Supplementary Material (ESI) for Dalton Transactions

Olefin Coordination in Copper(I) Complexes of *Bis*(2-pyridyl)amine

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Supplementary materials

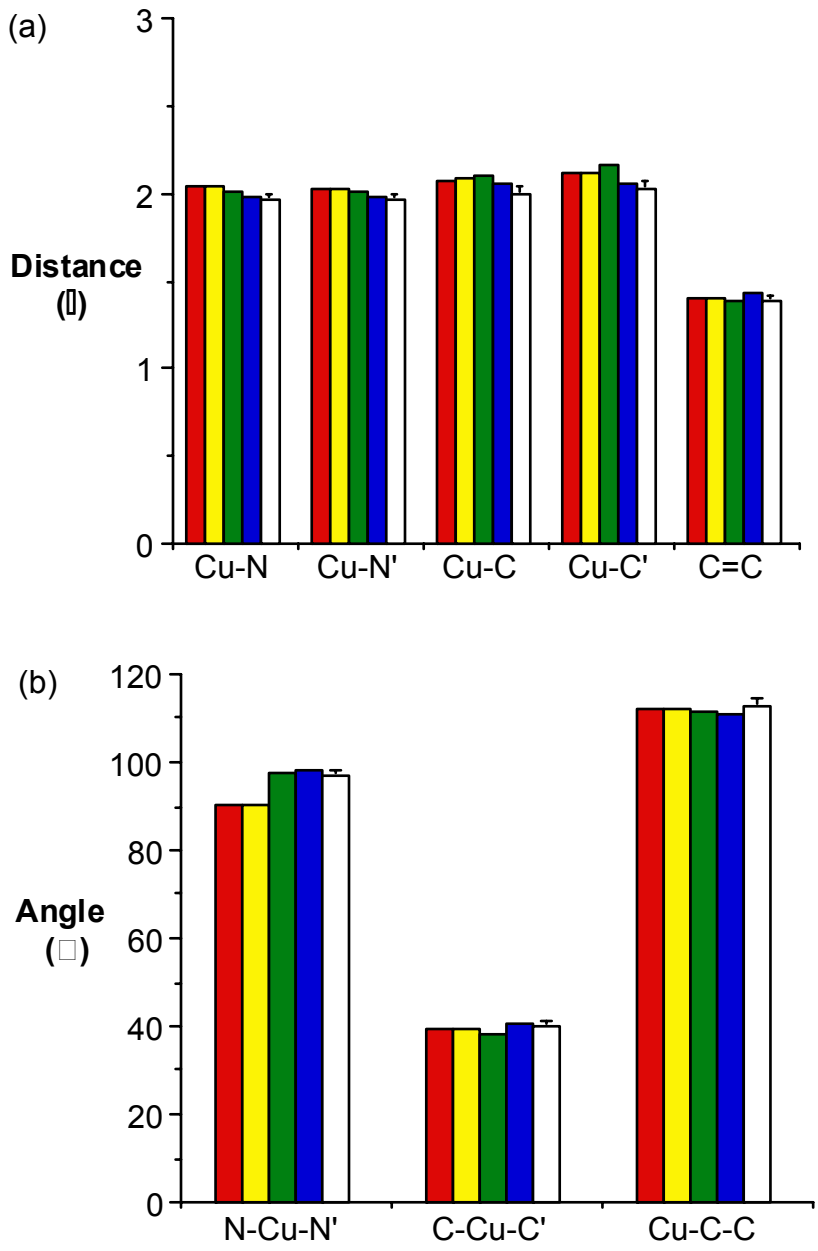

Figure S1. Plot of (a) bond lengths and (b) bond angles for calculated structure of [Cu(H-dpa)(1-octene)]$^{+}$, using MOPAC (■), RHF STO-3G (■), RB3LYP LANL2DZ/6-311++G* (■), and RMP2-FC LANL2DZ/6-311++G* (■) in comparison with experimentally determined values (□).

