

Title: Coordination Chemistry of the (eta(6)-p-Cymene)ruthenium(II) Fragment with Bis-, Tris-, andTetrakis(pyrazol-1-yl)borate Ligands: Synthesis, Structural, Electrochemical, and CatalyticDiastereoselective Nitroaldol Reaction Studies

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Abstract: Novel [Ru(eta(6)-p-cymene)(kappa(2)-L)X] and [Ru(eta(6)-p-cymene)(kappa(3)-L)]X center dot nH(2)O complexes (L = bis-, tris-, or tetrakis-pyrazolylborate; X = Cl, N-3, PF6, or CF3SO3) are prepared by treatment of [Ru(eta(6)-p-cymene)Cl-2](2) with poly-(pyrazolyl)borate derivatives [M(L)] (L in general; in detail L = Ph(2)Bp = diphenylbis-(pyrazol-1-yl)borate; L = Tp = hydrotris(pyrazol-1-yl)borate; L = pzTp = tetrakis(pyrazol-1-yl)borate; L = Tp(4Bo) = hydrotris(indazol-1-yl)borate, L = T-p4Bo,T-5Me = (5-methylindazol-1-yl)borate; L = Tp(Bn,4Ph) = hydrotris(3-benzyl-4-phenylpyrazol-1-yl)borate; M = Na, K, or Tl) and characterized by analytical and spectral data (IR, ESIMS, H-1 and C-13 NMR). The structures of [Ru(eta(6)-p-cymene)(Ph(2)Bp)Cl] (1) and [Ru(eta(6)-p-cymene)(Tp)Cl] (3) have been established by single-crystal X-ray diffraction analysis. Electrochemical studies allowed comparing the electron-donor characters of Tp and related ligands and estimating the corresponding values of the Lever E-L ligand parameter. The complexes [Ru(eta(6)-p-cymene)-(kappa(2)-L)X] and [Ru(eta(6)-p-cymene)(kappa(3)-L)]X center dot nH(2)O act as catalyst precursors for the diastereoselective nitroaldol reaction of benzaldehyde and nitroethane to the corresponding beta-nitroalkanol (up to 82% yield, at room temperature) with diastereoselectivity toward the formation of the threo isomer.

KeyWords Plus: Asymmetric Reaction; Ruthenium(II) Arene Complexes; Boron-Pyrazole Chemistry; Human Ovarian-Cancer; PI-Acceptor Ligands; Crystal-Structure; Ferrocene Derivatives; Sulfinato Complexes; Transition-Metals; Anticancer Drugs

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