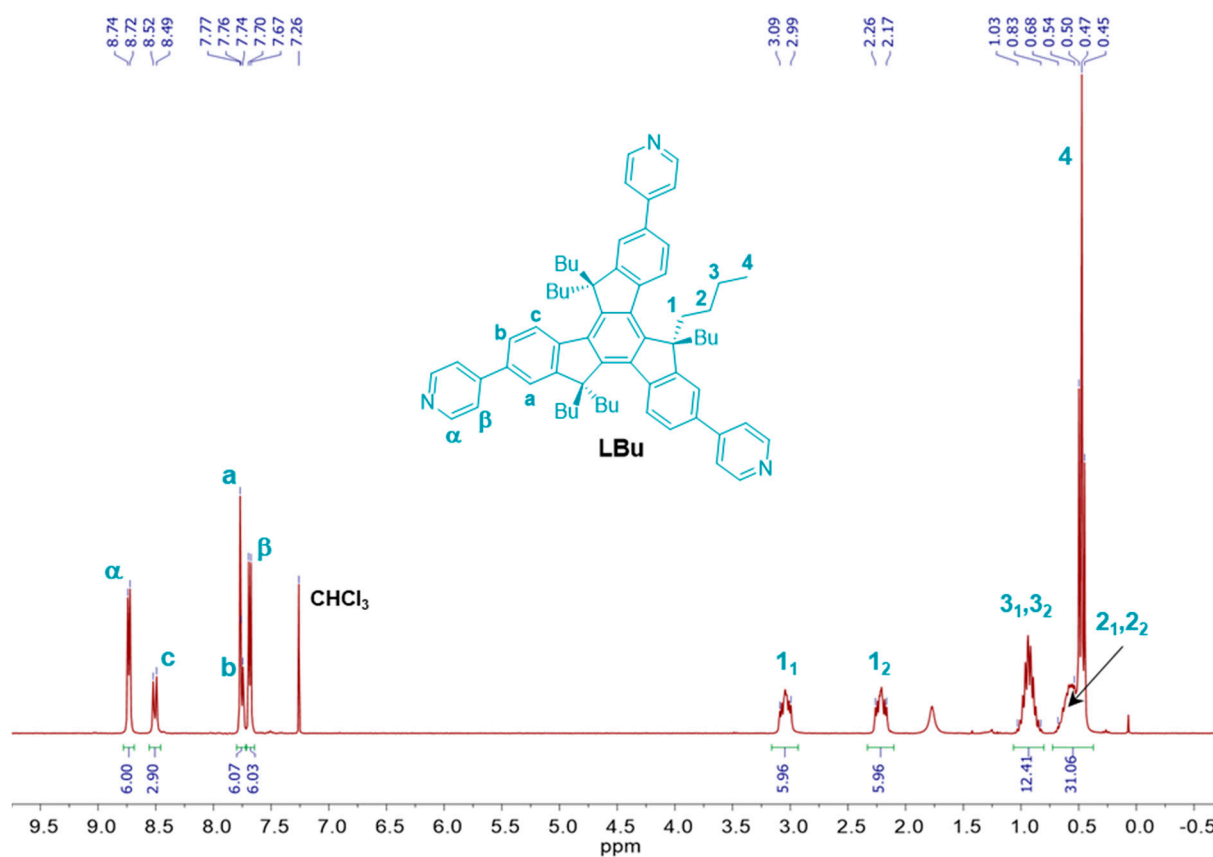
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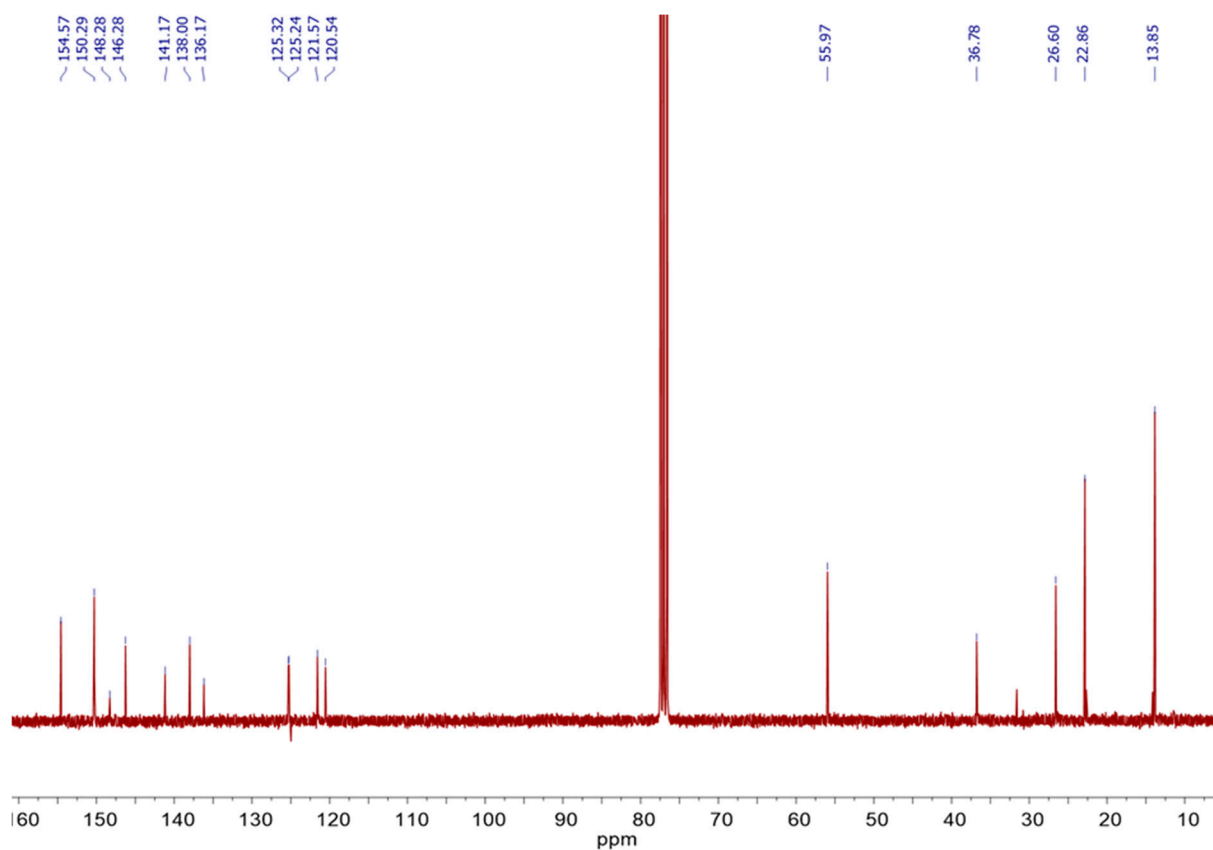
**Figure S1.** <sup>1</sup>H NMR spectrum of ligand **LEt** in CDCl<sub>3</sub>.



