Supporting Information for

An $S_4$-Symmetric Mixed-Valent Decacopper Cage Comprised of $[\text{Cu}^{\text{II}}(L-S_2N_2)]$ Complexes Bridged by $\text{Cu}^{\text{I}}(\text{MeCN})_n$ ($n = 1$ or 2) Cations

by Skylar J. Ferrara, Bo Wang and James P. Donahue
UV-vis Spectrum in MeCN of

\[ [(\text{Cu}^{\text{II}}(L\text{-N}_2\text{S}_2))_4(\mu_2\text{-Cu}^{\text{I}}(\text{MeCN})_2)_2(\mu_3\text{-Cu}^{\text{I}}(\text{MeCN}))_4]\]

\[ [\text{BF}_4]_6 \cdot 2.25\text{MeCN} \]

Conc = $5.604 \times 10^{-5}$ M

321 (shoulder, 4310),
365 (shoulder, 3830)
569 (1690)
Atom Labeling for Cation 1 of 
$[\text{Cu}_{10}(\text{S(CH}_2)_2\text{N(Me)CH}_2^-)_2(\text{MeCN})_8][\text{BF}_4]_6 \cdot (\text{MeCN})_{2.25}$

Thermal ellipsoid plot is drawn at the 40% probability level. Hydrogen atoms are omitted for clarity.
Partial Atom Labeling for Cation 1 of

\[ \text{[Cu}_{10}(S(CH_2)_2N(Me)CH_2^-)_2(\text{MeCN})_8][BF}_4]_6 \cdot \text{(MeCN)}_{2.25} \]

Thermal ellipsoid plot is drawn at the 40% probability level. Hydrogen atoms are omitted for clarity.
Atom Labeling for Cation 2 of
$\left[\text{Cu}_{10}(S(\text{CH}_2)_2 N(\text{Me})\text{CH}_2^-)_2(\text{MeCN})_8\right]\left[\text{BF}_4\right]_6 \cdot (\text{MeCN})_{2.25}$

Thermal ellipsoid plot is drawn at the 40% probability level. Hydrogen atoms are omitted for clarity.
Partial Atom Labeling for Cation 2 of $[\text{Cu}_{10}(\text{S(CH}_2)_2\text{N(Me)CH}_2\text{)}_2(\text{MeCN})_8][\text{BF}_4]_6 \cdot (\text{MeCN})_{2.25}]^{6+}$

Thermal ellipsoid plot is drawn at the 40% probability level. Hydrogen atoms are omitted for clarity.
Atom Labeling for $[\text{BF}_4]^{-}$ Anions and Interstitial MeCN $[\text{Cu}_{10}(\text{S(CH}_2)_2\text{N(Me)CH}_2^-)_2(\text{MeCN})_8][\text{BF}_4]_6\cdot(\text{MeCN})_{2.25}$

Thermal ellipsoid plot is drawn at the 40% probability level. Hydrogen atoms are omitted for clarity.