

A new mixed-valence Cu<sup>I</sup>/Cu<sup>II</sup> three-dimensional coordination polymer constructed with an *N,O*-donor ligand generated *via* solvothermal synthesis: structural features and magnetic properties.

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Streszczenie

A new mixed-valence Cu<sup>I</sup>/Cu<sup>II</sup> three-dimensional coordination polymer, poly[[diaquabis[μ<sub>4</sub>-2-(pyrazin-2-yl)quinoline-4-carboxylato]dicopper(I)copper(II)] bis(tetrafluoridoborate)], {[Cu<sub>3</sub>(C<sub>14</sub>H<sub>8</sub>N<sub>3</sub>O<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>](BF<sub>4</sub>)<sub>2</sub>]<sub>n</sub>, was synthesized and characterized, with 2-(pyrazin-2-yl)quinoline-4-carboxylic acid being employed as a linker ligand. The ligand was isolated as its hydrochloride salt, 4-carboxy-2-(pyrazin-2-yl)quinolin-1-ium chloride dihydrate, C<sub>14</sub>H<sub>10</sub>N<sub>3</sub>O<sub>2</sub><sup>+</sup>·Cl<sup>-</sup>·2H<sub>2</sub>O. The compounds show luminescence at 550 nm for the ligand and at 565 nm for the polymer at 297 K. The ligand structure was rationalized by means of quantum-chemical calculations, which led to a similar conformation to that determined from X-ray diffraction studies.

Słowa kluczowe

quinolinecarboxylic acid, quinolinium chloride, photoluminescence, magnetic properties, coordination polymer, crystal structure, quantum-chemical calculations.

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