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

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## Abstract

Schiff-base 1*H*-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 *i*Bu (**4**)) were synthesized. Complexes **2-4** were characterized by FT-IR, <sup>1</sup>H and <sup>13</sup>C{<sup>1</sup>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**<sub>tet-oct</sub> and **3**<sub>tbp-tbp</sub>. 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 Φ = 4%. Time dependent DFT

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