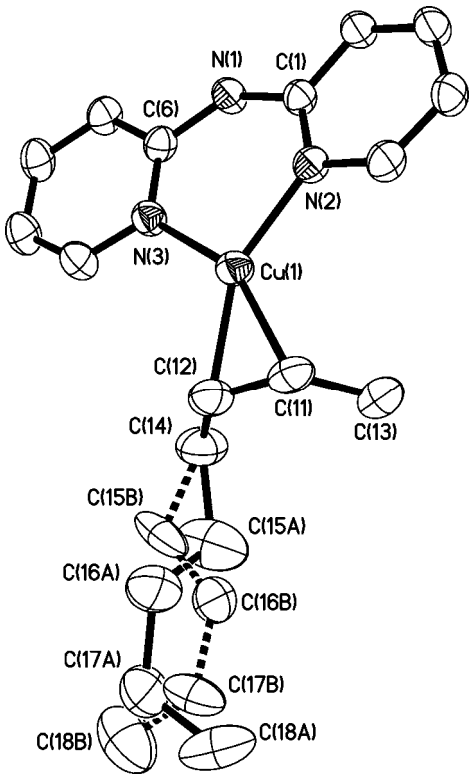

Figure S2. The structure of the $[Cu(H\text{-}dpa)(\textit{cis}\text{-}2\text{-octene})]^+$ cation in compound **6** showing the positional disorder of the C_5H_{11} group.

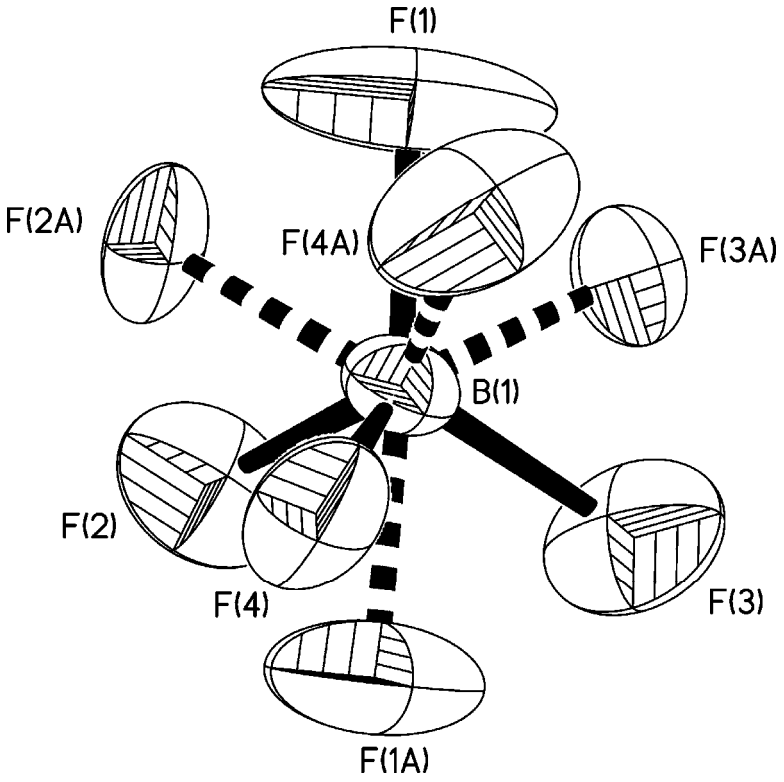

Figure S3. The structure of the BF_4^- anion in compound **8** showing the positional disorder.

