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# Synthesis, X-ray crystallographic and $^{1}$H NMR spectroscopic structural studies on cobalt(II) complexes of homoscorpionate, heteroscorpionates and chiral tris(pyrazolyl)borates obtained from 5(3)-*iso*propyl-3(5)-phenylpyrazole and 3,5-dimethylpyrazole.

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Streszczenie

Condensation of 5(3)-isopropyl-3(5)-phenylpyrazole with sodium borohydride led to a mixture of tris(pyrazolyl)borate ligands ($Tp^{x}$) − the homoscorpionate hydrotris(5-isopropyl-3-phenylpyrazolyl)borate and the heteroscorpionates hydro(3-isopropyl-5-phenylpyrazolyl)bis(5-isopropyl-3-phenylpyrazolyl)borate and hydrobis(3-isopropyl-5-phenylpyrazolyl)(5-isopropyl-3-phenylpyrazolyl)borate − that were converted into $Tp^{x}$Co(NCS) complexes. The molecular structures of pentacoordinate[hydrotris(5-isopropyl-3-phenylpyrazolyl)borato](tetrahydrofuran)(thiocyanato)cobalt(II) (**1-THF**) and [hydrobis(3-isopropyl-5-phenylpyrazolyl)(5-isopropyl-3-cobalt(II) (**3-THF**) were elucidated crystallographically. Hydro(3,5-dimethylpyrazolyl)bis(5-isopropyl-3-phenylpyrazolyl)borate was also obtained by condensation of 2.1 equiv. of 5(3)-isopropyl-3(5)-phenylpyrazole and 0.9 equiv. of 3,5-dimethylpyrazole with sodium borohydride, and it was converted into [hydro(3,5-dimethylpyrazolyl)bis(5-isopropyl-3-phenylpyrazolyl)borato] (thiocyanato)cobalt(II) (**4**), which was characterized by X-ray crystallography. The latter was converted thermally under mild conditions (358 K in toluene) into [hydro(3,5-dimethylpyrazolyl)(3-isopropyl-5-phenylpyrazolyl)(5-isopropyl-3-phenylpyrazolyl)borato](thiocyanato)cobalt(II) (**9**) in 45% yield, as was concluded from the $^{1}$H NMR spectrum of the post-reaction mixture. The dimer of **9** was obtained as single crystals from toluene/hexane and its structure was determined crystallographically. Two chiral $Tp^{x}$ ligands of opposite boron-centered configurations are coordinated to cobalt(II) ions in a $\kappa^{3}$ fashion. The pentacoordinate metal ions are bridged head-to-tail by the thiocyanate anions. This chiral $Tp^{x}$ ligand is the first example of a borate with fixed boron-centered chirality.

Adres publiczny

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