

Bromine versus chlorine substituent in breathing crystals of a copper(I) coordination compound with a triazolamine Schiff base

Autorzy

Emilia Ganczar

Agata Białońska

Rok wydania

2023

Czasopismo

Acta Crystallographica
Section B: Structural
Science, Crystal Engineering
and Materials

Numer woluminu

79

Strony

392-398

DOI

10.1107/s205252062300673x

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

It is known that *N*-[4-(chlorobenzylidene)-4*H*-1,2,4-triazol-4-amine in reaction with copper(I) perchlorate(VII) forms metastable breathing crystals built up of X-shaped binuclear units containing copper(I) ions in a trigonal coordination sphere. Using trifluoromethanesulfonate instead of perchlorate(VII) affects the self-assembly of the X-shaped units and the breathing function of the resulting crystals. The latter are not breathing crystals. Copper(I) trifluoromethanesulfonate with *N*-[4-(bromobenzylidene)-4*H*-1,2,4-triazol-4-amine crystallizes in two forms: open (with the presence of 1D channels) and closed (without 1D channels). Both are characterized by the presence of X-shaped binuclear cationic units and the trigonal coordination sphere of copper(I) ions. The open form has the ability to engage in reversible sorption. The desorption process is associated with the large reorientation of the binuclear units and the reorganization of the intermolecular interactions leading to the closure of the channels. The post-synthetically obtained channel-less form differs from the channel-less form obtained by direct crystallization, the latter being incapable of sorption. The mechanism of the desorption process of the open form is governed by the general principle of dense packing, and the main reason for the sorption process is the formation of directional halogen–halogen interactions. The halogen atom in the *para* position of the ligands influences the formation of different crystalline forms and also a different mechanism for the desorption process.

Słowa kluczowe

breathing crystals, copper(I) coordination compound, host-guest chemistry, halogen–halogen interaction

Adres publiczny

<http://dx.doi.org/10.1107/s205252062300673X>

Plik został wygenerowany dnia 2026-10-03 06:53:00

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/0yhvPjv>.