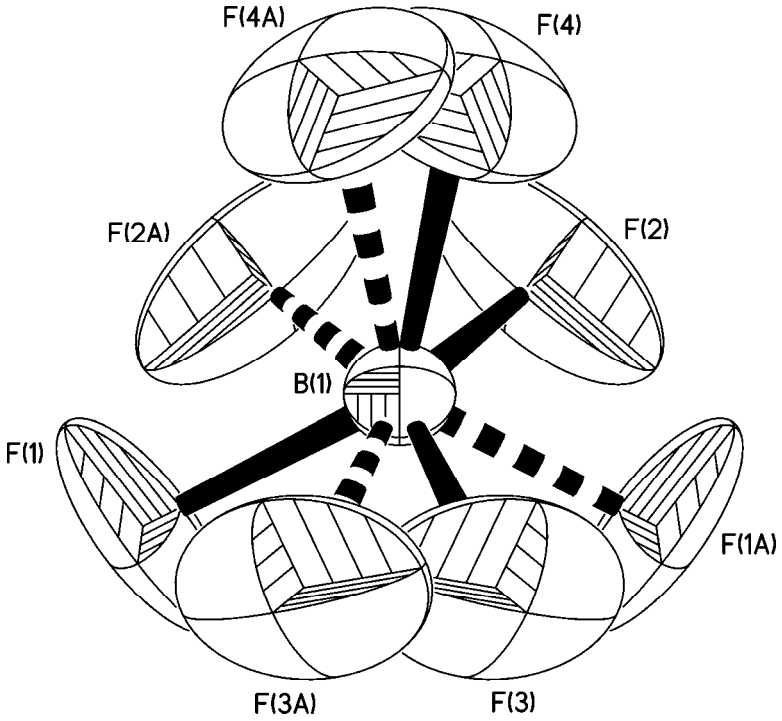

Figure S4. The structure of the BF_4^- anion in compound **11** showing the positional disorder.

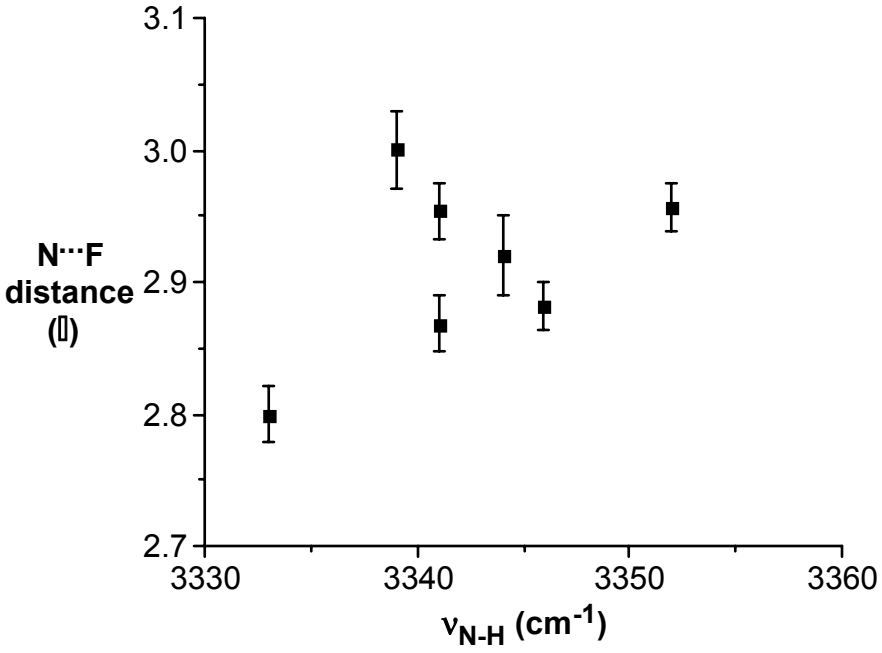

Figure S5. Plot of inter-ion N···F distance versus the IR N-H stretching frequency of the H-dpa ligand in [Cu(H-dpa)(olefin)]BF_4.

