

HS↔LS transition in iron(II) two-dimensional coordination networks containing tris(tetrazol-1-ylmethyl)methane as triconnected building block.

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Rok wydania

2012

Czasopismo

Inorganic Chemistry

Numer woluminu

51

Strony

237-245

DOI

10.1021/ic201535x

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Novel tripodal ligand 1,1',1''-tris(tetrazol-1-ylmethyl)methane (**111tz**) and products of its reactions with perchlorate as well as with tetrafluoroborate salts of iron(II) are presented. The isostructural complexes, $[\text{Fe}(\mathbf{111tz})_2](\text{ClO}_4)_2$ and $[\text{Fe}(\mathbf{111tz})_2](\text{BF}_4)_2$, were isolated as two-dimensional (2D) coordination networks revealing a honeycomb-like pattern with cages occupied by disordered anions. **111tz** molecules act as a tridentate ligand bridging three adjacent Fe(II) ions, and the nitrogen N4 atom of six tetrazole rings (tz) is placed in octahedron vertices of FeN_6 chromophores. The complexes, crystallizing in the $P\bar{3}$ space group, were characterized by variable-temperature single-crystal X-ray diffraction and variable-temperature magnetic susceptibility measurements. Variable-temperature magnetic susceptibility measurements show that both systems undergo abrupt and complete spin transition with $T_{1/2}^\uparrow = T_{1/2}^\downarrow = 176$ K for perchlorate and $T_{1/2}^\uparrow = 193.8$ and $T_{1/2}^\downarrow = 192.8$ K for the tetrafluoroborate analogue. Change of spin state in both complexes is accompanied by a thermochromic effect. The HS \rightarrow LS transition in $[\text{Fe}(\mathbf{111tz})_2](\text{ClO}_4)_2$ involves shortening of the Fe–N4 bond lengths from 2.171(2) Å (293 K) to 2.002(1) Å (100 K). In $[\text{Fe}(\mathbf{111tz})_2](\text{BF}_4)_2$, lowering of temperature from 293 to 100 K is accompanied by shortening of the Fe–N4 distances from 2.179(2) to 1.987(2) Å, respectively. Perchlorate in $[\text{Fe}(\mathbf{111tz})_2](\text{ClO}_4)_2$ or tetrafluoroborate anions in $[\text{Fe}(\mathbf{111tz})_2](\text{BF}_4)_2$ are engaged in the formation of intermolecular contacts within as well as with the neighboring 2D layer.

Adres publiczny

<http://dx.doi.org/10.1021/ic201535x>

Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>

Plik został wygenerowany dnia 2026-04-28 22:23:59

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