## **Supporting Information**

## Preparation of a Family of Hexanuclear Rhenium Cluster Complexes Containing 5-(Phenyl)tetrazol-2-yl Ligands and Alkylateion of 5-Substituted Tetrazolate Ligands

Jessica L. Durham<sup>†</sup>, Joan N. Tirado<sup>†</sup>, Stanley A. Knott<sup>†</sup>, Meghan K. Oh<sup>†</sup>, Robert McDonald<sup>‡</sup>, and

Lisa F. Szczepura<sup> $\dagger$ </sup>\*

<sup>†</sup>Department of Chemistry, Illinois State University, Normal, IL 61790-4160

<sup>‡</sup>Department of Chemistry, University of Alberta, Edmonton, Alberta T6G 2G2

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**Figure S1.** Cyclic voltammogram of 1 in  $CH_2Cl_2$ .



**Figure S2.** Cyclic voltammogram of **2** in CH<sub>2</sub>Cl<sub>2</sub>.



Figure S3. Cyclic voltammogram of 3 in  $CH_2Cl_2$ .



**Figure S4**. Cyclic voltammogram of 4 in  $CH_2Cl_2$ .



**Figure S5**. Cyclic voltammogram of **5** in CH<sub>2</sub>Cl<sub>2</sub>.



**Figure S6**. The <sup>31</sup>P NMR Spectra of **3** and **5** in CD<sub>3</sub>CN at 7 weeks.



**Figure S7.** <sup>31</sup>P NMR Spectra of  $[Re_6Se_8(PEt_3)_5(p-methoxybenzonitrile)](BF_4)_2$  in CD<sub>3</sub>CN taken at different time intervals.



**Figure S8**. <sup>31</sup>P NMR Spectra of  $[\text{Re}_6\text{Se}_8(\text{PEt}_3)_5(\text{NCPh})](\text{BF}_4)_2$  and NaN<sub>3</sub> in acetone- $d_6$  recorded at different time intervals.



**Figure S9.** Simulated and actual <sup>1</sup>H NMR spectra of the of  $[Re_6Se_8(PEt_3)_5(p-nitrophenyltetrazolate)](BF_4)$  complex. The simulation was obtained using Bruker Topspin 2.1 Daisy simulation software.





**Figure S10.** UV-Vis Spectra of 1 in CH<sub>2</sub>Cl<sub>2</sub>.



Figure S11. UV-Vis Spectra of 2 and 7 in  $CH_2Cl_2$ .



Figure S12. UV-Vis Spectra of 3 and 8 in  $CH_2Cl_2$ .



**Figure S13.** UV-Vis Spectra of 4 and 9 in  $CH_2Cl_2$ .



Figure S14. UV-Vis Spectra of 5 and 10 in  $CH_2Cl_2$ .



**Figure S15.** <sup>1</sup>H NMR spectra at different time intervals of the reaction mixture containing  $[Re_6Se_8(PEt_3)_5(2,5-phenyltetrazolate)](BF_4)$  and MeI in CDCl<sub>3</sub>.



**Figure S16.** <sup>31</sup>P NMR spectra at different time intervals of the reaction mixture containing  $[Re_6Se_8(PEt_3)_5(2,5-phenyltetrazolate)](BF_4)$  and BnBr in CDCl<sub>3</sub>.



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**Figure S17.** <sup>1</sup>H NMR spectrum of the reaction mixture containing  $[Re_6Se_8(PEt_3)_5(1,5-methyltetrazolate)](BF_4)$  and MeI in CDCl<sub>3</sub> taken at 24 h. Resonances marked with \* are assigned to the 1-methyl-5-methyltetrazole and 2-methyl-5-methyltetrazole.



**Figure S18.** <sup>31</sup>P NMR spectra at different time intervals of the reaction mixture containing  $[Re_6Se_8(PEt_3)_5(1,5-methyltetrazolate)](BF_4)$  and BnBr in CDCl<sub>3</sub>.

