

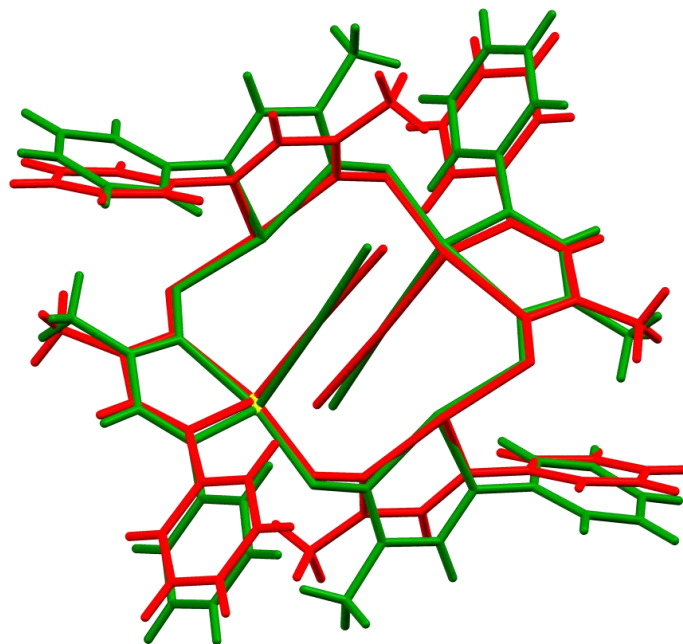
**Structural Diversity of the complexes of monovalent metal  $d^{10}$  ions  
with macrocyclic aggregates of iso-tellurazole *N*-oxides**

Jin Wang, Peter C. Ho, James F. Britten, Valerie Tomassetti and Ignacio Vargas-Baca\*

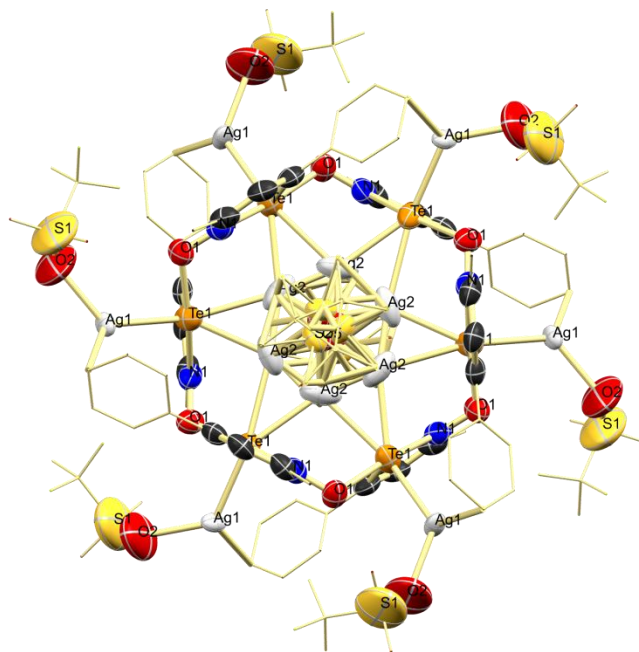
McMaster University, Department of Chemistry and Chemical Biology, 1280 Main Street West,  
Hamilton, Ontario, Canada L0R 1W0.

\* To whom correspondence should be addressed. E-mail: [vargas@chemistry.mcmaster.ca](mailto:vargas@chemistry.mcmaster.ca)

