Iron(III) bis(pyrazol-1-yl)acetate based decanuclear metallacycles : synthesis, structure, magnetic properties and DFT calculations.

Autorzy

Małgorzata J. Gajewska

Alina Bieńko

Radovan Herchel

Matti Haukka

Maria Jerzykiewicz

Andrew Ozarowski

Krzysztof Drabent

Chen-Hsiung Hung

Rok wydania

2016

Czasopismo

Dalton Transactions

Numer woluminu

45

Strony

15089-15096

DOI

10.1039/C6DT02333A

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The synthesis, structural aspects, magnetic interpretation and theoretical rationalizations for a new member of the ferric wheel family, a decanuclear iron(III) complex with the formula $[Fe_{10}(bdtbpza)_{10}(\mu_2\text{-}OCH_3)_{20}]$ (**1**), featuring the *N*,*N*,*O* tridentate bis(3,5-di-*tert*-butylpyrazol-1-yl)acetate ligand, are reported. The influence of the steric effect on both the core geometry and coordination mode is observed. Temperature dependent (2.0–300 K range) magnetic susceptibility studies carried out on complexes **1** established unequivocally antiferromagnetic (AF) interactions between high-spin iron(III) centers (S = 5/2), leading to a ground state S = 0. The mechanism of AF intramolecular coupling was proved using a broken-symmetry approach within the density functional method at the B3LYP/def2-TZVP(-f)/def2-SVP level of theory.

Adres publiczny

http://dx.doi.org/10.1039/C6DT02333A

Strona internetowa wydawcy

https://www.rsc.org/