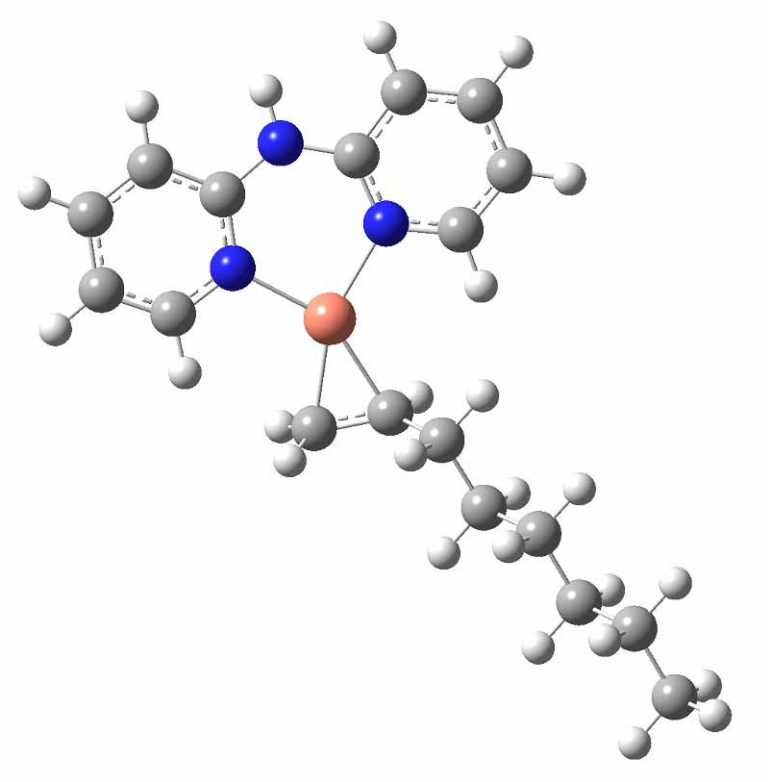

Figure S6. The structure of the $[Cu(H\text{-}dpa)(1\text{-octene})]^+$ cation calculated using MOPAC.

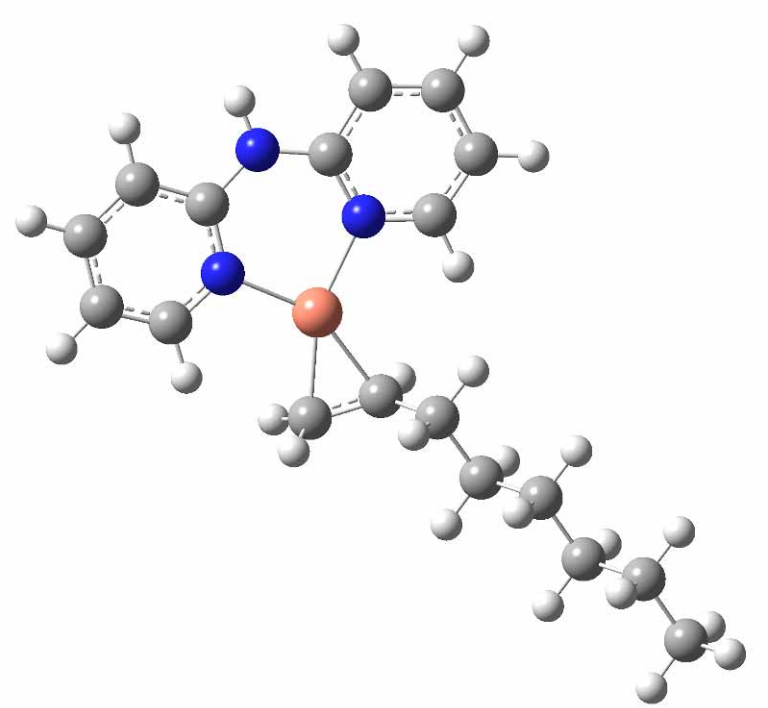

Figure S7. The structure of the $[Cu(H\text{-}dpa)(1\text{-}octene)]^{+}$ cation calculated using RHF STO-3G.

