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Monte Carlo and Exact Diagonalization of Copper (II) Trimer Spin Frustrated Systems[1] HAILEY X. EGIDO-BETANCOURT, LEONARD W. TER HAAR, CHRISTOPHER N. VARNEY, University of West Florida — We discuss the use and importance of trimer-based systems because of the spin frustration that may arise within extended lattices comprised of trimers. The possible intra- and inter-trimer exchange pathways they posses due to interconnections are evaluated using density functional theory (DFT) to identify the optimal structures that may be used in designing extended lattices. As example, trinuclear Cu_3^{6+}cores with each pair of copper atoms bridged by carboxylate ligands have three-fold symmetry. As trimers these structures have the potential to be modeled as a frustrated quantum spin-1/2 system. To analyze the magnetic ground state and topological properties, we utilize exact diagonalization on small clusters and compare with Monte Carlo simulations for a range of system sizes.

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