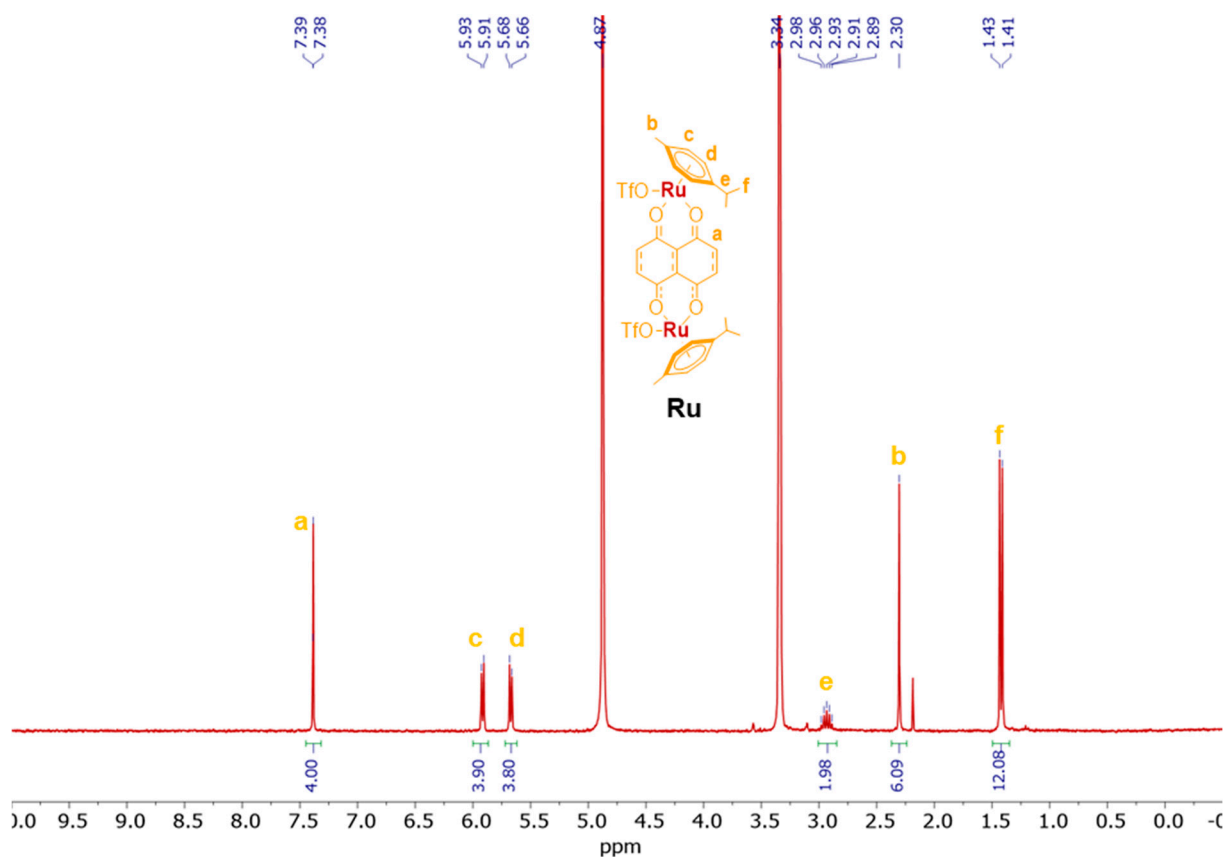
**Figure S2.** <sup>13</sup>C NMR spectrum of ligand **LEt** in CDCl<sub>3</sub>.



