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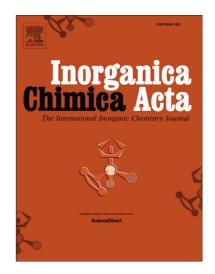
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### ACCEPTED MANUSCRIPT

# Isomerization and Luminescent Properties of Schiff-Base Aluminum Complexes Containing 1*H*-Pyrrole-2-Carbaldehyde Moieties

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#### **Abstract**

Schiff-base 1H-pyrrol-2-yl-methyleneamino-4,6-di-*tert*-butylphenol, ONNH<sub>2</sub> (1), and its aluminum complexes [(ONN<sub>2</sub>Al)AlR<sub>2</sub>] (R = Me (2), Et (3), and iBu (4)) were synthesized. Complexes 2-4 were characterized by FT-IR,  $^{1}H$  and  $^{13}C\{^{1}H\}$  NMR, and mass spectrometry. X-ray diffraction analysis shows that 2 is a bimetallic complex with one aluminum center in an octahedral environment and the other in a tetrahedral one, 3 and 4 are also bimetallic, but with both aluminum atoms in a trigonal bipyramidal geometry. In diluted solution, 3 coexists as two isomers, namely,  $3_{\text{tet-oct}}$  and  $3_{\text{tbp-tbp}}$ . The assignment of these isomers was complemented with Density Functional Theory (DFT) computations of the chemical shifts. The luminescent properties of 2 in CH<sub>2</sub>Cl<sub>2</sub> were investigated using UV-Vis and photoluminescence (PL) spectroscopies, showing emission in the green region with a quantum yield of  $\Phi = 4\%$ . Time dependent DFT

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