**SUPPLEMENTARY INFORMATION**

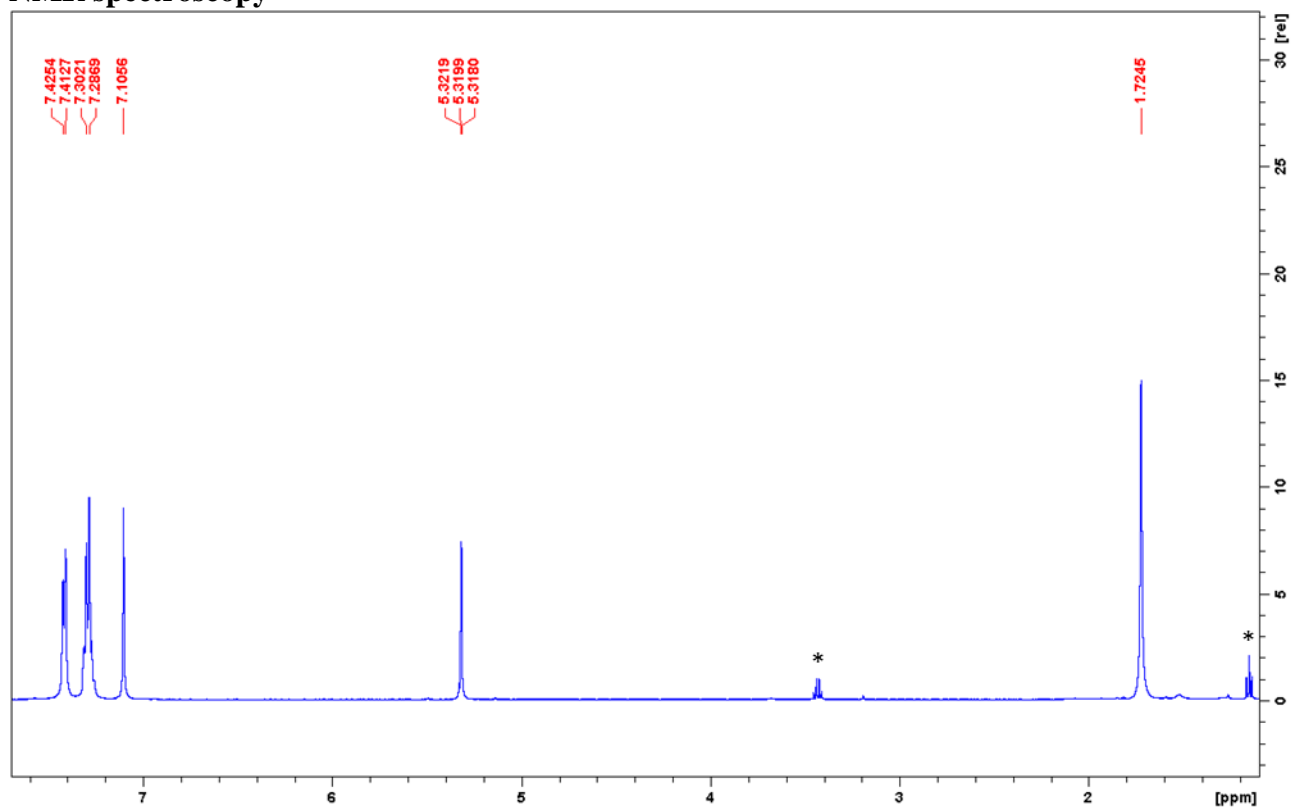


**Figure S1.** Superposition of the two crystallographically independent molecular structures in the crystal of [Au<sub>2</sub>Cl<sub>2</sub>(**1b**<sub>4</sub>)].