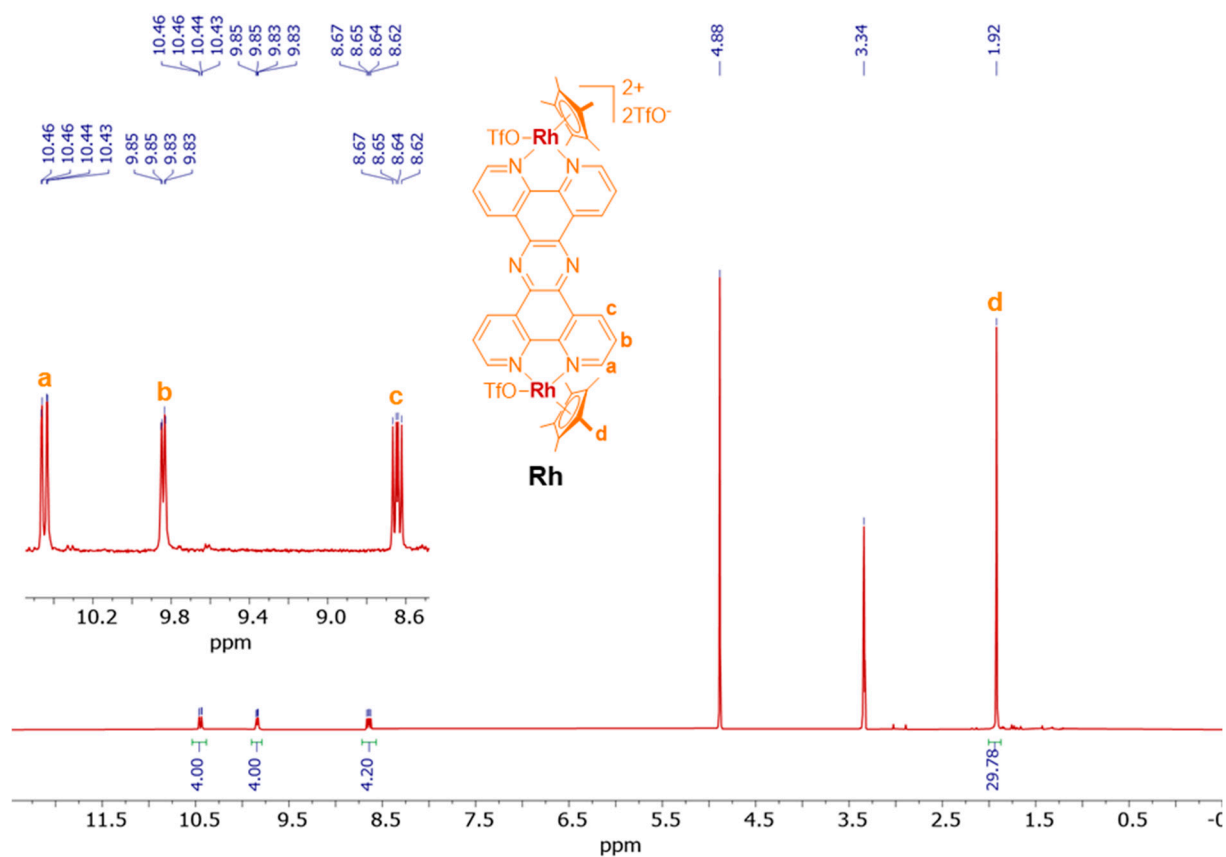
**Figure S3.** <sup>1</sup>H NMR spectrum of ligand **LBU** in CDCl<sub>3</sub>.



**Figure S4.** <sup>13</sup>C NMR spectrum of ligand **LBU** in CDCl<sub>3</sub>.



**Figure S5.**  $^1\text{H}$  NMR spectrum of **Ru** in MeOD.



**Figure S6.**  $^1\text{H}$  NMR spectrum of **Rh** in MeOD.

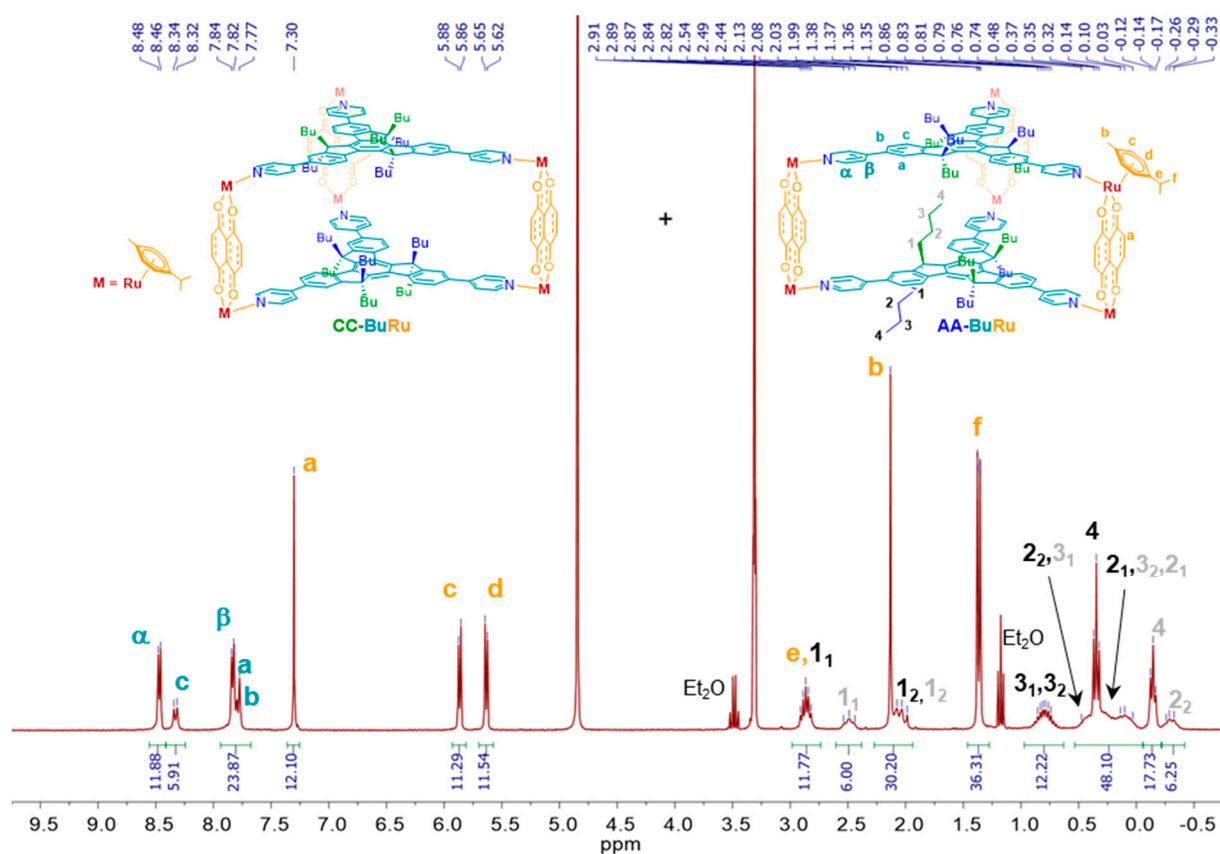


Figure S7.  $^1\text{H}$  NMR spectrum of **BuRu** in  $\text{MeOD}$ .

