Copper(II) complexes of 7-amino-2-methylchromone and 7-aminoflavone: magneto-structural, spectroscopic and DFT characterization.

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Streszczenie

Four new complexes of copper(II) consisting of two different chromone derivatives with carbonyl and amine donor atoms: 7-aminoflavone ($\mathbf{L^1}$) and 7-amino-2-methylchromone ($\mathbf{L^2}$), were synthesized and characterized by X-ray diffraction, UV–Vis, FT-IR, EPR spectroscopy, MS and elemental analysis. The complexes were synthesized using 2:1 ligand-to-metal ratio, but while three products $[Cu(\mathbf{L^2})_2Cl_2]_2$ (**1b**), $Cu(\mathbf{L^1})_2(ClO_4)_2(H_2O)_2$ (**2a**), $Cu(\mathbf{L^2})_2(ClO_4)_2(H_2O)_2$ (**2b**) maintained the applied stoichiometry, the fourth compound showed an unexpected 1:1 ratio and was identified as $[Cu(\mathbf{L^1})Cl_2]_n$ (**1a**). In all four compounds, the chromone derivatives were found to act as monodentate *O*- or *N*-ligands. Interestingly, in a doubly chloro-bridged dinuclear complex **1b** each Cu(II) cation interacts with one $\mathbf{L^2}$ ligand through the carbonyl *O*-donor, and with another $\mathbf{L^2}$ molecule through the amine *N*-donor, so the complex adopts a square pyramid geometry. According to a single-crystal X-ray diffraction analysis the complex **2b** is a distorted mononuclear octahedron with the central Cu(II) cation interacting only with oxygen donors (two perchlorate anions, two $\mathbf{L^2}$ ligands, and two water molecules). The structural characteristics of **1a** and **2a** complexes were elucidated from EPR measurements, where their g-tensor components were compared to those observed for **1b** and **2b**, the structures of which were determined by X-ray diffraction method. DFT calculations were performed to estimate the most favored mode of coordination, whereas comparative Hirshfeld surface studies were used to characterize intermolecular interactions in the studied complexes. Magnetic interactions of **1a** and **2a** were also analyzed.

Słowa kluczowe

Chromone derivatives, Copper(II) complexes, X-ray structure, DFT calculations, magnetic properties