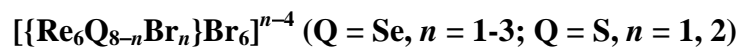


Photoluminescent Properties of Chalcobromide-capped Octahedral Hexarhenium(III) Complexes



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Supporting Information

Figures S1-S11

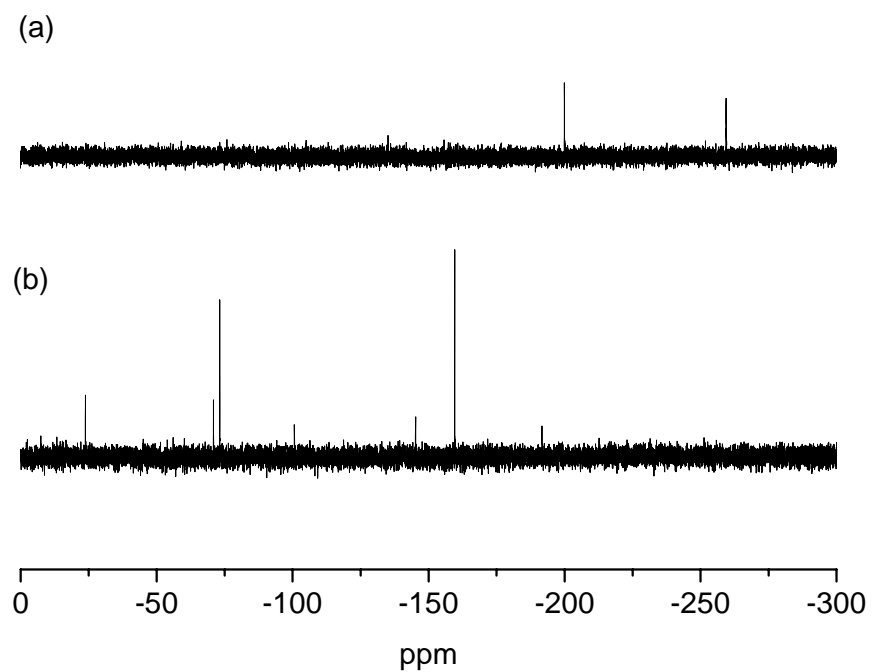


Figure S1. The ^{77}Se NMR spectra for $(\text{Bu}_4\text{N})_3[\{\text{Re}_6\text{Se}_7\text{Br}\}\text{Br}_6]$ (a) in CD_3CN and $(\text{Bu}_4\text{N})[\{\text{Re}_6\text{Se}_5\text{Br}_3\}\text{Br}_6]$ (b) in $\text{DMSO}-d_6$ at room temperature.

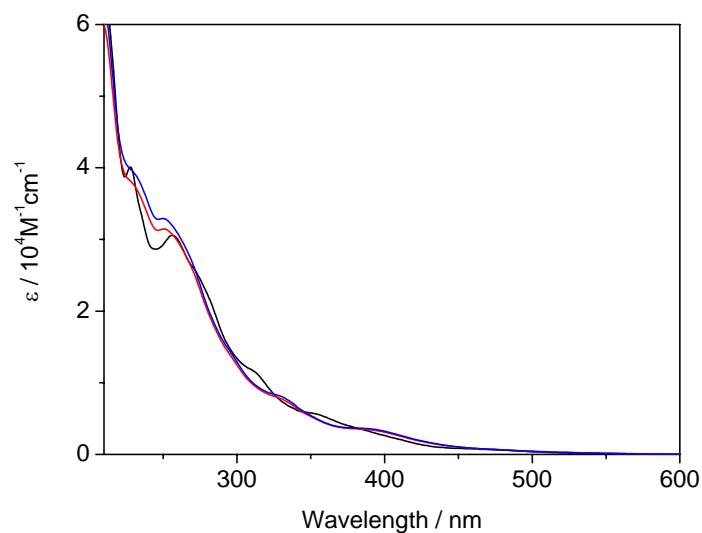


Figure S2. UV-vis absorption spectra of the D_{3d} ($[2\mathbf{a}\text{-Se}]^{2-}$, black) and C_{2v} ($[2\mathbf{b}\text{-Se}]^{2-}$, red; $[2\mathbf{b}\text{-Se}]^{2-}$, blue) isomers for $(\text{Bu}_4\text{N})_2[\{\text{Re}_6\text{S}_6\text{Br}_2\}\text{Br}_6]$ in acetonitrile at room temperature.