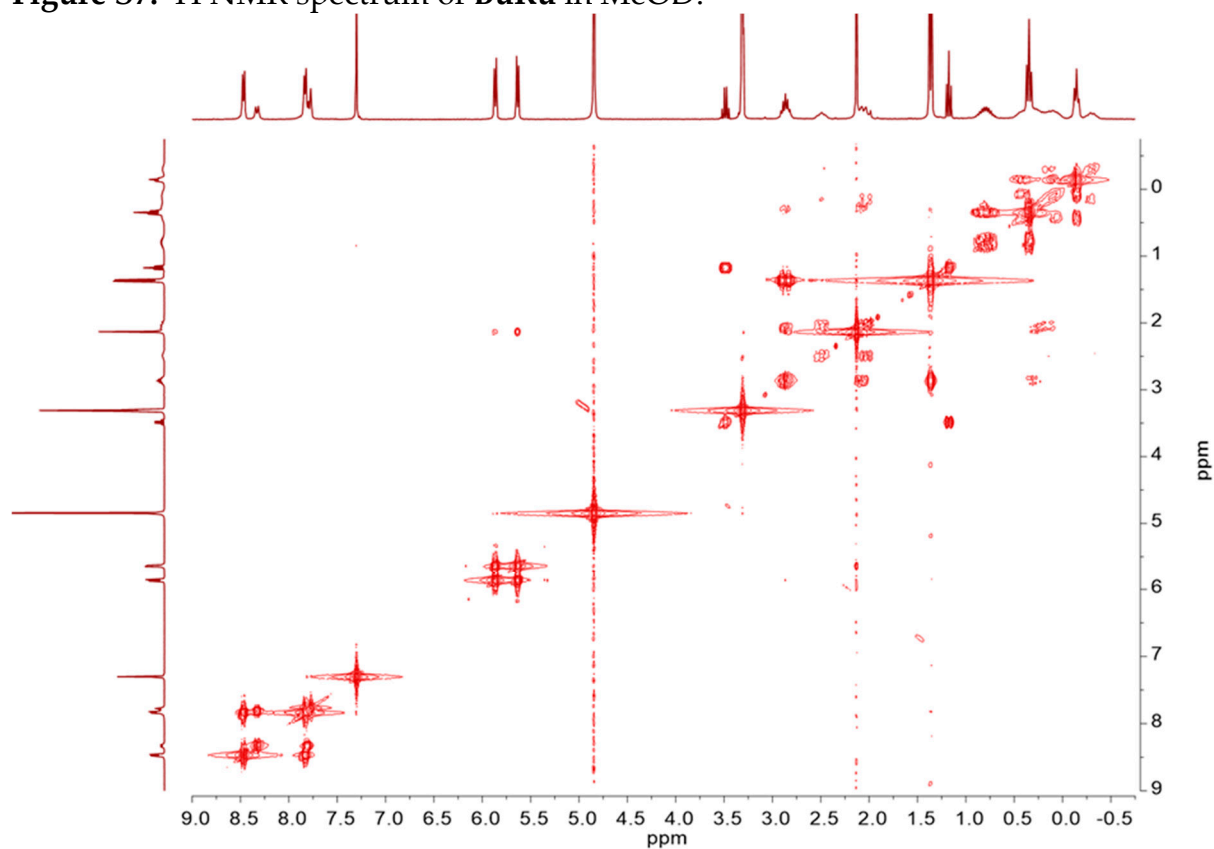
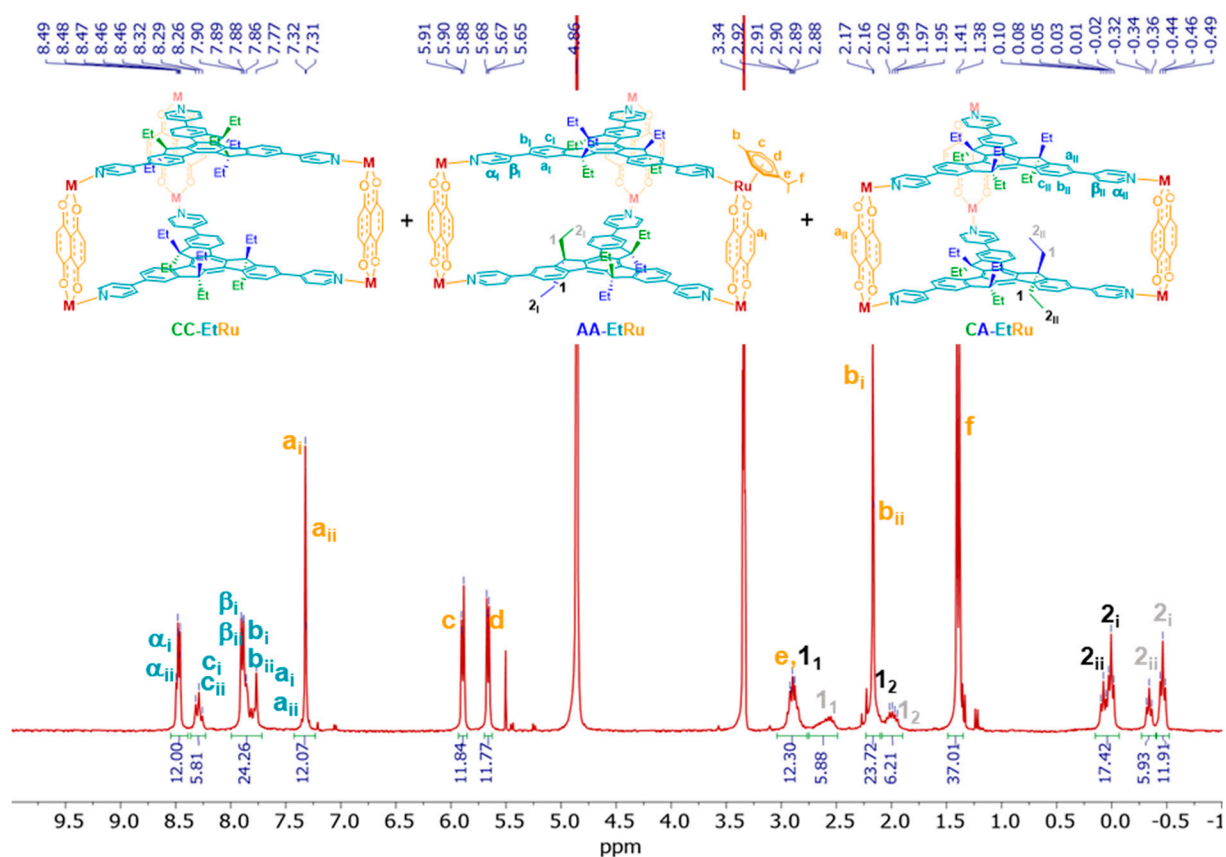
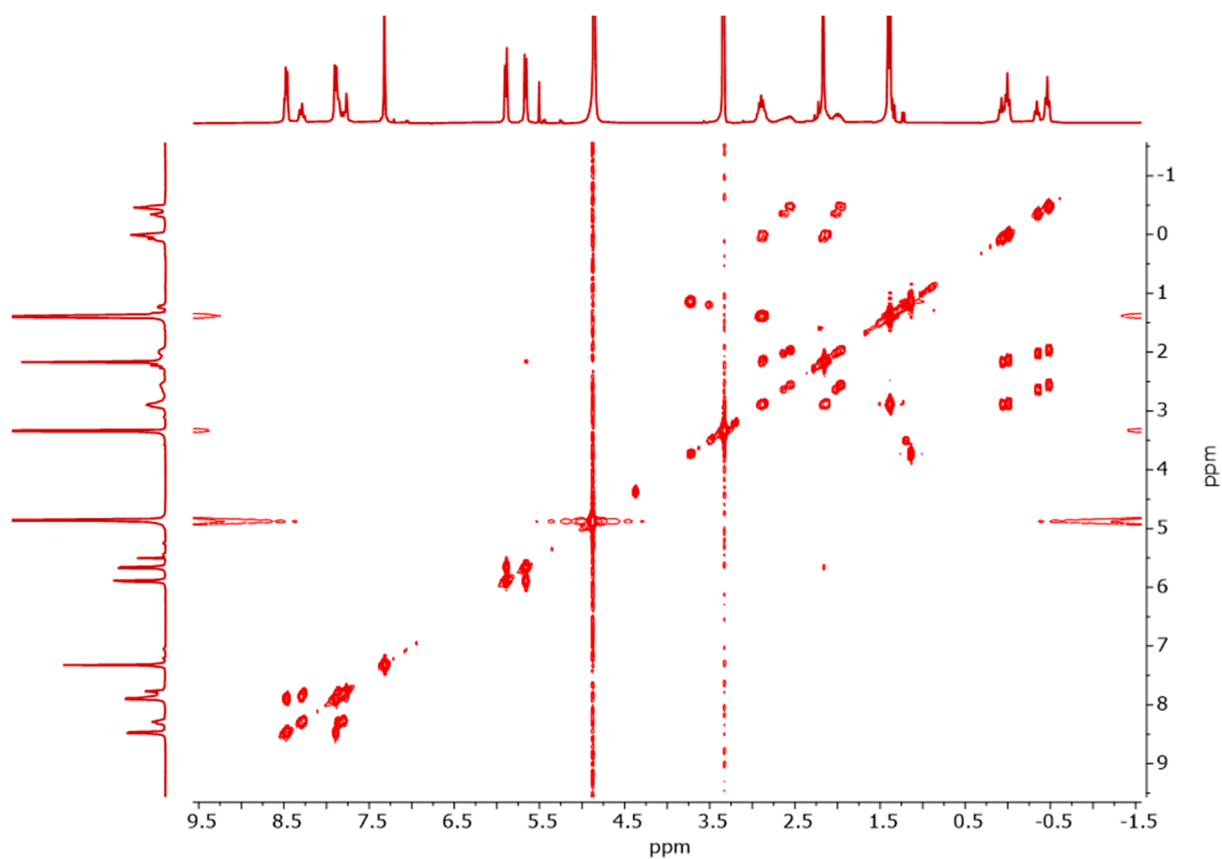


