

Supporting Information

Small Molecule Activation of Nitriles Coordinated to the $[\text{Re}_6\text{Se}_8]^{2+}$ Core: Formation of Carboxamide, Oxazine and Oxazoline Complexes

Colleen P. Chin, YiXin Ren, Joan Berry, Stanley A. Knott, Craig C. McLauchlan, Lisa F. Szczepura*

Department of Chemistry, Illinois State University, Normal, IL 61790-4160

Figure S1. 202.5 MHz ^{31}P $\{^1\text{H}\}$ NMR spectral data of samples taken at different time intervals in the room temperature UV-irradiation of $\mathbf{3}^{2+}$ in CD_3CN .

Figure S2. 500 MHz ^1H NMR spectral data of samples taken at different time intervals in the room temperature UV-irradiation of $\mathbf{3}^{2+}$ in CD_3CN .

Figure S3. 202.5 MHz ^{31}P $\{^1\text{H}\}$ NMR spectral data of samples taken at different time intervals in the room temperature UV-irradiation of $\mathbf{4}^{2+}$ in CD_3CN .

Figure S4. 500 MHz ^1H NMR spectral data of samples taken at different time intervals in the room temperature UV-irradiation of $\mathbf{4}^{2+}$ in CD_3CN .

Figure S5. 202.5 MHz ^{31}P $\{^1\text{H}\}$ NMR spectral data of samples taken at different time intervals in the room temperature UV-irradiation of $\mathbf{5}^{2+}$ in CD_3CN .

Figure S6. 500 MHz ^1H NMR spectral data of samples taken at different time intervals in the room temperature UV-irradiation of $\mathbf{5}^{2+}$ in CD_3CN .

Figure S7. 202.5 MHz ^{31}P $\{^1\text{H}\}$ NMR spectral data of samples taken at different time intervals in the heating of $\mathbf{3}^{2+}$ in CD_3CN (no reaction occurred).

Figure S8. 500 MHz ^1H NMR spectral data of samples taken at different time intervals in the heating of $\mathbf{3}^{2+}$ in CD_3CN (no reaction occurred).

Figure S9. 202.5 MHz ^{31}P $\{^1\text{H}\}$ NMR spectral data of samples taken at different time intervals in the heating of $\mathbf{4}^{2+}$ in CD_3CN .

Figure S10. 500 MHz ^1H NMR spectral data of samples taken at different time intervals in the heating of $\mathbf{4}^{2+}$ in CD_3CN .

Figure S11. 202.5 MHz ^{31}P $\{^1\text{H}\}$ NMR spectral data of samples taken at different time intervals in the heating of $\mathbf{5}^{2+}$ in CD_3CN .

Figure S12. 500 MHz ^1H NMR spectral data of samples taken at different time intervals in the heating of $\mathbf{5}^{2+}$ in CD_3CN .

Figure S13. Displacement ellipsoid plot (50%) of $\mathbf{5}(\text{BF}_4)_2$ showing the full disordered model of $\mathbf{5}^{2+}$ and the crystallographically unique BF_4^- .

Figure S14. Displacement ellipsoid plot (50%) of $\mathbf{7}(\text{BF}_4)$.

Figure S15. Space filling diagram of $\mathbf{5}^{2+}$.

Figure S16. UV-vis spectrum of $[\text{Re}_6\text{Se}_8(\text{PET}_3)_5(2\text{-methyloxazine})](\text{SbF}_6)_2$ ($\mathbf{5}(\text{SbF}_6)_2$) in CH_3CN with a concentration of 1.58×10^{-5} M.

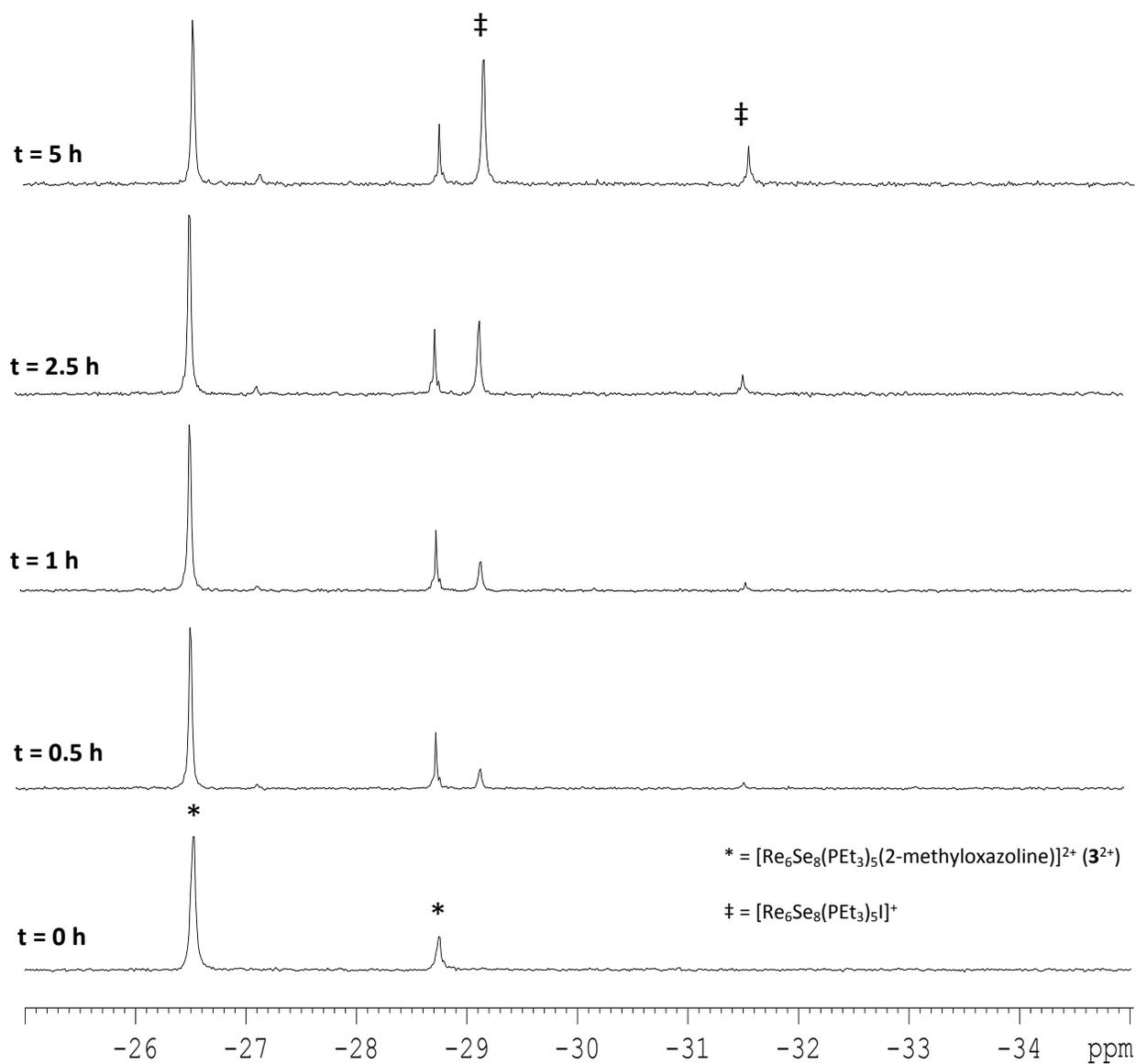


Figure S1. 202.5 MHz ^{31}P $\{^1\text{H}\}$ NMR spectral data of samples taken at different time intervals in room temperature the UV-irradiation of $\mathbf{3}^{2+}$ in CD_3CN .