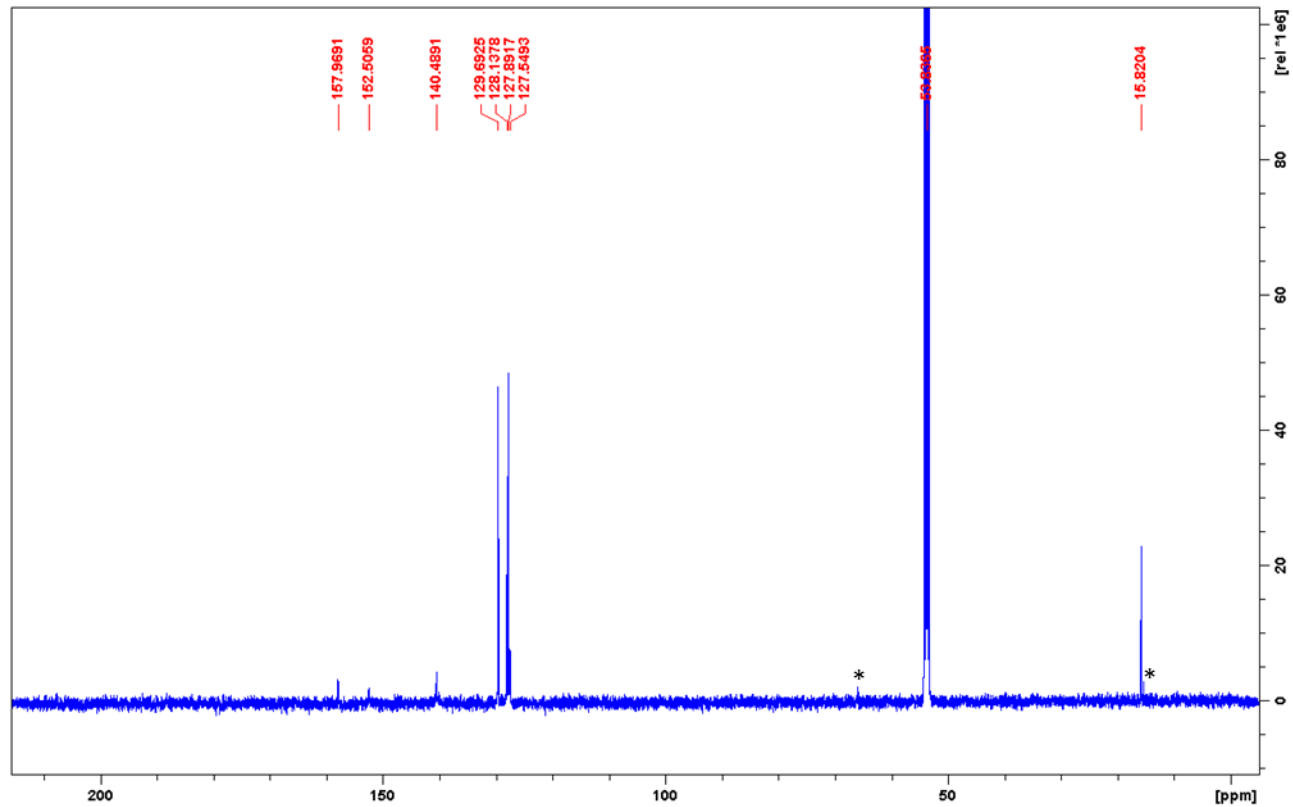


**Figure S2.** ORTEP displaying the superposition of three orientations of the molecular structure of the complex {[Ag<sub>2</sub>(μ-CF<sub>3</sub>SO<sub>3</sub>)<sub>2</sub>(**1b**<sub>6</sub>)]Ag<sub>2</sub>(CF<sub>3</sub>SO<sub>3</sub>)<sub>2</sub>}. Hydrogen atoms, are omitted for clarity; displacement ellipsoids calculated at 75%).