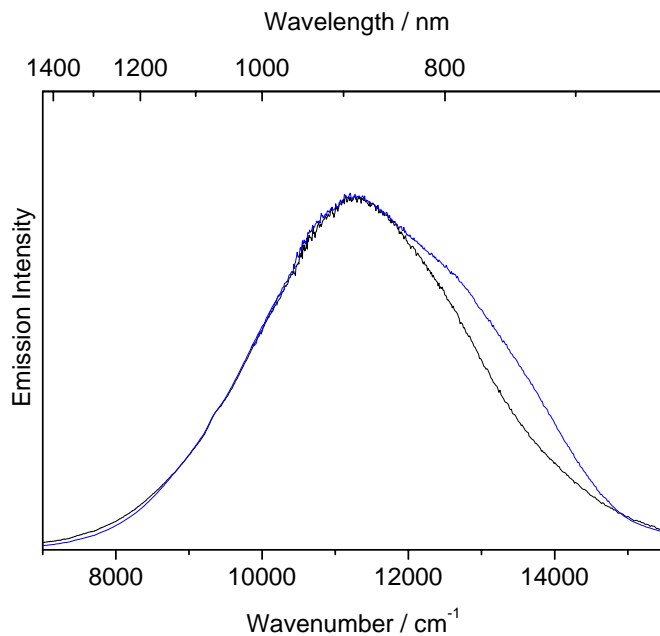


Figure S3. Emission spectra for $(\text{Bu}_4\text{N})_3[\{\text{Re}_6\text{Q}_7\text{Br}\}\text{Br}_6]$ ($\text{Q} = \text{S}$ (black), $\text{Q} = \text{Se}$ (blue)) in the crystalline phase at 296 K.

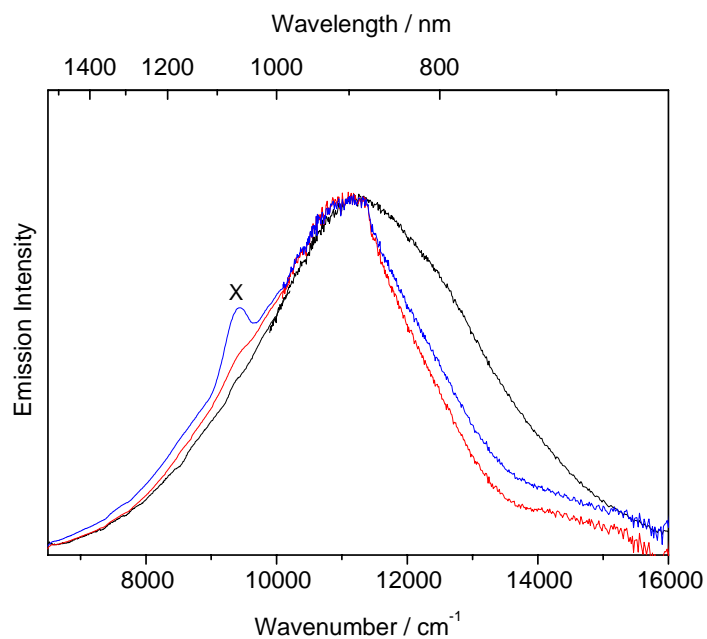


Figure S4. Emission spectra for $(\text{Bu}_4\text{N})_2[\{\text{Re}_6\text{S}_6\text{Br}_2\}\text{Br}_6]$ ($(\text{Bu}_4\text{N})_2[2\text{a-S}]$ (black), $(\text{Bu}_4\text{N})_2[2\text{b-S}]$ (red), and $(\text{Bu}_4\text{N})_2[2\text{c-S}]$ (blue)) in the crystalline phase at 296 K. The feature with x is due to instrumental artifact.