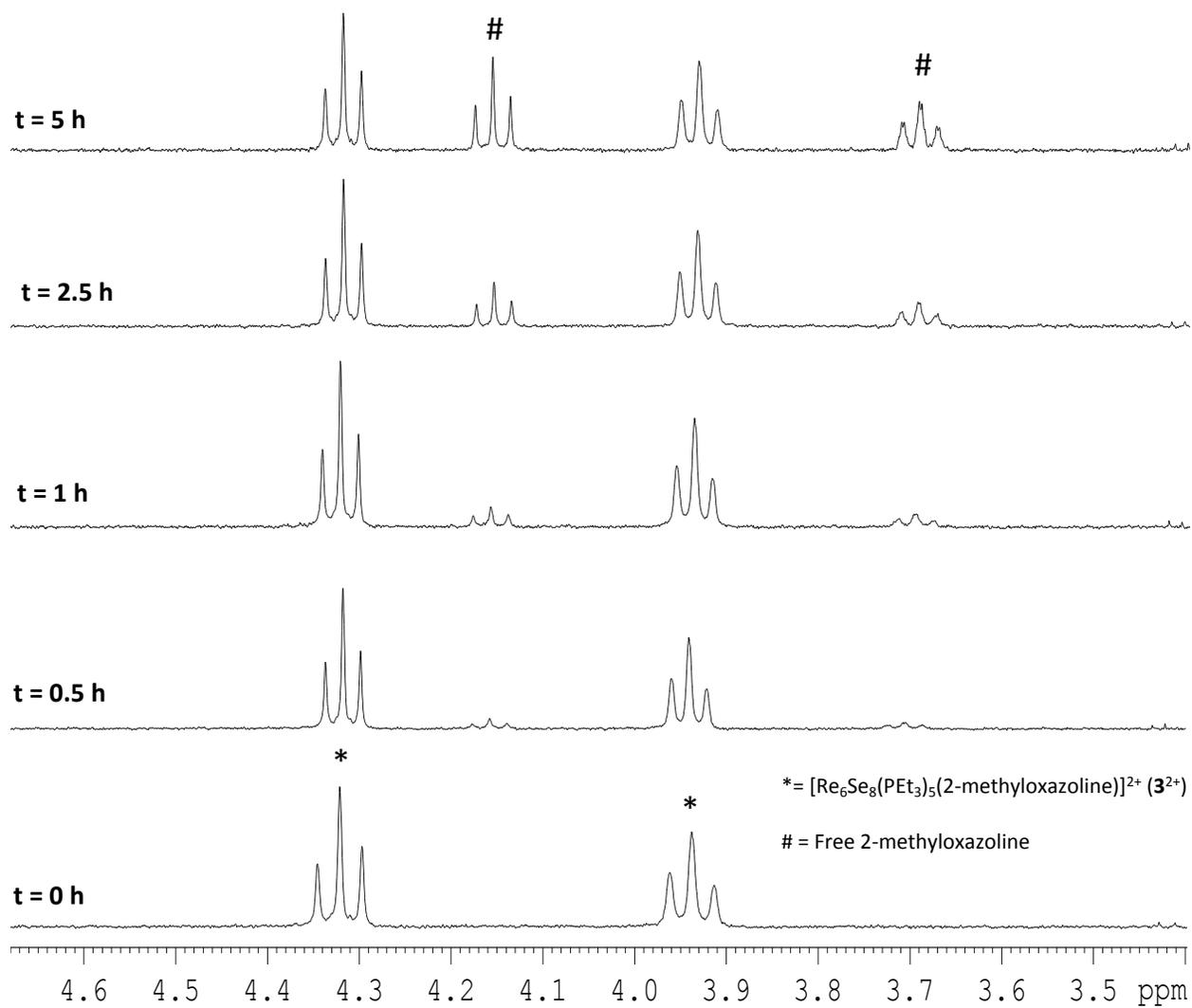


Figure S2. 500 MHz ^1H NMR spectral data of samples taken at different time intervals in the room temperature UV-irradiation of $\mathbf{3}^{2+}$ in CD_3CN .

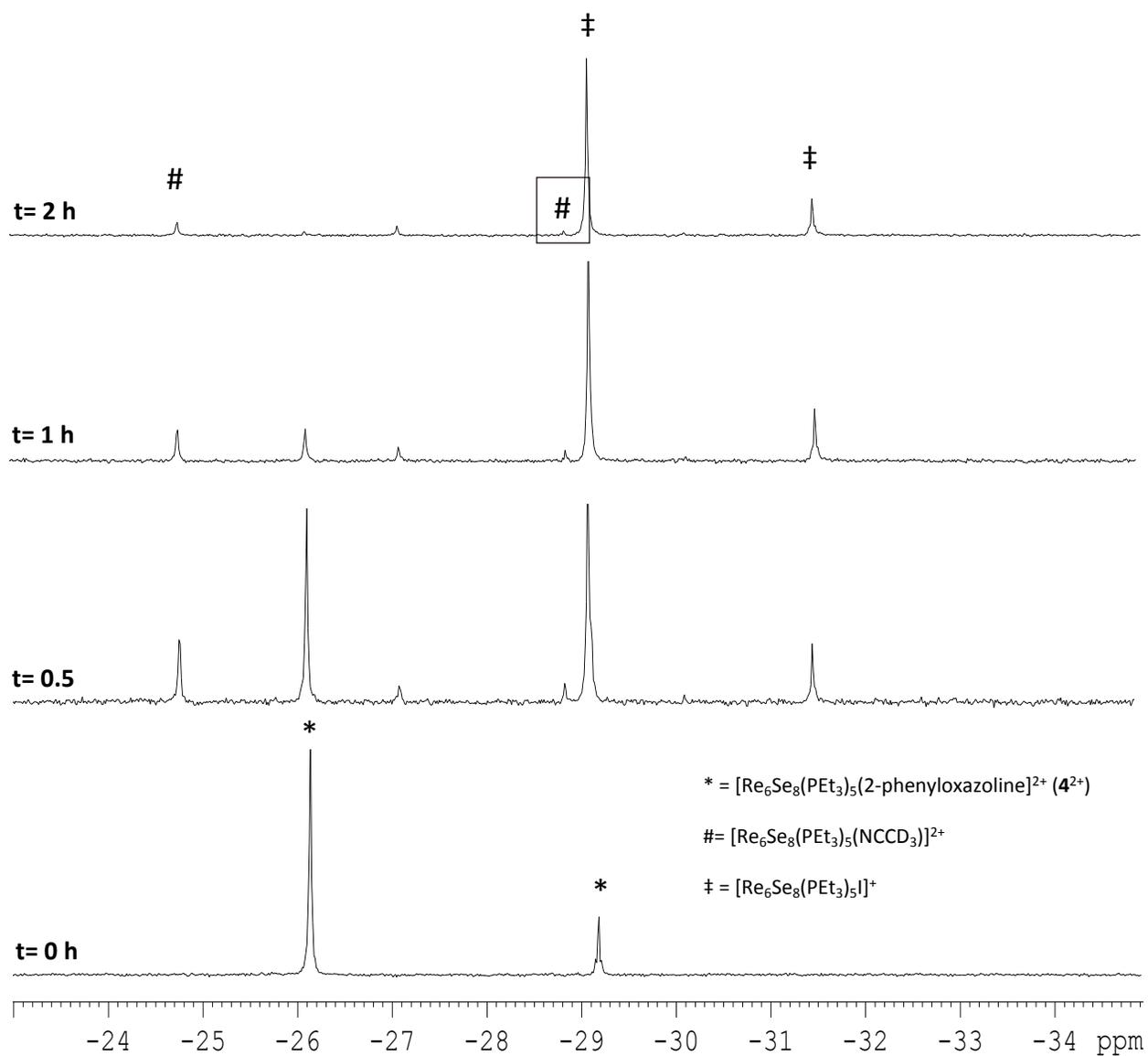


Figure S3. 202.5 MHz ^{31}P $\{^1\text{H}\}$ NMR spectral data of samples taken at different time intervals in room temperature the UV-irradiation of $\mathbf{4}^{2+}$ in CD_3CN .