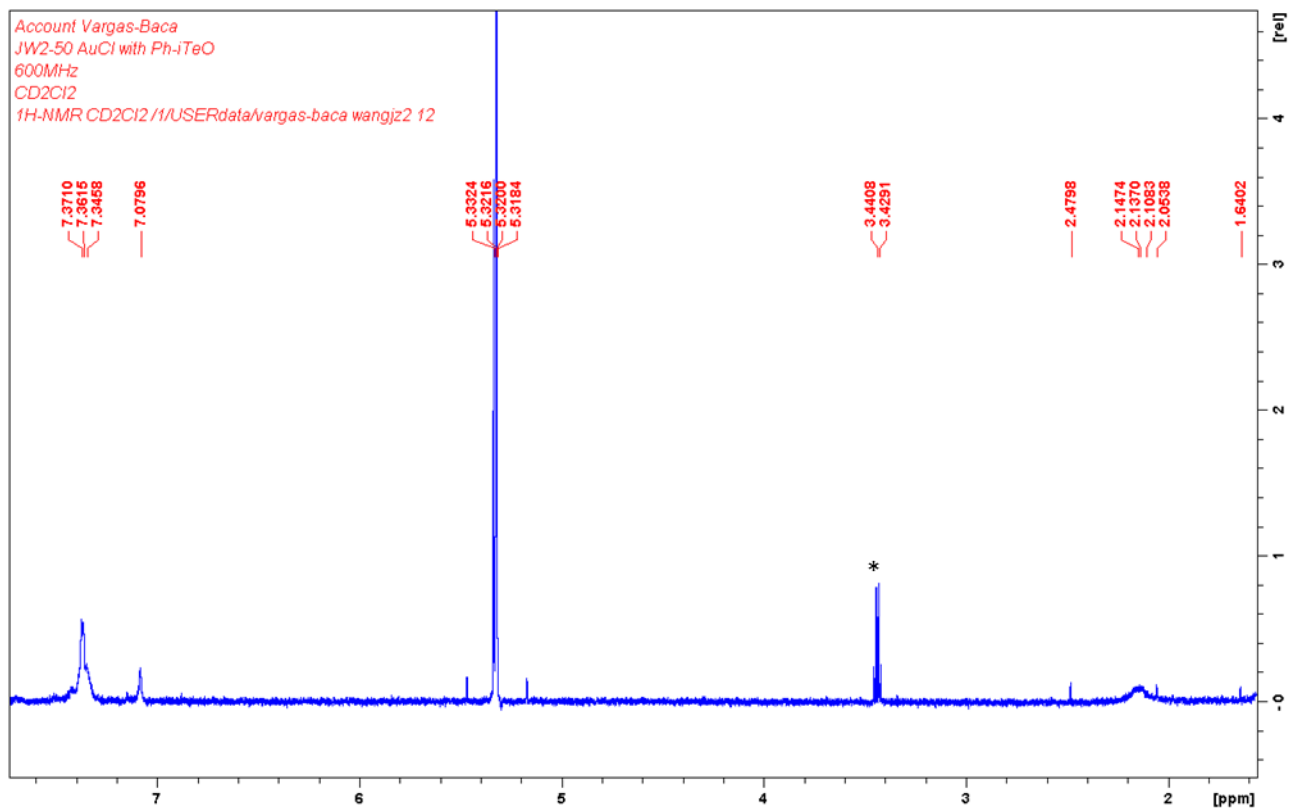
## NMR spectroscopy



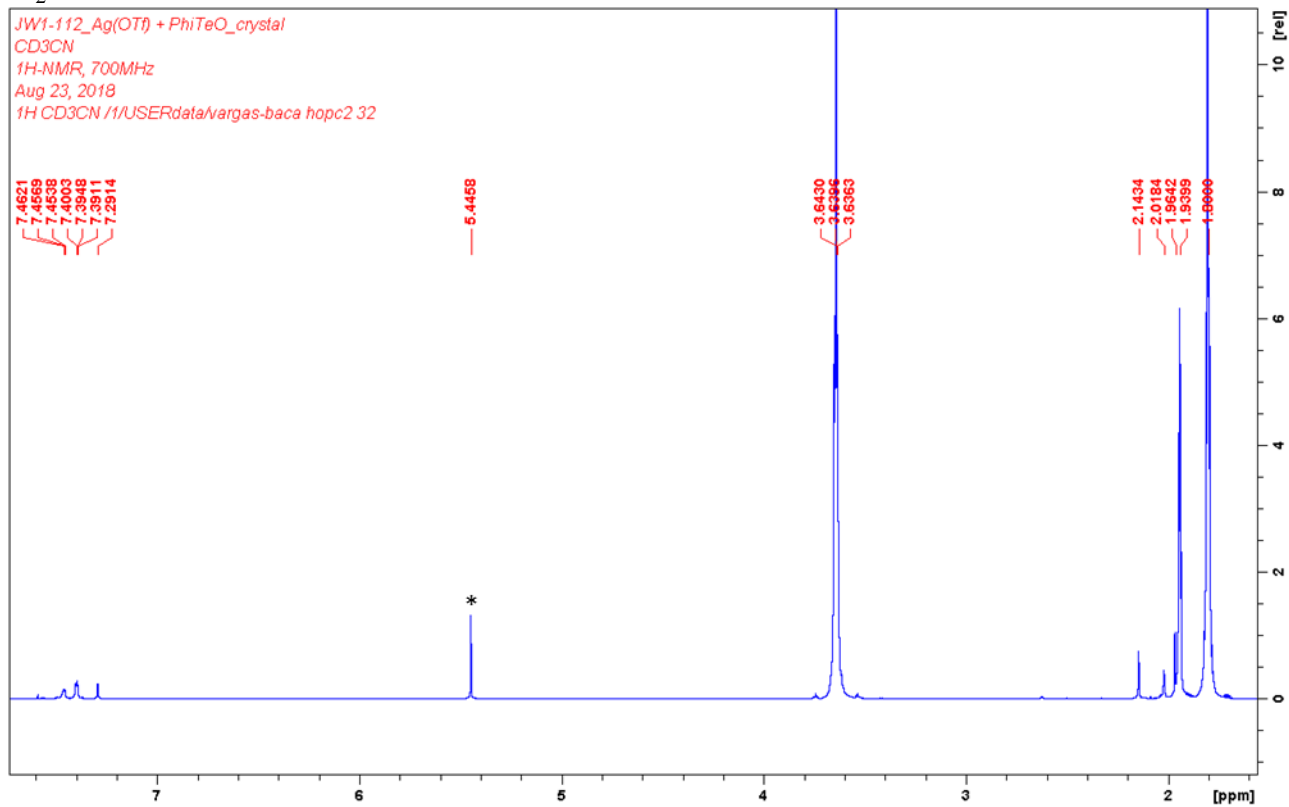
**Figure S3.**  $^1\text{H}$  spectrum of  $[\text{Cu}(\mathbf{1b}_4)(\text{CF}_3\text{SO}_3)]$  in  $\text{CD}_2\text{Cl}_2$ . Asterisks mark the resonances of  $\text{Et}_2\text{O}$  in trace amounts.



