Accepted Manuscript

Research paper

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PII: S0020-1693(18)30921-6

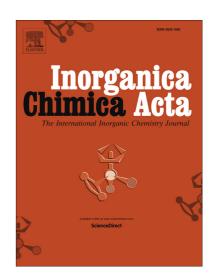
DOI: https://doi.org/10.1016/j.ica.2018.09.032

Reference: ICA 18490

To appear in: Inorganica Chimica Acta

Received Date: 13 June 2018

Revised Date: 10 September 2018 Accepted Date: 10 September 2018



Please cite this article as: B.J. Graziano, E.M. Collins, N.C. McCutcheon, C.L. Griffith, N.M. Braunscheidel, T.M. Perrine, B.M. Wile, Palladium complexes bearing κ^2 -N,N and κ^3 -N,N,O pendant amine bis(phenolate) ligands, *Inorganica Chimica Acta* (2018), doi: https://doi.org/10.1016/j.ica.2018.09.032

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ACCEPTED MANUSCRIPT

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 ω B97X-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 H21a-PdCl₂, H22a-PdCl₂, H1b-PdCl, H2b-PdCl, H1d-PdCl, and H1e-PdCl are reported.

Keywords: Palladium; X-ray; NMR; anagostic

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