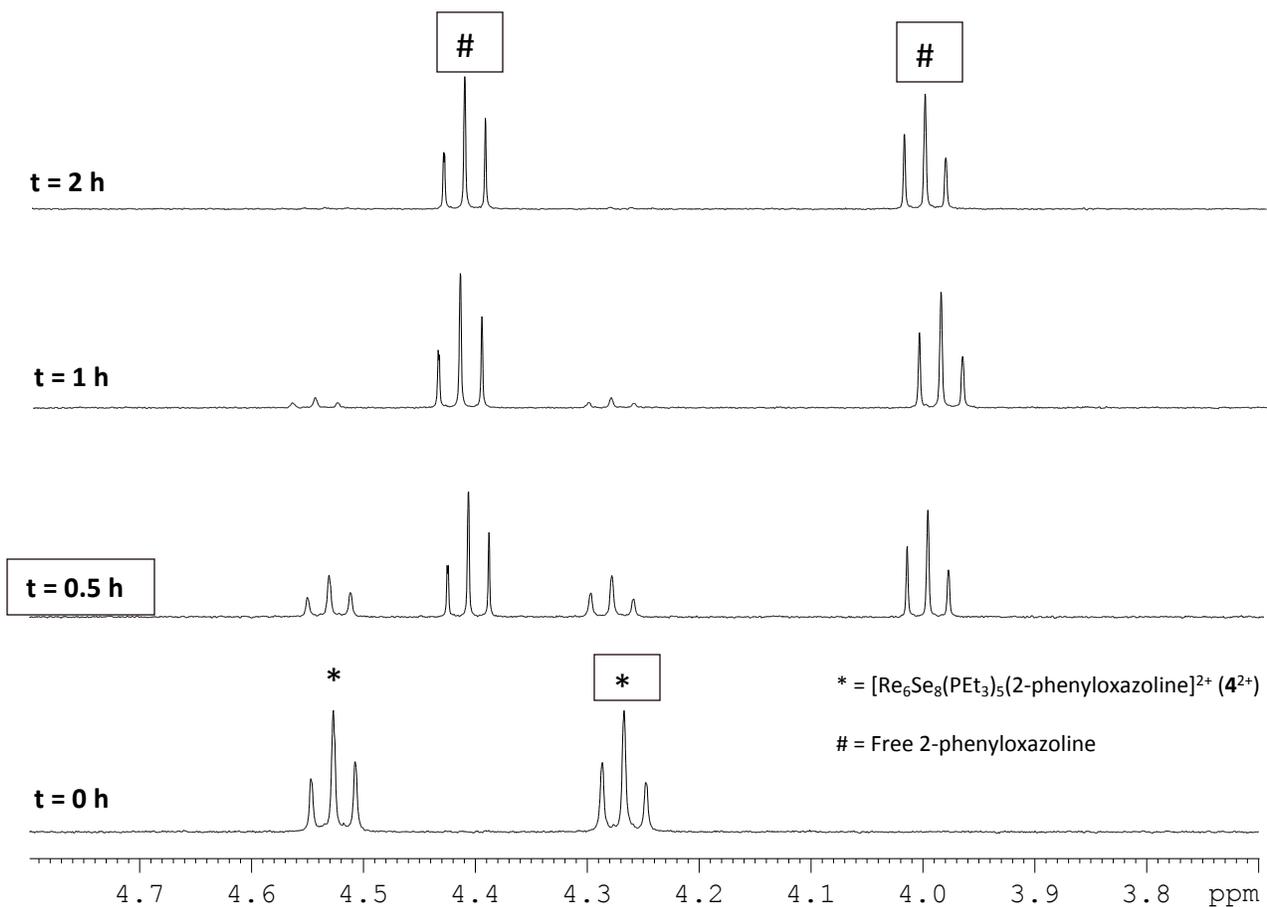


Figure S4. 500 MHz ^1H NMR spectral data of samples taken at different time intervals in the room temperature UV-irradiation of $\mathbf{4}^{2+}$ in CD_3CN .

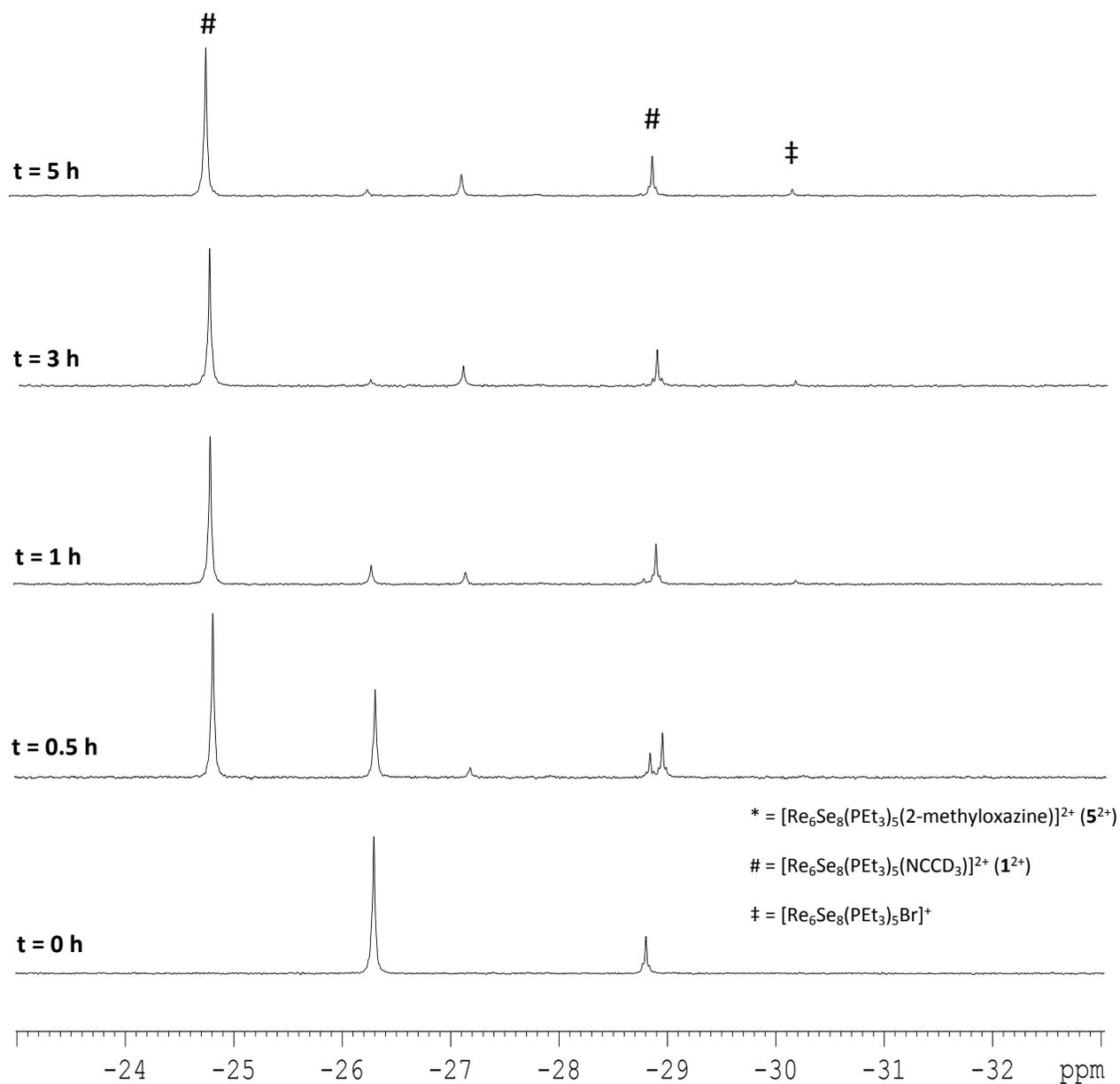


Figure S5. 202.5 MHz ^{31}P $\{^1\text{H}\}$ NMR spectral data of samples taken at different time intervals in the room temperature UV-irradiation of 5^{2+} in CD_3CN .