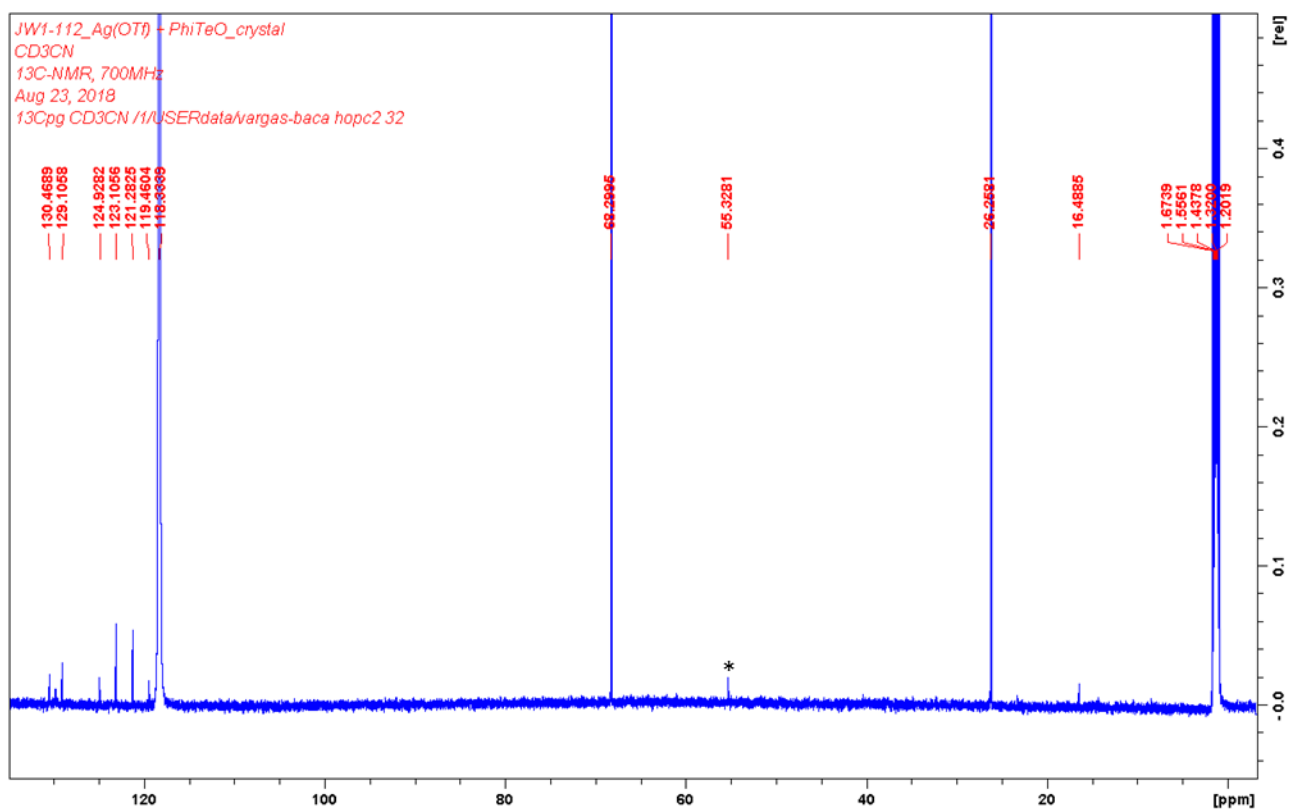
**Figure S4.**  $^{13}\text{C}$  spectrum of  $[\text{Cu}(\mathbf{1b}_4)(\text{CF}_3\text{SO}_3)]$  in  $\text{CD}_2\text{Cl}_2$ . Asterisks mark the resonances of  $\text{Et}_2\text{O}$  in trace amounts.



