New Dinuclear Macrocyclic Copper(II) Complexes as Potentially Fluorescent and Magnetic Materials

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Streszczenie

Two dinuclear copper(II) complexes with macrocyclic Schiff bases **K1** and **K2** were prepared by the template reaction of (R)-(+)-1,1′-binaphthalene-2,2′-diamine and 2-hydroxy-5-methyl-1,3-benzenedicarboxaldehyde **K1**, or 4-tert-butyl-2,6-diformylphenol **K2** with copper(II) chloride dihydrate. The compounds were characterized by spectroscopic methods. X-ray crystal structure determination and DFT calculations confirmed their geometry in solution and in the solid phase. Moreover, intermolecular interactions in the crystal structure of **K2** were analyzed using 3D Hirshfeld surfaces and the related 2D fingerprint plots. The magnetic study revealed very strong antiferromagnetic Cu^{II}-Cu^{II} exchange interactions, which were supported by magneto-structural correlation and DFT calculations conducted within a broken symmetry (BS) framework. Complexes **K1** and **K2** exhibited luminescent properties that may be of great importance in the search for new OLEDs. Both **K1** and **K2** complexes showed emissions in the range of 392–424 nm in solutions at various polarities. Thin materials of the studied compounds were deposited on Si(111) by the spin-coating method or by thermal vapor deposition and studied by scanning electron microscopy (SEM/EDS), atomic force microscopy (AFM), and fluorescence spectroscopy. The thermally deposited **K1** and **K2** materials showed high fluorescence intensity in the range of 318–531 nm for **K1**/Si and 326–472 nm for the **K2**/Si material, indicating that they could be used in optical devices.

Słowa kluczowe

oligonuclear complexes, magnetic properties, fluorescence, DFT, Hirshfeld analysis, EPR

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