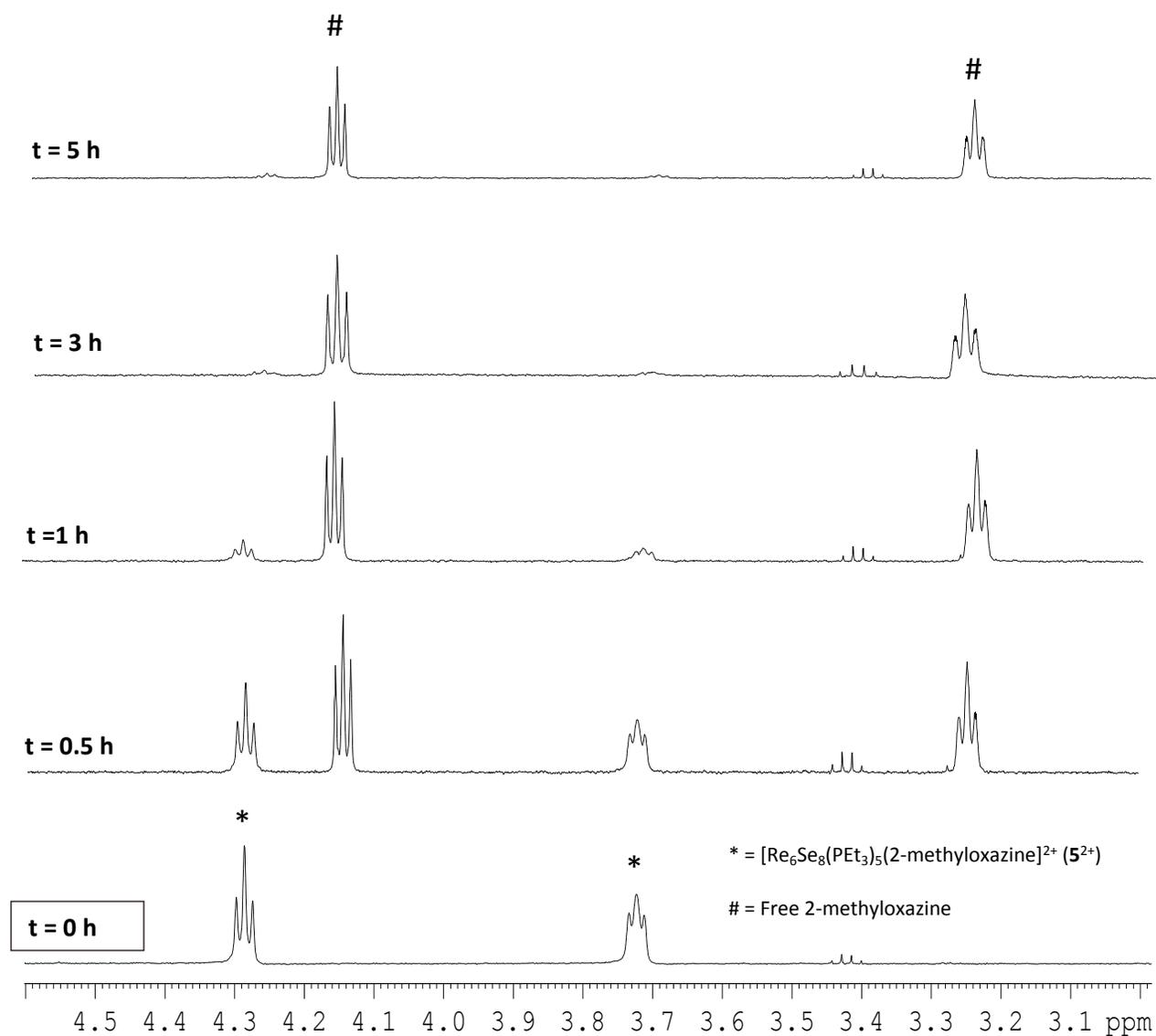


Figure S6. 500 MHz ¹H NMR spectral data of samples taken at different time intervals in the room temperature UV-irradiation of **5**²⁺ in CD₃CN.

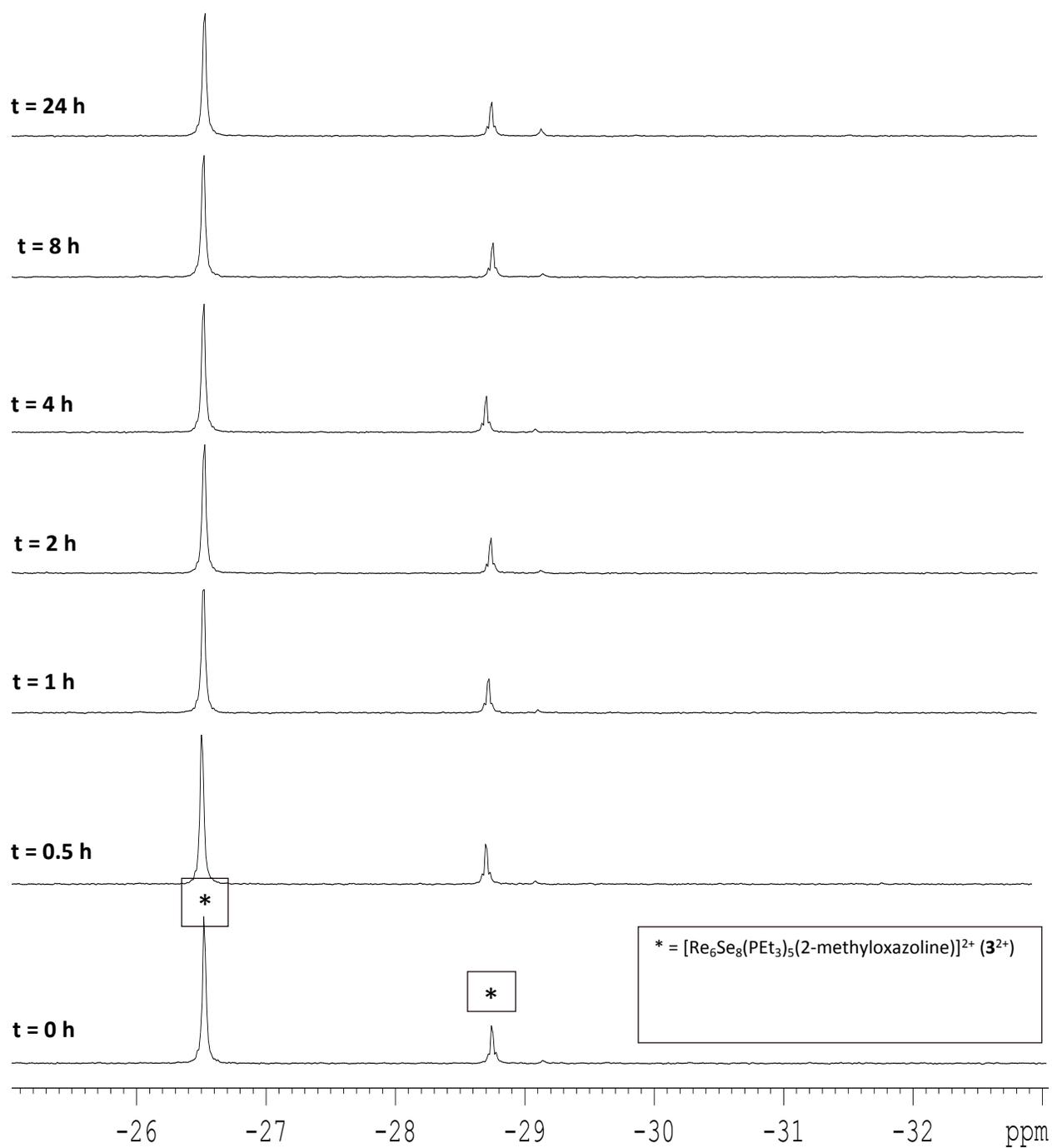


Figure S7. 202.5 MHz ^{31}P $\{^1\text{H}\}$ NMR spectral data of samples taken at different time intervals in the heating of $\mathbf{3}^{2+}$ in CD_3CN (no reaction occurred).

