Structural and electronic effects on the exchange interactions in dinuclear bis(phenoxo)-bridged copper(II) complexes

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Computational methods based on density functional theory have been employed to analyze the magnetic properties of dinuclear bis(phenoxo)-bridged CuII complexes. While the largest part of complexes in that family show antiferromagnetic coupling, we focus our study on those cases with distorted geometries that present ferromagnetic behaviour. The calculations reproduce such a magnetic behaviour, and a structural analysis reveals the main role played by several structural parameters, such as the Cu-O-Cu bridging angle. The out-of-plane shift of the phenoxo ring and the hinge distortion of the Cu2O2 central framework that are also important for similar hydroxo and alkoxo complexes. In this case the conformation of the phenoxo groups and the rotation of the phenyl rings can also play an important role. The last part of this work is dedicated to analyze the influence of the substituents of the phenoxo ring on the magnetic properties, which is especially important for structures with large ou