Scorpionate Complexes with the Main Group Elements Ca, Ba, Sr Riccardo Spagna², Carlo Santini¹, Maura Pellei¹, Giancarlo Gioia Lobbia¹, Massimo Pallotta¹, Simone Alidori¹, Mercedes Camalli², ¹Dipartimento di Scienze Chimiche, Università di Camerino, Italy. ²IC-CNR Sezione di Monterotondo, Roma, Italy. E-mail: riccardo.spagna@ic.cnr.it

The poly(pirazolyl)borate ligands together with various substituted forms have developed into one of the most versatile ancillary ligand in metal coordination chemistry. Particular attention is sometimes devoted to special azolyl rings, such as triazolyl, methylor trifluoromethyl-pyrazolyl rings. These ligands can exert quite different electronic and structural effects when compared with the analogues. Very little has been done on poly(pyrazolyl)borate systems bearing electron withdrawing substituents. The electron withdrawing groups in polyfluorinated ligands commonly improve the volatility, oxidation resistance, thermal stability, and solubility of metal complexes. To our knowledge, no poly(azolyl)borates containing a -NO₂ function have been prepared, presumably due to difficulties in the synthesis of ligands having both a hydride and a nitro group. However, a poly(azolyl)borate containing a -NO₂ substituent could be of interest due to its high coordinative flexibility from κ^4 - to μ^4 -N₂O₂ coordination ability.

We report here on the syntheses and structural investigations of main-group metal elements Ca, Ba and Sr with the hydrotris(3-methylpyrazolyl)borate, the hydrotris(1,2,4-triazolyl)borate and the new hydrotris(3-nitro-1,2,4-triazolyl)borate, an emerging category of electron withdrawing substituted scorpionate ligands.

Keywords: metalloorganic chemistry, pyrazolyl, crystal structures