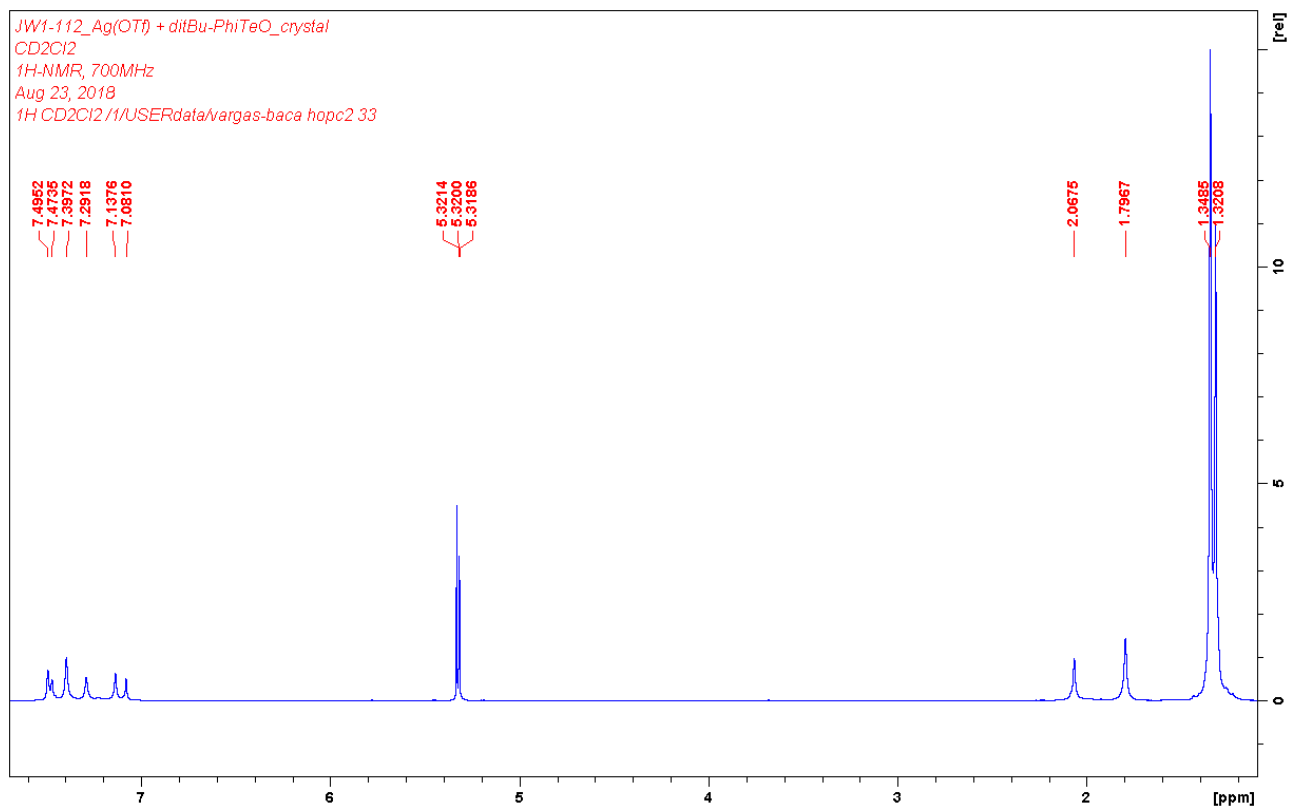
**Figure S5.**  $^1\text{H}$  spectrum of  $[\text{Au}_2\text{Cl}_2(\mathbf{1b}_4)]$  in  $\text{CD}_2\text{Cl}_2$ . The asterisk marks a resonance of residual  $\text{Et}_2\text{O}$ .



