Ligand-forced dimerization of copper(I)—olefin complexes bearing a 1,3,4-thiadiazole core.

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Streszczenie

As an important class of heterocyclic compounds, 1,3,4-thiadiazoles have a broad range of potential applications in medicine, agriculture and materials chemistry, and were found to be excellent precursors for the crystal engineering of organometallic materials. The coordinating behaviour of allyl derivatives of 1,3,4-thiadiazoles with respect to transition metal ions has been little studied. Five new crystalline copper(I) π-complexes have been obtained by means of an alternating current electrochemical technique and have been characterized by single-crystal X-ray diffraction and IR spectroscopy. The compounds are bis[μ-5-methyl-N-(prop-2-en-1-yl)-1,3,4-thiadiazol-2-amine]bis[nitratocopper(I)], [Cu2(NO3)2(C6H9N3S)2], (1), bis[μ-5-methyl-N-(prop-2-en-1-yl)-1,3,4-thiadiazol-2-amine]bis[(tetrafluoroborato)copper(I)], [Cu2(BF4)2(C6H9N3S)2], (2), μ-aqua-bis{μ-5-[(prop-2-en-1-yl)sulfanyl]-1,3,4-thiadiazol-2-amine}bis[nitratocopper(I)], [Cu2(NO3)2(C5H7N3S2)2(H2O)], (3), μ-aqua-(hexafluorosilicato)bis{μ-5-[(prop-2-en-1-yl)sulfanyl]-1,3,4-thiadiazol-2-amine}dicopper(I)-acetonitrile-water (2/1/4), [Cu2(SiF6)(C5H7N3S2)2(H2O)]·0.5CH3CN·2H2O, (4), and μ-benzenesulfonato-bis{μ-5-[(prop-2-en-1-yl)sulfanyl]-1,3,4-thiadiazol-2-amine}dicopper(I) benzenesulfonate-methanol-water (1/1/1), [Cu2(C6H5O3S)(C5H7N3S2)2](C6H5O3S)·CH3OH·H2O, (5). The structure of the ligand 5-methyl-N-(prop-2-en-1-yl)-1,3,4-thiadiazol-2-amine (Mepeta), C6H9N3S, was also structurally characterized. Both Mepeta and 5-[(prop-2-en-1-yl)sulfanyl]-1,3,4-thiadiazol-2-amine (Pesta) (denoted L) reveal a strong tendency to form dimeric {Cu2L2}2+ fragments, being attached to the metal atom in a chelating-bridging mode via two thiadiazole N atoms and an allylic C=C bond. Flexibility of the {Cu2(Pesta)2}2+ unit allows the CuI atom site to be split into two positions with different metal-coordination environments, thus enabling the competitive

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participation of different molecules in bonding to the metal centre. The Pesta ligand in (4) allows the CuI atom to vary between water O-atom and hexafluorosilicate F-atom coordination, resulting in the rare case of a direct CuI...FSiF52- interaction. Extensive three-dimensional hydrogen-bonding patterns are formed in the reported crystal structures. Complex (5) should be considered as the first known example of a CuI(C6H5SO3) coordination compound. To determine the hydrogen-bond interactions in the structures of (1) and (2), a Hirshfeld surface analysis has been performed.

Słowa kluczowe

1,3,4-thiadiazole, hirshfeld surface analysis, copper(I), crystal structure, electrochemical technique, π-complex

Adres publiczny

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