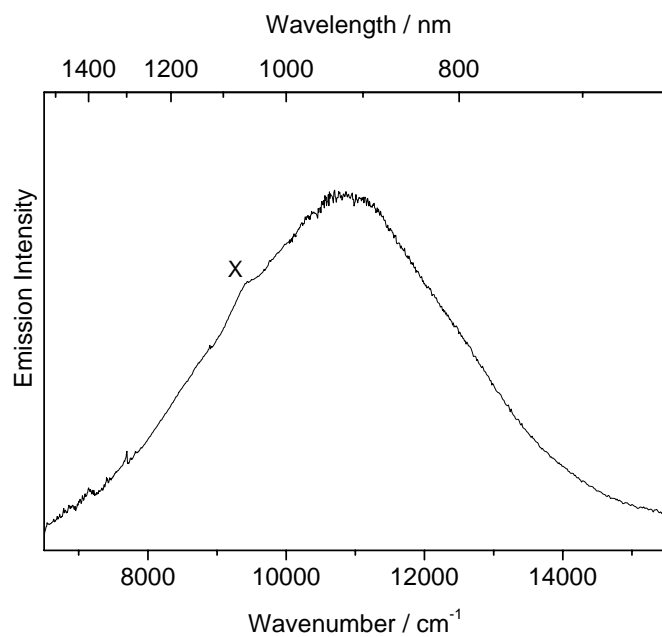


Figure S5. Emission spectrum for $(\text{Bu}_4\text{N})[\{\text{Re}_6\text{Se}_5\text{Br}_3\}\text{Br}_6]$ ($(\text{Bu}_4\text{N})[3\text{-Se}]$) in the crystalline phase at 296 K. The feature with x is due to instrumental artifact.

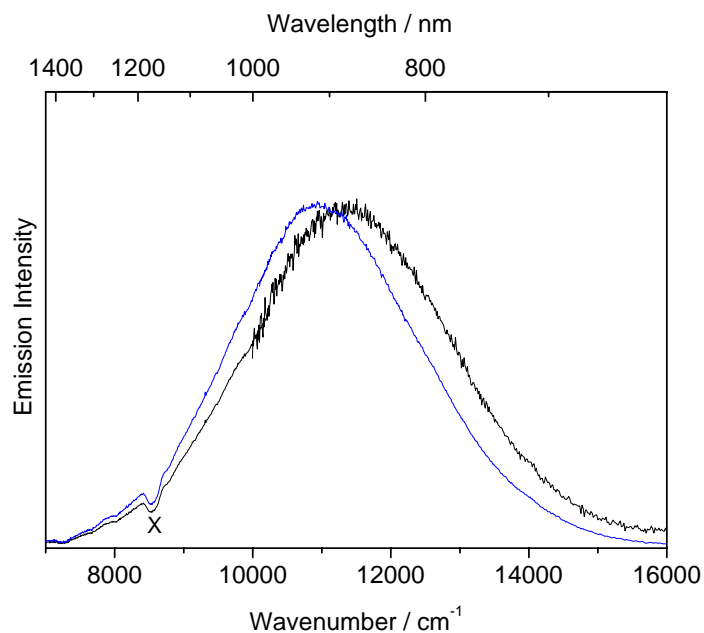


Figure S6. Emission spectra for $(\text{Bu}_4\text{N})_3[\{\text{Re}_6\text{Q}_7\text{Br}\}\text{Br}_6]$ ($\text{Q} = \text{S}$ (black), $\text{Q} = \text{Se}$ (blue)) in acetonitrile at 296 K. The feature with x is due to instrumental artifact.

