Supporting Material for "*Highly efficient perturbative+variational strategy for the evaluation of the magnetic coupling constants based on orthogonal valence bond theory. Application to the trinuclear Cu(II) site of the multicopper oxidases*"

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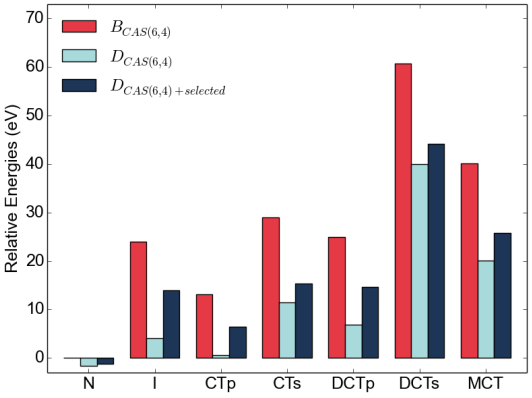
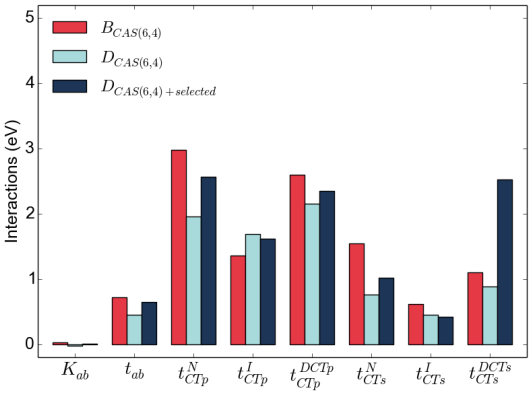
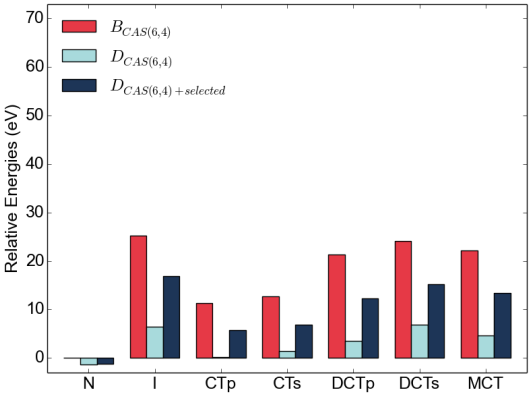


(a) Energies

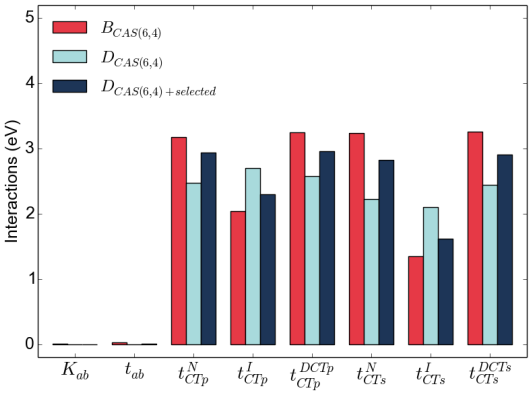


(b) Interactions

Figure S 1 – Bare (B) and dressed (D) Hamiltonian matrix elements for bisOH.



(a) Energies



(b) Interactions

Figure S 2 – Bare (B) and dressed (D) Hamiltonian matrix elements for $Cu_2(OH)_2$.