Supplementary Information

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

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**Figure S1.** Molecular geometry of the optimized structures of [Pt(Me₂pipdt)₂]²⁺ and [Pt(Et₃dazdt)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).
Figure S3. The linear correlation between $E_{\text{IPCT}}$ and $\Delta G_{12}$ in [Pt(mnt)$_2$]$^{2-}$ salts of [Pt(Et$_2$azd)]$^{2+}$ and [Pt(R$_2$pipdt)]$^{2+}$. 

The linear correlation is given by:

$$y = 3.5556 + 0.30556x \quad R = 0.98783$$