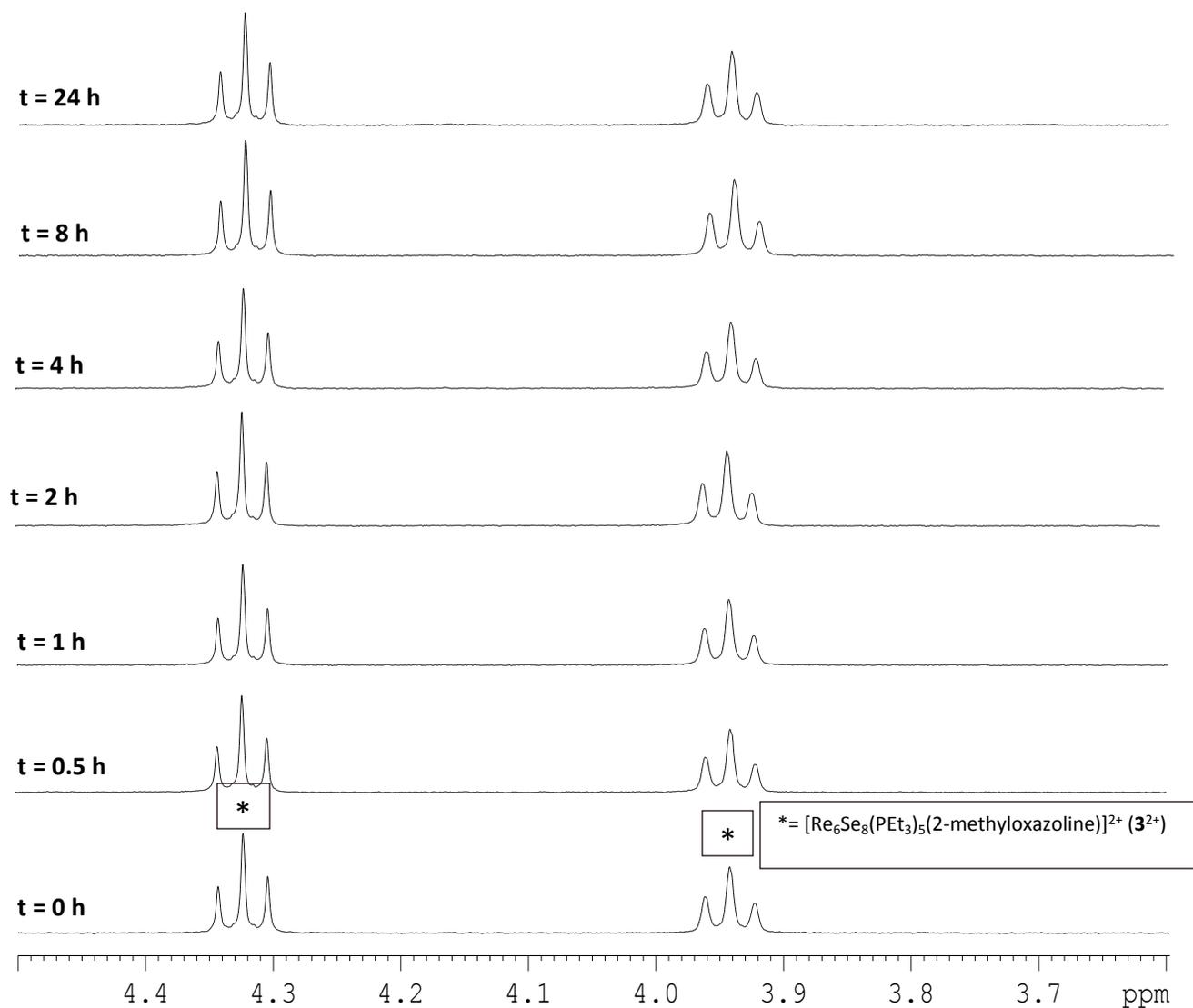


Figure S8. 500 MHz ^1H NMR spectral data of samples taken at different time intervals in the heating of $\mathbf{3}^{2+}$ in CD_3CN (no reaction occurred).

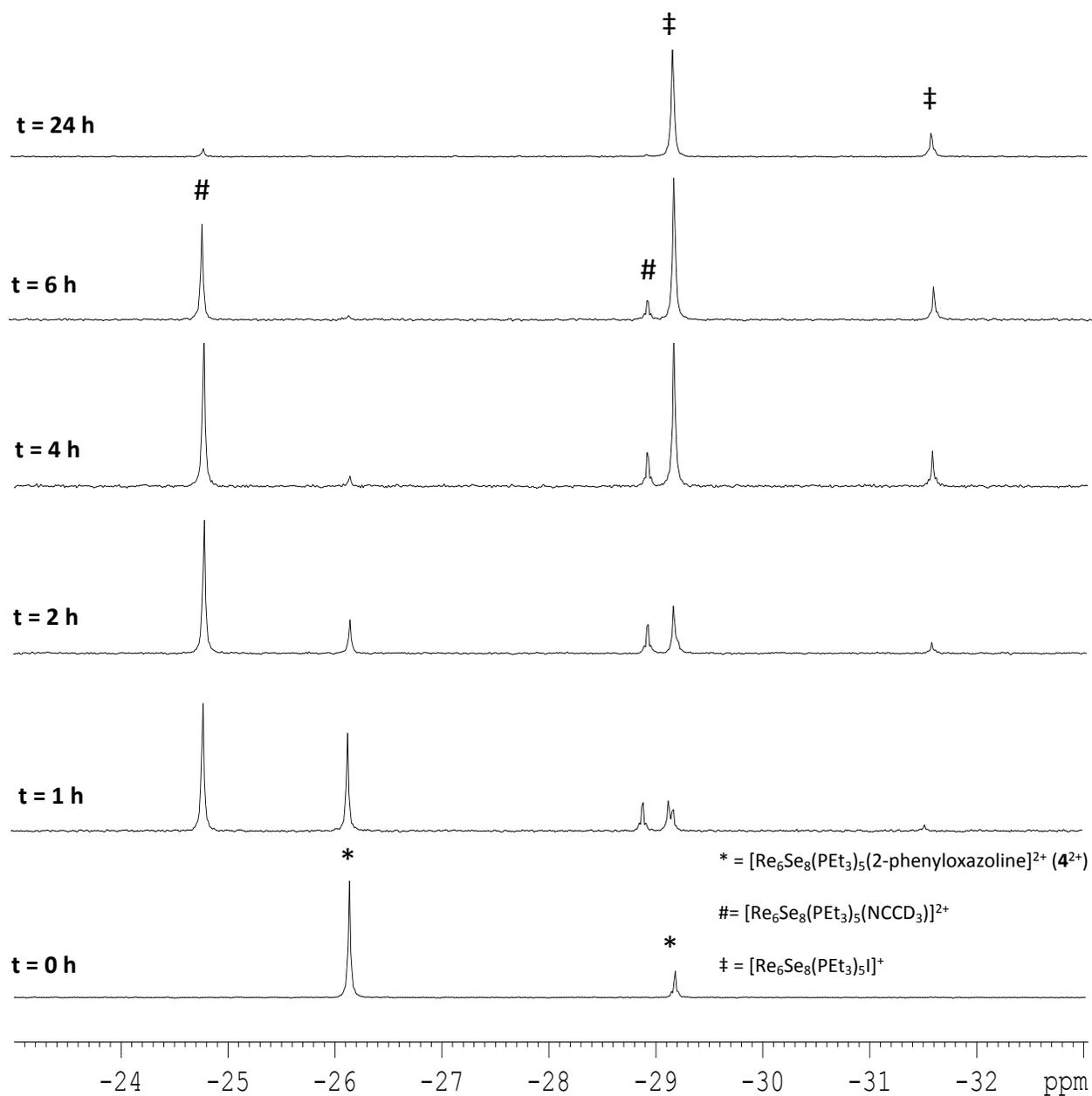


Figure S9. 202.5 MHz ^{31}P $\{^1\text{H}\}$ NMR spectral data of samples taken at different time intervals in the heating of 4^{2+} in CD_3CN .