Figure S8.  $^1\text{H}$  COSY NMR spectrum of **BuRu** in  $\text{MeOD}$ .

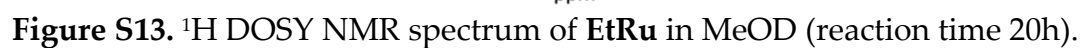




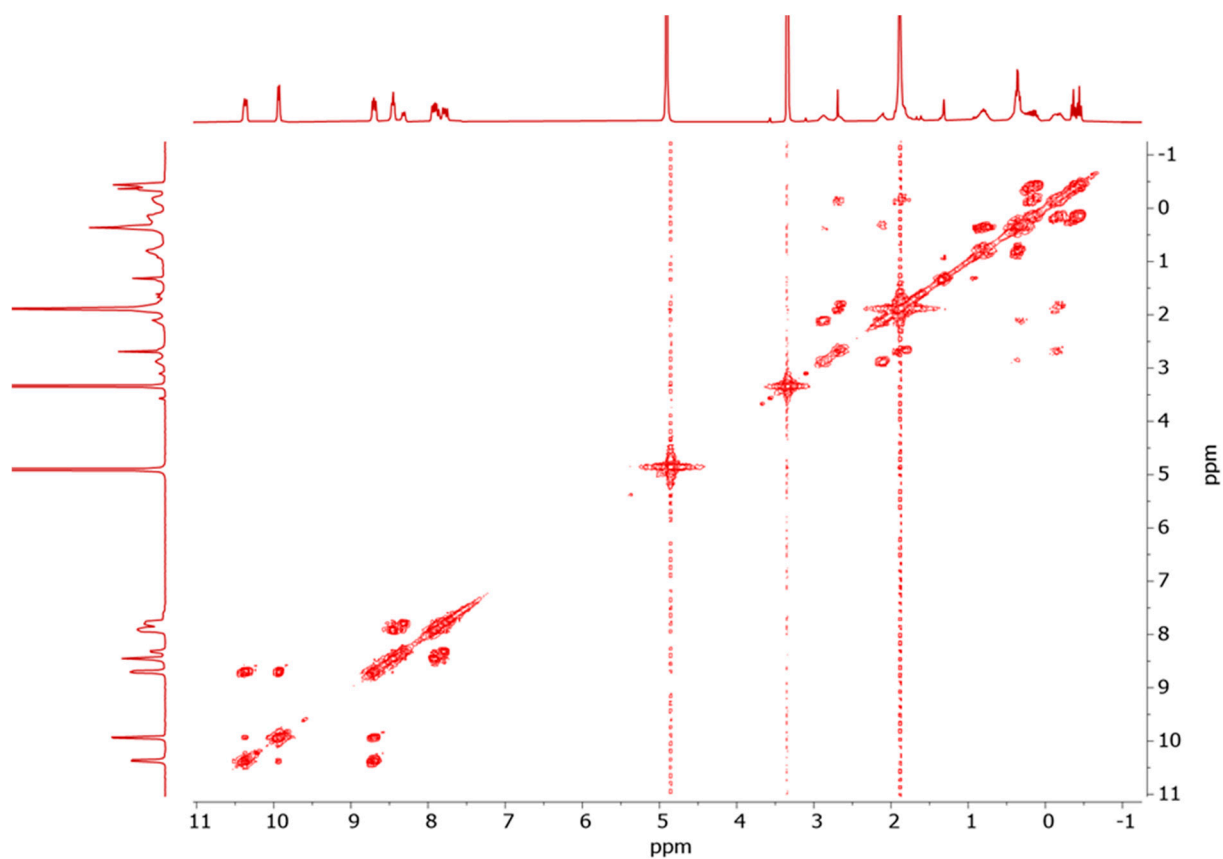
**Figure S11.** <sup>1</sup>H NMR spectrum of EtRu in MeOD (reaction time 20h).