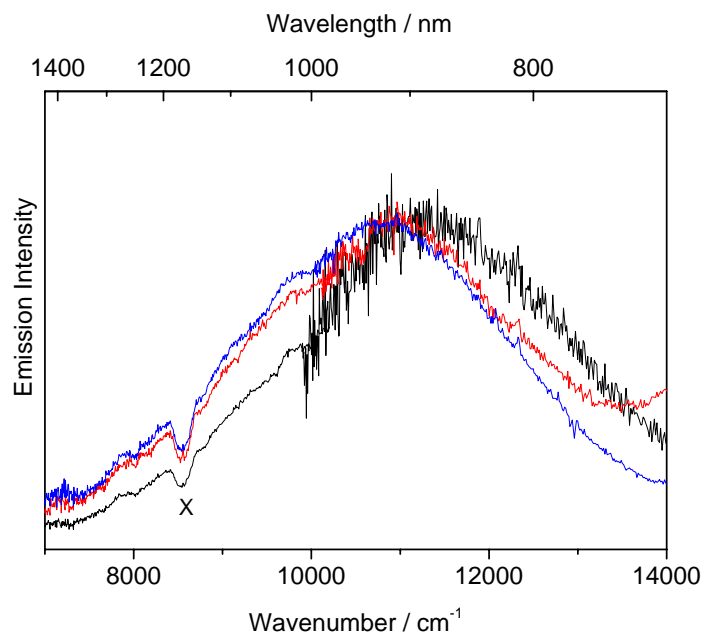


Figure S7. Emission spectra for $(\text{Bu}_4\text{N})_2[\{\text{Re}_6\text{S}_6\text{Br}_2\}\text{Br}_6]$ ($(\text{Bu}_4\text{N})_2[2\text{a-S}]$ (black), $(\text{Bu}_4\text{N})_2[2\text{b-S}]$ (red), and $(\text{Bu}_4\text{N})_2[2\text{c-S}]$ (blue)) in acetonitrile at 296 K. The feature with x is due to instrumental artifact.

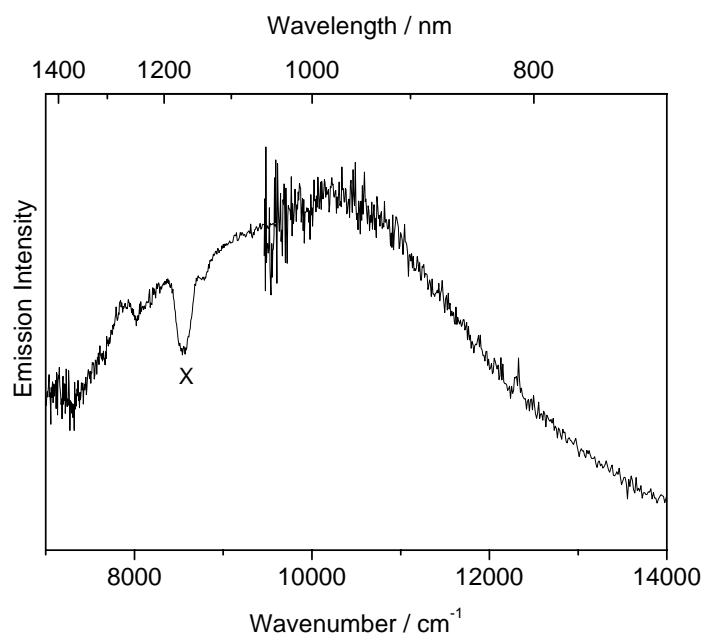


Figure S8. Emission spectrum for $(\text{Bu}_4\text{N})[\{\text{Re}_6\text{Se}_5\text{Br}_3\}\text{Br}_6]$ ($(\text{Bu}_4\text{N})[\mathbf{3-Se}]$) in acetonitrile at 296 K. The feature with x is due to instrumental artifact.

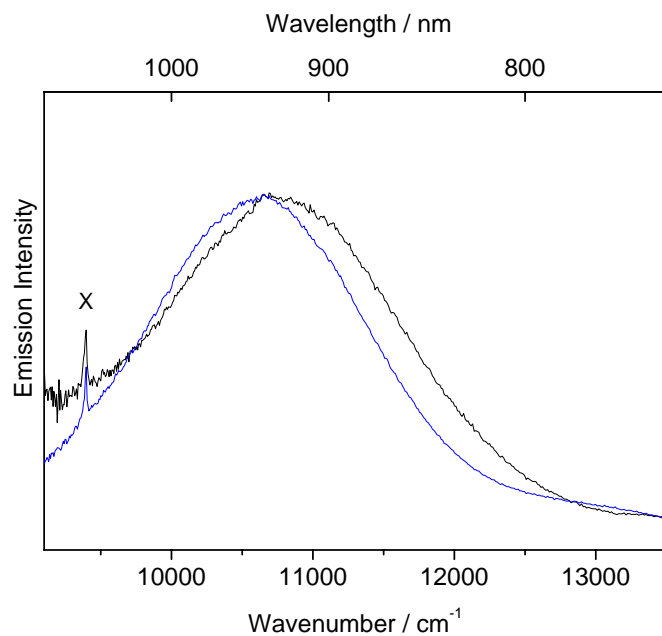


Figure S9. Emission Spectra for $(\text{Bu}_4\text{N})_3[\{\text{Re}_6\text{Q}_7\text{Br}\}\text{Br}_6]$ ($\text{Q} = \text{S}$ (black), $\text{Q} = \text{Se}$ (blue)) in the crystalline phase at 80 K. The feature with x is due to instrumental artifact.

