

X-ray structure of poly[aquabis(benzimidazole- N^3)copper(II)- μ -*trans*-2-butene-1,4-dicarboxylato- O,O' : O'' , O'''] (I) and magnetic and spectroscopic characterization of I and the isostructural copper(II)- μ adipato complex II.

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The title compounds $[\text{Cu}(\text{H}_2\text{O})(\text{C}_7\text{H}_6\text{N}_2)_2(\text{C}_6\text{H}_6\text{O}_4)]$ (I) and isostructural $[\text{Cu}(\text{H}_2\text{O})(\text{C}_7\text{H}_6\text{N}_2)_2(\text{C}_6\text{H}_8\text{O}_4)]$ (II) are the rarely observed seven-coordinate Cu(II) complexes of C_2 elongated square-pyramidal geometry with a double-capped base by two very long Cu–O(carboxylate) bonds. The valences of Cu–N and Cu–O bonds in I and II have been computed to confirm the assumed Cu(II) coordination number. The hydrogen bond system and Cu···Cu intra- and interpolymeric chain spacing in I and II have been analyzed to explain their magnetic properties. The magnetic susceptibility measurements of I and II in the range 1.7–300 K suggest weak antiferromagnetic interaction between Cu(II) centres. The EPR and d–d spectra of both complexes have been measured and analyzed.

The single-crystal X-ray structure analysis of I shows its isostructurality with the copper(II)- μ -adipato complex II. Both structures are the rarely observed seven-coordinate Cu(II) complexes of C_2 elongated square-pyramidal geometry with a double-capped base by two long Cu–O(carboxylate) bonds. The magnetic susceptibility measurements of I and II suggest weak antiferromagnetic interaction between Cu(II) centers. The EPR and d–d spectra of both complexes have been measured and analyzed.

Słowa kluczowe

Cu(II) stereochemistry, X-ray structures, Magnetism, EPR spectra

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