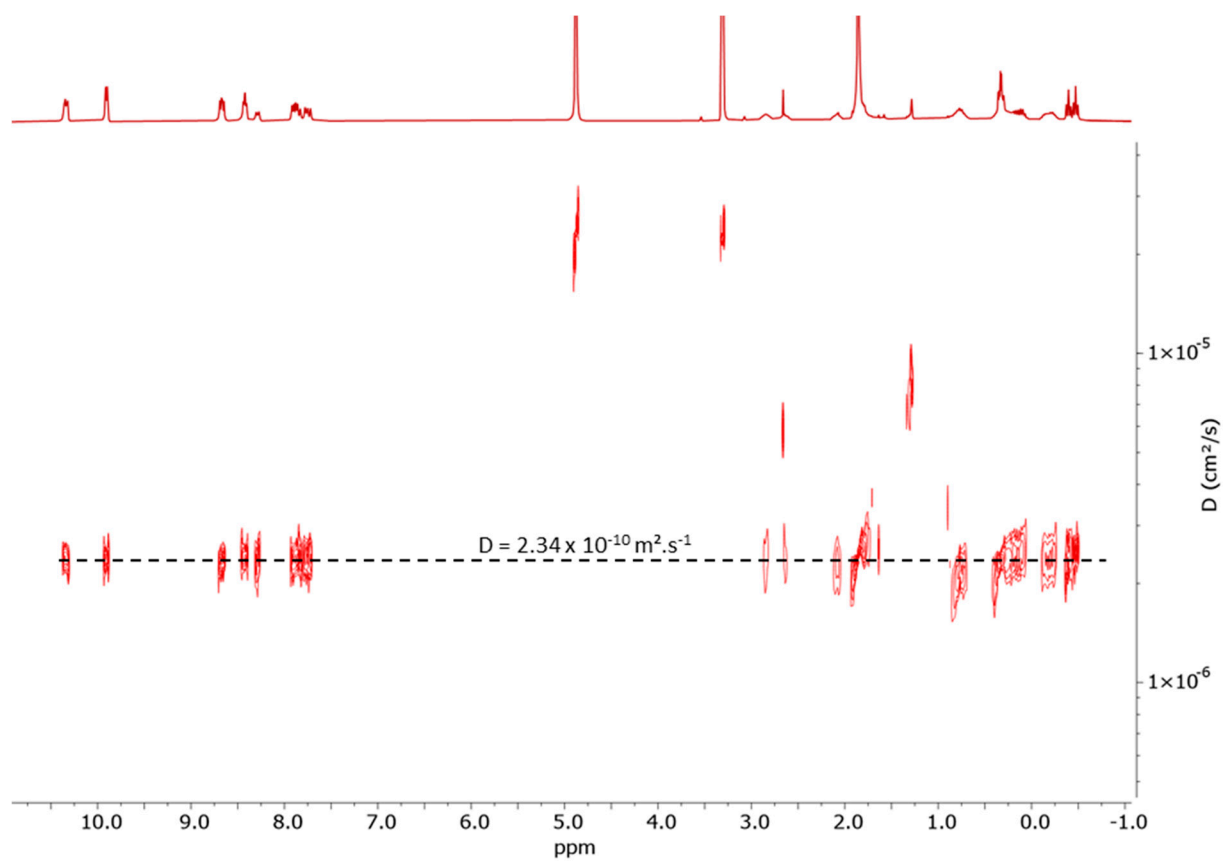
**Figure S12.** <sup>1</sup>H COSY NMR spectrum of EtRu in MeOD (reaction time 20h).