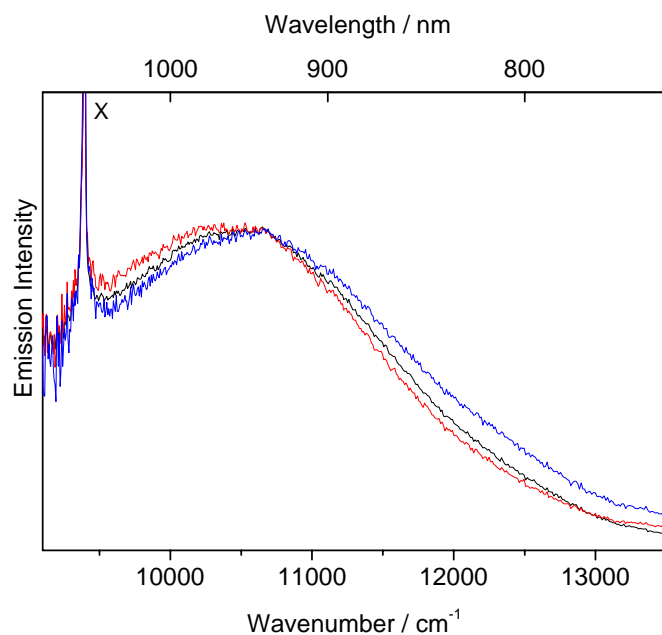


Figure S10. Emission Spectra for $(\text{Bu}_4\text{N})_2[\{\text{Re}_6\text{S}_6\text{Br}_2\}\text{Br}_6]$ ($(\text{Bu}_4\text{N})_2[\mathbf{2a-S}]$ (black), $(\text{Bu}_4\text{N})_2[\mathbf{2b-S}]$ (red), and $(\text{Bu}_4\text{N})_2[\mathbf{2c-S}]$ (blue)) in the crystalline phase at 80 K. The feature with x is due to instrumental artifact.

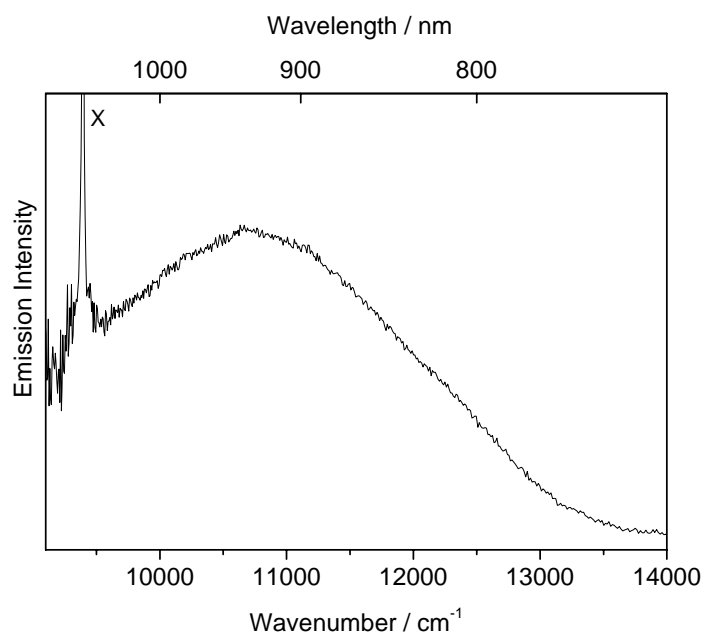


Figure S11. Emission Spectrum for $(\text{Bu}_4\text{N})[\{\text{Re}_6\text{Se}_5\text{Br}_3\}\text{Br}_6]$ in the crystalline phase at 95 K. The feature with x is due to instrumental artifact.