Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Magneto-structural analysis of metal-orotato coordination complexes based on N–H···O and O–H···O supramolecular synthon.

Autorzy

Kafeel Ahmad Siddiqui

Prem Lama

Alina Bieńko

Dariusz Bieńko

Rok wydania

2016

Czasopismo

Polyhedron

Numer woluminu

111

Strony

53-63

DOI

10.1016/j.poly.2016.03.003

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Two new supramolecular synthon induced single crystals of metal-orotato complexes of formula [Cu (Orotate).2H(2)O]2 (1), [Mn(Orotate)2.2H(2)O].2H(2)O] (2), have been engineefed and synthesized by self assembly of metal salts with orotic acid in presence of 25% ammonia solution. Although both complexes crystallize in similar crystal system and different coordination geometries [(square planar (1), octahedral (2)] but identical synthon patterns recur after complex formation. N-H center dot center dot center dot O, O-H center dot center dot center dot O synthons were the only artifact for both the hydrogen bonded metal-organic architecture. X-ray structural analysis, EPR, temperature independent paramagnetism (TIP) analysis, have been discussed. DFT calculation is used to rationalize the magnetic behavior of both the complexes. These calculations underline the pathway of magnetic exchange interactions through N-H center dot center dot center dot O, O-H center dot center dot center dot O supramolecular synthons and confirm, that the magnetic interactions propagate through such contacts in complex 1 and 2.

Słowa kluczowe

Crystal engineering, Metal-orotato complexes, hydrogen bonding, Magneto-structural analysis, density functional calculations

Adres publiczny

http://dx.doi.org/10.1016/j.poly.2016.03.003

Strona internetowa wydawcy

http://www.elsevier.com

Plik został wygenerowany dnia 2026-11-05 02:20:23

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/8YPg6TQ.