Intermolecular interaction energies and magnetic properties of spin-isolated multinuclear CuII complexes

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Dinuclear CuII complexes with 3,5-dinitrobenzoates and 2,2'-bipyridine (2) or 1,10-phenanthroline (3) were synthesized and characterized. A complete energy framework analysis using the HF/3-21G energy model was performed which found that dispersion forces and C - H?O interactions are responsible for the crystal structure features. The magnetic properties of the complexes show a weak magnetic exchange between spins, resulting in low exchange constants of -2.72(1)cm-1 and -1.10(1)cm-1 for complexes (2) and (3), respectively. This results from the low overlap between magnetic orbitals induced by 3,5-dinitrobenzoate bridges and the arrangement of the magnetic orbitals. Consequently, the dinuclear complexes (2) and (3) behave as spin-isolated multinuclear CuII species in contrast to the trinuclear complex with similar ligands. © 2020 International Union of Crystallography.

2,2'-bipyridine and 1,10-phenanthroline ligands

3,5-dinitrobenzoate ligand

multinuclear CuII complexes

spin-isolated behavior

Crystal structure

Magnetic properties

Magnetism

Synthesis (chemical)

1 ,10-phenanthroline

Dinuclear complex

Exchange constants

Intermolecular interaction energies

Magnetic exchange

Magnetic orbitals

Structure features

Trinuclear complex

Copper compounds