Unique Use of Dibromo–L–Tyrosine Ligand in Building of Cu(II) Coordination Polymer—Experimental and Theoretical Investigations

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Rok wydania

2024

Czasopismo

Molecules

Numer woluminu

29

Strony

2709/1-2709/17

DOI

10.3390/molecules29112709

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Although the crystals of coordination polymer {[CuCl(μ-O,O'-L-Br_2Tyr)]}n (1) (L-Br_2Tyr = 3,5-dibromo-L-tyrosine) were formed under basic conditions, crystallographic studies revealed that the OH group of the ligand remained protonated. Two adjacent [CuCl(L-Br_2Tyr)] monomers, bridged by the carboxylate group of the ligand in the syn-anti bidentate bridging mode, are differently oriented to form a polymeric chain; this specific bridging was detected also by FT-IR and EPR spectroscopy. Each Cu(II) ion in polymeric compound 1 is coordinated in the xy plane by the amino nitrogen and carboxyl oxygen of the parent ligand and the oxygen of the carboxyl group from the symmetry related ligand of the adjacent [Cu(L-Br_2Tyr)Cl] monomer, as well as an independent chlorine ion. In addition, the Cu(II) ion in the polymer chain participates in long-distance intermolecular contacts with the oxygen and bromine atoms of the ligands located in the adjacent chains; these intramolecular contacts were also supported by NCI and NBO quantum chemical calculations and Hirshfeld surface analysis. The resulting elongated octahedral geometry based on the [CuCl(L-Br_2Tyr)] monomer has a lower than axial symmetry, which is also reflected in the symmetry of the calculated molecular EPR g tensor. Consequently, the components of the d-d band obtained by analysis of the NIR-VIS-UV spectrum were assigned to the corresponding electronic transitions.

Słowa kluczowe

3,5–dibromo–L–tyrosine, copper(II), crystal structure, spectroscopies, theoretical calculations

Adres publiczny

http://dx.doi.org/10.3390/molecules29112709

Strona internetowa wydawcy

http://www.mdpi.com/journal/metals