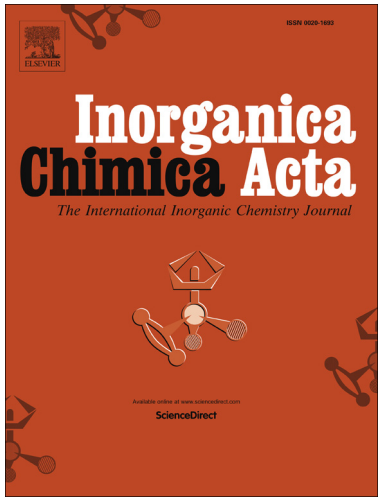

Research paper

Palladium complexes bearing κ ^{2}-*N*,*N* and κ ^{3}-*N*,*N*,*O* pendant amine bis(phenolate) ligands

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Palladium complexes bearing κ^2-*N*,*N* and κ^3-*N*,*N*,*O* pendant amine bis(phenolate) ligands

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Abstract

The synthesis and characterization of ten new palladium(II) amine bis(phenolate) complexes is reported. Solution and single-crystal X-ray diffraction studies reveal the presence of both κ^2-*N*,*N* and κ^3-*N*,*N*,*O* binding modes in these square planar complexes. For complexes with sterically less demanding phenolate donors, addition of external acidic or basic reagents allows for the selective masking of a coordination site at Pd. Complexes bearing bulky cumyl substituents on phenolate donors exhibited unusual ^{1}H NMR spectroscopic features that are consistent with an anagostic interaction with the palladium center. Computational analysis at the ωB97X-D/LAN2LDZ level of theory supported the assertion that such an anagostic interaction may play a role in stabilizing κ^2 complexes bearing a cumyl-substituted amine bis(phenolate) ligand. X-ray crystallographic data for **H$_2$1a-PdCl$_2$**, **H$_2$2a-PdCl$_2$**, **H1b-PdCl**, **H2b-PdCl**, **H1d-PdCl**, and **H1e-PdCl** are reported.

Keywords: Palladium; X-ray; NMR; anagostic