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

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Table of Contents

Figure S1.	Cyclic voltammogram of 1 in CH ₂ Cl ₂ .	S 3
Figure S2.	Cyclic voltammogram of 2 in CH ₂ Cl ₂ .	S 4
Figure S3.	Cyclic voltammogram of 3 in CH ₂ Cl ₂ .	S 5
Figure S4.	Cyclic voltammogram of 4 in CH ₂ Cl ₂ .	S 6
Figure S5.	Cyclic voltammogram of 5 in CH ₂ Cl ₂ .	S 7
Figure S6.	The ³¹ P NMR Spectra of 3 and 5 in CD_3CN at 7 weeks.	S 8
Figure S7.	³¹ P NMR Spectra of [Re ₆ Se ₈ (PEt ₃) ₅ (<i>p</i> -methoxybenzonitrile)](BF ₄) ₂	
	in CD ₃ CN taken at different time intervals.	S 9
Figure S8.	31 P NMR Spectra of [Re ₆ Se ₈ (PEt ₃) ₅ (NCPh)](BF ₄) ₂ and NaN ₃ in acetone-d	l_6
	recorded at different time intervals.	S 10
Figure S9.	Simulated and actual ¹ H NMR spectra of the of $[Re_6Se_8(PEt_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)_5(p-t_3)$	
	nitrophenyltetrazolate)](BF_4) complex. The simulation was obtained	
	using Bruker Topspin 2.1 Daisy simulation software.	S11
Figure S10.	UV-Vis Spectra of 1 in CH ₂ Cl ₂ .	S12
Figure S11.	UV-Vis Spectra of 2 and 7 in CH ₂ Cl ₂ .	S13

Figure S12.	UV-Vis Spectra of 3 and 8 in CH_2Cl_2 .	S14
Figure S13.	UV-Vis Spectra of 4 and 9 in CH_2Cl_2 .	S15
Figure S14.	UV-Vis Spectra of 5 and 10 in CH_2Cl_2 .	S16
Figure S15.	¹ H NMR spectra at different time intervals of the reaction	
	mixture containing [Re ₆ Se ₈ (PEt ₃) ₅ (2,5-phenyltetrazolate)](BF ₄)	
	and MeI in CDCl ₃ .	S17
Figure S16.	³¹ 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 ₃ .	S18
Figure S17.	¹ H NMR spectrum of the reaction mixture containing	
	$[Re_6Se_8(PEt_3)_5(1,5-methyltetrazolate)](BF_4)$ and MeI in CDCl ₃ taken	
	at 24 h. Resonances marked with * are assigned to the 1-methyl-5-	
	methyltetrazole and 2-methyl-5-methyltetrazole.	S19
Figure S18.	³¹ 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 ₃ .	S20

Figure S1. Cyclic voltammogram of 1 in CH_2Cl_2 .



Figure S2. Cyclic voltammogram of **2** in CH₂Cl₂.



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 CH₂Cl₂.



Figure S6. The ³¹P NMR Spectra of **3** and **5** in CD₃CN at 7 weeks.



Figure S7. ³¹P NMR Spectra of $[Re_6Se_8(PEt_3)_5(p-methoxybenzonitrile)](BF_4)_2$ in CD₃CN taken at different time intervals.



Figure S8. ³¹P NMR Spectra of $[\text{Re}_6\text{Se}_8(\text{PEt}_3)_5(\text{NCPh})](\text{BF}_4)_2$ and NaN₃ in acetone- d_6 recorded at different time intervals.



Figure S9. Simulated and actual ¹H 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 CH₂Cl₂.



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. ¹H 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 CDCl₃.



Figure S16. ³¹P 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 CDCl₃.



S18

Figure S17. ¹H NMR spectrum of the reaction mixture containing $[Re_6Se_8(PEt_3)_5(1,5-methyltetrazolate)](BF_4)$ and MeI in CDCl₃ taken at 24 h. Resonances marked with * are assigned to the 1-methyl-5-methyltetrazole and 2-methyl-5-methyltetrazole.



Figure S18. ³¹P 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 CDCl₃.