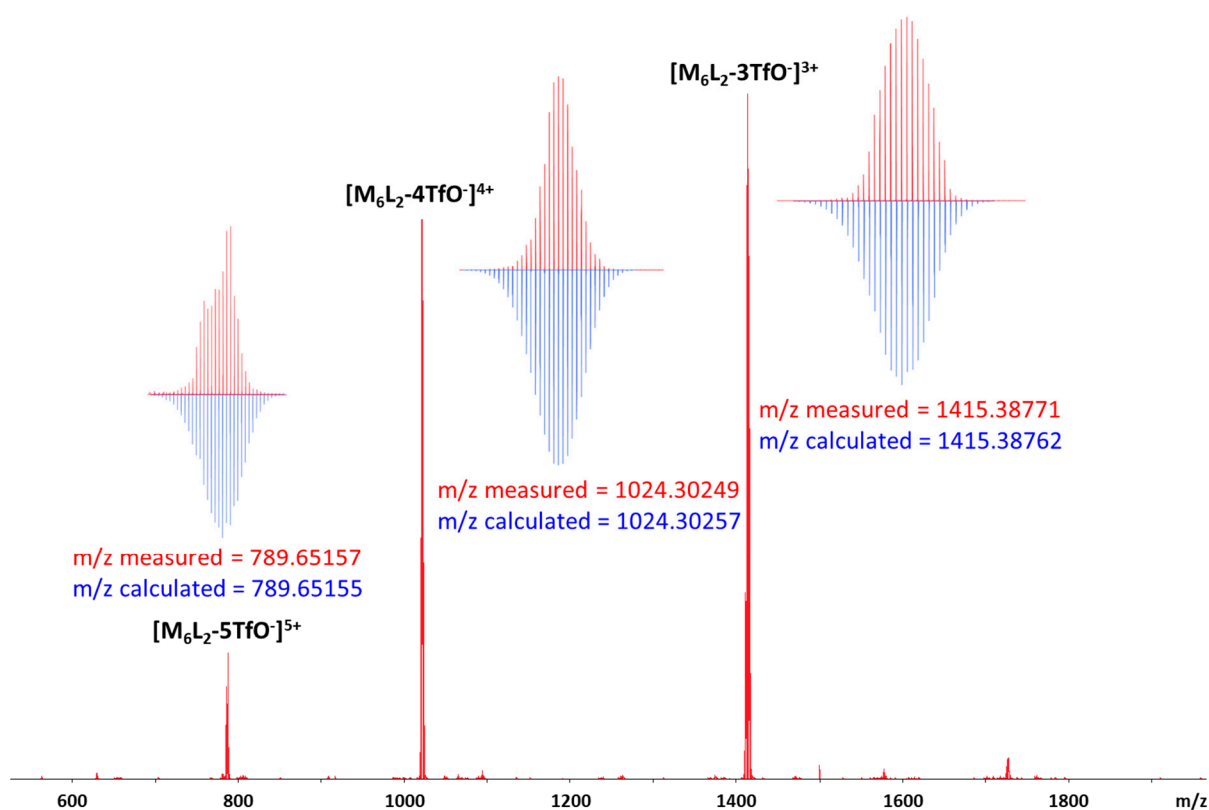




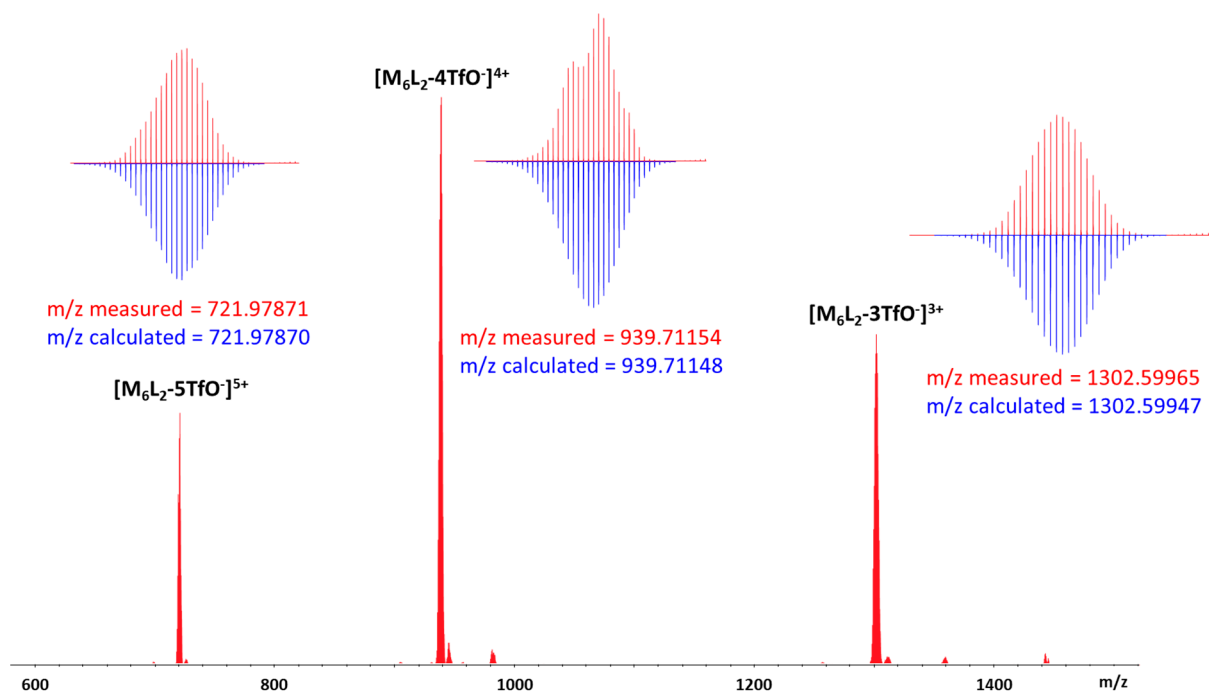
**Figure S15.**  $^1\text{H}$  COSY NMR spectrum of **BuRh** in MeOD.



