

Complexes of heteroscorpionate trispyrazolylborate anionic ligands. Part III. X-ray crystallographic and NMR studies on cobalt(II) complexes with tris(pyrazolyl)borate anionic ligands obtained from 3,5-di-methylpyrazole and 3(5)-methyl,5(3)-phenylpyrazole.

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Streszczenie

Condensation of 2 equiv. of 5(3)-methyl,3(5)-phenylpyrazole and 1 equiv. of 3,5-di-methylpyrazole with NaBH_4 resulted in the formation of sodium [hydrobis(3-phenyl,5-methylpyrazolyl)(3,5-di-methylpyrazolyl)borate]. The ligand was converted into the pentacoordinate $[\text{HB}(3,5\text{-di-Mepz})(3\text{-Ph},5\text{-Mepz})_2]\text{Co}(\text{NCS})(\text{THF})\cdot\text{THF}$ complex for which the molecular structure was determined by the X-ray crystallographic method. The geometry of the ligand in the cobalt(II) complex was compared with that of the homoscorpionate ligand in $[\text{HB}(3\text{-Ph},5\text{-Mepz})_3]\text{Co}(\text{NCS})(\text{THF})\cdot 0.5\text{THF}$ on the basis of X-ray structural data. The condition for the thermal conversion of the ligands in the studied $\text{Tp}'\text{Co}(\text{NCS})$ was established. The heating of the mentioned complexes at 428 K in propylbenzene resulted in a borotropic shift of 3-phenyl,5-methylpyrazolyl moieties resulting in the formation of new heteroscorpionates: the chiral $[\text{HB}(3,5\text{-di-Mepz})(3\text{-Ph},5\text{-Mepz})(3\text{-Me},5\text{-Phpz})]\text{Co}(\text{NCS})$ and $[\text{HB}(3\text{-Me},5\text{-Phpz})_2(3\text{-Ph},5\text{-Mepz})]\text{Co}(\text{NCS})$, which were characterized in solution by ^1H NMR spectroscopy. Heteroscorpionate anionic hydro(3,5-di-methylpyrazolyl)bis(3-phenyl,5-methylpyrazolyl)borate ligand (Tp') and its $\text{Tp}'\text{Co}(\text{NCS})(\text{THF})$ complex have been synthesized. The structure of the compound was compared with that of the corresponding homoscorpionate $\text{Tp}^{\text{Ph,Me}}\text{Co}(\text{NCS})(\text{THF})$ complex. Both complexes undergo borotropic shift of the 3-Ph,5-Mepz moiety to form new heteroscorpionate complexes: the chiral $[\text{HB}(3,5\text{-di-Mepz})(3\text{-Ph},5\text{-Mepz})(3\text{-Me},5\text{-Phpz})]\text{Co}(\text{NCS})$ and $[\text{HB}(3\text{-Ph},5\text{-Mepz})(3\text{-Me},5\text{-Phpz})_2]\text{Co}(\text{NCS})$.

Słowa kluczowe

Heteroscorpionate tris(3-R-pyrazolyl)borate cobalt(II) complexes, Structure, NMR

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