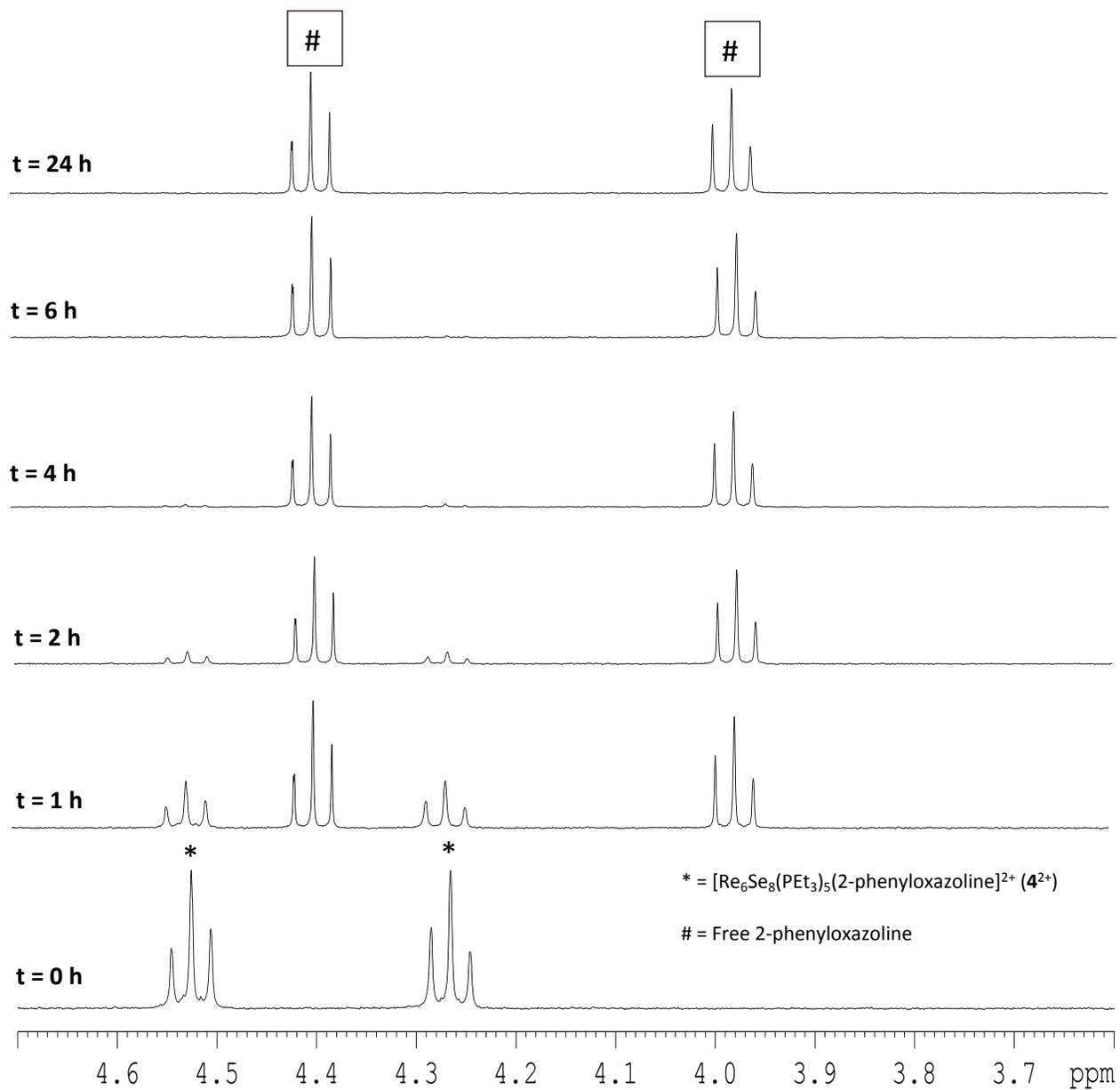


Figure S10. 500 MHz ^1H NMR spectral data of samples taken at different time intervals in the heating of $\mathbf{4}^{2+}$ in CD_3CN .

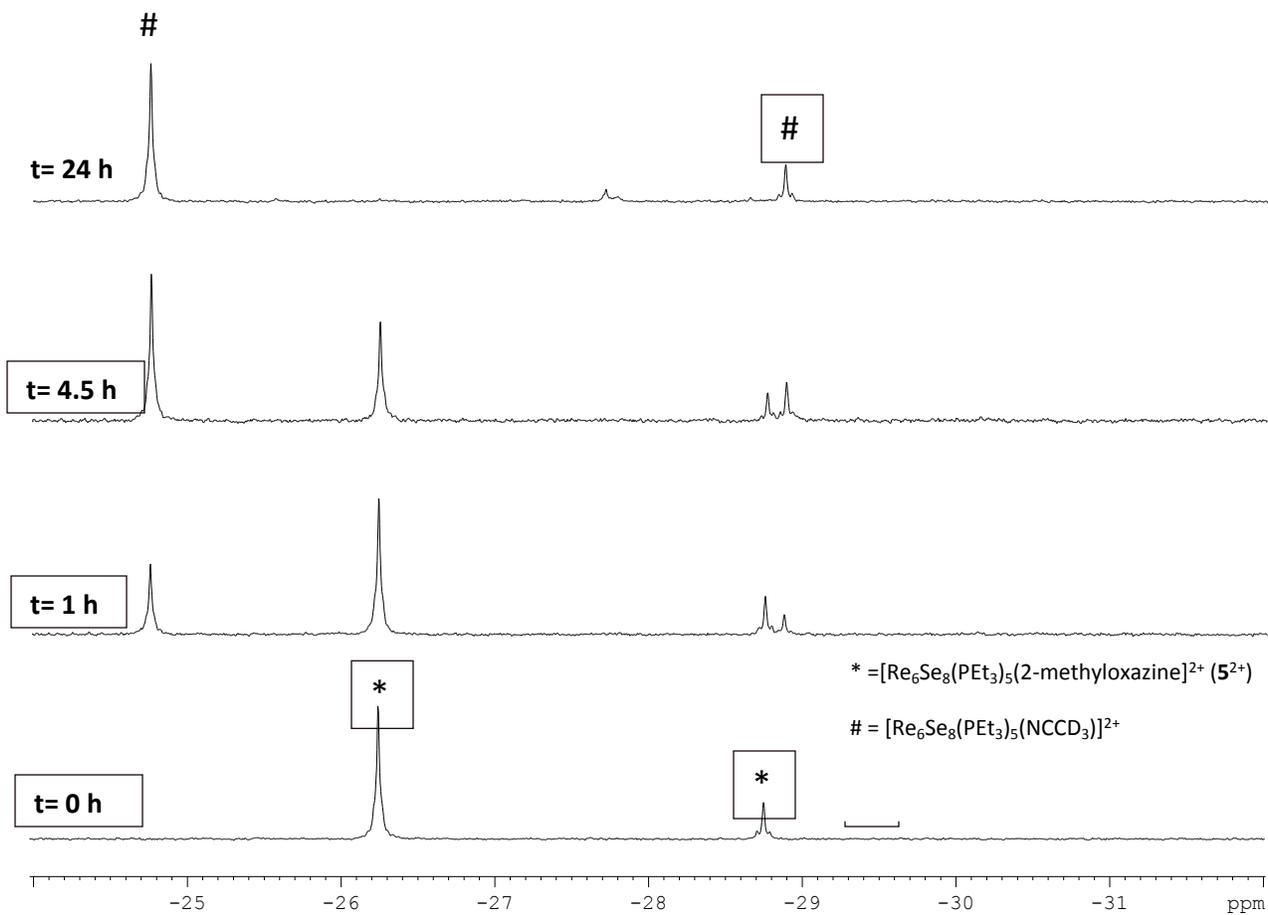


Figure S11. 202.5 MHz ^{31}P $\{^1\text{H}\}$ NMR spectral data of samples taken at different time intervals in the heating of $\mathbf{5}^{2+}$ in CD_3CN .