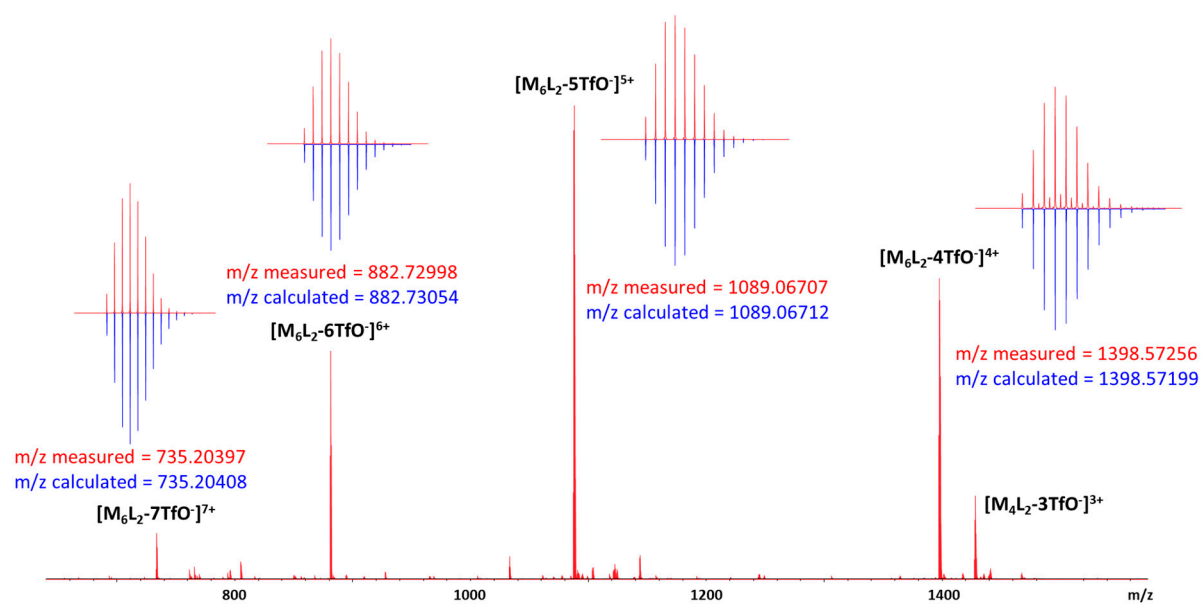
**Figure S16.**  $^1\text{H}$  DOSY NMR spectrum of **BuRh** in MeOD.



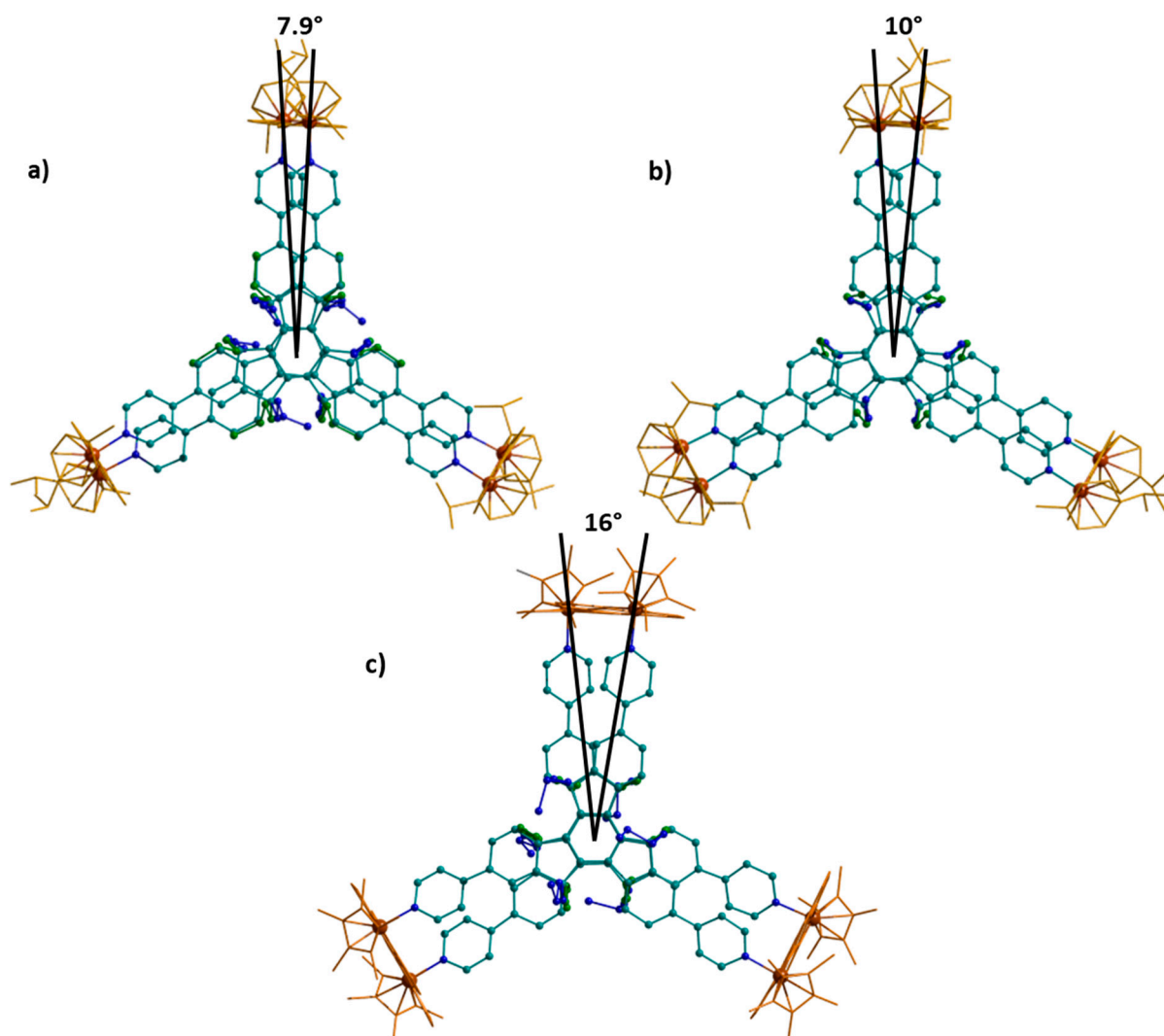
**Figure S17.** ESI-FTICR HRMS spectrum of **BuRu** in MeOH at  $C = 10^{-4}$  M.



**Figure S18.** ESI-FTICR HRMS spectrum of **EtRu** in MeOH at  $C = 10^{-4}$  M.



**Figure S19.** ESI-FTICR HRMS spectrum of **BuRh** in MeOH at  $C = 10^{-4}$  M.



**Figure S20.** Representation of Bailar twist angles in **BuRu** (X-Ray) (a), **EtRu** (MM+) (b) and **BuRh** (X-Ray) (c).