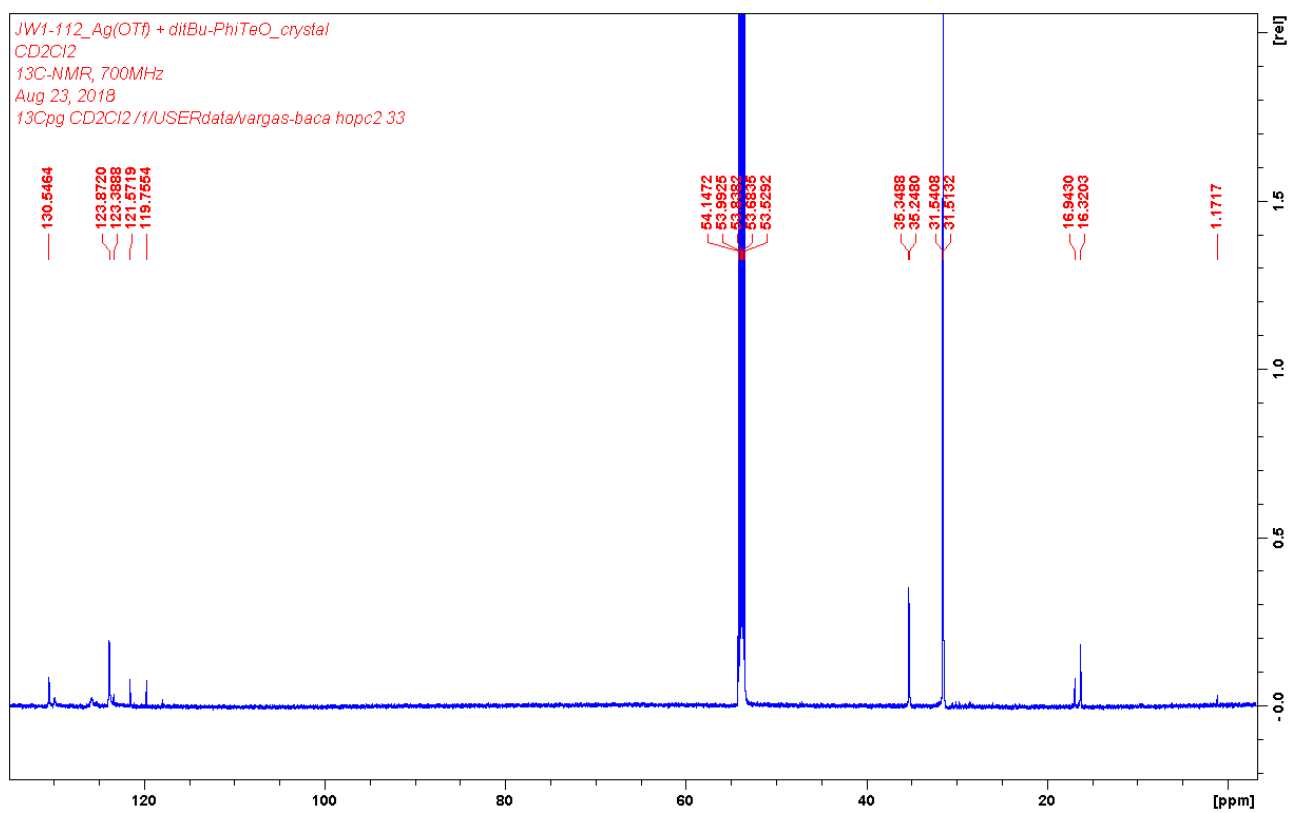
**Figure S6.**  $^1\text{H}$  spectrum of  $\{[\text{Ag}_2(\mu\text{-CF}_3\text{SO}_3)_2(\mathbf{1b}_6)]\text{Ag}_2(\text{CF}_3\text{SO}_3)_2\}$  in  $\text{CD}_3\text{CN}$ . The asterisk marks a resonance of crystallization  $\text{CH}_2\text{Cl}_2$ .



**Figure S7.**  $^{13}\text{C}$  spectrum of  $\{[\text{Ag}_2(\mu\text{-CF}_3\text{SO}_3)_2(\mathbf{1b}_6)]\text{Ag}_2(\text{CF}_3\text{SO}_3)_2\}$  in  $\text{CD}_3\text{CN}$ . The asterisk marks a resonance of crystallization  $\text{CH}_2\text{Cl}_2$ .



**Figure S8.**  $^1\text{H}$  spectrum of  $\{[\text{Ag}_2(\mu\text{-CF}_3\text{SO}_3)_2(\mathbf{1c}_6)]\text{Ag}_2(\text{CF}_3\text{SO}_3)_2\}$  in  $\text{CD}_2\text{Cl}_2$ .



**Figure S9.**  $^{13}\text{C}$  spectrum of  $\{[\text{Ag}_2(\mu\text{-CF}_3\text{SO}_3)_2(\mathbf{1c}_6)]\text{Ag}_2(\text{CF}_3\text{SO}_3)_2\}$  in  $\text{CD}_2\text{Cl}_2$ .