Electronic Supplementary Material (ESI) for Dalton Transactions
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Supplementary Information

Near-Infrared Pigments based on Ion-Pair Charge Transfer Salts of Dicationic and Dianionic Metal-Dithiolene [M(II)=Pd, Pt] Complexes

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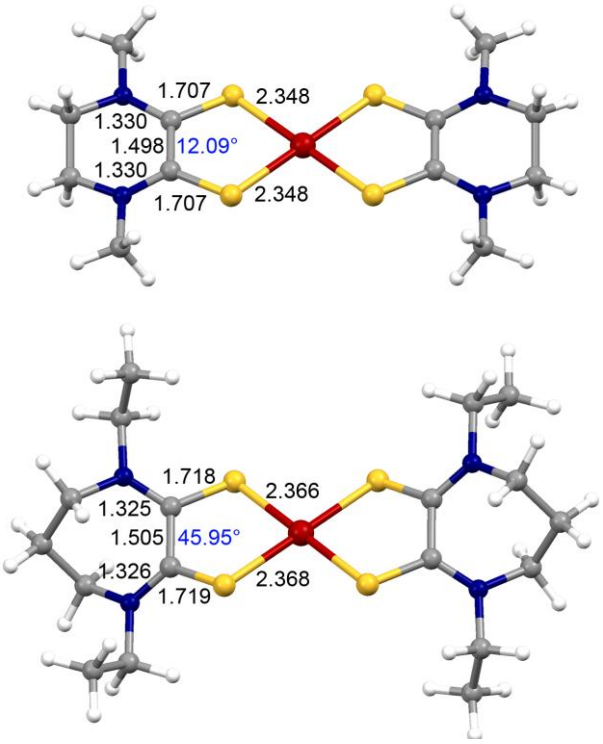

Figure S1. Molecular geometry of the optimized structures of $[Pt(Me_2pipdt)_2]^{2+}$ and $[Pt(Et_2dazdt)_2]^{2+}$ (B3LYP/6-31+G(d)-SDD). Bond distances in Å and the S-C-C-S torsion angle depicted in blue. For symmetry reasons only one set of parameters is reported.

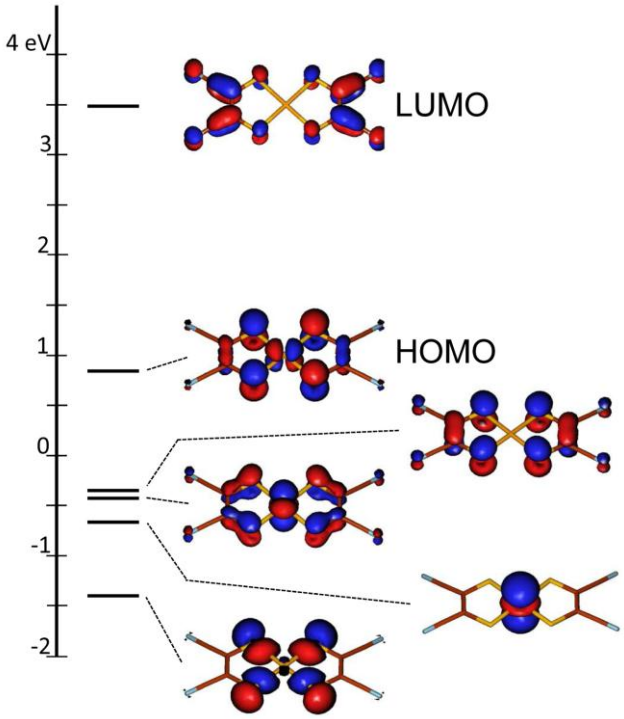

Figure S2. Spatial plots of the frontier molecular orbitals of $[Pt(mnt)_2]^{2-}$ in the gas-phase (B3LYP/6-31+G(d)-SDD, isovalue = 0.04).

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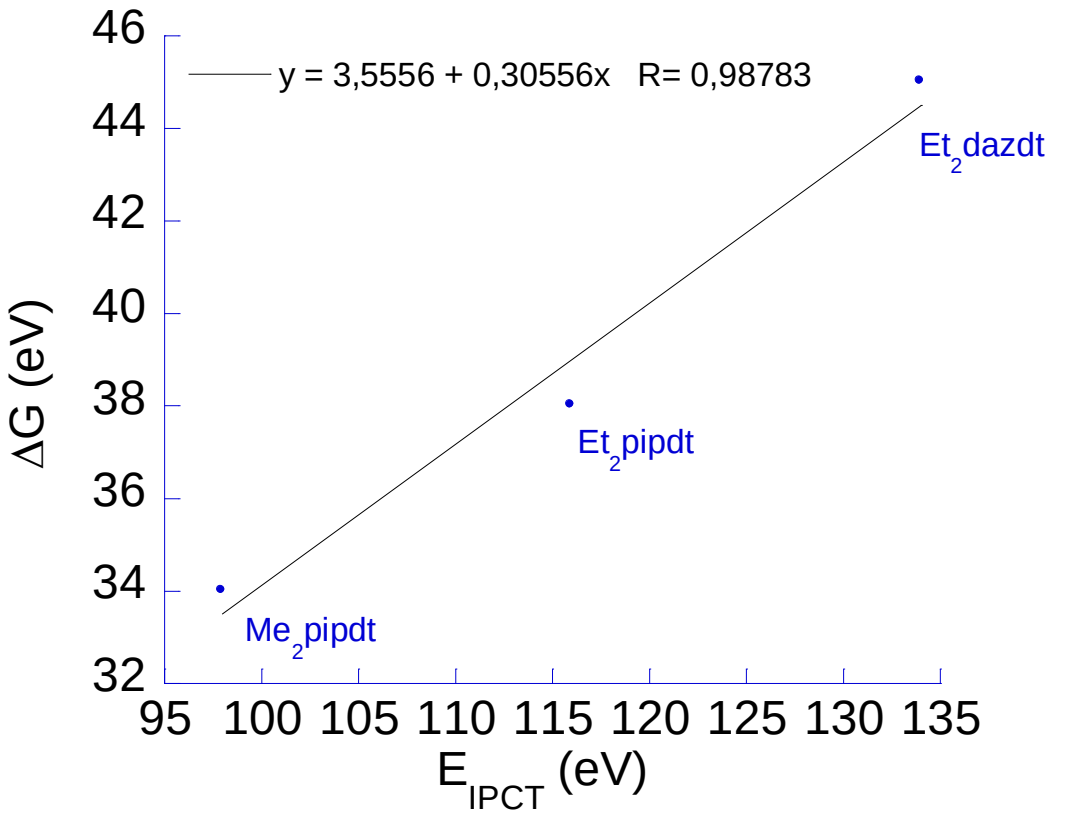

Figure S3. The linear correlation between E_{IPCT} and ΔG_{12} in $[Pt(mnt)_2]^{2-}$ salts of $[Pt(Et_2dazdt]^{2+}$ and $[Pt(R_2pipdt]^{2+}$