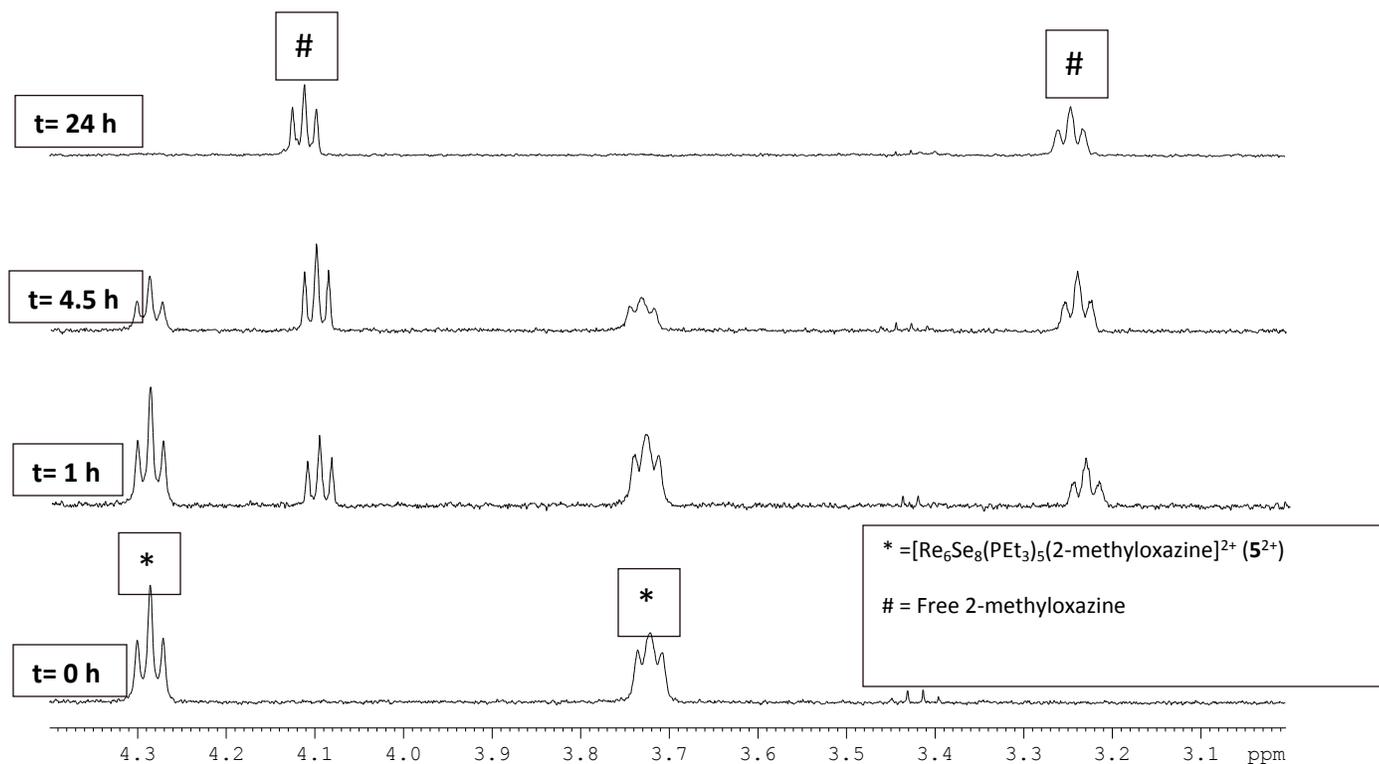
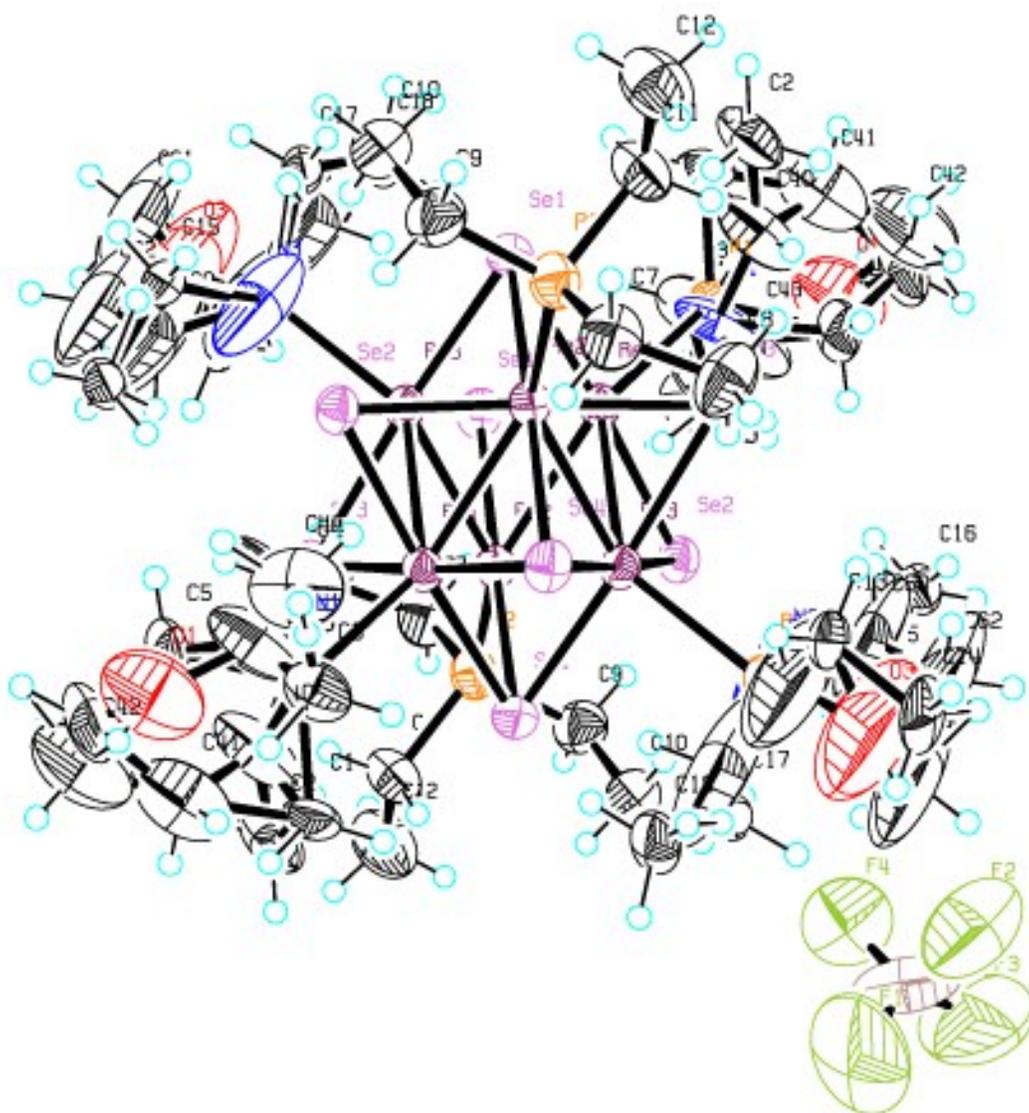


Figure S12. 500 MHz ¹H NMR spectral data of samples taken at different time intervals in the heating of 5²⁺ in CD₃CN.