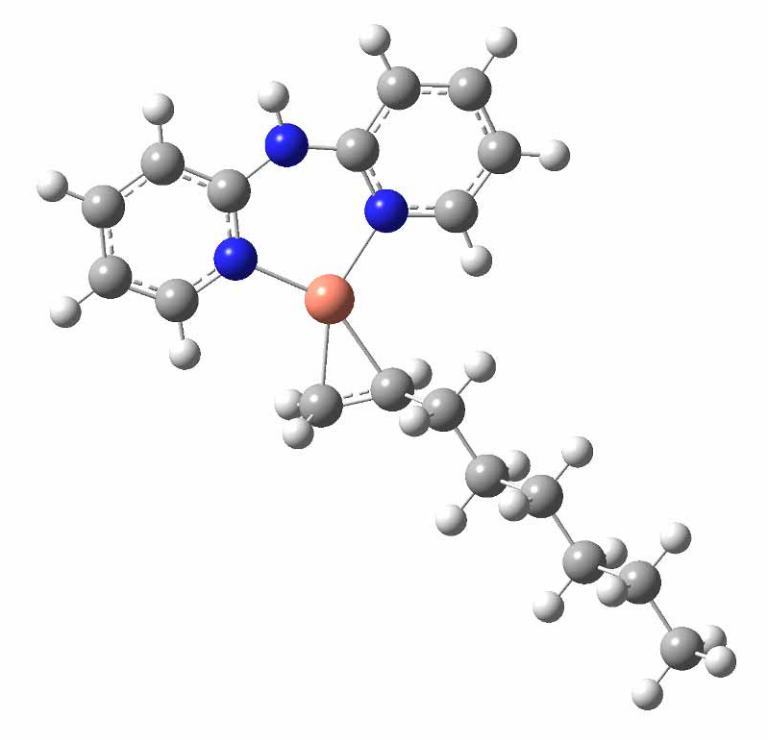

Figure S8. The structure of the $[Cu(H\text{-}dpa)(1\text{-octene})]^{+}$ cation calculated using RB3LYP LANL2DZ/6-311++G*.

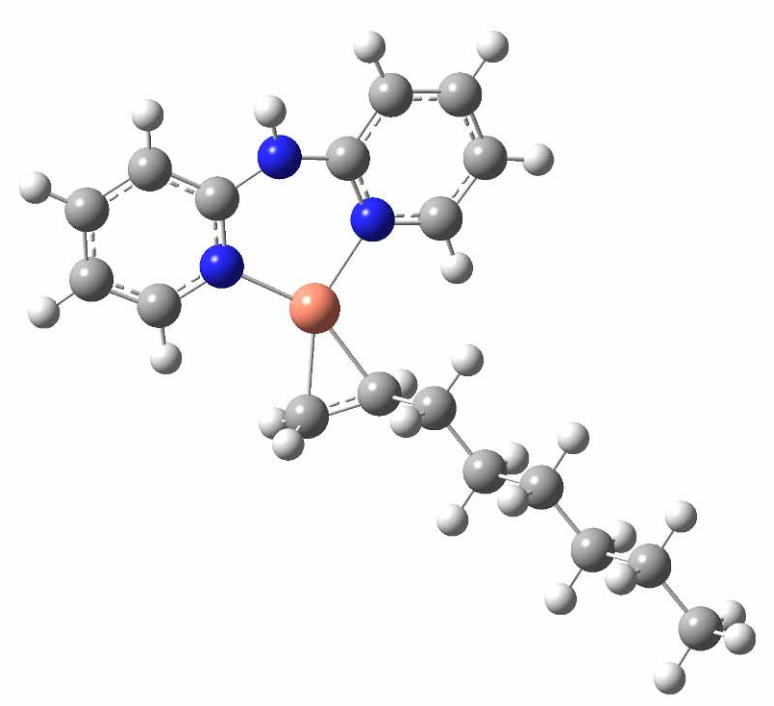

Figure S6. The structure of the $[Cu(H\text{-}dpa)(1\text{-octene})]^+$ cation calculated using RMP2-FC LANL2DZ/6-311++G*.