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

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Source: Organometallics

Volume: 30 Issue: 6 Pages: 1616-1626 DOI: 10.1021/om101146q Published: Mar 28 2011

Document Type: Article

Language: English

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)Cl2]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(4Ph) = hydrotris(3-benzyl-4-phenylpyrazol-1-yl)borate; M = Na, K, or Ti) 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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Funding:

<table>
<thead>
<tr>
<th>Funding Agency</th>
<th>Grant Number</th>
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<tbody>
<tr>
<td>Foundation for Science and Technology (FCT)</td>
<td>BPD/46812/2008</td>
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<td>University of Camerino</td>
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Publisher: Amer Chemical
Publisher Address: 1155 16th ST, NW, Washington, DC 20036 USA

ISSN: 0276-7333

Citation: PETTINARI, Claudio; MARCHETTI, Fabio; CERQUETELLA, Adele; PETTINARI, Riccardo; MONARI, Magda; MAC LEOD, Tatiana C. O.; MARTINS, Luísa M. D. R. S.; POMBEIRO, Armando J. L. - Coordination Chemistry of the (eta(6)-p-Cymene)ruthenium(II) Fragment with Bis-, Tris-, and Tetrakis(pyrazol-1-yl)borate Ligands: Synthesis, Structural, Electrochemical, and Catalysis Diastereoselective Nitroaldol Reaction Studies. Organometallics. ISSN 0276-7333. Vol. 30, n.º 6 (2011) p. 1616-1626.