Supplementary Material

Computational Spectroscopic Characterization of Bistable Binuclear Complex

\[(\text{CO})_2(\text{benzoate})\text{Fe}^\text{II/III}(-\text{terephthalate-})\text{Co}^\text{III/II}(\text{benzoate})(\text{CO})_2]^{1+}\]

Hossein Shirani \(^A\) and Hassan Sabzyan \(^B\)*

\(^B\)Department of Chemistry, College of Science, Arak Branch, Islamic Azad University, Arak, I. R. Iran.
\(^A\)Department of Chemistry, University of Isfahan, Isfahan 81746-73441, I. R. Iran.

*Email: sabzyan@sci.ui.ac.ir
Fig. S-1. Displacement vectors of some selected vibrational modes (the bold numbers in the first column, as highlighted Table 3) of the cis/trans isomers and IMCT Fe$^{II}$-Co$^{III}$ and Fe$^{III}$-Co$^{II}$ states of the bistable binuclear complexes studied in this work. Continued …
Fig. S-1. … Continued.