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Maura Pellei, Carlo Santini, Marika Marinelli, Andrea Trasatti, H.V. Rasika Dias

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The hydridotris(3-nitro-1,2,4-triazol-1-yl)borate, a new nitro-substituted electron withdrawing polydentate "scorpionate"-type ligand and related copper and silver phosphane complexes

Maura Pellei,^a Carlo Santini,^{a*} Marika Marinelli,^a Andrea Trasatti^a and H. V. Rasika Dias^b

^bSchool of Science and Technology – Chemistry Division, University of Camerino, via S. Agostino
1, 62032 Camerino (MC), Italy
^bDepartment of Chemistry and Biochemistry, Box 19065, The University of Texas at Arlington,

Arlington, Texas 76019-0065; USA

E-mail: carlo.santini@unicam.it (Carlo Santini)

Abstract

The new tripodal "scorpionate"-type ligand, the sodium hydridotris(3-nitro-1,2,4-triazol-1-yl)borate Na[HB(tz^{NO2})₃] (1), containing electron withdrawing nitro functional groups on the azolyl moiety, has been synthesized in high yield starting from 3-nitro-1,2,4-triazole and sodium borohydride. New copper(I) and silver(I) complexes, $[HB(tz^{NO2})_3]M(PR_3)_2$ (M = Cu or Ag; PR₃= P(C₆H₅)₃, or P(*p*-C₆H₄CH₃)₃) have been synthesized from the reaction of CuCl or AgNO₃ with Na[HB(tz^{NO2})_3] and triphenylphosphane or tri(*p*-tolyl)phosphane, respectively. These compounds have been characterized by elemental analyses, FT-IR, ESI-MS and multinuclear NMR spectroscopy. X-ray crystal structure of Na[HB(tz^{NO2})₃] (1) shows that it has polymeric network structure resulting from sodium atoms of tripodal Na[HB(tz^{NO2})₃] forming inter-molecular Na-N bonds to three nitrogen atoms of three neighboring triazolyl moieties of Na[HB(tz^{NO2})₃]. Each sodium center has distorted octahedral geometry with three short Na-N (inter-molecular) and three long Na-N bonds (to chelating N-atoms of [HB(tz^{NO2})₃]⁻ ligand). This nitro-substituted scorpionate ligand could be of interest due to its high coordinative flexibility from endo- to exo-polydentate coordination mode.

KEYWORDS. Silver(I); Copper(I); Chelate ligands; Scorpionates; X-ray; Phosphanes; Spectroscopy

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