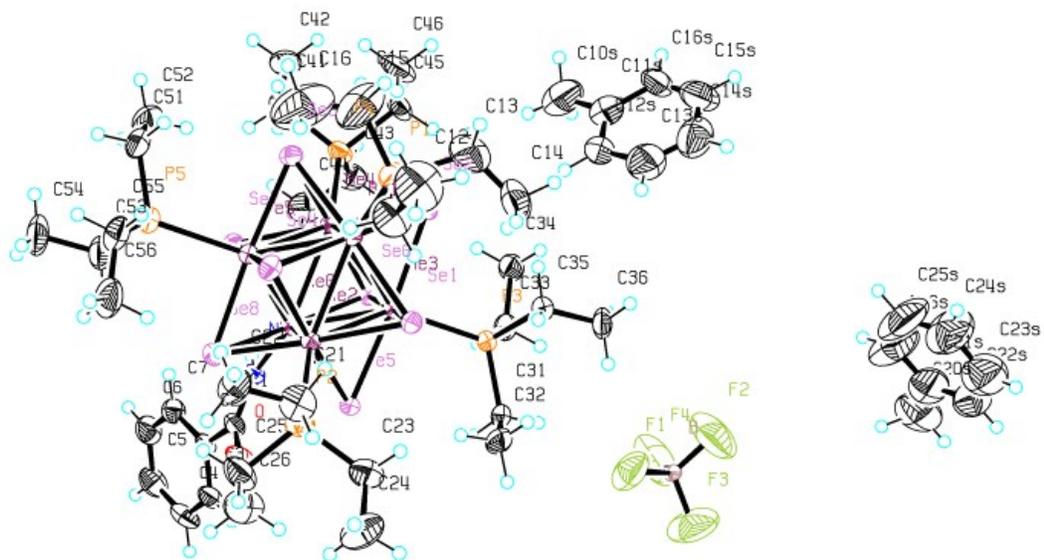


Figure S14. Displacement ellipsoid plot (50%) of 7(BF₄).

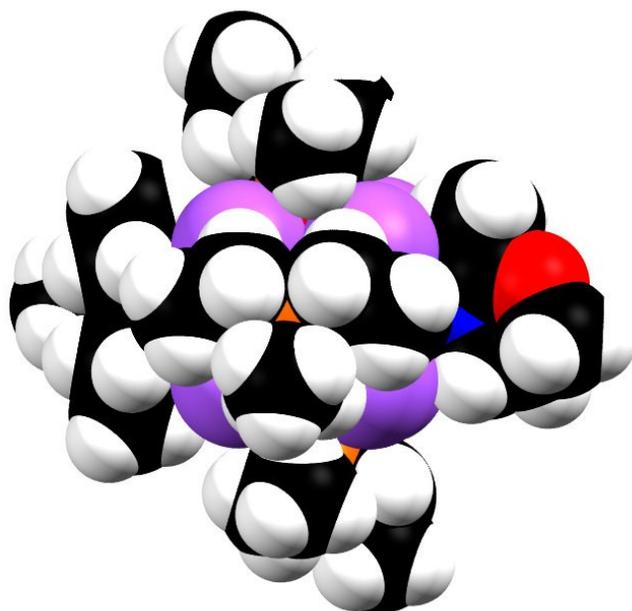


Figure S15. Space filling diagram of 5^{2+} .

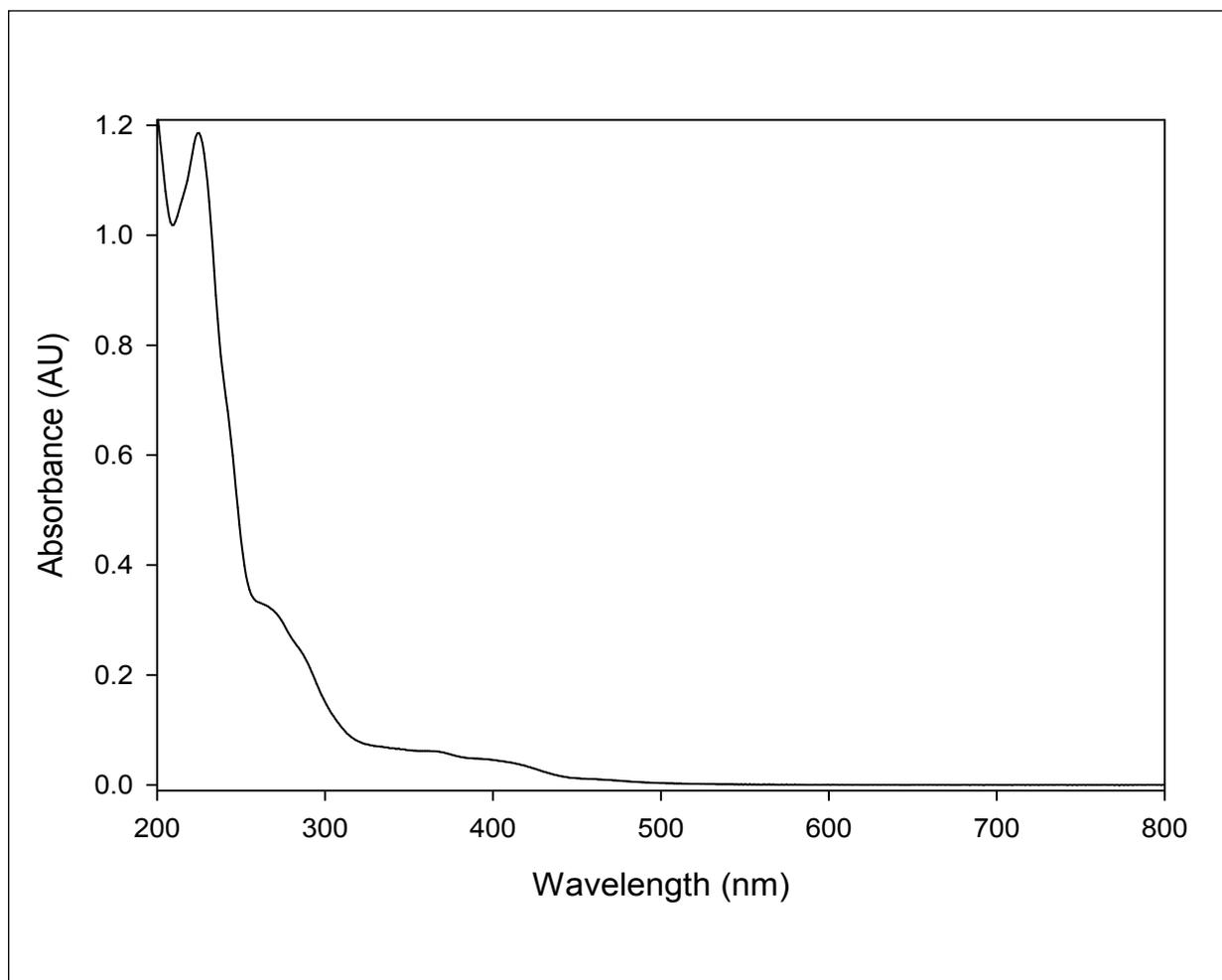


Figure S16. UV-vis spectrum of $[\text{Re}_6\text{Se}_8(\text{PEt}_3)_5(2\text{-methyloxazine})](\text{SbF}_6)_2$ (**5(SbF₆)₂**) in CH_3CN with a concentration of 1.58×10^{-5} M.