

Structural and photophysical properties of

$[(\text{CO})_3(\text{phen})\text{Re}(\text{-Br})\text{Re}(\text{phen})(\text{CO})_3]^+[(\text{CO})_3\text{Re}(\text{-Br})_3\text{Re}(\text{CO})_3]^-$: Where does its luminescence come from?

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$[(\text{CO})_3(\text{phen})\text{Re}(\text{-Br})\text{Re}(\text{phen})(\text{CO})_3][(\text{CO})_3\text{Re}(\text{-Br})_3\text{Re}(\text{CO})_3]\cdot\text{CH}_2\text{Cl}_2$ was prepared by direct reaction of $(\text{Re}(\text{CO})_3(\text{THF})\text{Br})_2$ (THF: tetrahydrofuran) and 1,10-phenanthroline in a 1:1 ratio, followed by recrystallization in dichloromethane. The compound is an ionic salt where both, cation and anion, are bimetallic complexes. Inside both of them the Re^I centers are bridged by one or three bromides respectively. The compound has an absorption band centered at 375 nm in CH_2Cl_2 , which has been assigned to a MLCT band. Excitation at 375 nm produces luminescent emission at 608 nm. Comparison of these results with closely related rhenium complexes, in addition to Time Dependent-DFT analysis, allow us to propose the $[(\text{CO})_3(\text{phen})\text{Re}(\text{-Br})\text{Re}(\text{phen})(\text{CO})_3]^+$ cation as main respons