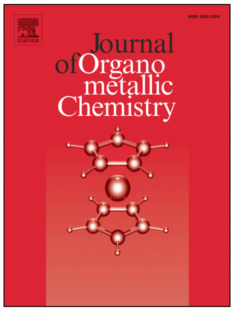

Borate-based ligands with soft heterocycles and their ruthenium complexes

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Borate-based ligands with soft heterocycles and their ruthenium complexes

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Abstract:

In a quest for effective synthetic precursors for the preparation of B-agostic complexes of ruthenium, we have shown that the reaction of $[Cp^*RuCl_2]_2$ ($Cp^* = \eta5\text{-}C_5Me_5$) with [NaBt] or [NaBo] (Bt = dihydrobis(2-mercaptobenzthiazolyl)borate; Bo = dihydrobis(2-mercapto-benzoxazolyl)borate) led to the formation of B-agostic complexes $[Cp^*RuBH_2L_2]$, **1a,b** (**1a**: L = 2-mercaptobenzthiazol, **1b**: L = 2-mercaptobenzoxazol) and $[Cp^*RuBH_3L]$, **2a,b** (**2a**: L = 2-mercaptobenzthiazol, **2b**: L = 2-mercaptobenzoxazol) in good yields. In parallel to the formation of **1a,b** and **2a,b**, this method also allowed the formation of ruthenium hydrotrisborate complexes $[Cp^*RuBYL_3]$, **3a-c** (**3a**: L = 2-mercaptobenzthiazol, Y = H; **3b**: L = 2-mercaptobenzoxazol, Y = H; **3c**: L = 2-mercaptobenzoxazol, Y = Cl). The key feature of complexes **3a-c** is the coordination of one of the 2-mercaptobenzothiazole ligand that connects to the metal and the boron centre through a common sulfur atom. Upon heating, compounds **3a,b** change into their corresponding S→N linkage isomers, in which the boron atom is bonded to three nitrogen atoms. The cyclic voltametric studies on compounds **3a-c** and **4a,b** suggest that a deviation in coordination of the